Chapter- 4

Chemical Bonding& Molecular structure

STUDY NOTE

Chemical Bonding:-It is the forces of attraction which binds the constituent atom in a molecule.

e.g NaCl, H_2O

$$\begin{tikzcd}[row sep=small] Na - e^- \rightarrow Na^+ \arrow[dr] & \\ & NaCl(s) \\ Cl + e^- \rightarrow Cl^- \arrow[ur] & \end{tikzcd}$$

Question:-Why do certain element combine, while some other element like noble gases do not combine in normal state?

Solution:-Every element/ atom want to be stable either by losing or by gaining or by mutually sharing or donating a pair of electrons from one atom to other atom. But elements like, He, Ne, Ar, Kr, Xe and Rn, except Helium all other elements having eight electrons in their valency shell. So, attaining eight electron in their valency shell known as octet rule due to stable electronic configuration, they do not loss or gain electron easily. That's why these gases do not take part in bond formation in normal state.

Types of Chemical Bonding:-

(a) Electrovalent or Ionic bond (b) Covalent bond (c) Co-ordinate bond

(d) Hydrogen bond (e) Metallic bond

Nacl, Mgcl2, $BaSO_4$, HF, HCl, Br_2, F_2

Electrovalent or Ionic bond:-

This type of bond is formed by transference or transfer of an electron takes place from one atom to other atom and both will attain the stable electronic configuration of nearest inert gas.

Formation of Sodium Chloride ($NaCl_{(s)}$):-

$Na_{11} \rightarrow 2,8,1$

$Cl_{17} \rightarrow 2,8,7$

$Na_{(2,8,1)} - e^- \rightarrow Na^+_{(2,8)} \equiv Ne$

$C_{(2,8,7)} + e^- \rightarrow Cl^-_{(2,8,8)} \equiv Ar$

$Na^+ + Cl^- \xrightarrow{\text{Coulombic force of attraction}} NaCl_{(s)} + U$

Where U =Lattice energy

It is the amount of energy released ,when one mole of ionic solid is formed from its constituent ions.

CaO:-

$Ca_{(20)} \rightarrow 2,8,8,2$

$O_8 \rightarrow 2,6$

$Ca_{(2,8,8,2)} - 2e^- \rightarrow Ca^{2+} \equiv Ar$

$O_{2,6} + 2e^- \rightarrow O^{2-} \equiv Ne$

$Ca^{2-} + O^{2-} \xrightarrow{\text{Coulombic force of attraction}} CaO_{(s)} + U$

$Ca^{2+} + O^{2-} \rightarrow CaO_{(s)} + U$

MgF₂ :-

$Mg_{12} \rightarrow 2,8,2$

$Mg_{(2,8,2)} - 2e^- \rightarrow Mg^{2+} \equiv Ne$

$F_9 \rightarrow 2,7$

$F_{(2,7)} + e^- \rightarrow F^- \equiv Ne$

$F_9 + 2e^- = 2F^- \equiv Ne$

$Mg^{2+} + 2F^- \xrightarrow{\text{Coulombic force of attraction}} MgF_2 + U$

$Mg^{2+} + 2F^- \rightarrow MgF_2 + U$

Electrovalency:-Number of electrons lost or gain during formations of 1 mole of ionic compound.

Characteristic of Ionic or electrovalent compound:-

Compound form by electrovalent or ionic compound is called electrovalent compound or ionic compound.

(a) These are generally hard and rigid due to strong forces of attraction

(b) High melting point and boiling point, due to hardness

(c) Good conductor of electricity only in fused or molten state or aqueous solution of that compound.

(d) Ionic compounds or electrovalent compounds are soluble in polar solvent like H_2O, but insoluble in non polar solvent like (cs_2, CCl_4, benzene, ether etc)

When some solute particles dissolved in water, the energy released is called hydration energy.

Lattice energy:- It is the amount of heat required to break 1 mole of anionic compound into its constituent ions.

Criteria for forming ionic bond:-

(a) Atom should have low ionisation enthalpy (Group - 1 and Group – 2)

(b) Atom should have high electron affinity (Group – 16 and 17)

(c) High lattice energy

$AlCl_3 \rightarrow$ Ionic bond formation

$Al_{13} \rightarrow 2,8,3$

$Al_{(2,8,3)} - 3r^- \rightarrow Al^{3+} \equiv Ne$

$Cl_{(17)} \rightarrow 2,8,7$

$Cl_{(2,8,7)} + 3e^- \rightarrow 3Cl^- \equiv Ar$

$$Al^{3+} + 3Cl^- \xrightarrow{\text{Colombic forces of attraction}} AlCl_3(s) + U$$

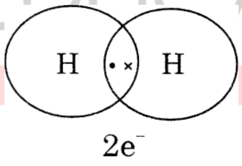
$$Al^{3+} + 3Cl^- \rightarrow AlCl_3(s) + U$$

Electrovalency:-No.of electron transfer during formation of 1 mole of ionic solid is known as electrovalency

Covalent Bond:-

When both the combing atom are deficient of some electrons, in this case only mutual sharing of an electron takes place in between two atom or among atoms present in a molecule and both the combining atom attain octet state except helium which attain duplet state.

Formation of H_2:- H_2 molecule is formed by combination of two H atom



$H_1 \rightarrow 1 or 1s^1$

i.e H atom is deficient of one electroni.e to attain duplet state

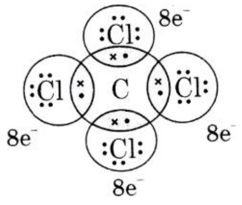
Carbon Tetra Chloride (CCl_4) :-

A methane molecule contain one atom of carbon and 4 atoms of hydrogen

$C_6 \rightarrow 2,4$

$Cl \rightarrow 2,8,7$

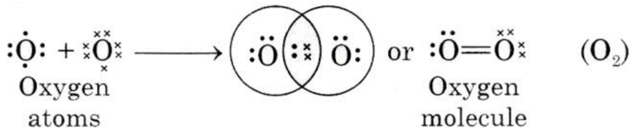
Carbon is deficient of 4 electrons where as each chlorine is deficient of One electron. So mutual sharing of electrons occur.



Formation of double covalent bond:-

O_2 molecule (oxygen molecule)

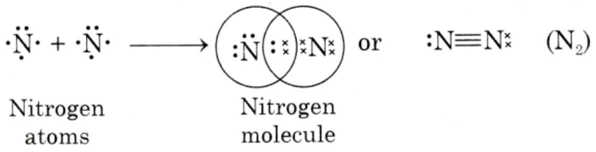
$_8O \rightarrow 2,6$



Triple Covalent bond:-

N_2 molecule

$_7N \rightarrow 2,5$



Characteristics of Covalent Compound:-

(a) Generally, these are gases, soft

(b) Low melting and boiling point

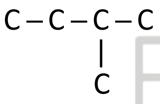
(c) Poor conductor of electricity

(d) Soluble in non-polar solvent but insoluble in polar solvent like H_2O

(e) Some covalent compounds shows isomerism

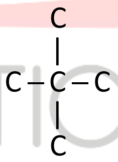
Isomerism:- Two or more compound having some molecular formula but different structure, physical and chemical properties are known as isomers to each other and this phenomenon is called isomerism.

e.g C_5H1_2 :- $H_3C-CH_2-CH_2-CH_2-CH_3$ (n – pentane)



$$\begin{array}{l} C-C-C-C \\ \quad\quad\;\; | \\ \quad\quad\;\; C \end{array}$$

(isopentane)



$$\begin{array}{c} C \\ | \\ C-C-C \\ | \\ C \end{array}$$

(Neopentane)

Formation of sigma and pi covalent bond on basis of overlapping of orbitals:-

Sigma Covalent bond & Pi Covalent bond

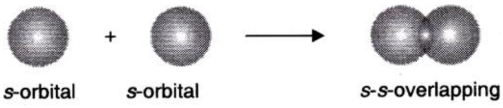
It is formed by overlapping of s-s, s-p and p-p atomic orbital in their internuclear axis

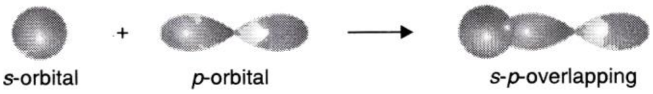
The atomic orbital should be half filled before overlapping.

Sigma bond is stronger than Pi covalent bond

Free rotation occur in sigma bond but not in pi bond

Sigma covalent bond:-



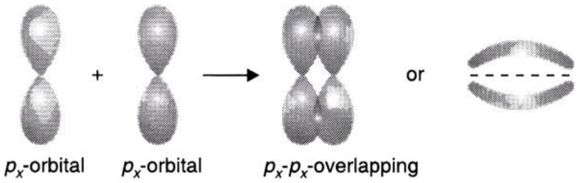


How HF molecule forms ?

$H \rightarrow 1s^1$

$_9F \rightarrow 1s^2\ 2s^2\ 2p_x^2\ 2p_y^2\ 2p_z^1$

Formation of Pi bond



Pi-bond:- O_2 and N_2 molecule

Formation of O_2(draw orbital diagram)

$_8O \rightarrow 1s^2\ 2s^2\ 2p_x^2\ 2p_y^1\ 2p_z^1$

Conclusion:- A double bond contains 1 sigma and 1 pi bond

Formation of N_2

$_7N \rightarrow 1s^2\ 2s^2\ 2p_x^1\ 2p_y^1\ 2p_y^1$

Lewis dot structure:-

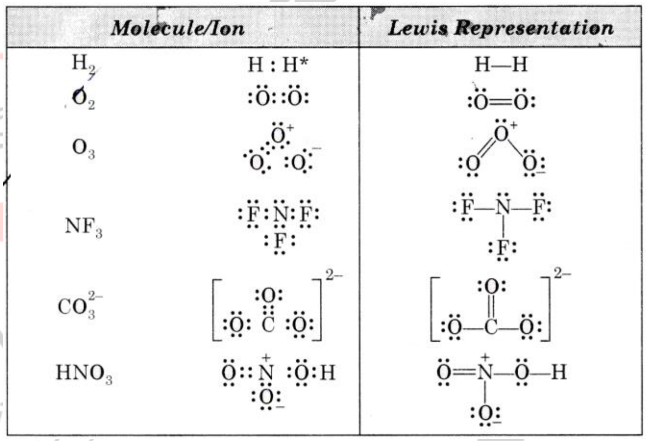
CH_4 :- Total no. Of valency $e^- = 4+4=8$

HNO_3 :- Total no. Of valency $e^- = 1+8+18=24$

HNO_2 :- Total no. Of valency $cl^- = 18$

CO_3^{2-} :- Total no. Of valency $Cl^- = 4+18+2=24$

NO_3^- :- Total no. Of valency $e^- = 5+18+1=24$



Molecule/Ion		Lewis Representation
H_2	H : H*	H—H
O_2	:Ö::Ö:	:Ö=Ö:
O_3	$\ddot{O}^+$ ·Ö· :Ö:⁻	$\ddot{O}^+$:O= Ö:⁻
NF_3	:F:N:F: :F:	:F—N—F: :F:
CO_3^{2-}	$[$:O: :Ö: C :Ö: $]^{2-}$	$[$:O: ‖ :Ö—C—Ö: $]^{2-}$
HNO_3	Ö::$\overset{+}{N}$:Ö:H :Ö:⁻	Ö=$\overset{+}{N}$—Ö—H :Ö:⁻

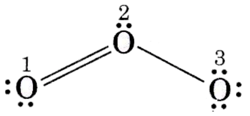
Limitations of octet rule:-

1. There are some covalent compounds in which central atom do not satisfy octet rule.
   e.g- BeH_2,BeF_2,$Becl_2$,BF_3,BBr_3,BCl_3,BI_3
2. There are some compounds in which the central atom contains odd electrons. e,g NO, NO_2
3. There are some covalent compounds in which the central atom contains more than 8 electrons. This is called expanded octet, containing 10, 12, 14, 16,
   PF_5, SF_6, H_2SO_4, SO_3
4. Lewis structure unable to explain about the shape of the molecule
   Octect rule gives inertness of noble gases, but there are some compounds of xenon like XeF_2, XeF_4, XeF_6

Formal Charges:-

Let us consider, O_3molecule.

Formal Charges:- Total no. Of valency electrons around each atoms – no.Of unshared $e^{-}s - \frac{1}{2}$ (no. Of shared e^{-})



Formal charge of 1st oxygen

$= 6 - 2 - \frac{1}{2}(6)$

$= 6 - 2 - 3$

$= 6 - 5 = 1$

Formal charge of 2nd oxygen

$= 6 - 4 - \frac{1}{4}(4)$

$= 6 - 4 - 2 = 0$

Formal charge around of 3rd oxygen

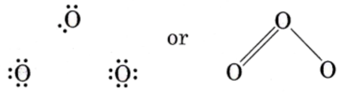
$= 6 - 6 - \frac{1}{2} \times 2$

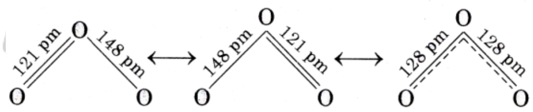
$= 6 - 7 = -1$

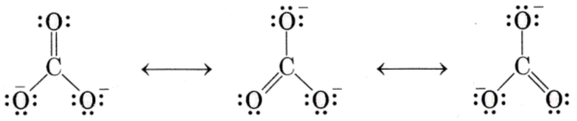
Resonance:-

When the single Lewi's dot structure unable to explain the geometry of the molecule accurately, in this case we have to consider more than one similar structure, bonding and non bonding electrons used to explain the shape of molecule accurately.

A resonating structure can be obtaining by delocalisation of pi electron.(diagram)

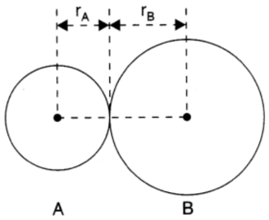




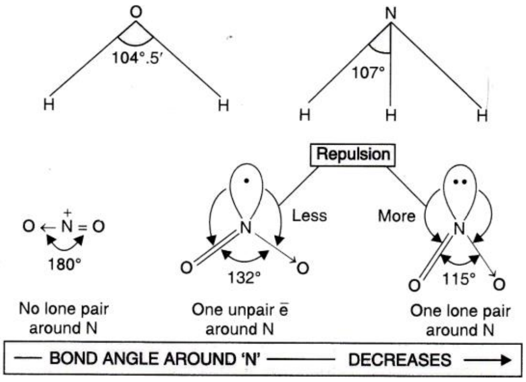


Bond Parameters:-

(a) Bond length:- It is the distance between two atom in a bond. It is measure in pico metre (P_m).bondlengths of different covalent bonds '−' > =>≡'−' > =>≡



(b) Bond angle: - The angle between two bond pair in a compound i.e H_2O, NH_3



(c) Bond order:- it is the number of bond formed between two atoms.

i.e $H-H \rightarrow$ the bond order is 1

$O=O \rightarrow$ The bond order is 2

$N \equiv N \rightarrow$ The bond order is 3

Polar and non-polar covalent bond:-

Polar Covalent bond:- When a covalent compound formed between two atoms which differ much value in their electronegativity,then the electron cloud will be shifted more towards more electronegative atom than the other. As a result charge separation occur.

The atom which is more electronegative acquire fractional negative charge and the less electro negative atom acquires fractional positive charge and this phenomenon is known as polarity in a covalent bond.

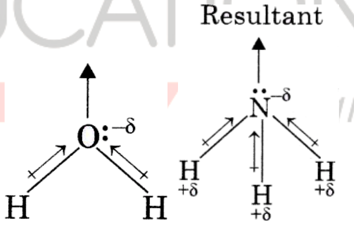
Non-Polar Covalent bond:- When a covalent compound formed between two atoms which do not differ value of their electronegativity, then the shared paired of e^-s remain in between two atom and in this case no charge separation occur.

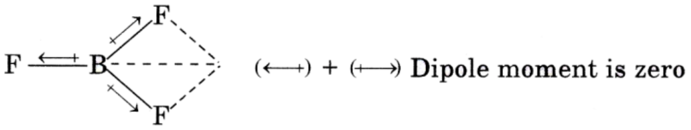
Dipole Moment:-It is a vector quantity having magnitude as well as direction.

It is defined as the product of the net positive and negative charges and the distance of charge separation.

Dipole moment = Net charges X Distance of the charge separation

Mathematically, $\mu = e \times d$





(Non-polar)

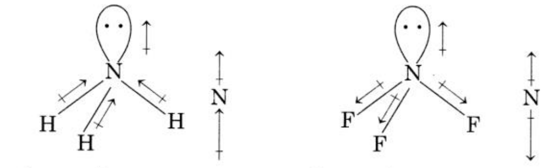
Unit of dipole moment is Debye (D)

$\mu = e \times d$

$= 10^{-10}\text{esu} \times 10^{-8}\text{cm}$

$= 18^{-18}\text{esucm}$

$= 3.33 \times 10^{-30}\text{cm}$



Lone pair moment reinforces bond moments (μ = 1.46 D)

Lone pair moment goes against the bond moments (μ = 0.25 D)

1 Debye = 10^8esu cm = 3.33×10^{-30}cm (coulomb .meter)

Application of Dipole moment (μ) :-

1. Dipole moment gives the shape of the molecule

2. Dipole moment gives idea about the extent of polarity in a molecule

Question:-

Although carbon dioxide contain 2 polar covalent bond but why CO_2 is a non-polar compound? $O=C=O$

Ans:-Due to linear geometry the two dipole moment cancel to each other and the net dipole moment becomes zero. Hence, this is treated as a non-polar compound.

Q:- Compare the Dipole moment of NH_3, NF_3 whose, dipole moment is more and why?

Solution:-

Dipole moment of NH_3 is more than NF_3

Hybridisation:-

The process of intermixing of two or more atomic orbital having nearly same energy and rearrange them- selves to give rise to new type of orbitals called hybrid orbitals. This phenomenon is known as hybridisation.

Criteria for Hybridisation:-

- Atomic orbital which takes part in hybridisation should contain atleast one electron.
- Atomic orbital having nearly same or equivalent energy can intermix with each other & rearrange with themselves to form the hybrid orbital.
- The orbital of one & same atom take part in hybridisation.

e.g $_6C \rightarrow 1s^2\ 2s^2\ 2p_x^1\ 2p_y^1\ 2p_z^0$ (ground state)

$_6C^* \rightarrow 1s^2\ 2s^1\ 2p_x^1\ 2p_y^1\ 2p_z^1$ (excited state)

Characteristics of hybrid orbital:-

(a) Number of atomic orbitals (hybridising) intermix is equal to number of hybrid orbitals formed.

(b) The hybrid orbital formed are all equivalent in shape and energy.

(c) The hybrid orbital formed at least contain single electron which is available for bond formation.

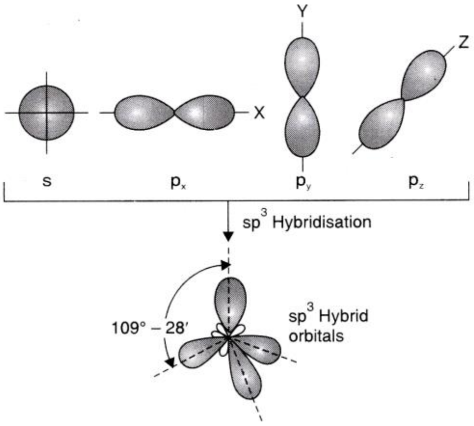
(d) The hybrid orbital formed, arranged themselves in such a way the repulsive interaction should be minimum.

(e) The repulsive interaction should be minimum when they are far away from each other.

Types of Hybridisation:-

sp^3 Hybridisation	sp^2 hybridisation
sp hybridisation	sp^3d hybridisation
$sp^3\ d^2$ hybridisation	

Sp^3 Hybridisation:-



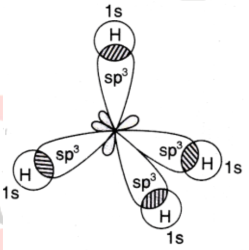
When 2s and 2px,2py,2pz atomic orbital intermix with each other and re-arranged with themselves .

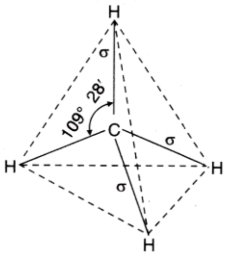
They give rise to four sp^3 hybrid orbitals. The four sp^3 hybrid orbitals formed are all equivalent in shape and energy.

For Example, All alkanes(CH_4, ...)

$_6C \rightarrow 1s^2\ 2s^2\ 2p_x^1\ 2p_y^1\ 2p_z^0$ (ground state)

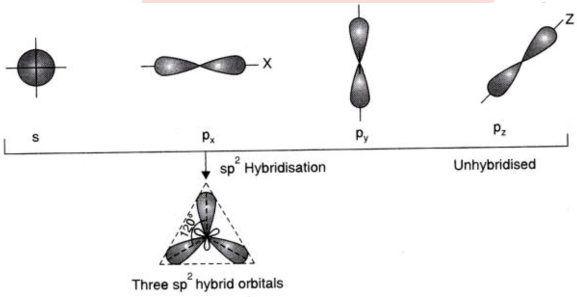
$_6C^* \rightarrow 1s^2\ 2s^1\ 2p_x^1\ 2p_y^1\ 2p_z^1$ (excited state)

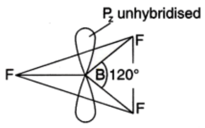


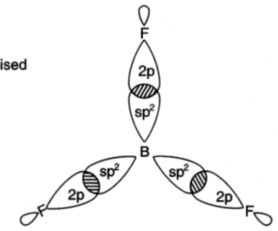


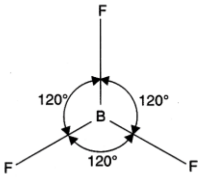
Now four half filled atomic orbital inter mix with each other and rearrange with themselves to form sp3 hybrid orbital.Hydrogen having single electron and single 1s orbital which is unpaired and available for overlapping.

SP² Hybridisation:- When one 2s and two 2p atomic orbital intermix with each other and rearrange with themselves, they give rise to three SP^2 hybrid orbitals.









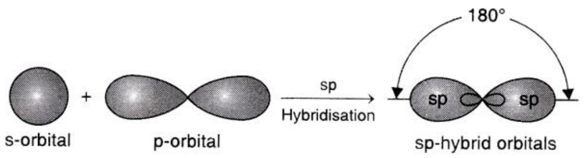
Example:-BF_3molecule

$_5B \rightarrow 1s^2\ 2s^2\ 2p_x^1$

$_5B^* \rightarrow 1s^2\ 2s^1\ 2p_x^1\ 2p_y^1$

$_9F \rightarrow 1s^2\ 2s^2\ 2p_x^2\ 2p_y^2\ 2p_z^1$

SP Hybridisation:-When one 2s and one $2P_x$ atomic orbital intermix with each other and rearrange with themselves, they give rise to two sp hybrid orbital. The two sp hybrid orbitals arrange themselves in such a way that the repulsive interaction becomes minimum i.e by creating 180^0 or linear shape



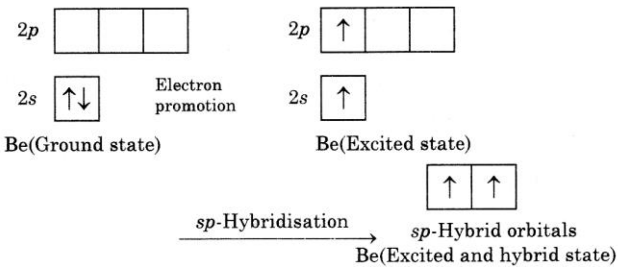
$$\frac{360}{2} = 180^0$$

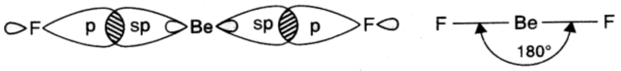
Shape is linear

BeF$_2$:- $_4Be \rightarrow 1s^2\ 2s^2$

$_4Be^* \rightarrow 1s^2\ 2s^1\ 2p_x^1$

$_9F \rightarrow 1s^2\ 2s^2\ 2p_x^2\ 2p_y^2\ 2p_z^1$





C$_2$H$_2$:- $_6C \rightarrow 1s^2\ 2s^2\ 2p_x^1\ 2p_y^1\ 2p_z^0$

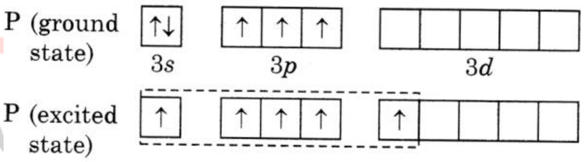
$_6C^* \rightarrow 1s^2\ 2s^1\ 2p_x^1\ 2p_y^1\ 2p_z^1$

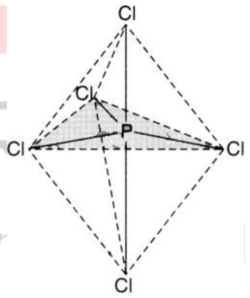
SP^{3}d Hybridisation:-

PCl$_5$, $_{15}P \rightarrow 1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^3\ 3d^0$

$_{15}P \rightarrow 1s^2\ 2s^2\ 2p^6\ 3s^1\ 3p_x^1\ 3p_y^1\ 3p_z^1\ 3d_{xy}^1$

$_{17}Cl \rightarrow (10Ne)3s^2\ 3p_x^2\ 3p_y^2\ 3p_z^1$





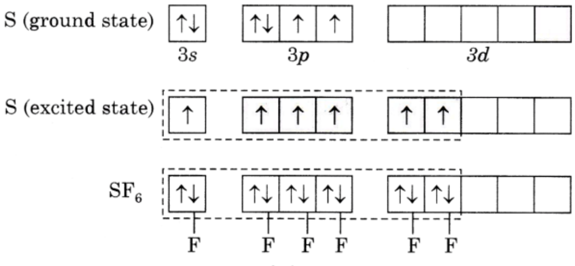
sp^{3}d^2 Hybridisation:-

SF$_6$

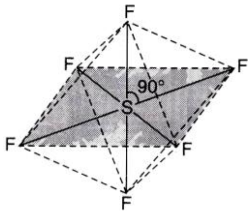
$_{16}S$- $[Ne]_{10}\ 3S^2\ 3P_x^2\ 3P_y^1\ 3p_z^1$

$_{16}S$- $[Ne]_{10} 3S^1\ 3P_x^1\ 3P_y^1\ 3P_z^1\ 3d_{xy}^1\ 3d_{yz}^1$

$_9F \rightarrow 1s^2\ 2s^2\ 2px^2\ 2py^2\ 2pz^1$



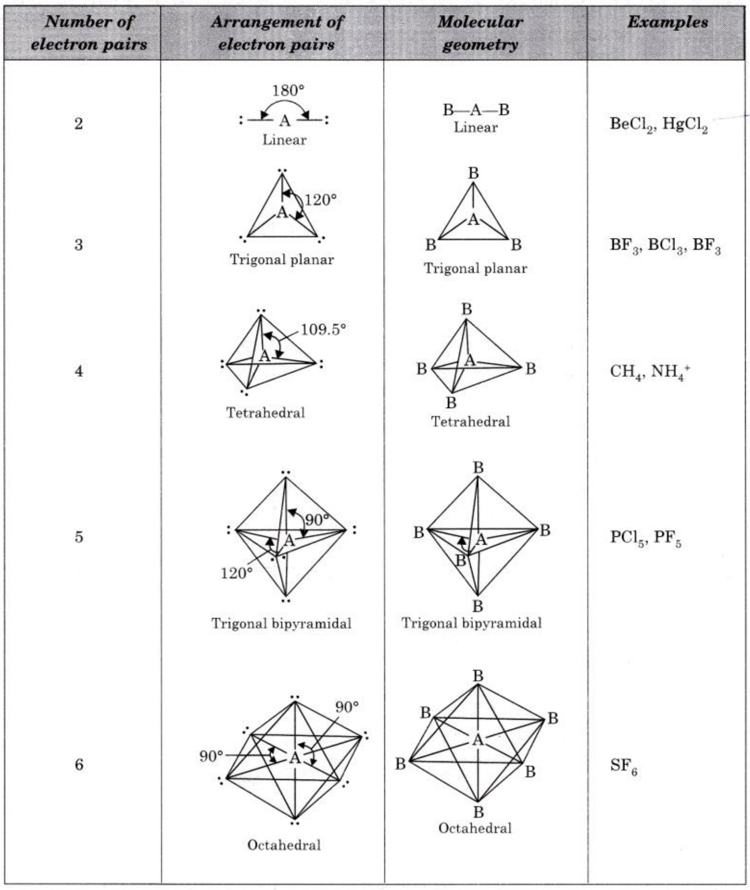
sp^{3}d^2 hybridisation



VSEPER Theory (Valency shell electron pair repulsion theory):-

Postulates:-

- The unpaired electron present around central atom make bond pair with the unpaired electron of surrounding atom while the paired electron remains as lone pair.
- Being similarly charged the lone pair as well as bond pair repels to each other.
- The repulsive interactions are not equal in magnitude i.e there magnitude are lp-lp >lp – bp>bp – bp
- Lone pair as well as bond pair arrange themselves in such a way the repulsive interaction should be minimum. The repulsive interaction should be minimum when they are far away from each other.
- Due to presence of lone pair of electrons.it disturb the regular geometry of the molecule. inspite of getting regular geometry the geometry become irregular we can say it as disturbed tetrahedral or pyramidal in case of ammonia.



Number of electron pairs	*Arrangement of electron pairs*	*Molecular geometry*	*Examples*
2	180° Linear	B—A—B Linear	$BeCl_2$, $HgCl_2$
3	120° Trigonal planar	Trigonal planar	BF_3, BCl_3, BF_3
4	109.5° Tetrahedral	Tetrahedral	CH_4, NH_4^+
5	90° 120° Trigonal bipyramidal	Trigonal bipyramidal	PCl_5, PF_5
6	90° 90° Octahedral	Octahedral	SF_6

As result the bond angle also changes due to LP – BP the angle reduce to 107^0 from 109^0.

MOLECULAR ORBITAL THEORY:-

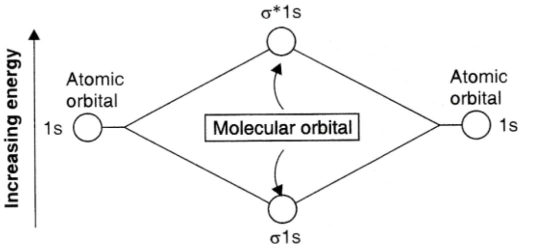
Salient Features of Molecular Orbital Theory:-

(a) According to molecular orbital theory, a molecular orbital is formed by linear combinations of atomic orbital .(LCAO- Linear combination of atomic orbital)

(b)A molecular orbital embraces the nuclei of two bonded atom

(c) The number of atomic orbitals linearly combined is equal to the number of molecular orbitalsformed.

(d) When two atomic orbitals are linearly combined they give rise to two molecular orbitals, these molecular orbitals are named as a bonding molecular orbital represented by sigma and pi bond. Anti-bonding molecular orbital represented by $\sigma *$andπ^*.



(e) One of the molecular orbital having lower energy than the other molecular orbital.

i.e BMO has lower energy then ABMO.

(f) BMO is formed by addition overlapping of atomic orbitals where as ABMO formed by subtraction overlapping of two atomic orbitals. For example if ψA and ΨB are two wave functions,

then BMO = $\psi A + \Psi B$

and ABMO = $\psi A - \Psi B$

(g) The MO diagram represented as above.

(h) Each MO obeys:-Aufbau's principle, Pauli's exclusion principle and Hund's rule of maximum multiplicity.

(i) Formations of Molecular orbital

Atomc orbital	Atomic orbital	B.molecular	ABMorbital
1s	1s	$\sigma 1s$	$\sigma * 1s$
2s	2s	$\sigma 2s$	$\sigma * 2s$
$2p_y$	$2p_y$	$\sigma 2p_y$	$\sigma * 2p_y$
2px	2px	$\pi 2px$	$\pi * 2px$
2py	2py	$\pi 2py$	$\pi * 2py$

Energy level of molecular orbitals:-Atomic No. – 1 to 7 same energy level

$\sigma 1s < \sigma *1s < \sigma 2s < \sigma *2s < \pi 2px = \pi 2py < \sigma 2py < \pi * 2px = \pi * 2py < \sigma * 2py$

Atomic No. – 8 and 8 onwards

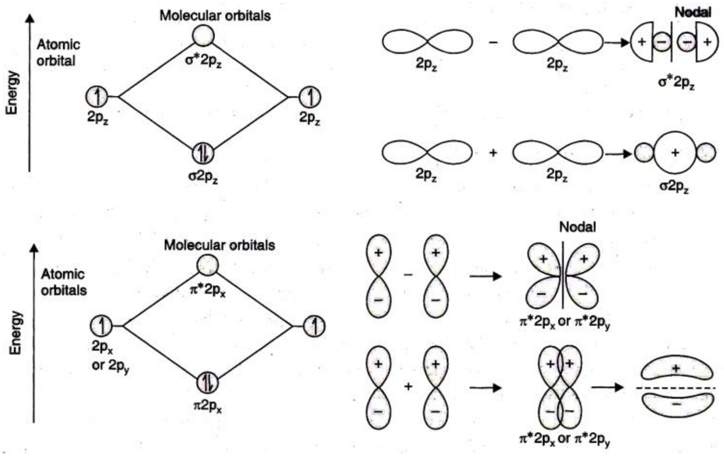
Write energy level.

LCAO method:-

BMO (Addition overlapping)

$\sigma *$ ABMO (subtraction over lapping)

BMO and ABMO



Question:-Draw the MO diagram of H_2 molecule

H_2 Total no. Of e^-s = 2

$\text{MOEC} \Rightarrow (\sigma 1st)^2 (\sigma^* 1s)^0$

He_2 – Total no. Of e^- s = 4

M. O. E. C - $(\sigma 1s)^2 (\sigma^* 1s)^2$

$Li_2 \rightarrow \text{MOEC} \rightarrow (\sigma 1s)^2 (\sigma^* 1s)^2 (\sigma 2s)^2$

$Be_2 \rightarrow \text{MOEC} \rightarrow (\sigma 1s)^2 (\sigma^* 1s)^2 (\sigma 2s)^2 (\sigma^* 2s)^2$

$B_2 \rightarrow \text{MOEC} \rightarrow (\sigma 1s)^2 (\sigma^* 1s)^2 (\sigma 2s)^2 (\sigma^* 2s)^2 (\sigma 2py)^2$

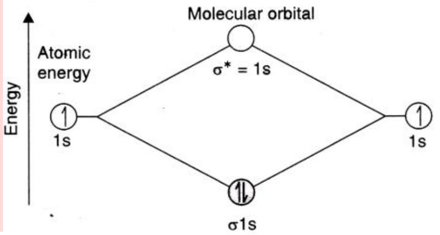
$C_2 \rightarrow \text{MOEC} \rightarrow (\sigma 1s)^2 (\sigma^* 1s)^2 (\sigma 2s)^2 (\sigma^* 2s)^2 (\sigma 2py)^2 (\pi 2px = \pi 2py)^2$

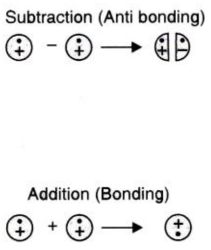
Bond Order = $\frac{1}{2}(Nb - Na)$

(a) $\underline{H_2 \rightarrow \text{MOEC} \rightarrow (\sigma 1s)^2 (\sigma^* 1s)^0}$

Bond order= $\frac{1}{2}(Nb - Na)$

$= \frac{1}{2}(2 - 0) = 1$





Stability if Nb> Na (it is stable)

If Nb = Na (it is unstable)

If Nb< Na (it is unstable)

Presence of any unpaired electrons indicates the property of paramagnetic. No presence of unpaired electrons indicates the property of diamagnetism.

He_2 Total no. Of e^-s = 4

$\text{MOEC} \rightarrow (\sigma 1s)^2 (\sigma^* 1s)^2$

Bond order = $\frac{1}{2}(Nb - Na)$

$= \frac{1}{2}(2 - 2) = \frac{0}{2} = 0$

As the bond order came zero (0) that means there is no bond formed between two helium atom, hence it is hypothetical (so practically there is no. Bond between two helium atom)

Li_2, Total no. Of e^- s = 6

$$\text{MOEC} = (\sigma 1s)^2 (\sigma^* 1s)^2 (\sigma 2s)^2$$

Bond order = $\frac{1}{2}(4-2)=1$

Stable because,Nb> Na, diamagnetism

Be_2 :- Total no. Of electrons = 8

$$\text{MOEC} = (\sigma 1s)^2 (\sigma^* 1s)^2 (\sigma 2s)^2 (\sigma^* 2s)^2$$

Bond order = $\frac{1}{2}(4-4)=0$

Unstable because Nb = Na

B_2 :- Total no. Of e^-s = 10

$$\text{MOEC} = (\sigma 1s)^2 (\sigma^* 1s)^2 (\sigma 2s)^2 (\sigma^* 2s)^2 (\pi 2px)^1 = (\pi 2py)^1$$

Bond order = $\frac{1}{2}(6-4)=\frac{2}{2}=1$

Stability because Nb> Na

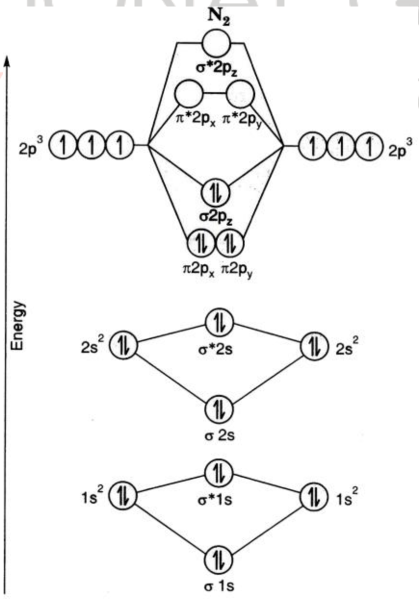
Para magnetism

C_2 :- Total no. Of e^-s = 10

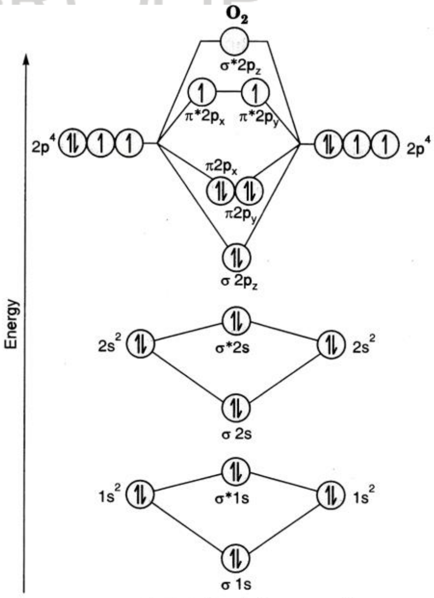
$$\text{MOEC} = (\sigma 1s)^2 (\sigma^* 1s)^2 (\sigma 2s)^2 (\sigma^* 2s)^2 (\pi 2px)^2 = (\pi 2py)^2$$

Bond order = $\frac{1}{2}(8-4)=2$

N_2 :- Total e^-s = 14



Energy level diagrams of B_2, C_2, Li_2 are similar to N_2



Energy level diagrams of F_2 and Ne_2 are similar to O_2

$$\text{MOEC}=(\sigma 1s)^2(\sigma^*1s)^2(\sigma 2s)^2(\sigma^*2s)^2(\pi 2px)^2=(\pi 2py)^2(\sigma 2py)^2$$

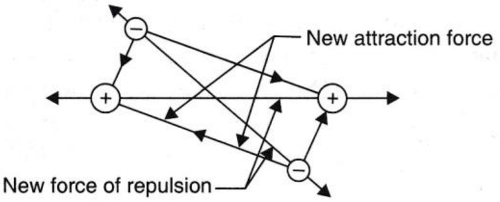
$$\text{Bond order}=\frac{1}{2}(\text{Nb}-\text{Na})$$

$$=\frac{1}{2}(10-4)=3$$

$$\text{MOEC}\rightarrow \text{K.K}(\sigma 2s)^2(\sigma^*2s)^2(\pi 2px)^2=(\pi 2py)^2(\sigma 2pz)^2$$

Qualitative/ Non mathematical treatment of valence bond theory:-

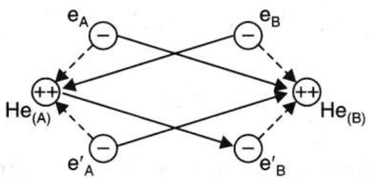
Formation of H_2 molecule by VBT

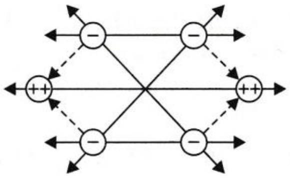


$H+H\rightarrow H_2$

(a) 2 types of attractive interaction

(b) 2 types of repulsive interaction





Let us consider two H atom having nucleus of NA and NB and their electrons are e_A and e_B

(a) The two attractive interaction arises due to N_A and e_A (old interaction) and NB and eB

NA – e_B and N_B – e_A new interaction

(-) old attractive interaction.

(.....) new attractive interaction

(b) The repulsive interaction are also of two types

Experimentally it has been observed that magnitude of new attractive forces is more than the magnitude of new repulsive forces, as a result, the two atoms approaches each other, as a result the net potential energy decreases.

Ultimately a stage came when the net forces of attraction balances the new repulsive interactions. At this stage two hydrogen atoms are said to bonded together to form a stable molecule having bond length 74 PM.

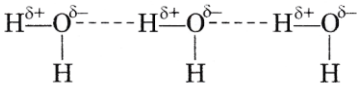
Hydrogen Bond:-It can be defined as the partial attractive force which binds hydrogen atom of one molecule with the electronegative atom (F, O or N) of another molecule. Hydrogen bond is represented by a dotted line (.......) while a solid line represents a covalent bond. For example:

(a) In HF molecule, the hydrogen bond exists between hydrogen atom of one molecule and fluorine atom of another molecule as depicted below.

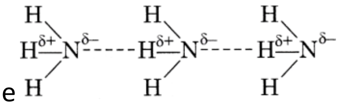
$$---H^{\delta+}-F^{\delta-}---H^{\delta+}-F^{\delta-}---H^{\delta+}-F^{\delta-}$$

Here, hydrogen bond acts as a bridge between two atoms which holds one atom by covalent bond and the other by hydrogen bond.

(b) H_2O molecule



(c) NH_3 molecule



Cause of Formation of Hydrogen Bond:- When hydrogen is bonded to a strongly electronegative element 'X', the electron pair shared between the two atoms moves far away from hydrogen atom. As a result the hydrogen atom becomes highly electropositive with respect to the other atom 'X'. Since there is displacement of electrons towards X, the hydrogen acquires fractional positive charge $\left(\delta^{+}\right)$ while 'X' attains fractional negative charge $\left(\delta^{-}\right)$. This results in the formation of a polar molecule having electrostatic force of attraction which can be represented as.

$H^{\delta+}-X^{\delta-}------H^{\delta+}-X^{\delta-}----H^{\delta+}-X^{\delta-}$

The magnitude of H-bonding depends on the physical state of the compound. It is maximum in the solid state and minimum in the gaseous state. Thus, the hydrogen bonds have a strong influence on the structure and properties of the compounds.

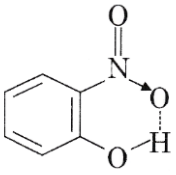
Types of H-Bonds:-

There are two types H-bonds

(a) Intermolecular hydrogen bond:- It is formed between two different molecules of the same or different compounds. For example, H-bond in case of HF molecule, alcohol or water molecules, etc.

$---H^{\delta+}-F^{\delta-}---H^{\delta+}-F^{\delta-}---H^{\delta+}-F^{\delta-}---H^{\delta+}-F^{\delta-}$

(b) Intramolecular hydrogen bond:- It is formed when hydrogen atom is situated between the two highly electronegative (F, O, N) atoms present within the same planar molecule. For example, o-nitrphenol.



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