Lewis Kossel Theory:

According to Lewis, every atom tends to have 8 electrons in their valence shell as inert gas have. This is called octet theory / rule.

Li Be B C N O F

Kossel proposed the idea of ionic bond that first (alkali metals) and second (alkaline earth metals) group can give their electrons and form cation and 15, 16, 17 (Nitrogen, chalcogens, Halogens) group can take electrons and form anion.

$Na \xrightarrow{e^-} Na^+$

$Cl \xrightarrow{e^-} Cl^-$

NaCl → Ionic bond

Exception of Octet:

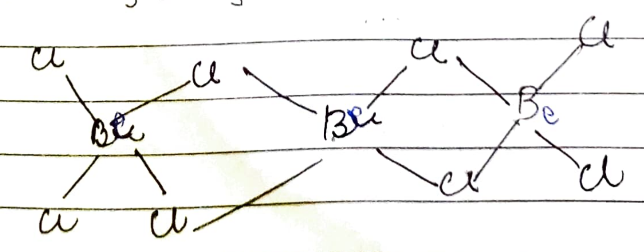
i) Hypovalent compounds or electron deficient or Lewis acids are stable inspite of the fact that they have incomplete octet.

Lewis's acids are stable despite being hypovalent

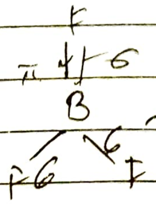
eg $LiCl$, BeX_2, AlX_3, etc.

BF_3, BCl_3, BBr_3, BI_3 etc

$BeCl_2$ → g
→ solid



BF_3 (Back bonding होता है)



→ completes octet through back-bonding

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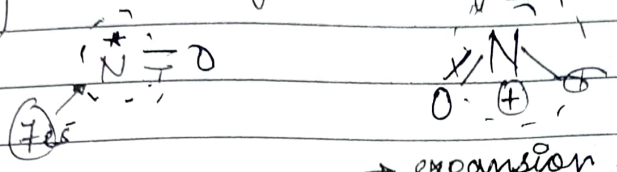
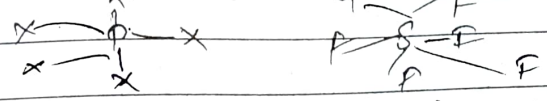
odd electronic species.

ii) Odd electrons are also stable despite of the fact that they don't obey octet rule.

e.g. 

iii) Hypervalent species → expansion of octet & species which have expansion of octet are also stable.

e.g. PX_5, SF_6, SiF_6^{2-}, SO_4^{2-}, IF_7, $XeOF_4$



→ Octet rule is based on inertness of noble gases. But Kr & Xe forms compound. with F & O.

Kr & Xe → Noble gases which react with F & O → $XeOF_4$

→ Octet rule doesn't explain, shape, stability energy, colour of compounds etc.

COVALENT BOND:

→ It is formed by mutual sharing of e⁻ pair. b/w two atoms.

mutual sharing pair

* CONDITION:

i) Physical state:
They are solid, liquid & gas.

N_2 → Gas ← O_2 ; F_2 → Gas
P_4, As_4, Sb_4, Bi → solid ← S_8, Se_8, Te_8, Po ; Cl_2 → Gas, Br → Liquid, I_2 → solid

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• weak intermolecular forces

i) covalent compounds have weak intermolecular force of attraction so they have low M.P & B.P & low density (low M.P, B.P)

ii) Down the group B.P ↑ M.P ↑ density (↑)
DTC, covalent character ↓ thermal staurity ↑

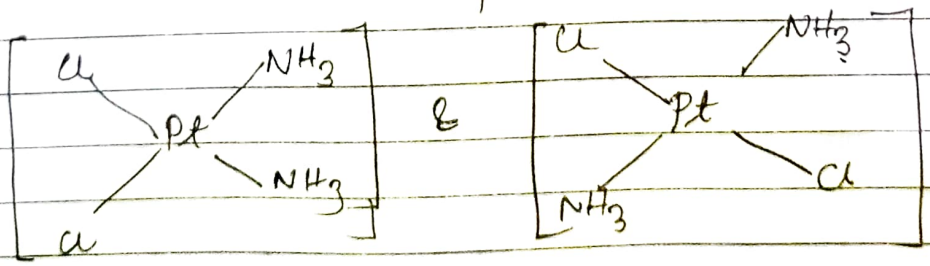
iii) Solubility:
covalent compounds are non-polar or less polar. so they are insoluble or less soluble in water. while more soluble in organic solvent.
↳ like acetone, toluene

iv) Electrical conductivity:
They have low conductivity & they are bad conductor except H_2O, ammonia & graphite
↑ due to localization of e⁻

v) Isomerism:
Directional character → isomerism.

covalent bond has directional character so covalent compound can exhibit isomerism e.g.

$[PtCl_2(NH_3)_2]$ has chemical formula as.



Covalent → directional
Ionic → non-

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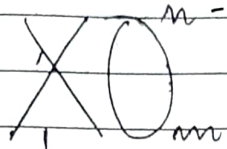
Structure:



Note : Consider ONLY negative charge on O

central atom

NOTE: Flourine & Hydrogen can never act as central atom

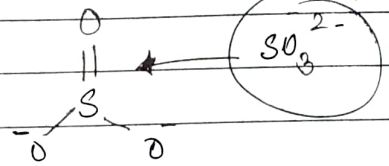
How to select a central atom?

a) less EN no. ✓
b) less electronegative ✓
c) More covalency ✓

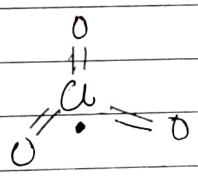
** No. of π-bonds : m - n* — no. of -ve charge

L.P = (valency - tot bonds) / 2

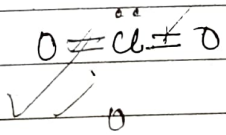
e.g. SO_3^{2-}



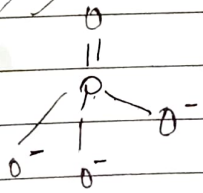
ClO_3^- →



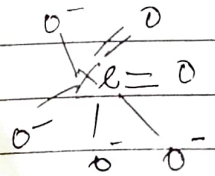
ClO_2 →



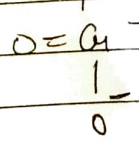
PO_4^{3-} →



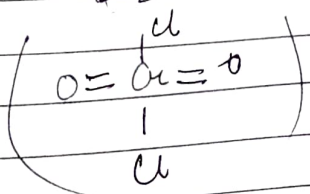
XeO_6^{4-} →



CrO_4^{2-} →



$C_4O_2Cl_4$



Basic requirement:

Each bonded atom gets an octet of electrons.

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Total lone → $\frac{1}{2}$ shares

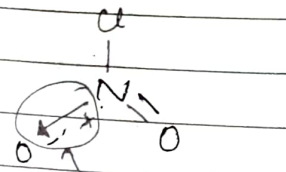
lone pair: $\frac{\text{Valency} - \text{total bond}}{2} = \frac{V - t_b}{2}$

Nitrogen, Oxygen, Halogen

N O X

1 2 3

NO_2Cl =



Hybridisation (Skip these pages)

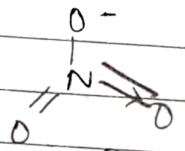
sp^2

Co-ordinate bond: Donor → (+) Recipient → (−)

NO_2^+ =

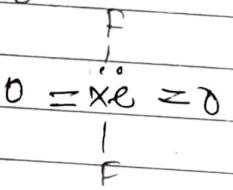
Hybridisation sp → ($\sigma + \pi_p$)

NO_3^- =



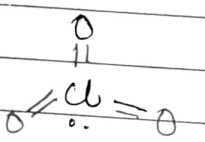
sp^2

XeO_2F_2 =



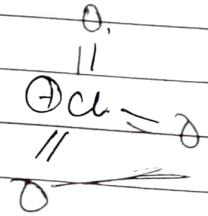
sp^3

ClO_3

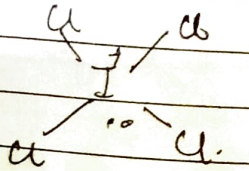


sp^3

ClO_3^+



$[ICl_4]^+$:



sp^3d

helps in selection of lowest energy structure.

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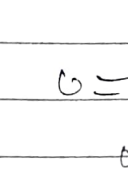
Formal Charge on an atom in a lewis Structure :

$$F.C = \left[\begin{matrix}\text{tot no. of valence} \\ e^- \text{ in free atom}\end{matrix}\right] - \left[\begin{matrix}\text{tot lone} \\ \text{pairs}\end{matrix}\right] - \frac{1}{2}[\text{shared } e^-s]$$

e.g. O_3 : $6 - 2 - \frac{1}{2}(6) = +1$

$F_C = [\text{valency} - \{\text{total no. of surrounding } e^-s\}]$

Note: SO_4^{2-} (perfectly tetrahedral)



Finding sigma bond & lone-pair :

XeF_5^+ = 8 + 7 × 5 − 1 = 42

Inert gas ← Valence electron

8 → to attain octet.

42 − 40 = 2 → 5 ← σ bond no.

2 → 1/2 → 2/2 → 1 lone pair.

Note :

XeF_2 → F − Xe − F (linear) (NO × 3)

XeF_4 → (square planar)

ClF_3 → (T-shaped)

NH_3 → (pyramidal)

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Hybridisation: $\sigma + lp =$ (steric no.) Hybridisation

steric no. ($\sigma + lp$)

2	sp → linear
3	sp^2 → Trigonal planar
4	sp^3 → Tetrahedron
5	sp^3d → TBP
6	sp^3d^2 → Oh.
7	sp^3d^3
8	sp^3d^4

Valence shell electron pair theory

VSEPR THEORY:

→ It decides shape of molecule on basis by electron pair repulsion.

ORDER OF VSEPR:

$l\text{-}p - l\text{-}p > lp - \pi$ bond pair $> lp - \sigma > \pi - \pi > \pi - \sigma > \sigma - \sigma$

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Resonance :

Delocalisation of (π e⁻)

π e⁻ → (e⁻) of π bond & conjugate lone pair.

conjugate lone pair:

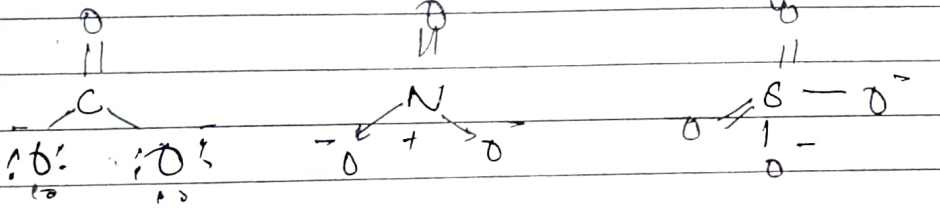
Condition :-

(i) π bonds must be conjugated

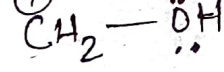
$CH_2=CH-CH=CH_2$

$CH_2=CH-CH=NO$

(ii) π bonds & lone-pair are conjugated.



(iii) l.p and vacant ('p' or 'd') orbitals must be conjugated



Resonance energy: (Metacardic) → one central atom

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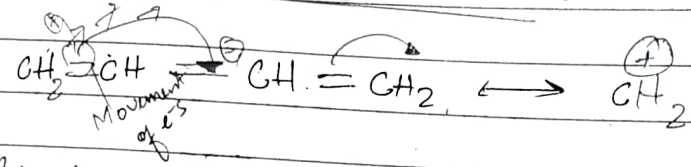
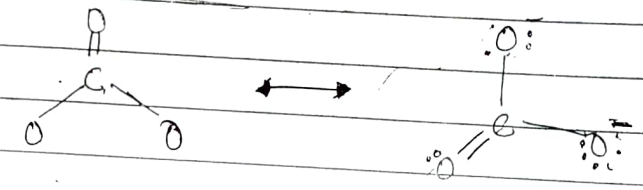
▲ Actual B.E – energy of most stable resonating structure

How to draw Resonating structure (or Canonical form)

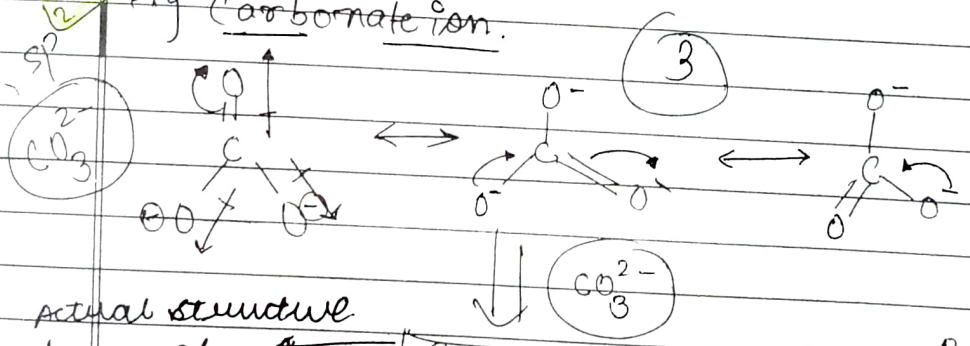
i) π bond to π bond movement



ii) lp to π bond

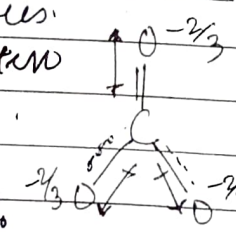


e.g Carbonate ion.



Actual structure of all different possible structures that can be written for the molecule.

(Resonance hybrid)



Partial π-character over the

Bond order $(\sigma+\pi) = \left(1+\frac{1}{3}\right) = \frac{4}{3}$

extra stabilized!

- Resonance energy ↑ Molecule ↑ Stability ↑
- R.E ∝ no. of resonating structures.
  ∝ no. of covalent bonds in a molecule.

formal charge: Respective charge on an atom.

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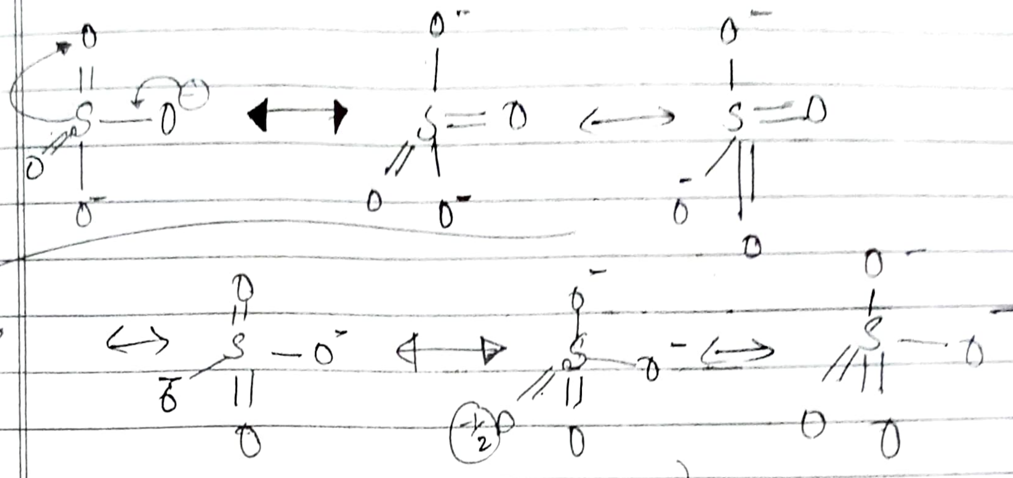
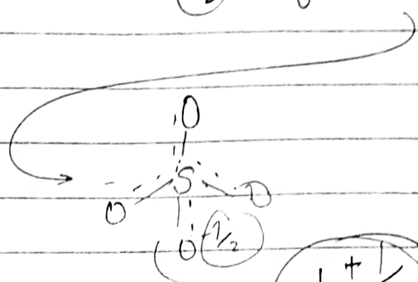


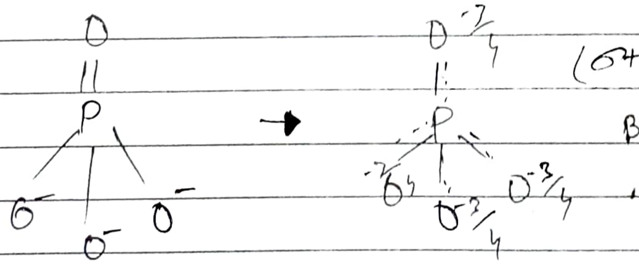


$1 + \frac{1}{2} = 1.5$

Bond order : Total no. of bonds / Surrounding atom in Reso...

Bond order : Total no. of bonds / No. of Surrounding atoms Involved in Resonance

PO_4^{3-}



$(\sigma + \pi)$

B.O (P–O)

$1 + \frac{3}{4} = \frac{5}{4}$

How to remember:

Borden = FB / SA

FB ← only those involved in resonance

SA ← only those involved in resonance

Borden ← Bond order.

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Calculated oxdn state → Maxm oxdn state

If C < M — X - X

(Calculated oxdn state < Maxm oxdn state)

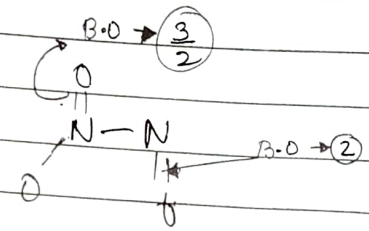
C = M — X - O - X

C > M — X - O - O - X

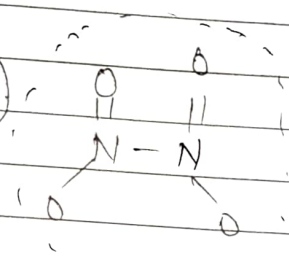
Peroxy linkage

NOTE:
An electron in an atomic orbital is influenced by one nucleus while in a MO it is influenced by two or more nuclei

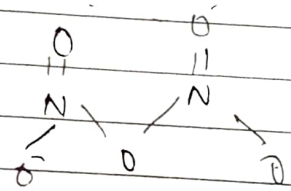
N_2O_3



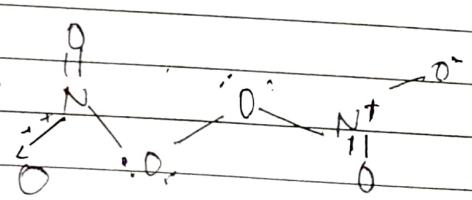
N_2O_4



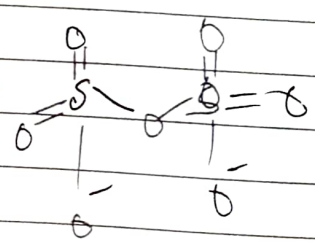
N_2O_5



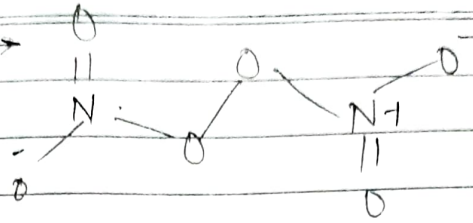
N_2O_6 →



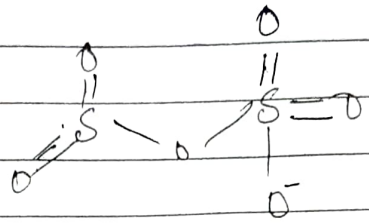
$S_2O_7^{2-}$ →



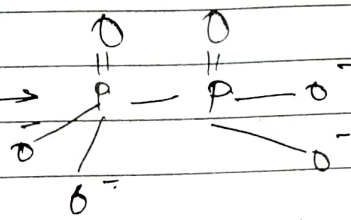
N_2O_6 →



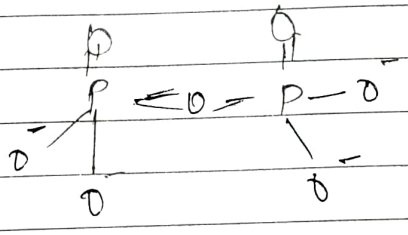
$S_2O_7^{2-}$ →



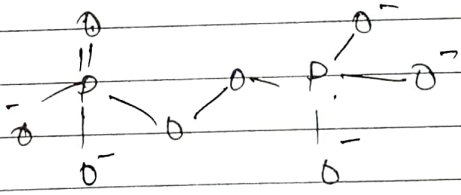
$P_2O_6^{4-}$ →



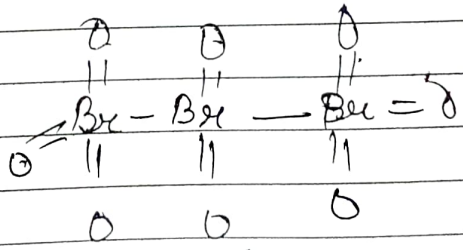
$P_2O_7^{4-}$



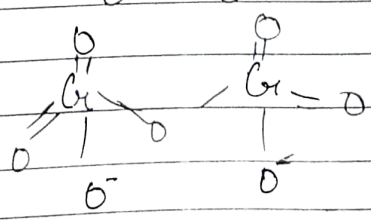
$P_2O_8^{4-}$



Br_3O_8 →



$Cr_2O_7^{2-}$



Factors:
* Hybridisation
* Lp
* E_N
* Size of surrounding atom

} for central atom

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i) If hybridisation same, then

No. of l.p at C.A $\propto \frac{1}{\text{Bond Angle.}}$

a) ClO_2^- < ClO_3^- < ClO_4^- | l.p at C.A ↑ B.A ↓

sp^3 sp^3 sp^3

l.p = 2 1 0

b) CH_4 > NH_3 > H_2O

sp^3 sp^3 sp^3

l.p 0 1 2

c) NO_2 < NO_2^- < NO_3^- ⇝ $NO_3^- > NO_2^- > NO_2$

sp^2 sp^2 sp^2

ii) E.N of C.A → E_N of C.A $\propto$ Bond angle.

A → E_N ↑ θ ↑ | E_N ↑ B.A ↑

B more B reputation

phosphine Arsine

$\ddot{N}H_3$ > PH_3 > AsH_3 > SbH_3

sp^3

No hybridisation

107° 93° 91° 90°

H_2O > H_2S > H_2Se > H_2Te

↓ 91°

104.5°

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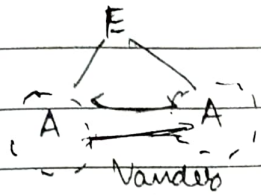
$NCl_3 > PCl_3 > AsCl_3 > SbCl_3$

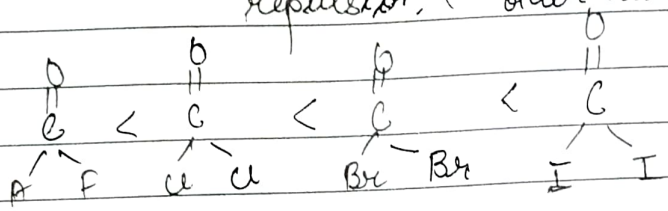
iv) Size of surrounding atoms $\propto$ Bond angle

Size ↑ B.A ↑

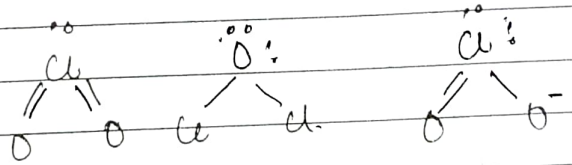


surrounding atom

repulsion, (encroach into each other Vander Waal's zone)



$ClO_2 > Cl_2O > ClO_2^-$



Surrounding atom same

L.P = 0

X

central atom

Regular Geometry :

In which L.P at C.A is zero and all surrounding atoms are same.

e.g. BF_3, BCl_3, BBr_3, BI_3, CO_3^{2-}, SO_4^{2-}, ClO_4^-, CrO_4^-, MnO_4^-, MnO_4^{2-}

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In the regular geometry having molecules bond ∠'s are same if they have same hybridisation.

sp^2 → then - 120°

sp^3 → then - 109°28'

Q> Order of bond angle :

a> CH_4, CCl_4, $SiCl_4$, PO_4^{3-} Ans :- $CH_4 = CCl_4 = SiCl_4 = PO_4^{3-}$

b> H_2O NH_3 PH_3 H_2S Ans → $NH_3 > H_2O > PH_3 > H_2S$

c> SO_2 SO_3 SO_3^{2-} SO_4^{2-} Ans :- $SO_3 > SO_2 > SO_4^{2-} > SO_3^{2-}$

	SO_2	SO_3	SO_3^{2-}	SO_4^{2-}
	sp^2	sp^2	sp^3	sp^3
lp	1	0	1	0

Q.) NO of 180° & 90° in B.A :

BrF_3

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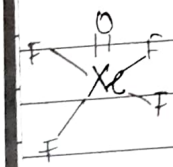
Q> No. of 120° B.A in.

Structure		lp	Hybridisation	6+4 Geometry	Shape	B.A
Q>	$POCl_3$	0	sp^3	Tetrahedron (To)	Tetrahedron (To)	< 109.5
	XeF_4	2	sp^3d^2	Oh	Square planar	
	$XeOF_4$	1	sp^3d^2	Oh	Square pyramidal	< 90
I—I—I	I_3^-	3	sp^3d	TBP	linear	180
Q	ClO_2^+	1	sp^2		V-shaped	

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Valence Shell Electron Pair Repulsion Theory

→ Proposed by ~~Sidwick~~ Sidgwick & Powell, Further it was developed by Gillespie & Nyholm.

* Geometry of molecule depends upon valence shell electrons i.e σ bond or π-bond or lone-pair.

* Valence shell electron pair i.e bonds repel each other in a molecule so they arrange themselves in such a way that repulsion becomes minimum & dist becomes maximum.

Double bond occupy more space

* Bond-pair occupy less space & lone pair occupy less space so bond-pair - lone pair exert more repulsion than bond pair (electron cloud of lone pair is dispersed)

why is e⁻ cloud of lone pair dispersed?

Sol: l-p - l-p repulsion ↑

Order of VSEPR:

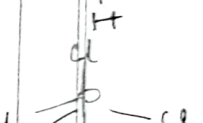
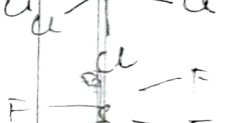
l.p > δ

l.p - l.p. > l.p - π > π - π. > π - δ > δ - δ

VSEPR → sp^3d → Trigonal Bi-pyramidal

equatorial | axial

* l.p occupy equatorial position
* More E.N → AXIAL
* Double bonds → More space → equatorial.

Molecule.	V.S.E.P.R.	Geometry	Shape	L.P.	B.A.	Examples	Structure.
AB_2	2 (6+4)	linear B-A-B	linear	0	180°	$BeCl_2$ (gas)	Cl—Be—Cl
AB_3	3	Trigonal planar	Trigonal planar.	0	120°	BX_3, AlX_3	
AB_4	4	Tetrahedral (& Td)	Td.	0	109°28'	CH_4, $SiCl_4$, CCl_4 etc	
* AB_5	5	Trigonal Bipyramidal (TBP)	(TBP).	0	120°, 180°	PCl_5, PF_5 etc.	
AB_6	6	Octahedron.	Oh	0	90°, ~~180°~~ (Axial)	SF_6, SiF_6^{2-}, PF_6^-	
$\ddot{A}B_2$	3	Trigonal planar	~~Trigonal~~ Bent (V-shaped)	1	<120°	SO_2.	
$\ddot{A}B_3$	4	Td	Pyramidal.	1	<109°28'	NH_3, PF_3 etc	

due to repulsion by L.P.

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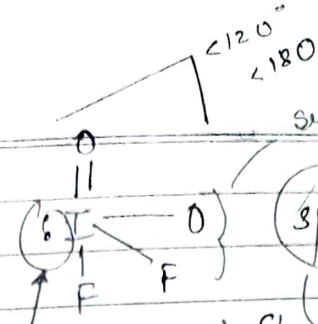
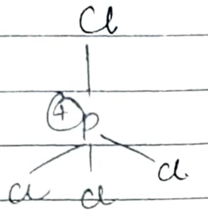
* $IO_2F_2^{\ominus}$ →



sp^3d

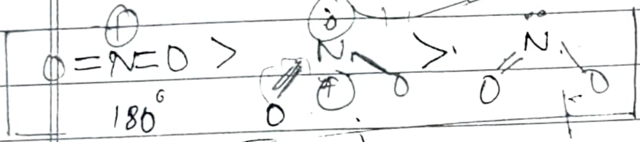
$\frac{7-(1+1+1+1+1)}{2} = 1 = lp$ Shape: See-saw. TBP

* $PCl_4^{\oplus}$ →



sp^3 Td

B.A Q) NO_2^+ NO_2 NO_2^- ?



Note:

* electron pair = 4 → AB_4 → Td, sp^3, R.G e.g ⇒ CH_4, CCl_4
  → $\ddot{A}B_3$ (Pyramidal), sp^3 e.g ⇒ NH_3, PCl_3
  → $\ddot{\ddot{A}}B_2$ → Bent or V-shaped, sp^3 e.g H_2O,

* $\bar{e}$ pair = 5 → AB_5 → TBP, sp^3d, eg, PCl_5, PF_5
  → $\ddot{A}B_4$ → See saw, sp^3d, eg → SF_4, $IO_2F_2^-$, $ICl_2^{\oplus}$
  → $\ddot{A}B_3$ → T-shaped, sp^3d eg ClF_3, $XeOF_2$
  → $\ddot{A}B_2$ → linear, sp^3d, e.g I_3^-

Internuclear axis should pass through (Max^m e⁻ density)

e⁻ cloud

orbitals

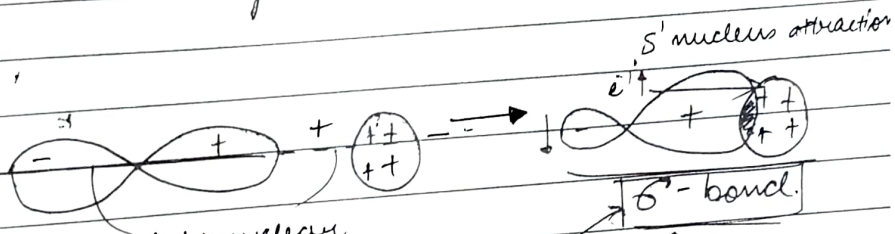
ATOME

Types of Overlapping:

a) Axial overlapping or Head-on overlapping: (AXIAL)

→ When atomic orbitals overlap along their internuclear axis then this is called axial overlapping. This forms σ bond and because in this type extent of overlapping is more so σ bonds are stronger than π bonds.

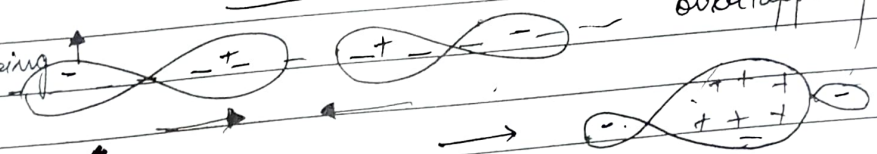
e.g.



Axial:

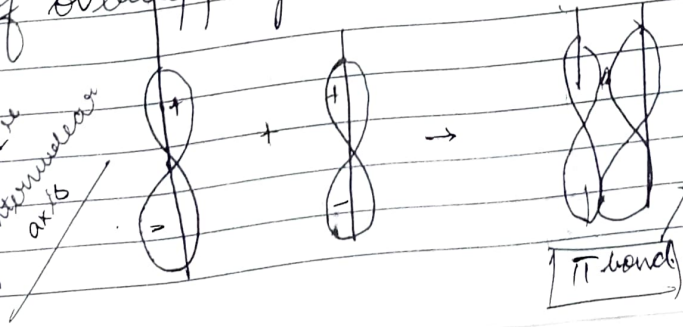
Extent of overlapping ↓

Bond Strength ↑



b) Sidwise overlapping: (Colateral overlapping) (CO-LATERAL)

→ When orbitals overlap along the Ir axis of inter-nucleus. This results in π-bond and in this extent of overlapping is less so π bond is weak.



Extent of $p\pi - p\pi$ overlapping $\propto$ $\frac{1}{\text{Lewis Acid character}}$

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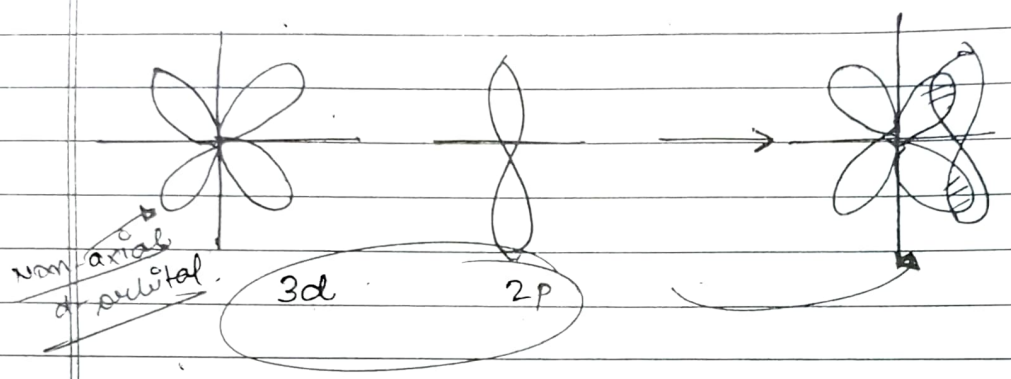
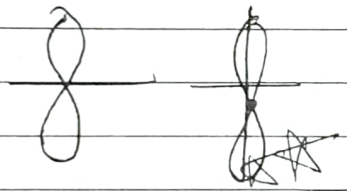
L.A ↑ $p\pi - p\pi$ overlapping ↓

Extent of side-wise overlapping:

$\boxed{2p-2p} > 2p-3p > 3p-3p$

↑ rarely seen





size ↑ overlapping ↓

$2p-2p > \boxed{2p-3d} > 2p-3p > 3p-3p$

Note: ** s-orbital always forms $\boxed{\sigma \text{ bond}}$.
They can never form π-bond while p and d orbitals can form, σ and π both.

Bond →
- σ } s-s, s-p, p-p } Axial
- π } p-p, p-d } Lateral
- δ → only d-d overlapping

(-ve overlapping) → no bond condition

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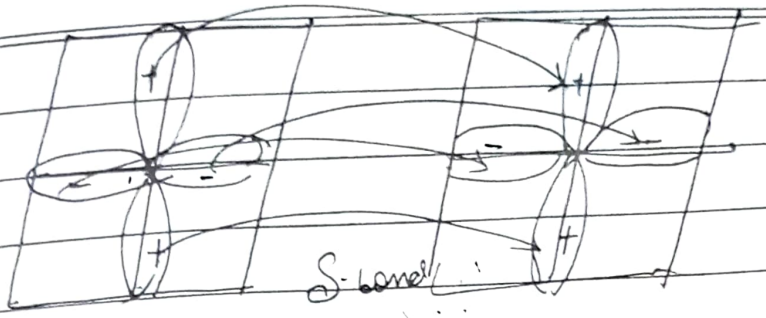
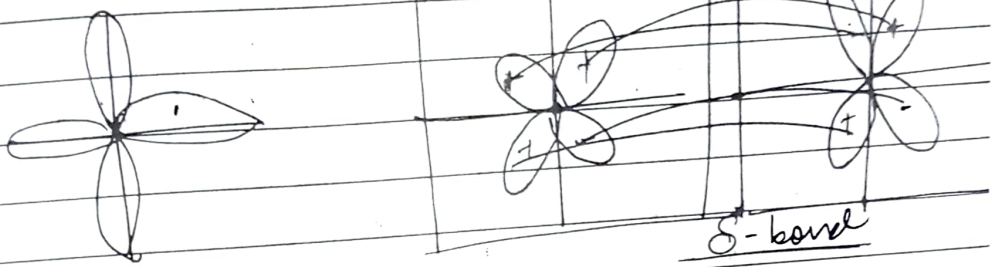


δ-bond



δ-bond

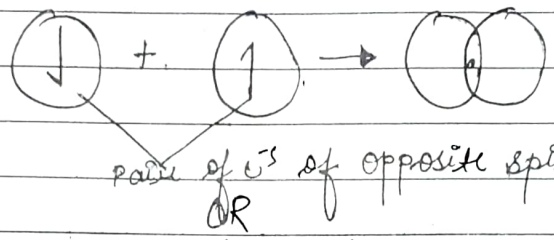
$p_x - p_y$ orbital can never overlap.

Orbitals.	Axis.	Type of bond.
p_x & p_x	x y z	~~No bond~~ π ~~No bond~~ π bond
p_x & p_y	x y z	No bond
p_x & d_{xy}	x y z	No bond π- bond No-bond
p_y & $d_{x^2-y^2}$	x y z	No bond π bond.
d_{xy} & d_{xy}	x y z	π π δ

(6)	$d_{z^2-y^2}$ & $d_{x^2-y^2}$	X Z Y	6 8 6

Condition of overlapping :-

* combining atomic orbital must have one electron each with opposite spin



pair of e⁻s of opposite spin

OR

One orbital is fully filled and another orbital is vacant.

(fully filled + vacant) orbital

fully filled + vacant

Drawbacks of VBT :

* It explains bond formation, strength of bond and stability of molecule but it does not explain shape and geometry of molecule.

Explained by VSEPR.

VBT:
* bond formation
* strength of bond
* stability of molecule

VSEPR:
Shape of molecule and geometry

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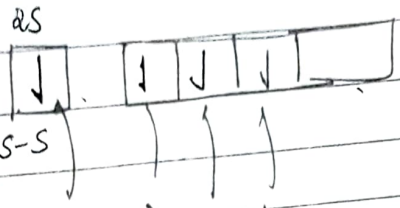
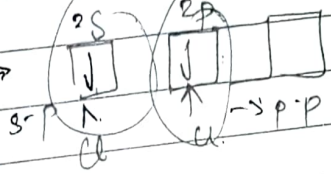
Formation of molecule according to VBT:

* H_2 → 

* CH_4 → C → 

* $BeCl_2$ → Be → 

Need of Hybridisation:

* According to VBT, methane or any other molecule should have different type of overlapping different bond strength but actually in a molecule all bonds are identical i.e explained by hybridisation

Hybridisation:

* It is the process in which atomic orbitals of an atom with nearly same energy are mixed and redistributed their energy and result equal no. of new orbitals with same energy, same size, same shape.
* These new orbitals are called hybrid orbitals.

Bonding lobe

Anti-bonding lobe

Note: Extent of overlapping ↑ More stronger bond ↑

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Characteristics

* It is a hypothetical process.

* Only valence orbitals but not e^-s take part in the hybridisation and final orbital may be fully-filled, half-filled or vacant

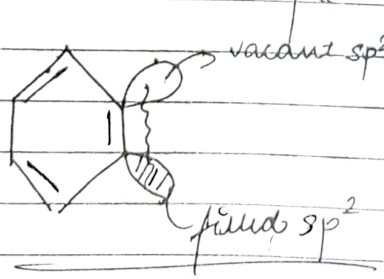
Participation of valence orbitals

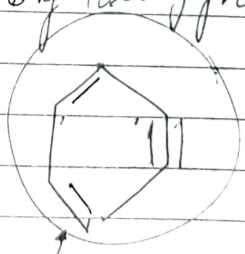
* No. of formed hybrid orbitals will be equal to no. of atomic orbitals which take part in the hybridisation.

* Hybrid orbitals are more directional than pure orbitals, so hybrid orbitals have more extent of overlapping. so they form more stronger bond.

Directional nature

* NOTE: Hybrid orbitals generally form σ bond. They do not form π bond. but there is some exception e.g Benzyne





Structure of Benzyne

(σ) strength > (π) bond

H·O

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examples of hybridisation

1) sp

e.g $BeCl_2$, CO_2, CS_2

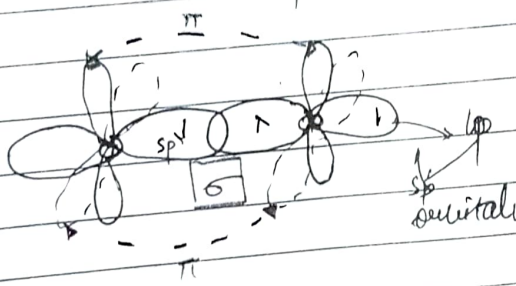
s + P_x / P_y + P_z

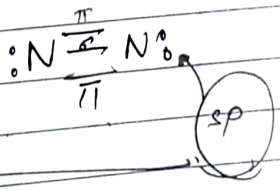
structure: linear

$:N \equiv N:$

N_2 → 1s | ↑↓ | ↑ | ↑ — Unhybridised: 2

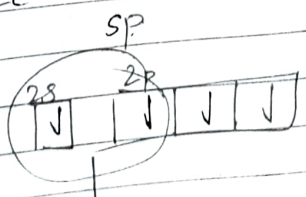
2sp





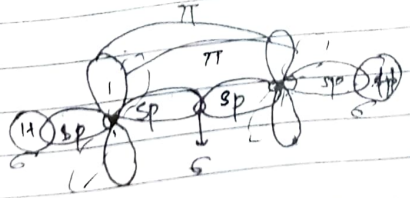
sp - sp

e.g $H-C \equiv C-H$



π-bonds are weak as extra p orbitals overlapping

2sp



Oxygen → e(-ve)

contraction of ~~orbitals~~

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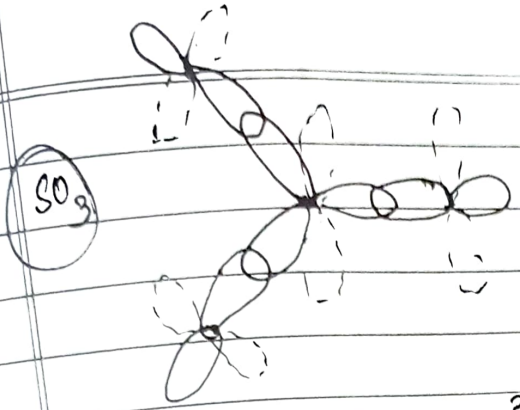

3σ

3π (1 p-π)
(2 - dπ - pπ)

a) if hybridisation is sp^3 then all π bonds are dπ-pπ.

b) if hybridisation < sp^3 then
no. of dπ-pπ = (n - 1)
↑ total π bonds

NOTE:

How to calculate no. of dπ-pπ bonds

↓

i) hybridisation → < sp^3
⇓
(n-1) total π bonds

sp^3d SO_2 → sp^2 → (1)

PO_4^{3-} → sp^3 → (1)

Cl_2O_7 → sp^3 → 6

ClO_4^- → sp^3 3

SO_3^{2-} → sp^3 → (1)

SO_4^{2-} → sp^3 → (2)

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* sp^3d → $s + p_x + p_y$ + $p_z + d_{z^2}$ (max...)

$3sp^2$ $2pd$

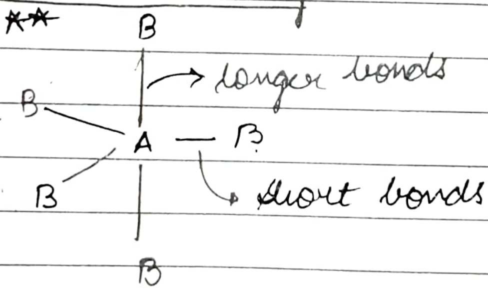
TBP

*** a) sp^3d or TBP molecules do not have all the bonds identical but 3 equitorial bonds have sp^2 & two axial bonds have pd hybridisation.

Equatorial bonds have s-character, so they are stronger bonds, less bond length while axial bonds are weaker & have longer bond length.

Take example of double bond

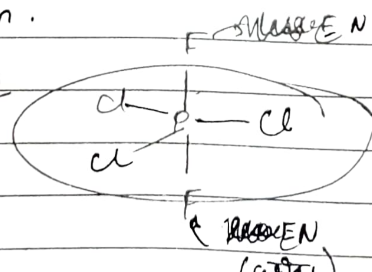
**



$EN\uparrow$ axial position

c) More EN atom occupy axial position while less EN atom occupy equatorial position.

e.g PCl_3F_2



← Cl → EN ↓ size ↑ (120° से है) less repulsion

$P(CH_3)_2F_3$ →

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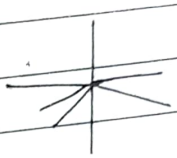
sp^3d^2 → Oh (Octahedron)

$$S + P_x + P_y + P_z + d_{x^2-y^2} + d_{z^2}$$

$\underbrace{\quad\quad\quad\quad\quad\quad}_{6\ sp^3d^2}$ → all are equal.

e.g SF_6, SiF_6^{2-}, PF_6^-, AsF_6^-, SbF_6^-

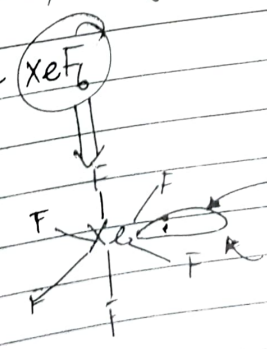
sp^3d^3 → Pentagonal bipyramidal



$$S + P_x + P_y + P_z + d_{x^2-y^2} + d_{xy} + d_{z^2}$$

$$S + \underbrace{P_x + P_y + d_{x^2-y^2} + d_{xy}}_{6\ sp^2d^2 \text{ form pentagon.}} \ \&\ \underbrace{P_z \ \&\ d_{z^2}}_{\text{axial.}}$$

e.g IF_7 & XeF_6



lp is stereochemically inert.

capped octahedral or distorted octahedral

B.P. → axial
→ equatorial

Bent's rule:

(Axial → P character ↑)

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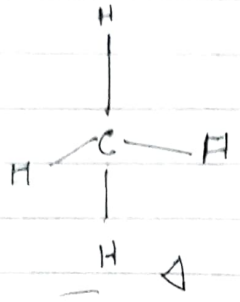


(BASIL)

S% ↑ L ↓

Bond length

Axial

→ More electronegative atom attached to hybrid orbital (H.O) that has more p-character & less s-character.

→ B.P and π bond occupy eq. hybrid orbitals (H.O) that has more s character and ~~more~~ less p-character

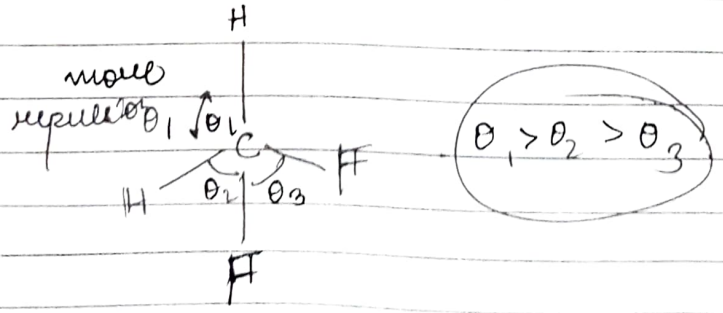
$$\cos\theta = \frac{s}{s-1} = \frac{p-1}{p}$$

→ As we know;

as θ ↑ % s character ↑ ~~size of HO ↓~~ ~~size of H~~

% p character ↓

B.E ↑ B.L ↓



$\theta_1 > \theta_2 > \theta_3$

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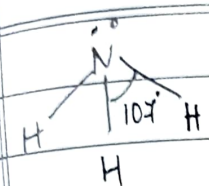


$\cos 107^\circ = -0.3$

$-0.3 = \frac{S}{S-1}$; $0.3 = \frac{P-1}{P}$

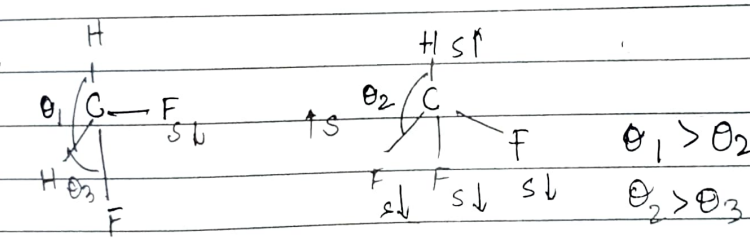
$P = 0.64$

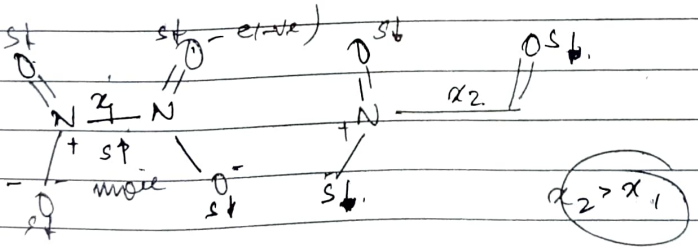
$S = 0.23$

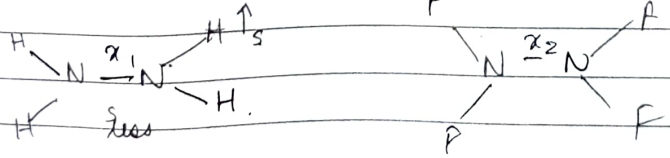
23 %.

(< 25 %.)

sp

(Q) 

(Q) 

(Q) 

NOTE: opp overlap → destructive
same overlap → constructive

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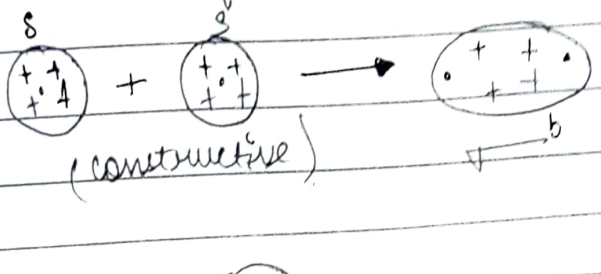
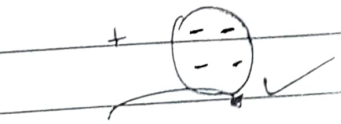
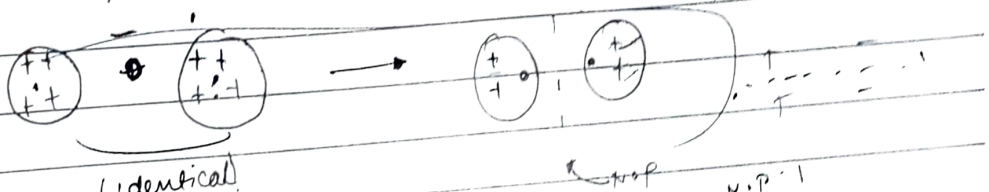
Formation of MO:

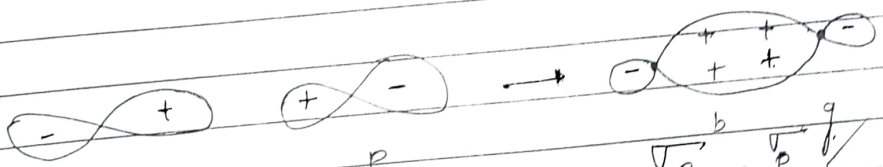


Gerade
→ same sign of Ψ along nucleus
→ Opp sign of Ψ along nucleus

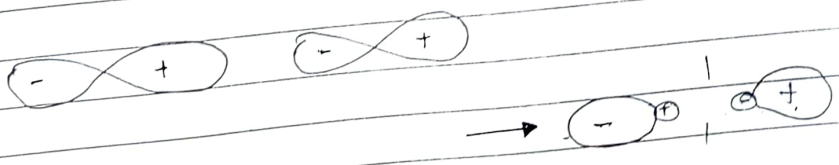


NO nodal plane

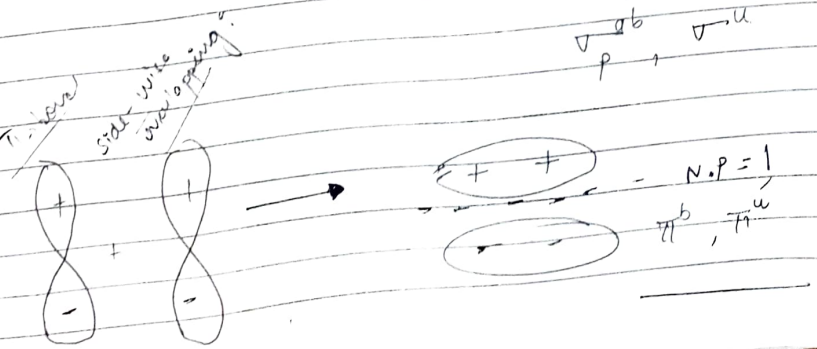




N.P = 0



N.P = 1



Gerade or ungerade orbitals are designated for identical ones.

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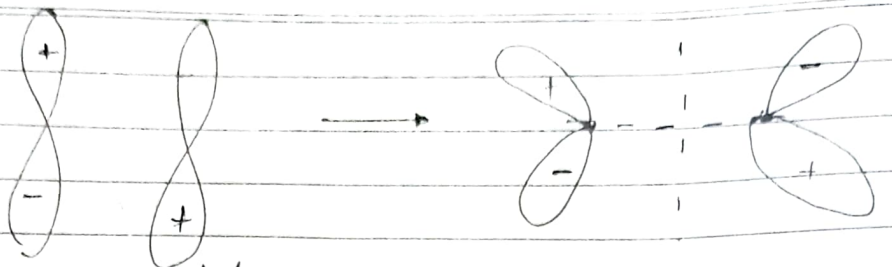
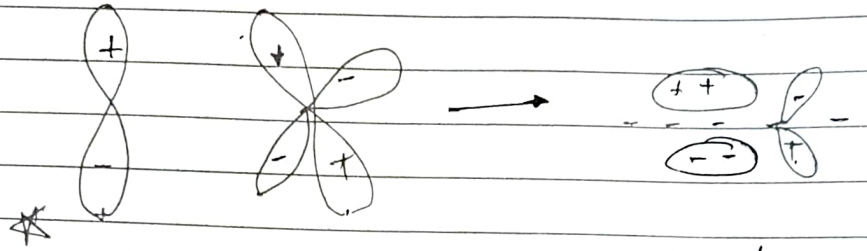


Negative overlapping → A·O ↑ favours major bonding part ξ

N·P : 2 ↑ e density ↓

π^{ab} or π^{*}, π^{g}



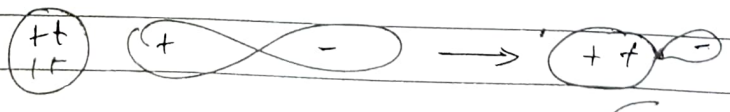
$p_\pi - d_\pi$

N·P : 1

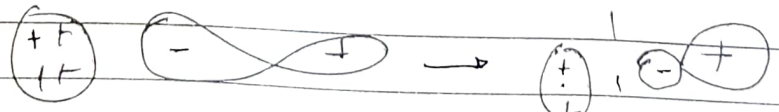
(σ). (σ^*)

σ — σ^{b}_{ab} - gerade
σ^{ab} - ungerade

π — π^{b} - ungerade
π^{ab} gerade



σ_{sp}



N·P

σ_{sp}

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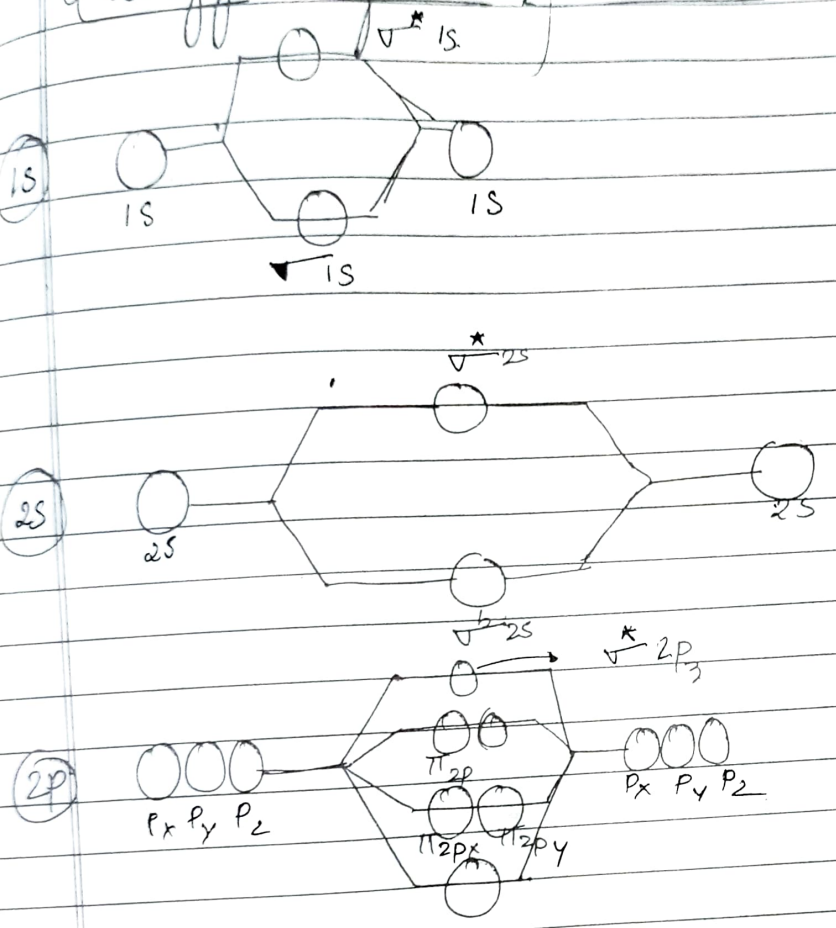
Energy diagram for M.O.



s-p mixing

excitation

Boron, Carbon, Nitrogen

For B_2, C_2, N_2 → 14 e⁻s system

$\sigma_{1s} < \sigma^*_{1s} < \sigma_{2s} < \sigma^*_{2s} < \pi_{2p_x} = \pi_{2p_y} < \sigma_{2p_z} < \pi^*_{2p_x} = \pi^*_{2p_y} < \sigma^*_{2p_z}$

Due to s-p mixing the energy of π_{2p_x} & π_{2p_y} is lowered than σ_{2p_z}

σ_{2p_z} is lowered than $\sigma^*_{2p_z}$