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11th Class Chemistry

**Chemical Bonding and Molecular
Structure**

By Palnivel ahir

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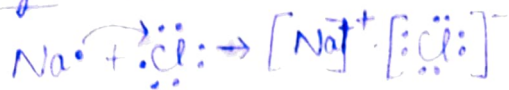
CHAPTER-4

Difference B/w Electrovalent bond (Ionic) and Covalent bond.

Ionic Bond

→ Ionic bond is a bond is formed by the complete transference of a certain number of e^- 's from one atom to another atom.

e.g:- NaCl.



↓
Electrostatic force of attraction.

→ They are Normally Solids.

→ There is strong force of attraction b/w ions.

→ Their Melting and boiling Points are high.

→ They conduct electricity in aqueous solution or in the molten state.

Covalent bond

→ It is formed of same or different elements combine by mutual sharing of electrons.

e.g:- H_2 , O_2 , HCl .



H H.

H-H.

→ They are Solid, liquid, or gas.

→ There is ~~also~~ relatively weak force of attraction.

→ Their Melting and boiling Points are very low.

→ They do not conduct or generally they are bad conductors.

Fajan rules [Ionic Compound]

=> In an Ionic Compound if the Polarising Power is high as well as Polarizability is high, there will be more of Covalent character less of Ionic character.

For Example:- NaCl :- it is a ionic compound.



In Na^+ ($P^+ = 11$, $e^- = 10$).

Now $P^+ > e^-$ \therefore the nuclear Power will be more.

Small

Size of

Cation

its nuclear Power is high

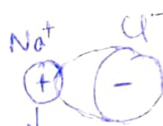
(Polarizing Power increases.)

In Cl^- ($P^+ = 17$, $e^- = 18$).

Now $P^+ < e^-$ \therefore the size will increase.

Large Size of Anion (Polarizability increases)

its nuclear Power is low.



Nuclear Power is higher than Cl^- nuclear Power. So it will start attract from Cl^- and it forms a bond like a Covalent bond.

Polarizing Power :- Tendency to attract electron cloud [e^- cloud].

Polarisability :- The tendency of an ion to get distorted. (or Tendency of e^- cloud to bend)

Cation :- Smaller Size of cation greater Polarizing Power.

Anion :- Greater Size of Anion greater Polarizability.

For Example :- (i) ~~NaCl~~, ~~LiCl~~ Here Li^+ has more Polarizing Power than Na^+ .
(Size of $\text{Li}^+ < \text{Size of Na}^+$) \therefore LiCl has more Covalent character than NaCl .

(ii) NaCl , NaBr .
(Size of Br^- is more than Cl^-) \therefore Br^- has more Polarizability than Cl^- .
 \therefore NaBr has more Covalent character than NaCl .

(iii) FeCl_2 , FeCl_3

Fe^{2+} , Fe^{3+}

(Size of $\text{Fe}^{3+} < \text{Fe}^{2+}$) \therefore Fe^{3+} has more Polarizing Power than Fe^{2+} .

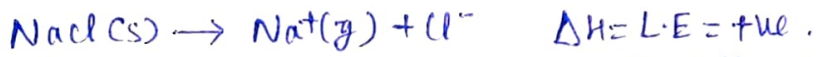
\therefore FeCl_3 has more Covalent character than FeCl_2 .

Lattice Energy :- The energy released when one mole of ionic compound is formed from its ions in their gaseous state. (3)



or.

The Energy required to completely separate a mole of solid ionic compound into gaseous ions.



(Endothermic Reax).

$$L.E = \frac{k q^+ q^-}{r_c + r_a}$$

where q^+ = charge of cation, r_c = Radius of cation, q^- = " " anion, r_a = " " Anion.

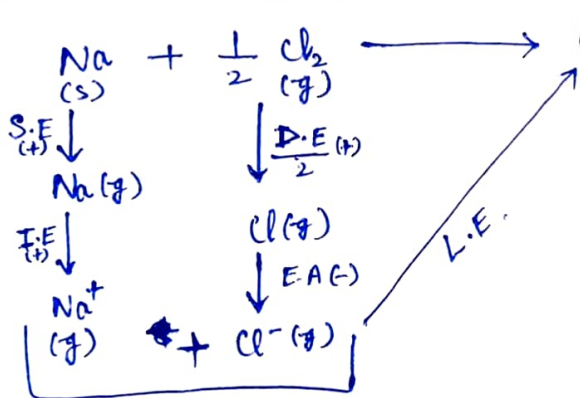
$L.E \propto q^+$ $2^+ \text{ MgCl}_2 < 3^+ \text{ AlCl}_3$	$L.E \propto q^-$ $\text{Al}_2\text{O}_3 < \text{AlN}$ $\downarrow \quad \quad \downarrow$ $\text{O}^{2-} \quad \quad \text{N}^{3-}$	$L.E \propto \frac{1}{r_c}$ Size of atom (cation) decreases. L.E increases. $\text{LiF} > \text{NaF}$.	$L.E \propto \frac{1}{r_a}$ Anion size decrease. L.E increases. $\text{KBr} > \text{KI}$ $\downarrow \quad \quad \downarrow$ Small than I.
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→ Lattice energy is directly proportional to charge of ion (cation ~~and~~ anion).
 (L.E $\propto q^+ q^-$)

→ Lattice energy is inversely proportional to size of ions.
 $L.E \propto \frac{1}{r_c + r_a}$

Born Haber Cycle :- For Formation of ionic compound e.g. Na^+Cl^- .

(ΔH_f = Heat of formation (Heat Released))



$$\Delta H_f = S.E + I.E + \frac{D.E}{2} - E.A - L.E.$$

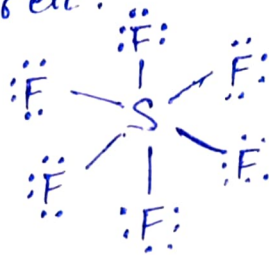
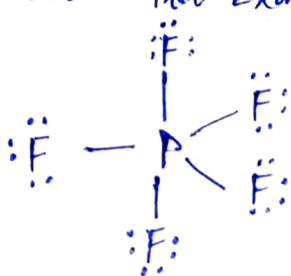
- Where S.E = Sublimation energy.
- I.E = Ionization energy.
- D.E = Bond Dissociation energy.
- E.A = Electron affinity.
- L.E = Lattice energy.

Limitations of octet Rule :-

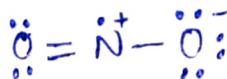
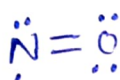
(5)

The Rule failed to predict the Shape and Relative Stability of molecules.

- It is based upon the inert nature of noble gases. However, some noble gases like Xenon and Krypton form compounds such as XeF_2 , KrF_2 etc.
- The element present in Third period have more than eight valence electrons around the central atom - For Example: PF_5 , SF_6 etc.



- The octet rule is not satisfied for all atoms in a molecule having an odd no. of e^- 's for Ex. :- NO and NO_2 .



- This rule cannot be applied to those compounds in which the no. of e^- 's surrounding the central atom is less than eight. Eg:- $LiCl$, BeH_2 , $AlCl_3$ etc.

Dipole Moment :-

It is the Product of the magnitude of charge on anyone of the atoms of distance b/w them.

$$\mu = e \times d$$

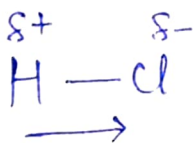
Where μ = Dipole moment.

e = charge on anyone of the atoms.

d = distance b/w the atoms.

Its unit in C.G.S system is Debye (D).

Example:-



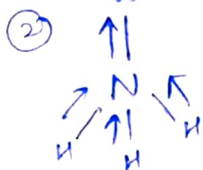
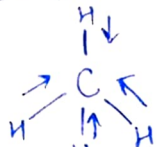
(Dipole moment has a magnitude and a Direction).

- (1) ⇒ It is vector quantity and Points towards more electronegative atom.



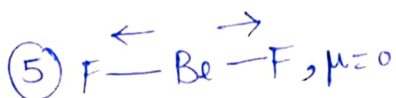
Example:-

(1) CH_4 .

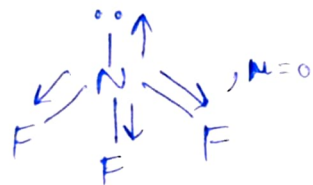


(vector sum in the same direction hence dipole moment will be more.)

(Same Reason)



(6)



(vector sum in the opposite direction, hence dipole moment will be zero).

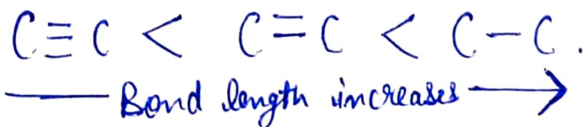
Bond Parameters

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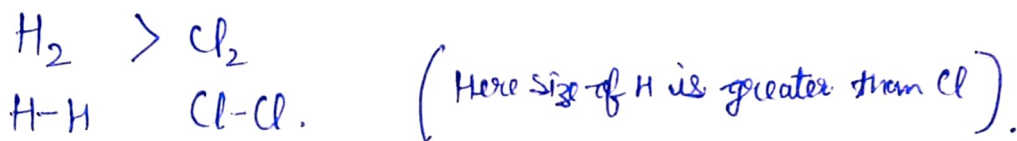
⇒ Bond length :- It is the average distance b/w the centres of the nuclei of two bonded atoms in a molecule.

⇒ Bond length depends upon the following factors :-

1) → Bond length decreases with increase in bond multiplicity.

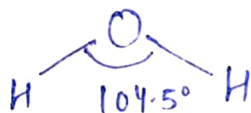


2) → Size of the Atom :- The bond length increases with increase in the size of the atom.



⇒ Bond angle :- It is the average angle b/w the orbitals of the central atom containing the bonding e⁻ pairs in the molecule. It is expressed in degree/minute/second.

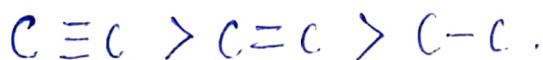
For Example :- The H-O-H (Bond angle in H₂O is 104.5°)



⇒ Bond Dissociation energy :- The amount of energy is required to break one mole of bonds of particular type b/w the atoms of a molecule in the gaseous state.

→ Depends upon following factors :-

1) Bond Multiplicity :- Bond dissociation energy increases with increase in Bond Multiplicity.



← Bond Dissociation energy →

2)

or It is no. of Bonds B/w two atoms in a molecule. (7)

Bond order :- It is a measurement of the number of e⁻s involved in bonds b/w two atoms in a molecule.

→ Most of the time, bond order is equal to the no. of bonds b/w two atoms. (Exception occur when the molecule contains antibonding orbitals).

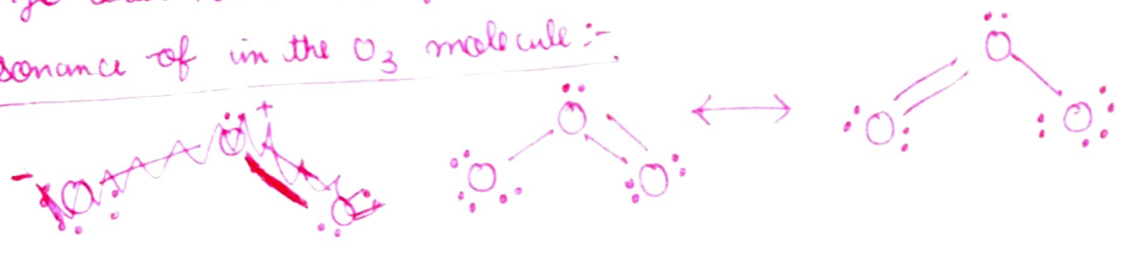
⇒ Bond order = $\frac{[\text{No. of Bonding e}^- - \text{no. of antibonding e}^-]}{2}$

If bond order = 0, the two atoms are not bonded.

~~For Example~~ For Example H-H, O=O, N≡N, C≡N
 B.O = 1 B.O = 2 B.O = 3 B.O = 3.

Resonance :- (The Displacement of e⁻ in this way that bond change their position to get more stable structure).

Resonance of in the O₃ molecule :-

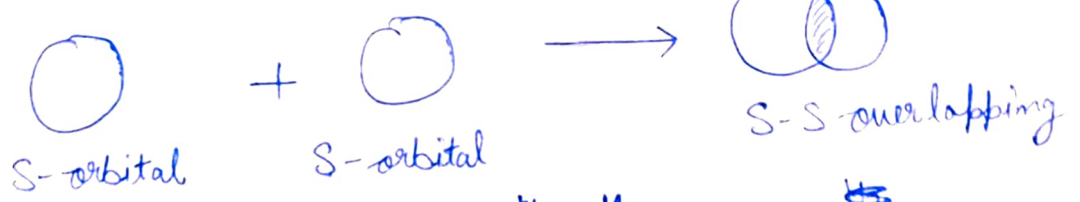


VBT (Valence Bond Theory) :- It is the overlap criteria of atomic orbitals. or [Covalent bond is formed by overlapping of atomic orbitals].

⇒ Types of overlap :-

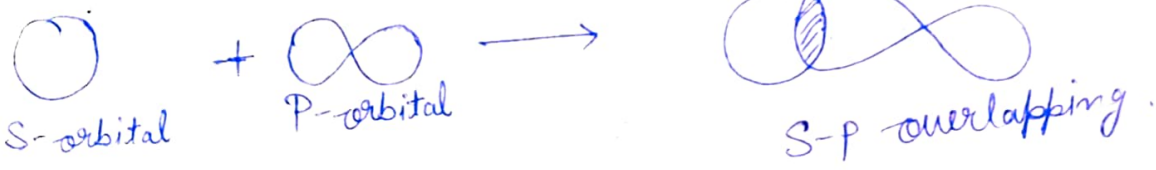
(i) Sigma bond :- A Covalent bond resulting from the formation of a molecular orbital by the end to end overlap of s along internuclear axis.

s-s overlapping :-

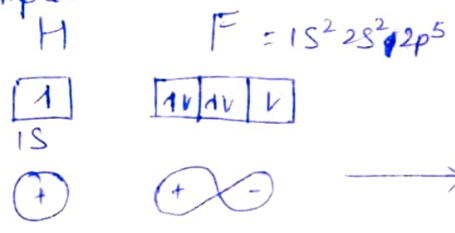


Example :- H₂ = (H-H)

(b) S-P overlapping :-

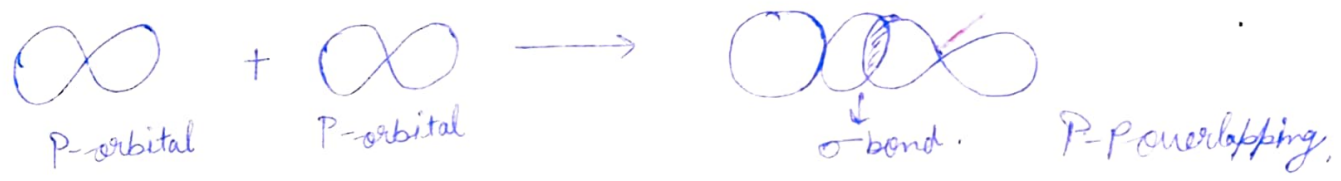


Example:-

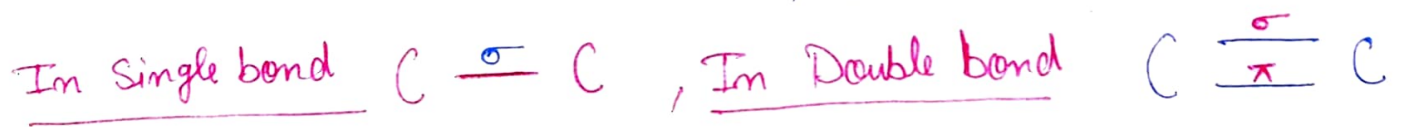
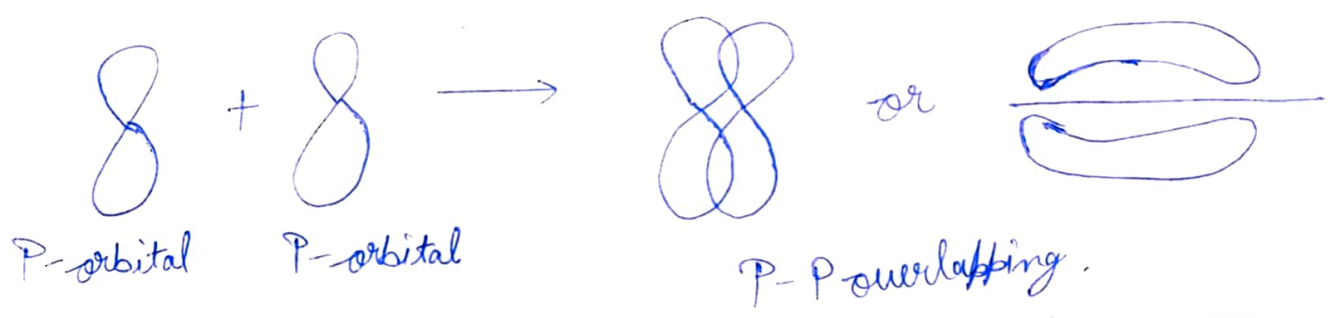


(Mostly Same Sign orbitals overlapping is Positive overlap (Most appropriate))

(c) P-P overlapping :-



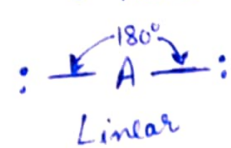
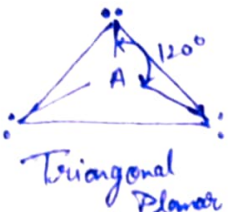
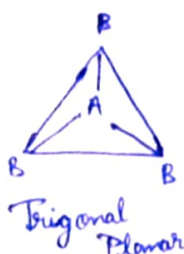
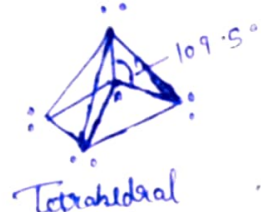
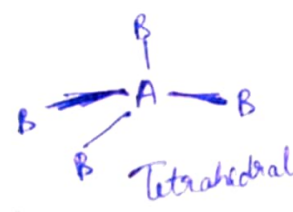
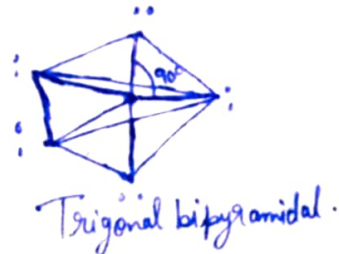
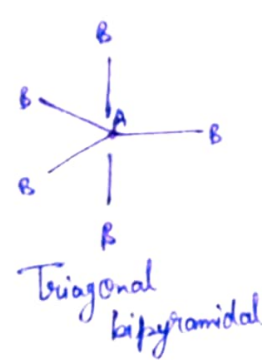
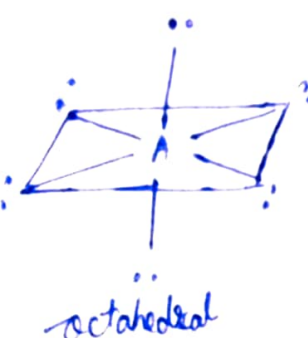
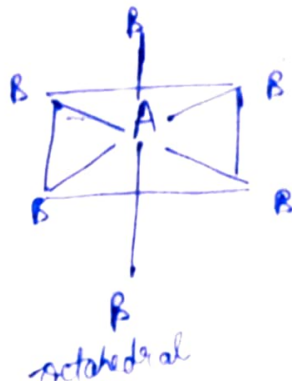
(ii) Pi (π) bond :- A Covalent bond formation of molecular orbitals by Side-to-Side overlap of atomic orbitals along a Plane Perpendicular to a line connecting the nuclei of the atoms.



[Note :- σ bond is stronger bond than π -bond (Because it overlaps internuclear axis).]

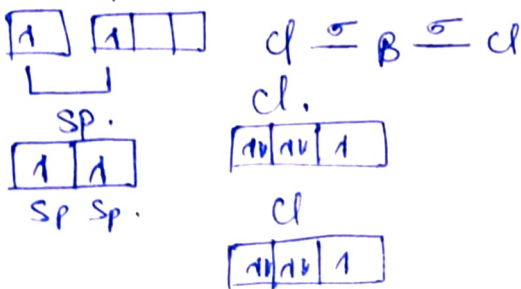
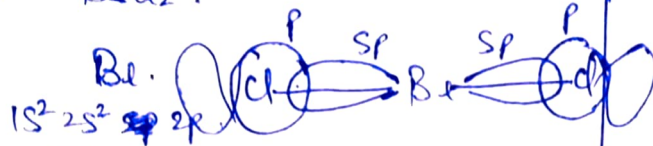
Hybridisation:- Inter mixing of Atomic orbitals of the same atom with nearly same energy, resulting in formation of new orbitals of equal and identical shape.

Table:- Geometry of Molecules in which the Central atom has no Lone Pair of electrons.

Number of e ⁻ Pairs	Arrangement of e ⁻ Pairs	Molecular geometry	Examples	Hybridisation
2	 <p>Linear</p>	$B - A - B$ Linear	$BeCl_2, HgCl_2$	sp
3	 <p>Trigonal Planar</p>	 <p>Trigonal Planar</p>	BF_3	sp^2
4	 <p>Tetrahedral</p>	 <p>Tetrahedral</p>	CH_4, NH_4^+	sp^3
5	 <p>Trigonal bipyramidal</p>	 <p>Trigonal bipyramidal</p>	PF_5	sp^3d
6	 <p>octahedral</p>	 <p>octahedral</p>	SF_6	sp^3d^2

⇒ Calculate $Z = \text{No. of } \sigma \text{ bond} + \text{L.P of Central Atom.}$

1) BeCl_2 .



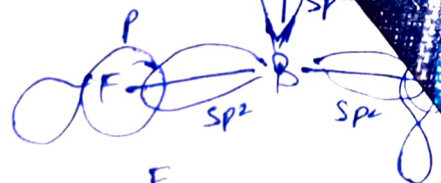
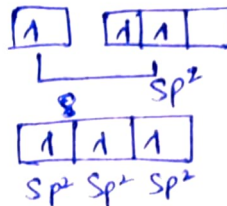
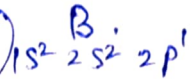
No. of σ bond is 2.

$Z = 2$.

→ Then Hybridisation is sp .

→ Geometry is Linear.

2) BF_3 .



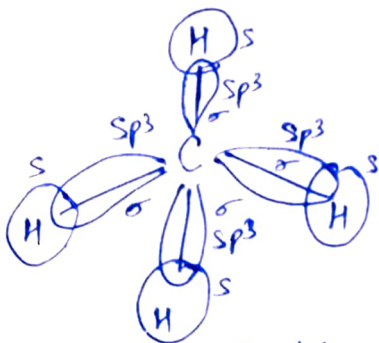
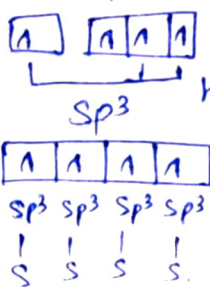
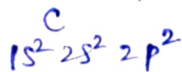
No. of σ bond is 3.

$Z = 3$.

→ Then Hybridisation is sp^2 .

→ Geometry is Trigonal Planar.

3) CH_4 .



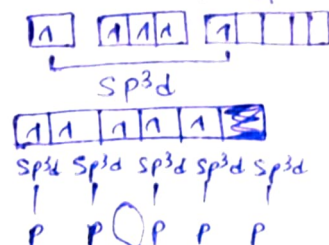
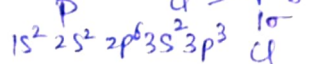
No. of σ bond is 4.

$Z = 4$.

Then Hybridisation is sp^3 .

Geometry is Tetrahedral.

4) PCl_5 .



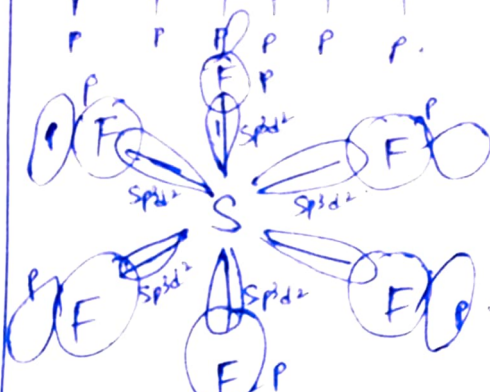
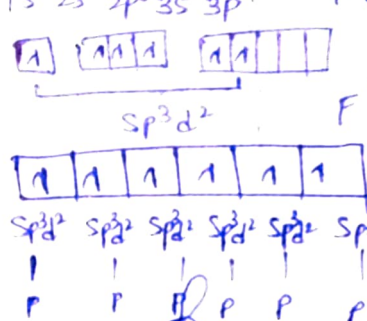
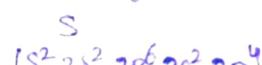
No. of σ bond is 5.

$Z = 5$.

Then Hybridisation is sp^3d .

Geometry is Trigonal Bipyramidal.

5) SF_6 .



No. of σ bond is 6.

The Hybridisation is sp^3d^2 .

Geometry is octahedral.

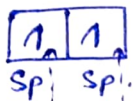
Hybridisation of BeCl_2 .

$\Rightarrow \text{Be} (Z=4)$

$1s^2 2s^2 2p^0$

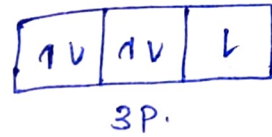


New Hybrid orbitals



(3p) Cl Cl.
(sp)

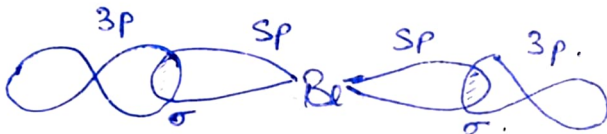
Cl.
 $1s^2 2s^2 2p^6 3s^2 3p^5$



There are 2 σ bonds. = 2.

Hybridisation is sp.

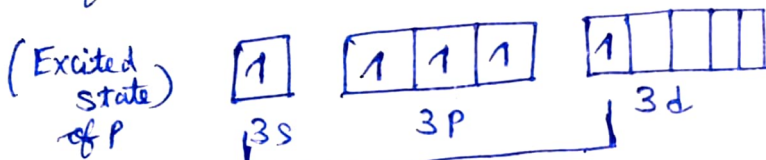
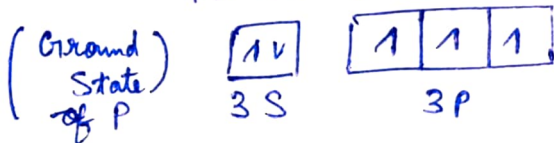
Geometry is Linear.



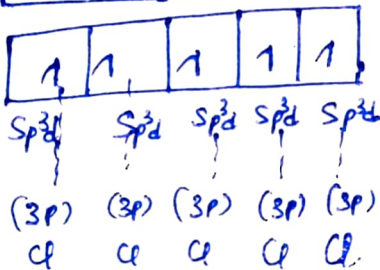
Hybridisation of PCl_5 .

$\Rightarrow \text{P} (Z=15)$

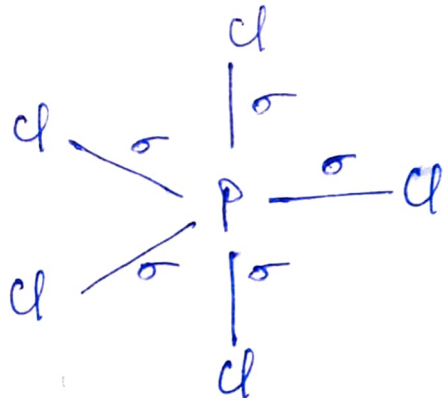
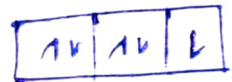
$1s^2 2s^2 2p^6 3s^2 3p^3$



New Hybrid orbitals



Cl.
 $1s^2 2s^2 2p^6 3s^2 3p^5$



No. of σ bonds are 5.

Then Hybridisation is sp^{3d}.

Geometry is Trigonal bipyramidal

VSEPR (Valence shell electron pair repulsion theory).

- => There are three types of repulsion in a covalent molecule
 $lp-lp > lp-b.p. > b.p-b.p.$
- => These repulsion depend upon difference in electronegativity between A and B.
- => The hybridisation of central atom decides geometry and VSEPR theory the shape of molecule.

Total no. of e ⁻ Pairs	Geometry of the e ⁻ Pairs.	B.P	L.P	Geometry (Shape) of the molecule	Examples
		(Molecule formula)			
2 Hybridisation = sp	 Linear.	2	0	 Linear	$BeF_2, BeCl_2, HgCl_2$.
3 $H = sp^2$	 Trigonal Planar	3	0	 Trigonal Planar	$BF_3, AlCl_3, SO_3$.
		2	1	 Bent (V-shape)	$SO_2, O_3, SnCl_2, NO_2$
4 $H = sp^3$	 Tetrahedral	4	0	 Tetrahedral	SiF_4, NH_4^+, CH_4 .
		3	1	 Trigonal Pyramidal	$NH_3, PCl_3, NCl_3, NF_3, PH_3, H_3O^+$
		2	2	 Bent	H_2S, NH_2^-, H_2O .

S
H

7
6

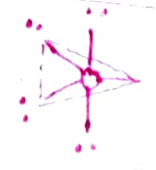
Number of lone
e⁻ Pairs.

B.P | L.P.

Geometry (Shape) of the
molecule.

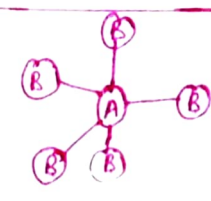
Example, 13

sp^{3d}



Trigonal
bipyramidal

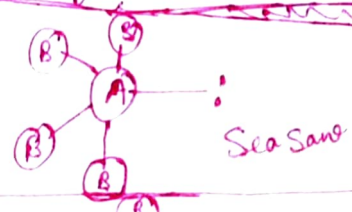
5 | 0
(AB₅)



Trigonal bipyramidal

PCl₅,
PF₅, SbCl₅

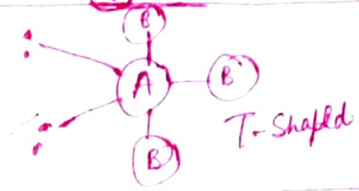
4 | 1
(AB₄L)



Seesaw

SF₄

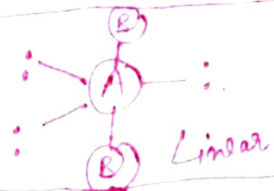
3 | 2
(AB₃L₂)



T-shaped

ClF₃

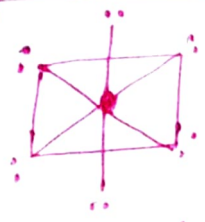
2 | 3
(AB₂L₃)



Linear

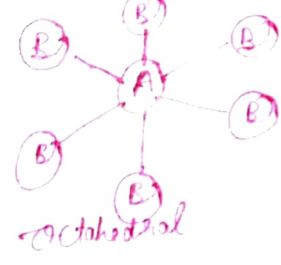
XeF₂

6
H = sp^{3d²}



octahedral

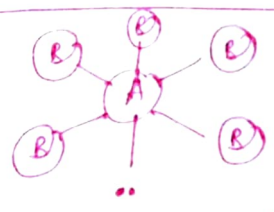
6 | 0
(AB₆)



octahedral

SF₆

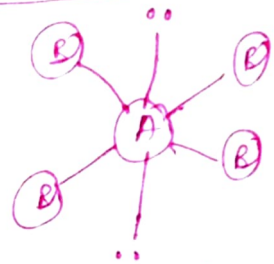
5 | 1
(AB₅L)



Square pyramidal

ClF₅

4 | 2
(AB₄L₂)



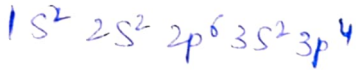
Square Planar

XeF₄

Example :-

(i) SO₂

~~S (Z=16)~~ S (Z=16)



O (Z=8)



Number of e⁻ Pair = Number of σ Bond + Lone pair

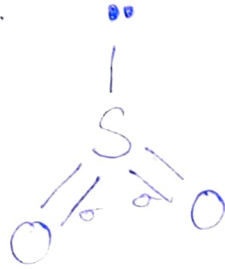
= 2 + 1 = 3.

Hybridisation = Sp²

Molecular formula = AB₂L

Geometry = Triangular Planar.

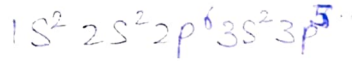
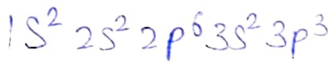
Shape = Bent (V-Shape).



(ii) Pcl₃

P (Z=15)

Cl (Z=17)



No. of e⁻ Pair = No. of σ Bond + Lone pair

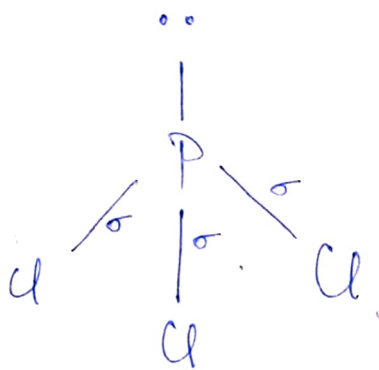
= 3 + 1 = 4.

Hybridisation = Sp³

Molecular formula = AB₃L

Geometry = Tetrahedral.

Shape = Trigonal Pyramidal

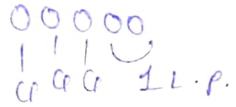


Rough

S (V.E) = 6.



AB₂L



AB₃L

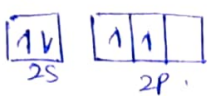
Hybridisation in C₂H₆ molecule. (Ethane)

C (Z=6).

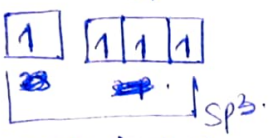
H (Z=1).

1s² 2s² 2p²

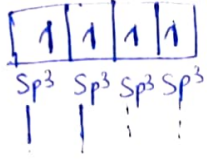
Ground State



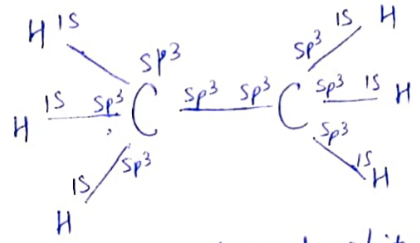
Excited State



New hybrid orbitals.

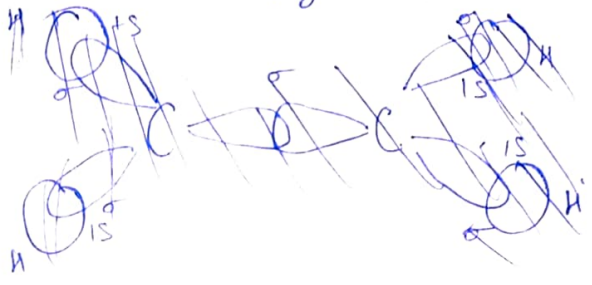


1s¹



unhybrid orbital = 0.

Hybrid orbital = 4.



Hybridisation in C₂H₄ molecule. (Ethene)

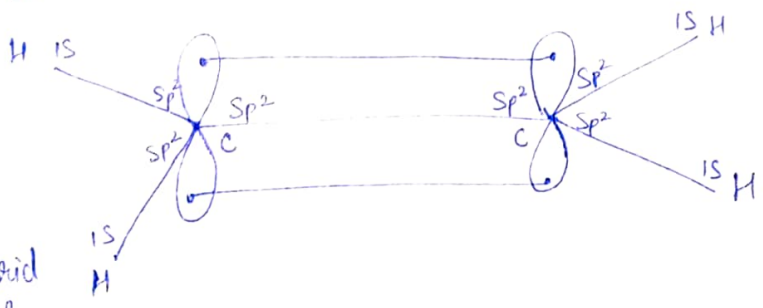
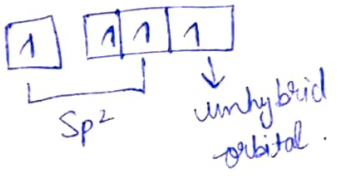
CH₂=CH₂.

C (Z=6).

Ground State



Excited State



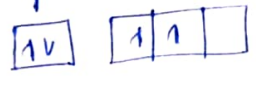
Hybridisation of C₂H₂ molecule. (Ethyne).

HC≡CH.

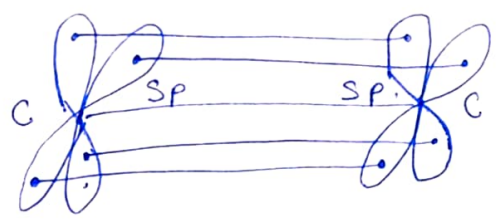
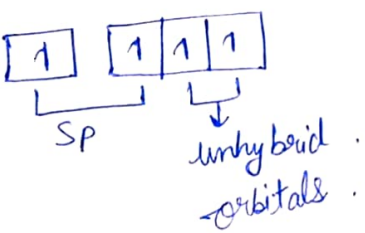
C (Z=6).

1s² 2s² 2p²

Ground State



Excited State



Atomic orbital (V.B.T)

- Atomic orbital is the region having the highest Probability of finding an e^- in an atom.
- Schrodinger equation is used.
- It fails to explain Paramagnetic character of O_2 .
- It fails to explain the existence of H_2^+

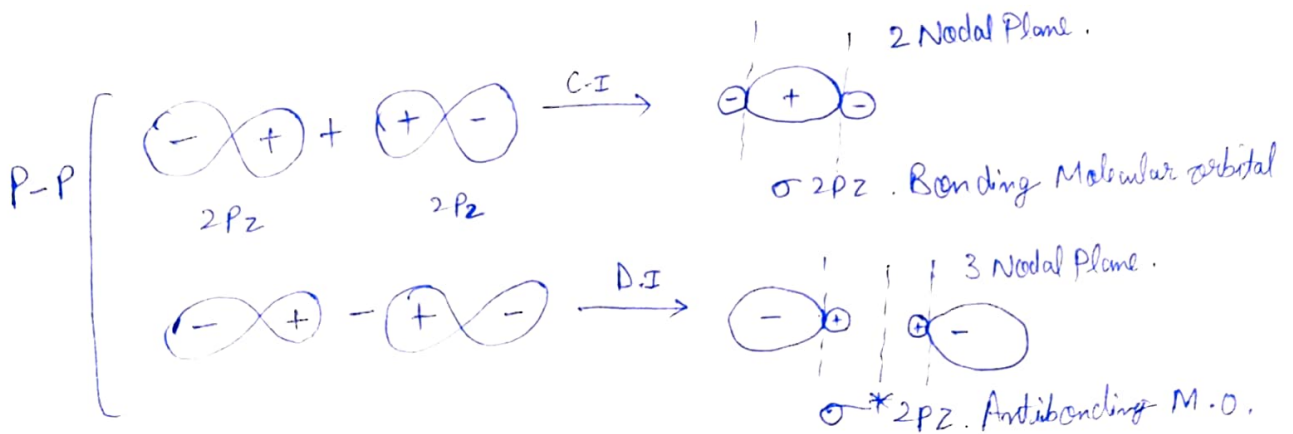
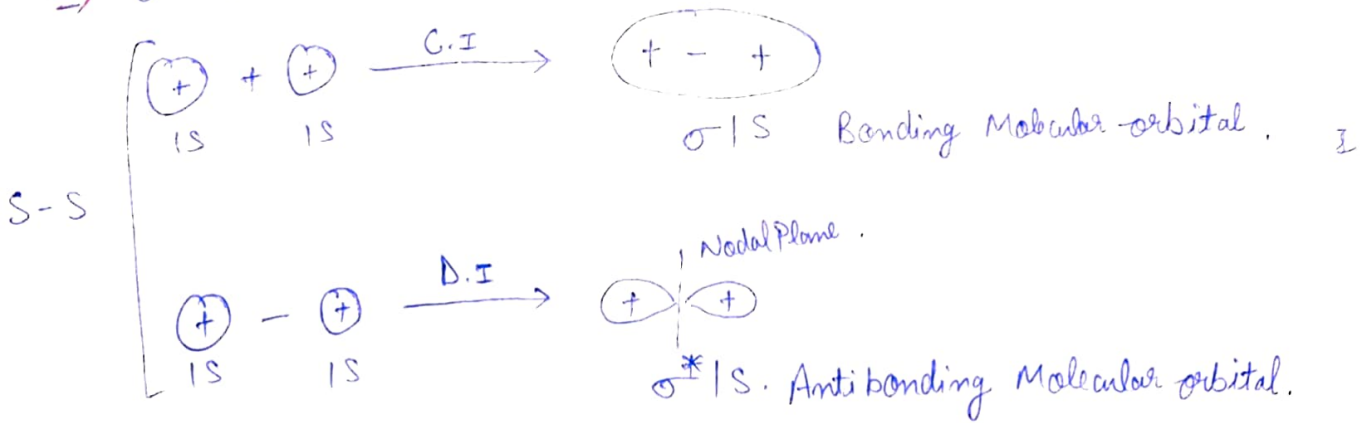
Molecular orbital

- Molecular orbital is the region having the highest Probability of finding an electron of a molecule.
- Linear Combination of atomic orbitals (LCAO) is used.
- It explains the Para magnetic character of O_2 .
- It explains the existence of H_2^+ .

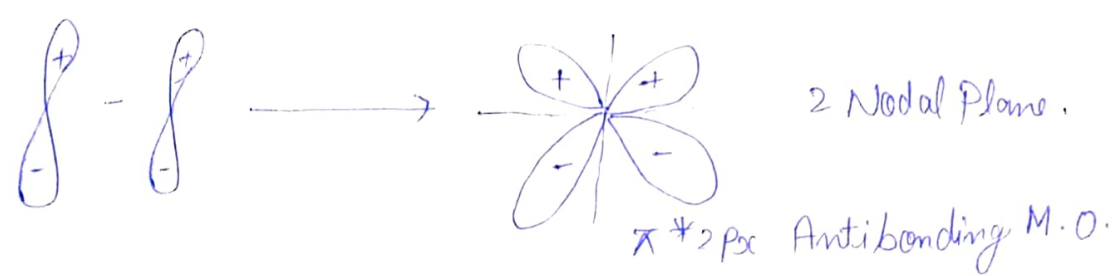
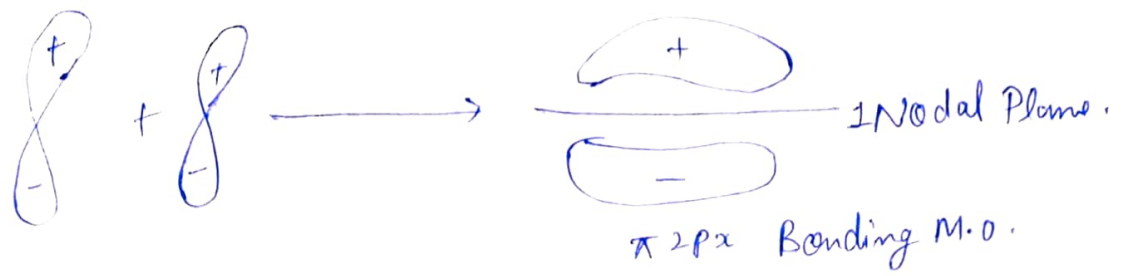
Formation of ~~Molecular orbital~~ Bonding molecular orbital and Antibonding molecular orbital.

[we have two (σ, π) Molecular orbitals].

\Rightarrow σ Molecular orbital :- Axial Atomic orbital overlapping.



π Molecular orbital :- (where Sidewise overlapping of p orbitals)



Bonding Molecular orbital

- These orbitals have less energy.
- They are More Stable.

→ Like :- $\sigma 1s, \sigma 2p_z, \pi 2p_x, \pi 2p_y$ etc

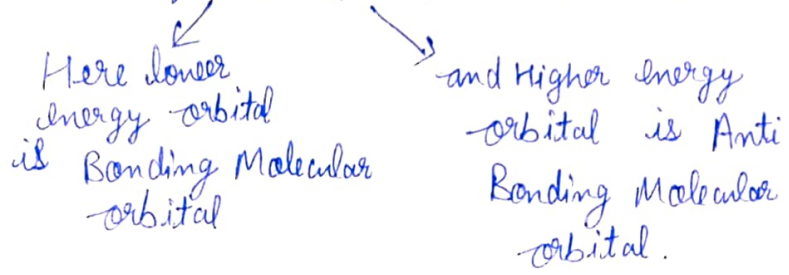
Anti Bonding Molecular orbital

- These orbitals have high energy.
- They are less Stable.

→ orbitals like :- $\sigma^* 1s, \sigma^* 2p_z$ etc.

How to do e- Configuration of molecules :-

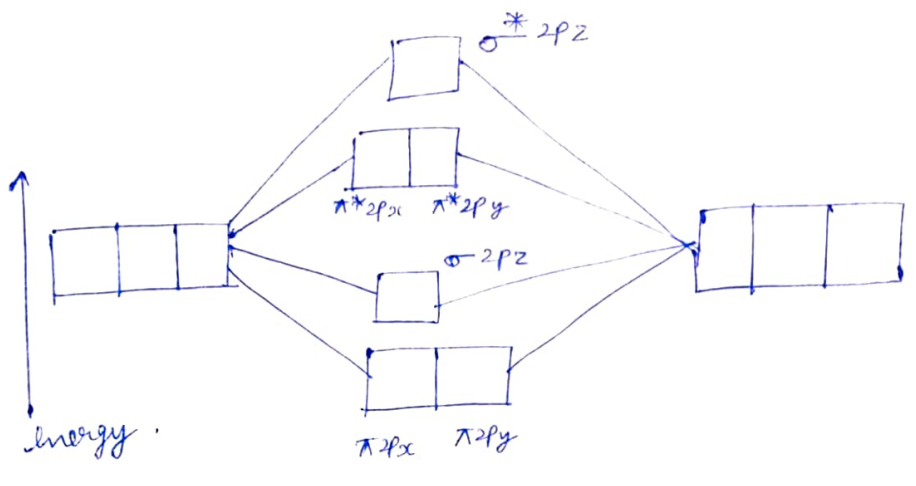
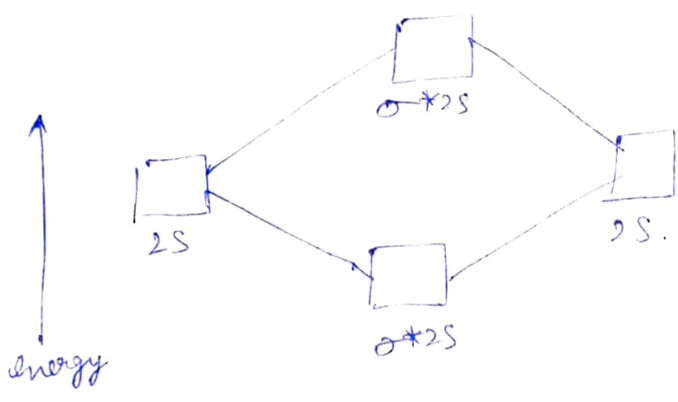
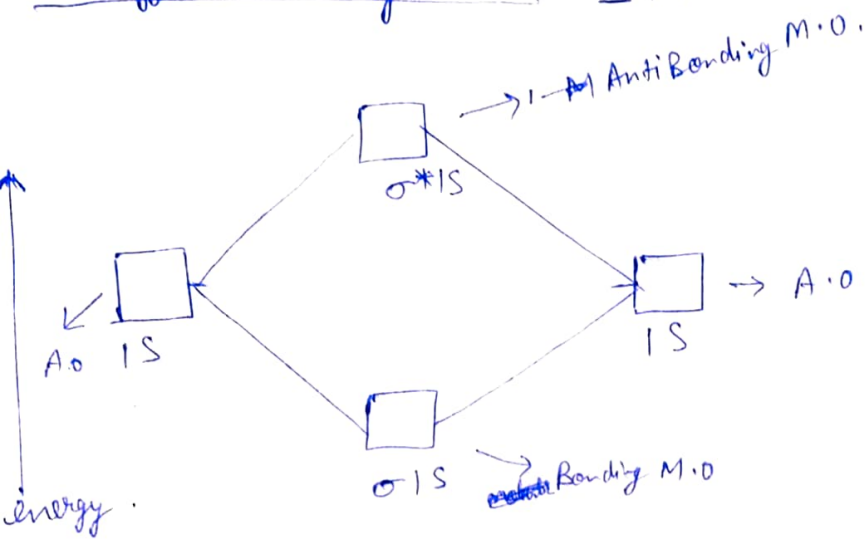
- Some Rules follow to fill the electrons in orbitals.
- (a) Aufbau Principle, (b) Pauli's Exclusion, (c) Hund's Rule.



→ ~~the~~ The electronic Configuration is for the molecule which have (less than or equal to $14e^-$ or ~~less than~~ ≥ 14).

$(\sigma 1s \sigma^* 1s) (\sigma 2s \sigma^* 2s) (\pi 2p_x = \pi 2p_y) \sigma 2p_z (\pi^* 2p_x = \pi^* 2p_y) \sigma^* 2p_z$.

Energy level diagram :- $\geq 14e^-$



For Example:-

E.C of Li_2 . (No. of $e^- = 6$).



→ Paired e^- .

∴ it is diamagnetic character.

Li_2^+ (No. of $e^- = 7$).

$$\rightarrow B.O = \frac{N_b - N_a}{2} = \frac{4 - 2}{2} = 1$$



(Magnetic nature \Rightarrow it is Paramagnetic).

$$\rightarrow B.O = \frac{N_b - N_a}{2} = \frac{4 - 3}{2} = \frac{1}{2}$$

Li_2^+ (No. of $e^- = 5$).



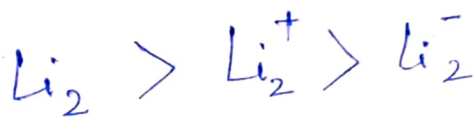
→ unpaired e^- .

∴ it is Paramagnetic.

$$\rightarrow B.O = \frac{N_b - N_a}{2} = \frac{3 - 2}{2} = \frac{1}{2}$$

B.O \propto Stability.

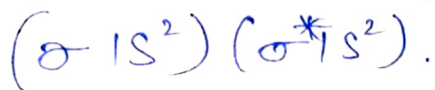
[Note :- If we get same B.O of the molecule. then we have to check its antibonding e^- 's. if antibonding e^- will be less. it will be more stable].



← Stability increases.

He molecule (He_2).

(No. of $e^- = 4$).



$$B.O = \frac{N_b - N_a}{2} = \frac{2 - 2}{2} = \frac{0}{2} = 0.$$

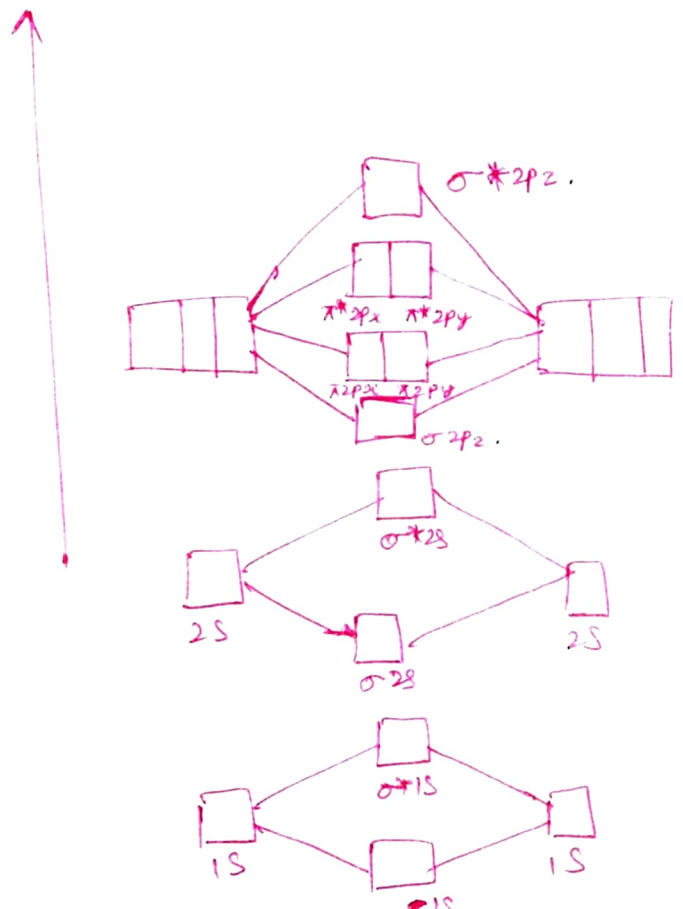
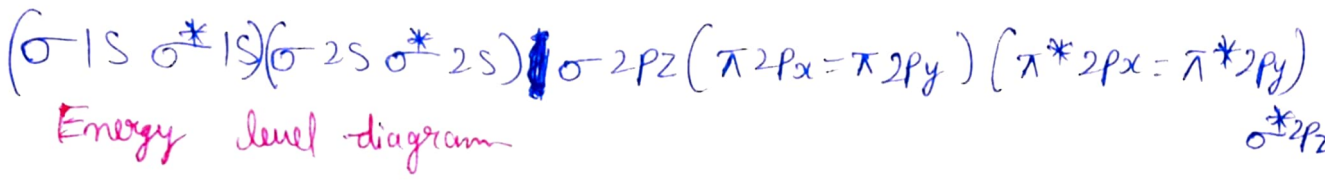
He molecule does not exist.

(if any molecule B.O will be zero. the molecule will not exist).

If molecule contain $e^-s > 15$ and < 20 .
 (15-20).

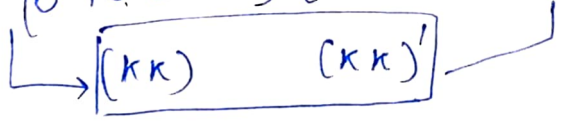
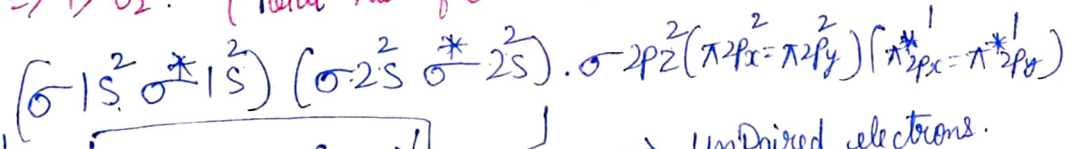
(20)

Then, the E.C will be.



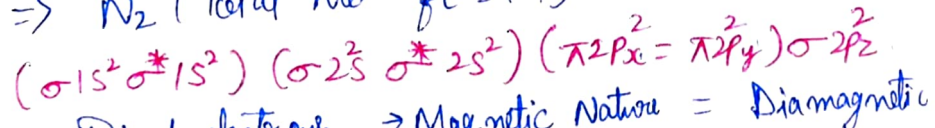
write e^- configuration :- O_2 and N_2 .

$\Rightarrow O_2$. (Total No. of $e^- = 16$).



- \rightarrow Unpaired electrons.
- \rightarrow Magnetic Nature :- Paramagnetic.
- $\rightarrow B.O = \frac{N_b - N_a}{2} = \frac{10 - 5}{2} = \frac{5}{2} = 2.5$.

$\Rightarrow N_2$ (Total No. of $e^- = 14$).



\rightarrow Paired electrons, \rightarrow Magnetic Nature = Diamagnetic

$\rightarrow B.O = \frac{N_b - N_a}{2} = \frac{10 - 4}{2} = \frac{6}{2} = 3$.