Hybridisation -

It is given by Pauling.
acc. to overlapping theory diff. covalent bond in molecule are different
e.g - in $BeCl_2$

$$Cl \overset{S-P}{—} Be \overset{P-P}{—} Cl,$$

both Be - Cl are different in nature but experimentally it is found that both bond are same in nature so it does not explain by overlapping theory so new concept for explation of formation of covalent bond given by pauling and that is hybridisation

→ mixing of diff. orbitals and redistribution of energy to form same no. of new orbitals those have same energy and shape. This new orbitals are called Hybrid orbitals. In case of $BeCl_2$

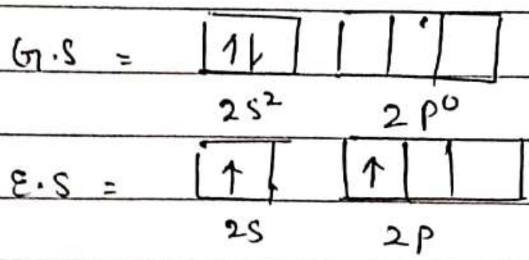
$$Cl \overset{P-SP}{—} Be \overset{SP-P}{—} Cl$$

Type of Hybridisation -

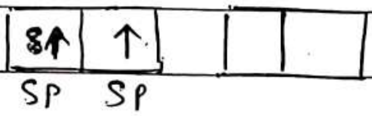
1) S-P hybridisation.
1 no S + 1 no P ⟶ 2 no. S-P hybrid orbitals

for e.g. Formation of $BeCl_2$
(Be)(4) :-

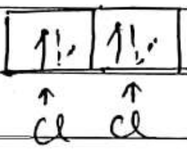
★ shape linear bond angle - 180



At hybridisation state



formation of $BeCl_2$ =



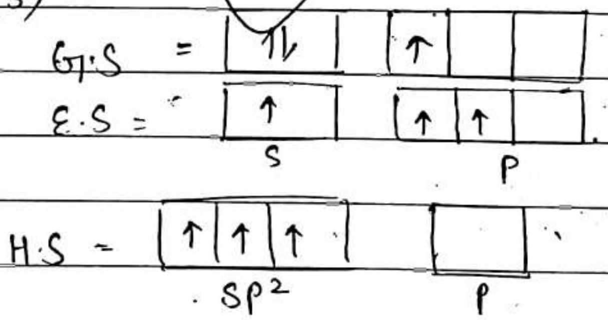
2) SP^2 hybridisation

1S + 2P ⟶ 3 no. of SP^2 Hybrid orbitals

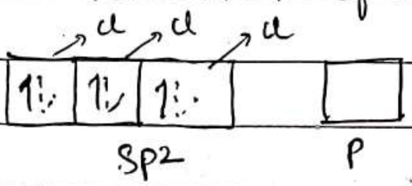
Shape - trigonal planes - bond angle - 120°

ex - BCl_3

B(5)



formation of BCl_3

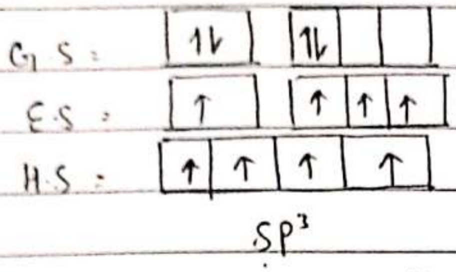


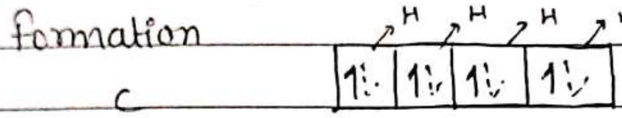
3) sp^3 Hybridisation

1S + 3P ⟶ $4sp^3$ hybrid orbitals

example CH_4

C(6)





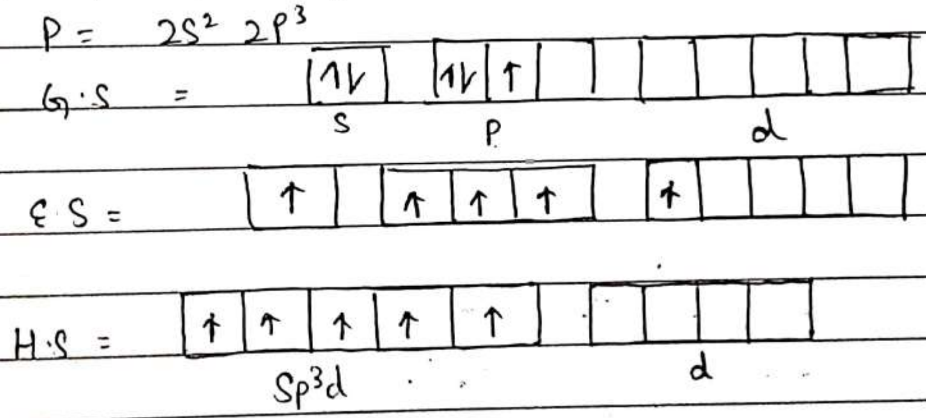
Shape - tetrahedral bond angle - 109°28'

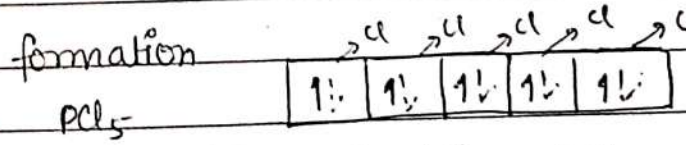
4) Sp³d Hybridisation

1S + 3P + 1d ⟶ 5 sp³d hybrid orbitals

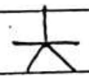
example PCl_5

P = $2S^2$ $2P^3$





Shape - Trigonal bipyramid



Note - In hybridisation process empty orbitals, unpaired e⁻ orbitals, lone pair orbitals can be participant.

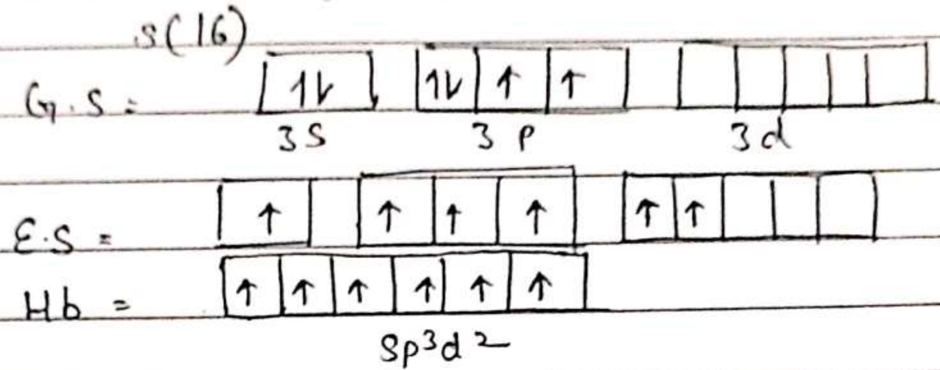
In coordination compound - empty orbitals participate in hybridisation process

★ Hybridisation - No. of bond atom + no. of lone pair

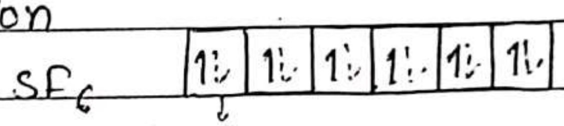
lone pair - valence e⁻ - bond atom + (-ve charge) - (+ve charge)

5) sp^3d^2 Hybridisation -

e.g. formation of SF_6



formation



Shape — octahedral

Some Examples are :-

i) NH_4^+

$4 + (5-4) - 1$

sp^3

ii) SO_4^{-2}

$4 + (6-8) + 2$

$4 - 2 + 2 = 4$

sp^3

iii) I_3^-

$3 + (7-3) + 1$

$3 + 2 + 1 = 6$

sp^3d^2

iv) CO_3^{2-} ✓

$3 + (4-6) + 2$

sp^2

v) N_3^-

$3 + (5-3) + 1$

$3 + 1 + 1$

sp^3d^1

vi) BF_3

$3 + (5-3)$

$3 + 1$

sp^3

vii) PCl_5

$5+(5-5)$

sp^3d

viii) IF_5

$5+(7-5)$

$5+1=6$

sp^3d^2

ix) IF_7

$7+(7-7)$

sp^3d^3

x) H_3O^+

$3+(6-3)-1$

$3+3-1$

$3+\textcircled{2} \rightarrow$ lone e^-

$3+\underset{\downarrow}{1} = sp^3$

lone pair

xi) NO_3^-

$3+(5-6)+1$

$3+2$

sp^2

xii) SO_4^{2-}

$4+(6-8)+2$

$=4$

sp^3

xiii) ClO_4^-

$4+(7-8)+1$

$4+3+1$

$4+2=6$

sp^3d^2

xiv) CH_3^-

$3+(4-3)+1$

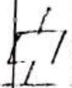
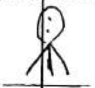
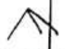
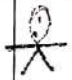
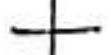
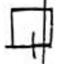
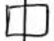
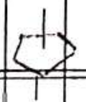
sp^3

☺ VSEPR : Valence shell Electron Pair Repulsion Theory :-

Acc. to this theory if any lone pair available in molecule than lone – pair – lone pair repulsion is higher as compare to lone pair – ~~lone~~ bond pair and bond – pair – bond pair subsequently.

$l.p - l.p > l.p - b.p > b.p - b.p.$

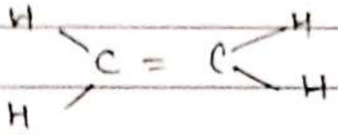
14/08

Types of molecules	No. of bond atom	No. of lone pair	H.B	electronical Geometry	Molecular Geometry (shape)	Bond Angle	Example
AB_2	2	0	SP	Linear		180	$BeCl_2$
AB_3	3	0	Sp^2	Trigonal planer		120	BCl_3
AB_4	4	0	Sp^3	T.H		109°28'	CH_4
AB_5	5	0	Sp^3d	Trigonal pyramid			
AB_6	0	0	Sp^3d^2	Octahedral			SF_6
AB_2L	2	1	Sp^2		 bend shape		SO_2
AB_3L	3	1	Sp^3		 Pyramidal	≅ 108	NH_3
AB_2L_2	2	2	Sp^3		 bent		H_2O
AB_4L	4	1	Sp^3d		 See saw		
AB_2L_3	3	2	Sp^3d		T. shape		
AB_2L_3	2	3	Sp^3d		 linear	180'	I_3^-
AB_5L	5	1	Sp^3d		 square pyramidal		
AB_4L_2	4	2	Sp^3d^2		 square planer		
AB_7	7	0	Sp^3d^2		Pentagonal biplanar		

i) CH_4

$4\sigma \rightarrow sp^3$

ii) $CH_2 = CH_2$



3σ bond of Carbon

$- sp^2$

iii) C_2H_2 or $H-\overset{sp}{C}\equiv\overset{sp}{C}-H$

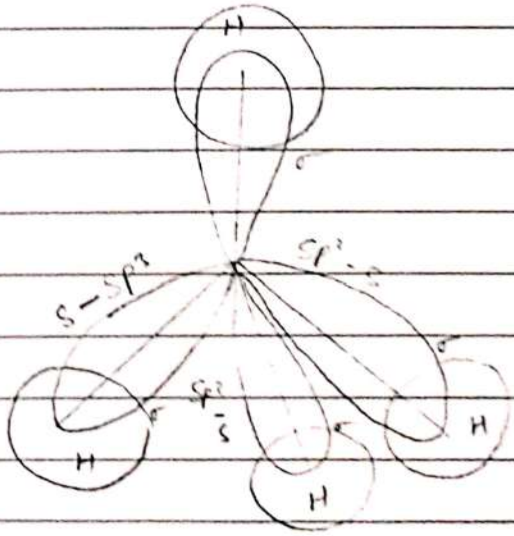
$2\sigma \rightarrow sp$

iv) C_3O_2 (Carbon suboxide)

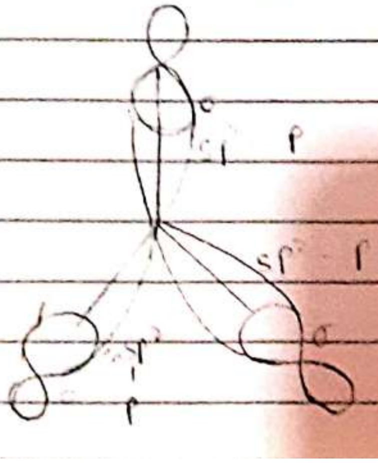
$O=\overset{sp}{C}=\overset{sp}{C}=\overset{sp}{C}=O$

Hybrid Molecular structure of CH_4 :→

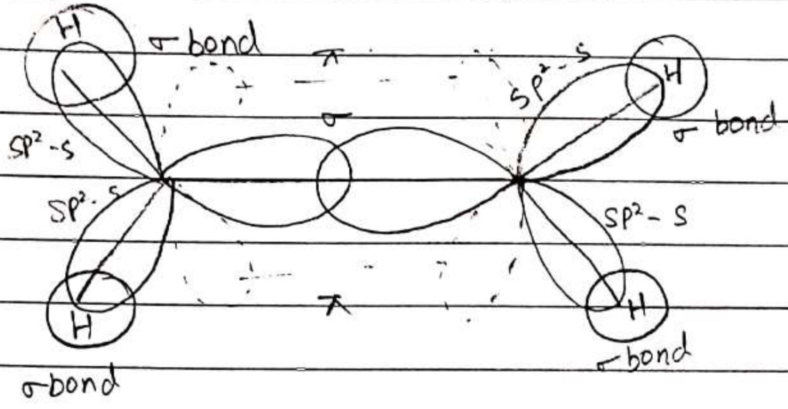
a) CH_4



b) BCl_3

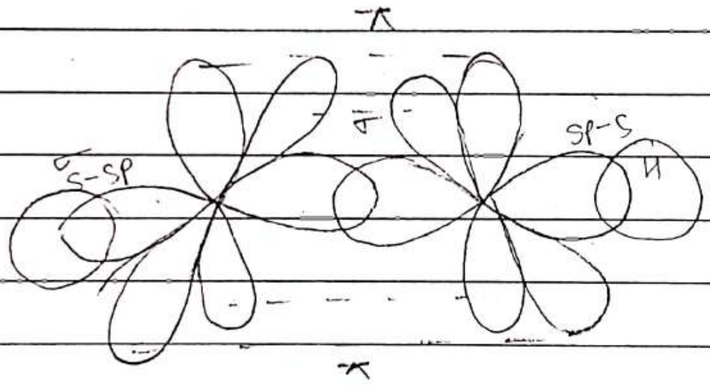


c) $\overset{sp^2}{CH_2} = \overset{sp^2}{CH_2}$

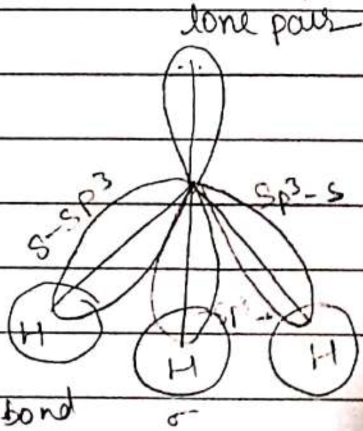


p_z forms π bond side - side.

d) C_2H_2 (CH = CH)



e) NH_3
sp^3



✓

Que Methane, Ammonia and water have sp^3 hybridisation but bond angle and shape are different in all three molecules. Why?

Ans Due to lone pair.

CH_4 - 0
NH_3 - 1
H_2O - 2

Que CO_2 and linear but SO_2 is bent in nature. Why?

no lone pair — 1 lone pair

sp, Linear. — sp^2, bent shape

Limitations of Hybridisation theory (V.B.T) -

a) It does not explain magnetic properties of molecules or ions.

b) It does not tell us why bond order of molecules or ions should be in fraction.

c) It does not explain increasing or decreasing order of stability of molecules or ions.

* Molecular Orbital Theory :-

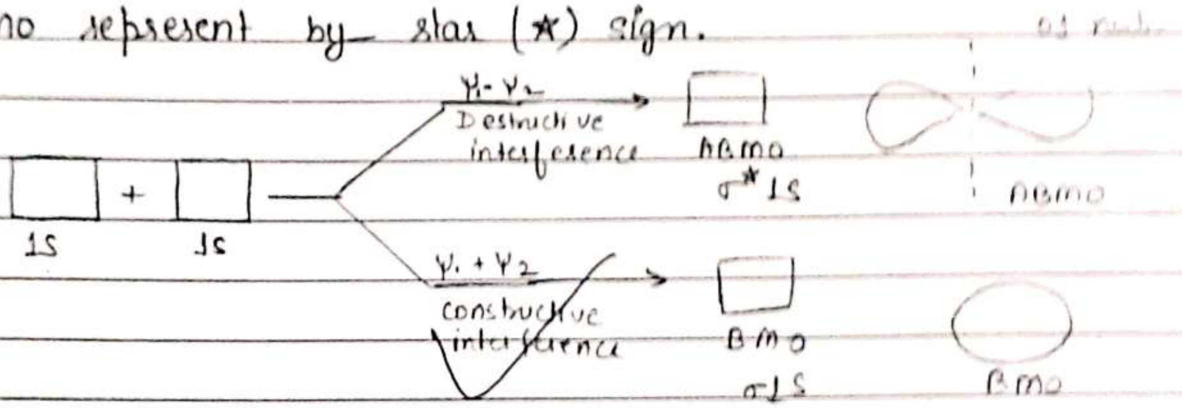
a) This concept is given by Hund.

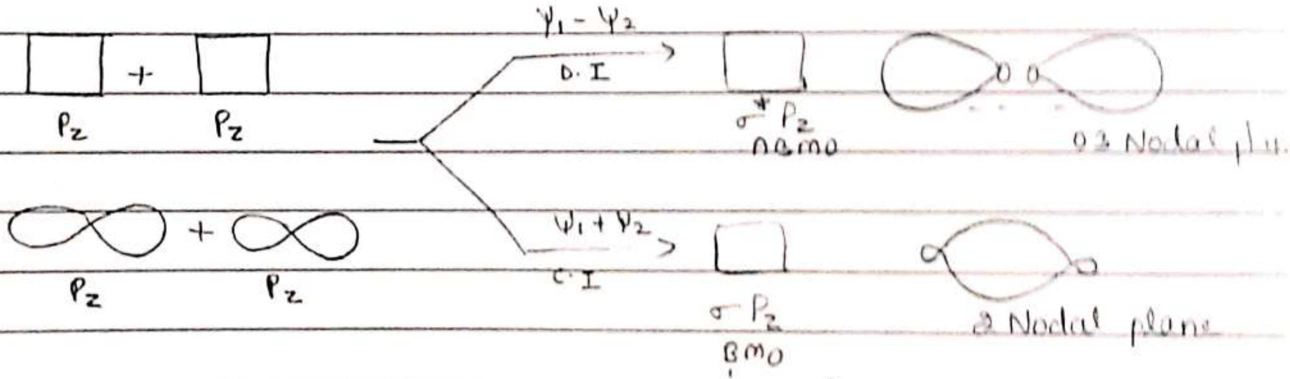
b) Acc. to this theory, atomic orbitals form same no. of bonding molecular orbital (B.M.O) and anti-bonding molecular orbital (ABMO)

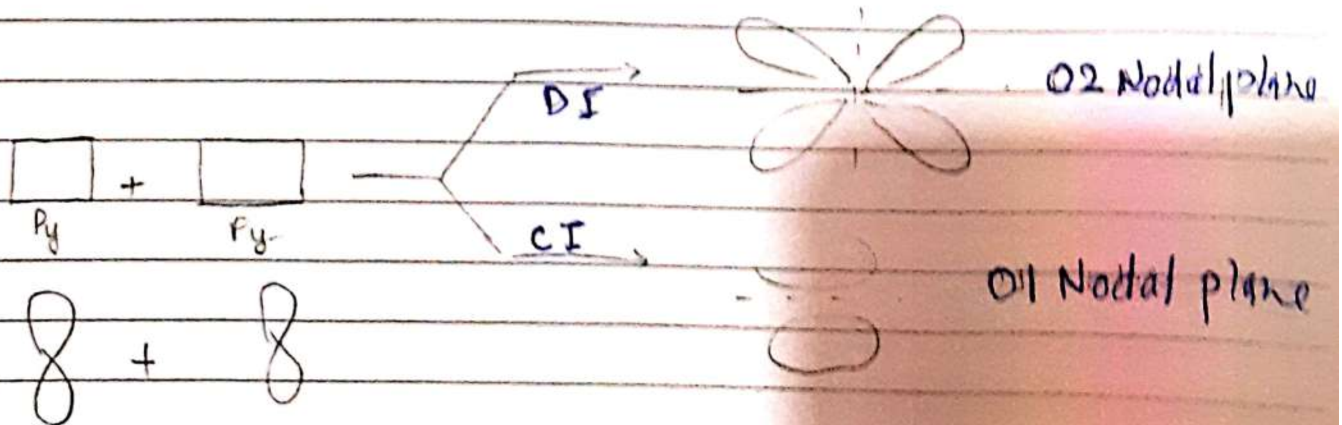
c) B.M.O form due to constructive interference of atomic orbitals and ABMO formed due to destructive interfere of atomic orbitals.

d) B.M.O have lower energy as compare to A.B.M.O So B.M.O is more stable and favour formation of molecule

e) A.B.MO represent by star (★) sign.



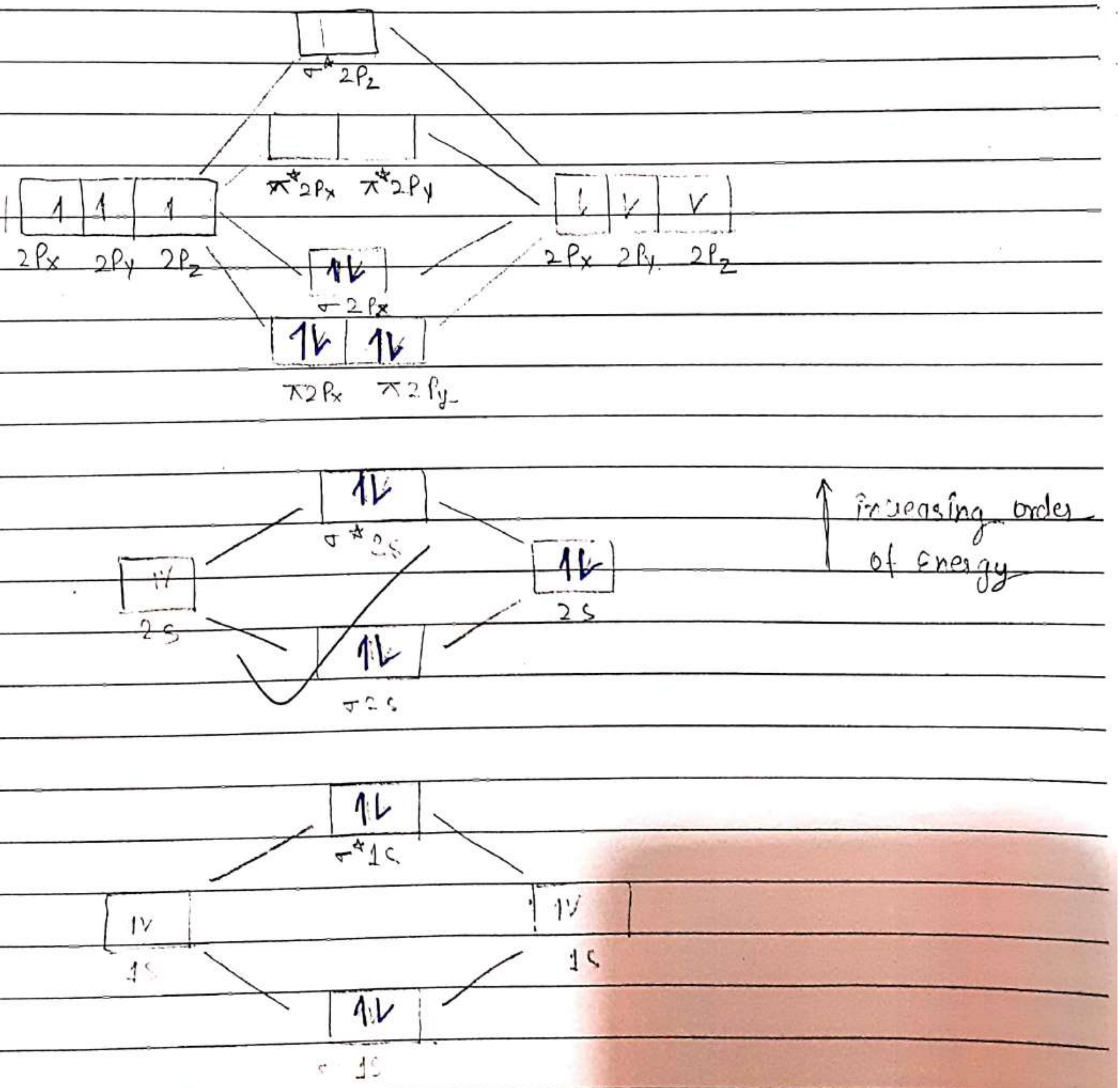




→ Electrons are filled in molecular orbital acc. to Afbau Principle, Hund's rule and Pauli Exclusion rule.

→ (n+l) rule not follow in M.O.T

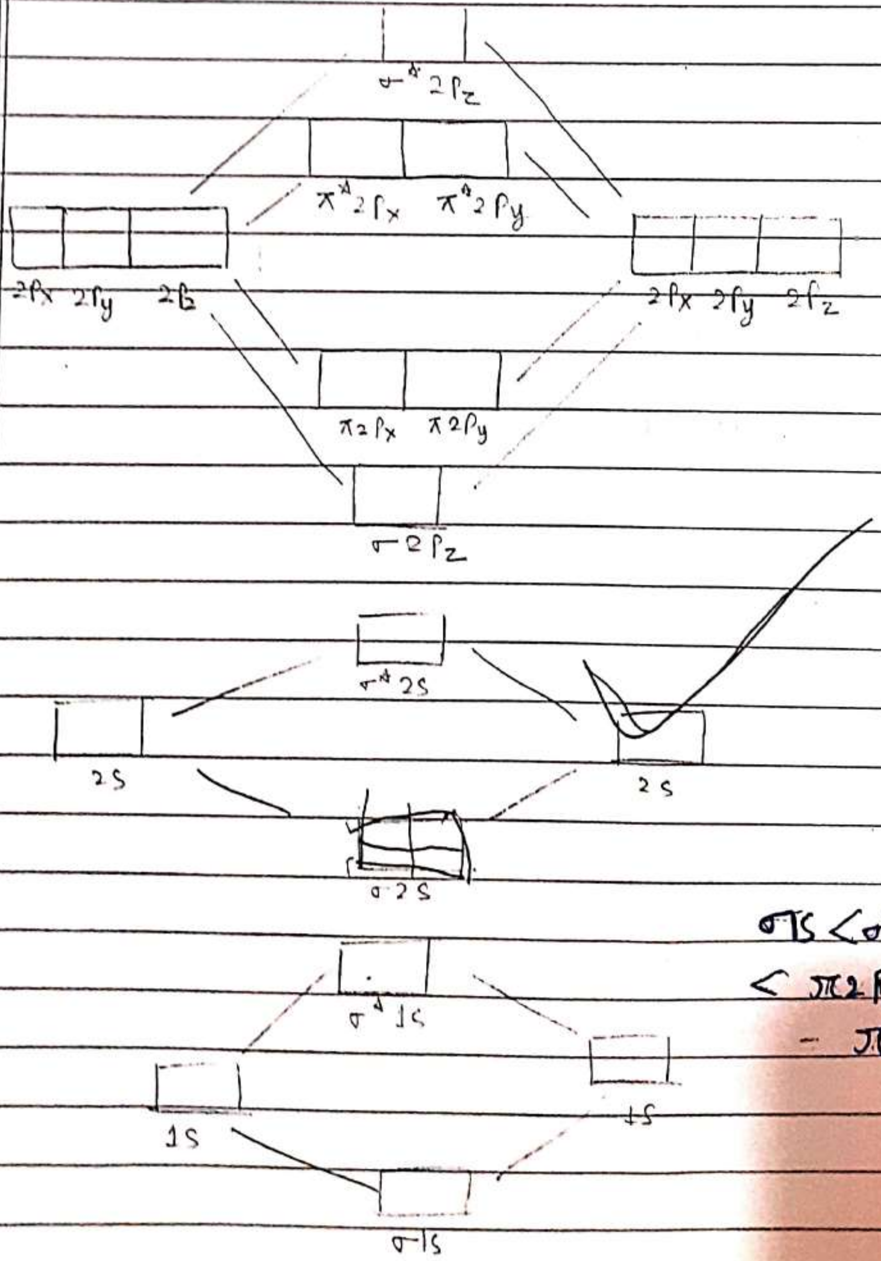
→ Molecular orbital diagram for Hydrogen to Nitrogen can be ~~drop~~ draw as following –



$\sigma 1s < \sigma^* 1s < \sigma 2s < \sigma^* 2s < \pi 2p_x = \pi 2p_y < \sigma 2p_z < \pi^* 2p_x$
$= \pi^* 2p_y < \sigma^* 2p_z$

The correct electronic configuration for molecular orbital till Nitrogen can be written as ↑

→ for oxygen and Flourine molecule, Molecular orbital diagram written as.



$\sigma 1s < \sigma^* 1s < \sigma 2s < \sigma^* 2s < \sigma 2p_z$
$< \pi 2p_x = \pi 2p_y < \pi^* 2p_x =$
$= \pi^* 2p_y < \sigma^* 2p_z$

According to molecular orbital theory diagram, we can find out bond order of molecules or ions.

$$\text{Bond order} = \frac{N_B - N_A}{2}$$

Here,

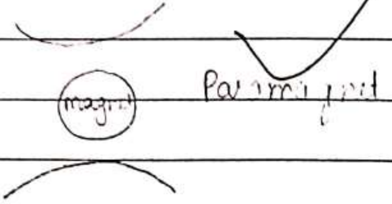
N_B = no. of e^- in bonding molecular orbital
N_A = no. of e^- in Anti bonding M.O

We can also find out that molecule or ions should be stable or unstable

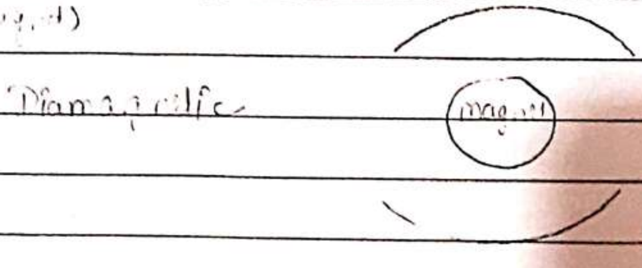
If ....

$N_B > N_A \longrightarrow$ Stable
$N_B < N_A \longrightarrow$ unstable
(does not exist)

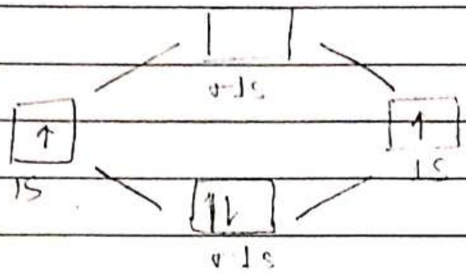
→ If unpaired e^- are available in M.O.T diagram then molecules or ions are paramagnetic in nature.
(Those substance which attract towards magnet in presence of magnetic field)



→ If paired e^- are available then atoms or molecules are diamagnetic in nature.
(repulsion of magnet)

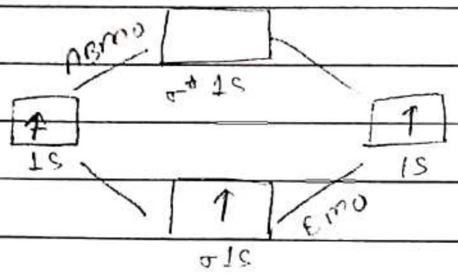


Que Write down the increasing order of stability, bond order, bond length in following - H_2, H_2^+, H_2^-



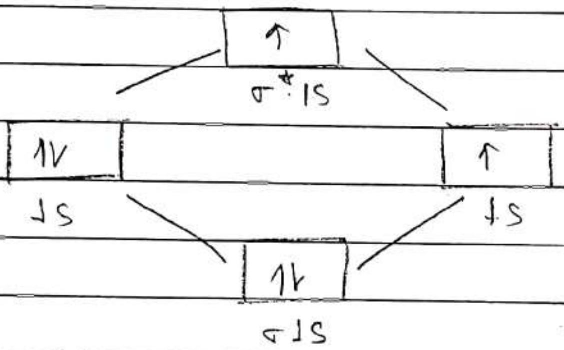
B. order = $\frac{2-0}{2} = 1$

H — H



Bond order = $\frac{1-0}{2}$

$= 0.5$



Bond order = $\frac{2-1}{2}$

$= 0.5$

★ Bond order ↑ Bond length ↓ Stability ↑

Increasing order of bond order :-

$H_2^- = H_2^+ < H_2$

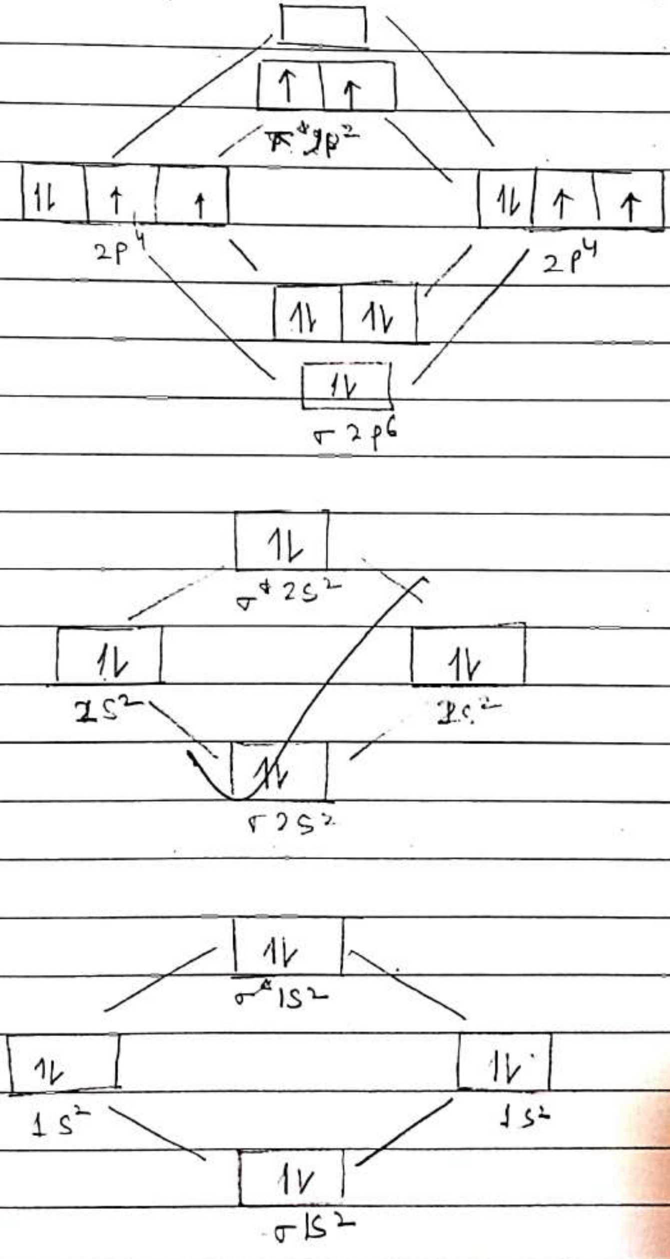
Bond length = $H_2 < H_2^+ < H_2^+$

~~Note :-~~

Stability = $H_2^- < H_2^+ < H_2$

Note :- If bond order is equal then those molecule or ions are more stable which have less no. of antibonding molecular orbital electron or which having highes positive charge.

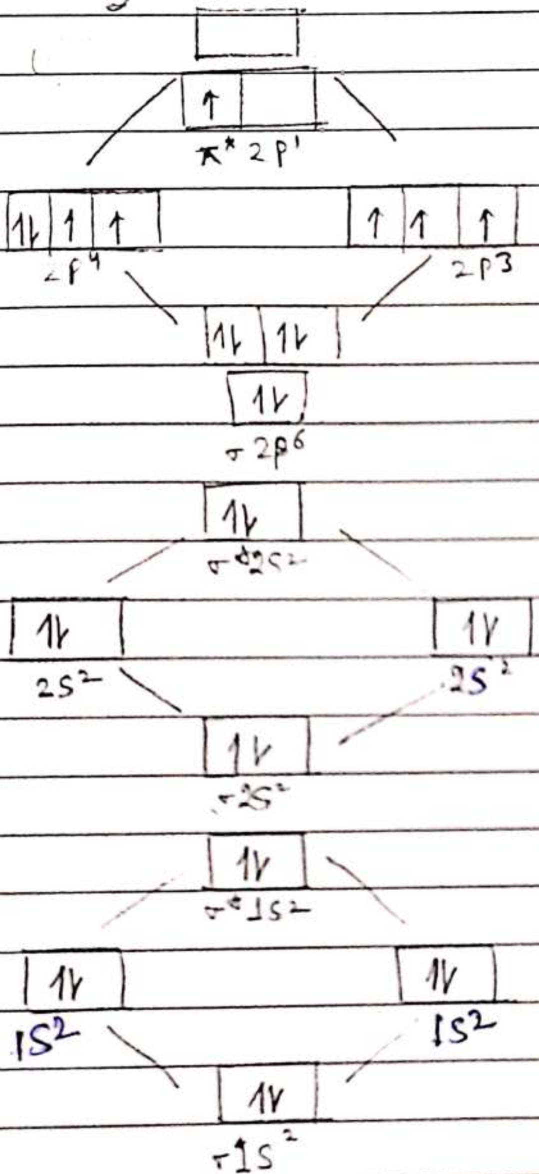
Que O_2, O_2^{+1} are paramagnetic but O_2^{-2} is diamagnetic in nature. Explain with M.O.T



2 unpaired e^- ∴ paramagnetic

$$B.O = \frac{10-6}{2} = 2.$$

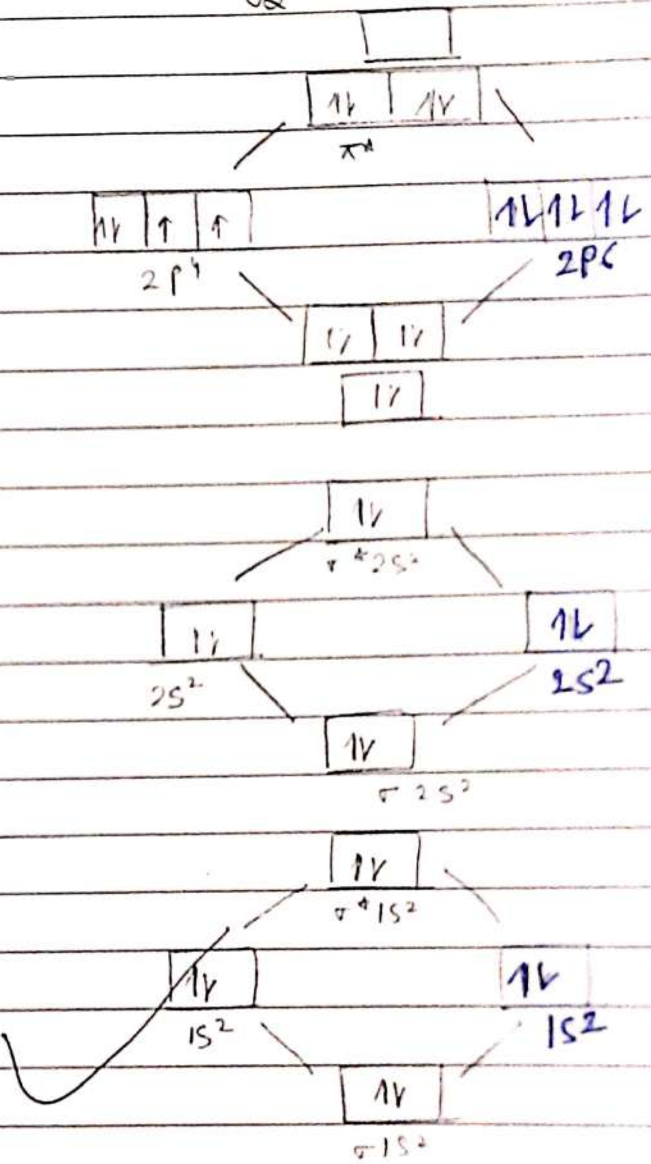
O_2^+



$B.O = \frac{10-5}{2} = 2.5$

1 unpaired e^- - paramagnetic

O_2^{-2}



$B.O = \frac{10-8}{2} = 1$

No unpaired e^-

diamagnetic

→ O_2 have 2 unpaired e^- and O_2^+ have 1 unpaired e^- so those are paramagnetic in nature but O_2^{-2} have paired e^- so that is diamagnetic in nature

Qu Write down the molecular orbital Electronic configuration for O_2 gas.

Ans $\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \sigma 2p_z^2, \pi 2p_y^2 = \pi 2p_x^2 ; \pi^* 2p_y^1 = \pi^*$

molecule/ ions	molecular Orbital Electronic confi.	N_B	N_A	B.O	Stability	mag. Property
B_2	$\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \pi 2p_x^1 = \pi 2p_y^1$	6	4	1	Stable	Paramagnetic
C_2	$\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \pi 2p_x^2 = \pi 2p_y^2$	10	4	3	Stable	Diamagnetic
N_2	$\sigma 1, \sigma^* 1$ [illegible] $, \pi 2p_x^2 = \pi 2p_y^2, \sigma 2p_z^2$	12	4	4	Stable	Diamagnetic
N_2^+	[illegible] $\sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \pi 2p_x^2 = \pi 2p_y^2, \sigma 2p_z^1$	9	4	2.5	Stable	Paramagnetic
[illegible] 14 N_2^-	$\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \pi 2p_x^2 = \pi 2p_y^2, \sigma 2p_z^2, \pi^* 2p_x^1$	10	5	2.5	Stable	Paramagnetic
NO	$\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \sigma 2p_z^2, \pi 2p_x^2 = \pi 2p_y^2, \pi^* 2p_x^1$	10	5	2.2	Stable	Paramagnetic
NO^+	$\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \sigma 2p_z^2, \pi 2p_x^2 = \pi 2p_y^2$	12	4	4	Stable	Diamagnetic
NO^-	$\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \sigma 2p_z^2, \pi 2p_x^2 = \pi 2p_y^2, \pi^* 2p_x^2$	12	6	3	Stable	Diamagnetic

Magnetic Moment

$$\mu = \sqrt{n(n+2)} \text{ BM}$$

(Bohr Magneton)

Here n = no. of unpaired e^-