

3. CHEMICAL BOND

Electronic - Valency theory:-

In periodic table inert gas elements are having a stable electronic configuration. Except Helium (He) the remaining elements have got $ns^2 np^6$ configuration known to be Octet configuration. The remaining elements are not at all having this type of configuration. So that all the elements are ready to achieve this configuration by losing electrons (8+) by gaining electrons (8-) Sharing electrons is known to be electronic - Valency theory.

* Ionic Bond

Due to the migration of electron(s) from one atom to another atom cation and anion results to give an ionic bond by strong Electro-static attraction forces

Ex:- (i) Sodium chloride NaCl:-

Atomic No. of Sodium (Na) = 11

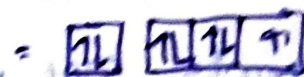
Its electronic configuration = $1s^2 2s^2 2p^6 3s^1$

To attain stability 'Na' atom gives up one electron by 1st Ionisation Enthalpy.



Atomic number of chlorine (Cl) = 17

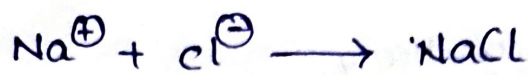
Valency configuration = $3s^2 3p^5$



To attain stability 'Cl' atom takes up one electron to get stable configuration



Then, Due to strong electrostatic attraction forces Na^+ and Cl^- combines to give NaCl .

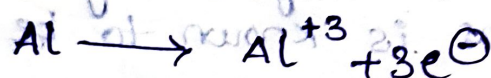


(ii) AlCl_3

Atomic no. of Al = 13

Valency configuration = $2s^2 2p^6 3s^2 3p^1$

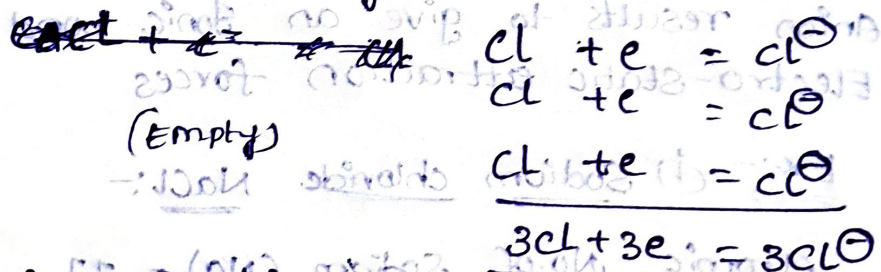
To attain stability Aluminium atom give up '3' electrons.



Atomic no. of chlorine (Cl) = 17

Valency configuration = $2s^2 2p^6 3s^2 3p^5$

To attain stability 'Cl' atom up '8' electrons to get stable configuration.

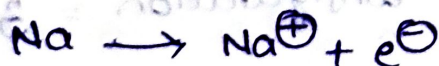


Aluminium combines with 3 chloride ions to give an ionic compound aluminium chloride.

* Lewis dot method

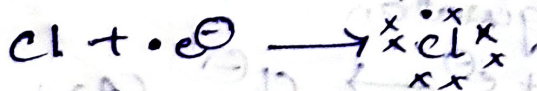
Na = 11

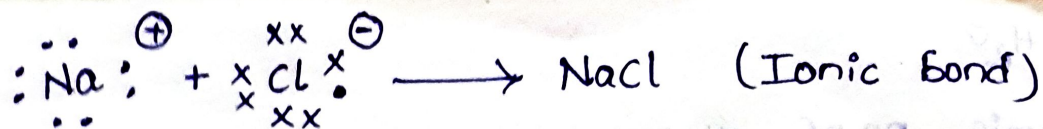
Valency configuration = $2s^2 2p^6 (3s^1)$



Lewis Dot method = $\text{Na} \longrightarrow :\text{Na}: + \cdot (\text{e}^-)$

Chlorine = $3s^2 3p^5 \Rightarrow \boxed{\uparrow\downarrow} \boxed{\uparrow\downarrow} \boxed{\uparrow}$

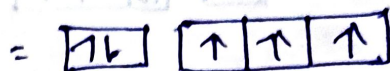




* (i) NF_3

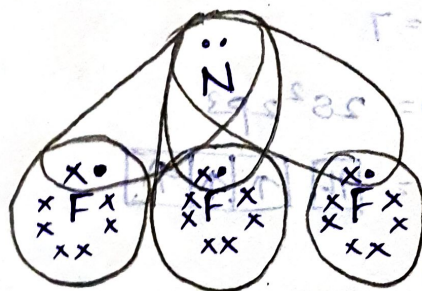
Nitrogen = 7

Valency configuration = $2s^2 2p^3$



F = 9

Valency configuration = $2s^2 2p^5$



Covalent bond:-

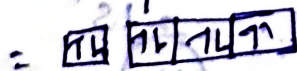
The sharing of electron pair(s) b/w two atoms is known to be covalent bond.

Ex:- (i) $\text{H}-\text{Cl}$ (Hydrogen chloride)

Atomic number of Hydrogen = 1
configuration = $1s^1$

Atomic no. of chlorine = 17

Configuration = $3s^2 3p^5$



$\text{H}-\text{Cl}$

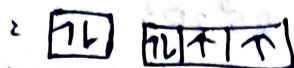
(ii) H_2O

Atomic no. of Hydrogen = 1

Configuration = $1s^1$

Atomic no. of Oxygen = 8

Configuration = $2s^2 2p^4$



(iii) NH_3 (Ammonia)

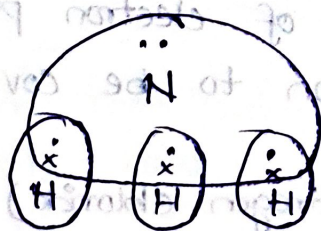
Atomic no. of Nitrogen = 7

Electronic configuration = $2s^2 2p^3$



Atomic no. of (H) = 1

Valency configuration = $1s^1$

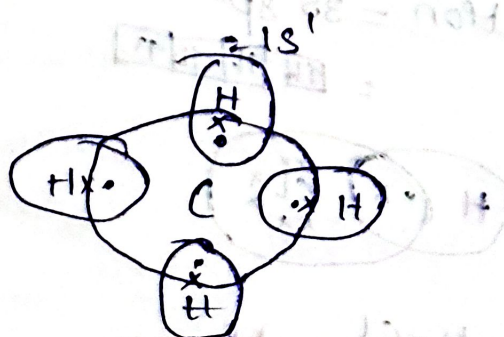


(iv) CH_4 (Methane)

Atomic no. of Carbon = 6

configuration = $2s^2 2p^2$

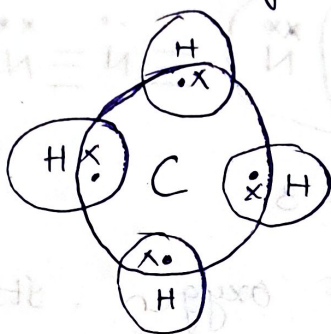
Atomic no. of Hydrogen = 1



According to Ground State configuration, carbon atom has two unpaired electrons only. That's why it is capable to form two bonds only. In reality carbon forms '4' bonds with 4 Hydrogen atoms (CH_4). So, ground state configuration is not applicable. In the presence of high energy the $2s^2$ electrons are excited to vacant p_z orbital to give '4' unpaired electrons



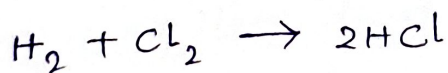
Excited electronic configuration = 



* Properties of covalent bond:-

) Bond distance:-

In the case of covalent bonded molecules the half of the distance b/w two centers of two nuclei is known to be covalent radius



In the case of Hydrogen chloride

$\text{H}-\text{Cl}$. The bond distance is given by 1.275 pm. This is not at all considered as atomic radius of individuals.

In the case of Homo-Nuclear molecules (CH_4 , Cl_2 , N_2 , F_2) The covalent radius said to be individual atomic radii

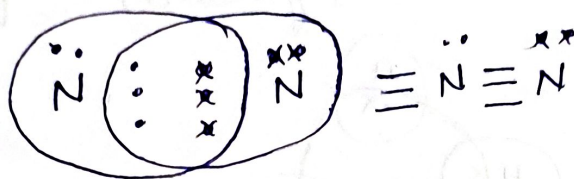
② Bond order:-

In the case of di-atomic molecules the no. of bonds placed b/w two atoms is known to be Bond order.

Ex: i) In the case of Nitrogen (N), its Bond order is '3'

Nitrogen atomic number = 7

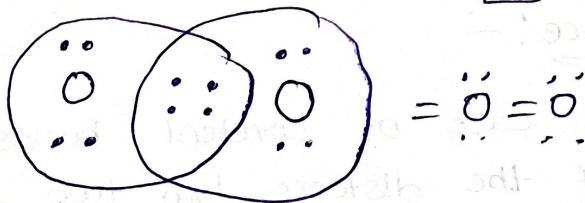
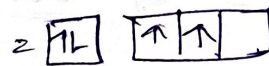
Electronic configuration = $2s^2 2p^3$



Bond order = 3

ii) In the case of Oxygen, its Bond order is 2.

atomic number of oxygen = $2s^2 2p^2$



Bond order = 2

③ Bond Angle:-

In given molecule the practice calculation of Bond angle towards adjacent orbitals is known to be bond angle. At this stage all the repulsions are minimised in molecule.

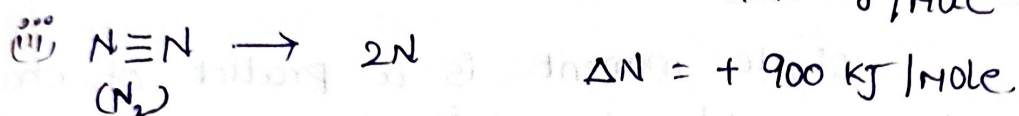
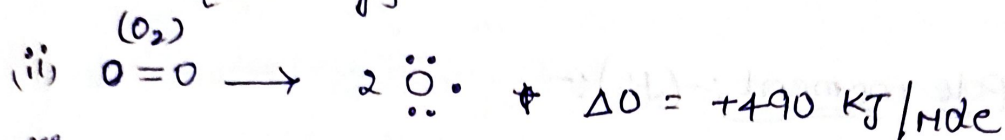
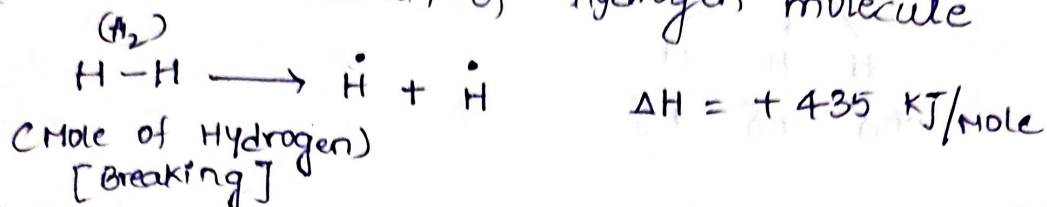
Ex:- i) In water molecule bond angle is " $104^\circ 30'$ "

ii) In Ammonia molecule bond angle is " 107° "

Bond Dissociation Energy

The energy required to break one mole of bonds is known to be Bond Dissociation Energy.

Ex: (i) Bond Dissociation of Hydrogen molecule

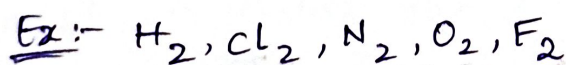


~~Polar and~~

Types of covalent bond:-

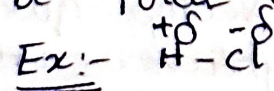
Non polar covalent bond:-

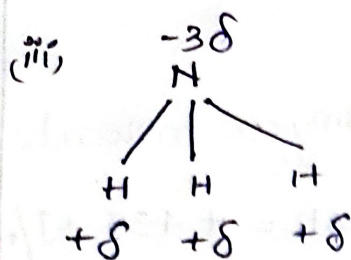
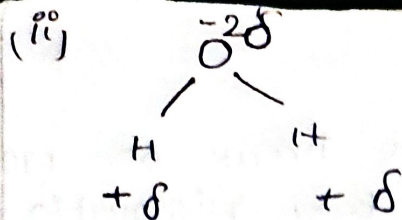
If covalent bond placed b/w two similar atoms. Then, the bond pair always between two centers of two atoms. That's why the molecule doesn't attain positive & negative charges (Di-pole)



Polar covalent bond:-

When covalent bond is placed b/w two dissimilar atoms ("hetero"). Then, the bond pair of electrons shift towards (Partially) one particular atom which has got high electronegativity. then this atom attains partial -ve charge, and other atom gets partial +ve charge. Due to the formation of this charges the covalent bond is known to be Polar covalent bond.





(m)

* Dipole moment :- (μ) :-

Dipole moment is a product of charge and distance b/w two poles. therefore, Dipole

Dipole moment $\mu = \delta \cdot L$

= charge . Distance

$\therefore \mu = \text{colomb meter} \rightarrow \text{units}$

The units for dipole moment is "DEBYE"

$1 \text{ Debye} = 10 = 3.33 \times 10^{-30} \text{ colomb meter}$

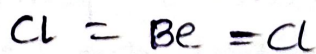
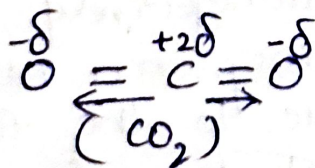
Ex: - (i) 1.875 D

It means $1.875 \times 3.33 \times 10^{-30} \text{ colomb meter}$

(ii) 2 D

$\rightarrow 2 \times 3.33 \times 10^{-30}$

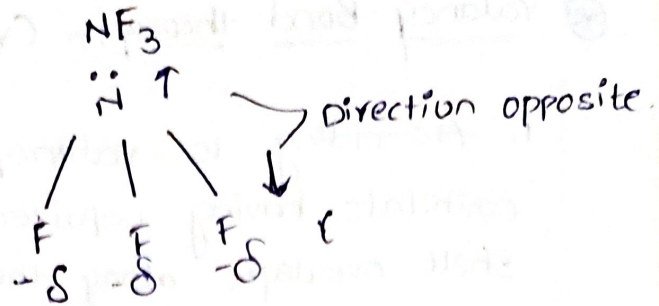
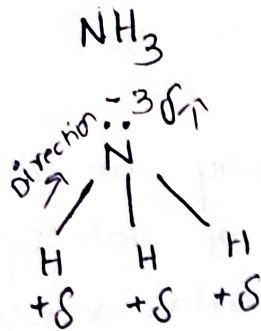
In the case of linear molecules like carbon dioxide and (CO_2) and BeCl_2



Since, Dipole moment is a vector quantity which is a product of magnitude and direction that's why in the case of linear molecules equal & opposite Di-Pole moment

values in algebraic sum is said to be zero.

* Discuss the Dipole moment of NH_3 and NF_3 :-



In the case of ammonia 'N' has got high electronegativity. That's why the bond pair of electrons moves towards nitrogen, and the same time the lone pair on 'N' atom (is) also moves tries to move in the same direction (forward) so that the bond pair of electrons in ammonia and the lone pair travels in same direction. So that the molecule is having good dipole moment.

In contrast to this, in the case of NF_3 molecules. The bond pair of electrons moves towards fluorine atom and the same time. The lone pair of electrons on nitrogen atom moves forward direction. this results a disturbance in charge and hence, the calculated dipole moment is higher for NH_3 (Ammonia) than, NF_3 molecule.

Am * Fajans law:-

1. (Fajans law), in given cations, which cation has got low atomic radii comes under covalent character.
2. In given cations which one is having high Ionization Enthalpy are favourable for covalent bond.
3. In given cations which is having high charge comes under covalent character.
4. In given cations which cation has got "Pseudo inert gas configuration" comes under covalent character.

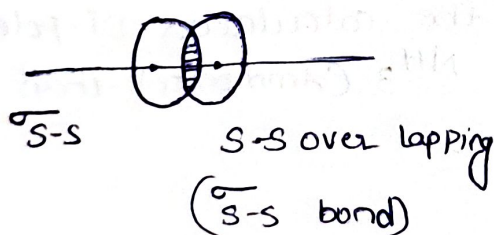
Similarly, we can explain covalent bond for anions.

* Valency Bond theory:- (VB theory)

1. According to valency bond theory the atomic orbitals having unpaired electrons of valency shell overlaps along the inter-nuclear axis to give covalent bond.
2. As the overlapping increases strong covalent bond results as the overlapping is minimum weak covalent bond results.
3. If the overlapping of p-orbitals takes place perpendicular to the inter-nuclear axis to give a weak ' π '-bond takes place. on the other hand the strong covalent bond results on internuclear axis to give "sigma" (σ) bond takes place.

Ex: ① H_2 molecule

According to VB theory the overlapping of '2' 1s orbital along the inter-nuclear axis gives covalent bond

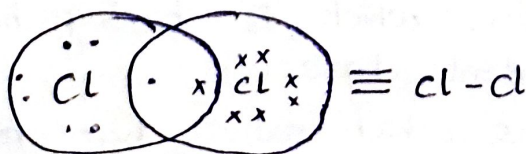
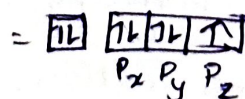


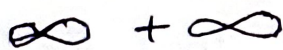
- [Inter-nuclear axis:- means an imaginary line passes through 2 centers of 2 nuclei]

② Cl_2 molecule

Chlorine Atomic no. = 17

Electronic configuration = $3s^2 3p^5$

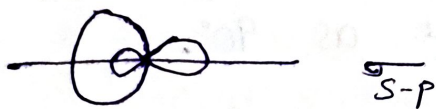
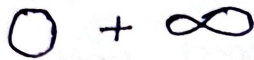
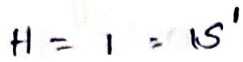




$\overline{P-P}$ CP-P over lapping)

3)

HCl molecule :-



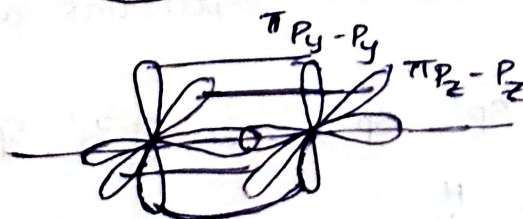
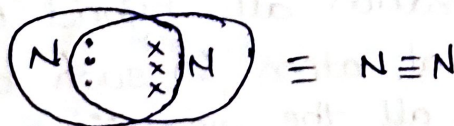
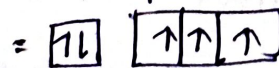
$\overline{SP}$ (S-P over lapping)

During the formation of covalent bond two atomic orbitals placed with single electrons overlap along the internuclear axis results "sigma bond". It is a strong bond because the newly formed electron pair placed b/w two centers of two nuclei.

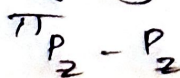
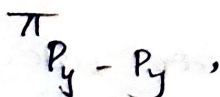
4) N_2 molecule :-

Atomic number of Nitrogen = 7

Electronic configuration = $2s^2 2p^3$



π bond



In the case of p_x orbitals. They overlap along internuclear axis to give a sigma bond ($\sigma_{p_x-p_x}$) then two, p_y orbitals, two, p_z orbitals overlap laterally (sideways) overlapping to be two, π Bonds results. π -Bond is always a Weak bond. Because, the electron density spreads perpendicular to the internuclear axis. So that it is easily "exposed to the environment".

VB theory couldn't explain bond angles in NH_3 and in water molecule (H_2O). But it explained the bond angle as 90° .

* Hybridization:-

* (1) The process of mixing of atomic orbitals of same energy leads to formation of same numbered hybrid orbital is known to be Hybridization.

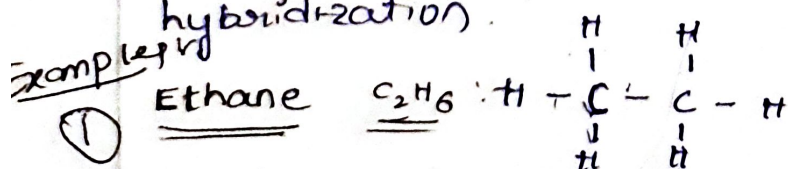
(2) according to Hybridization paired valency orbital is also allowed for hybridization. But, these hybrid orbitals not allowed for chemical reaction.

(3) Hybrid orbitals with unpaired electrons are only allowed for sigma bond (σ) formation.

(4) To explain π -Bond formation 'unhybridized' pure p-orbitals are allowed for π -bond formation.

(5) After the hybridization all hybrid orbitals are placed on central atom in such a way such that at which all the repulsions are minimised.

(6) There are sp^3 , sp^2 , sp , sp^3d , sp^3d^2 , sp^3d^3 hybridization.



In Ethane two carbon atoms are undergoes sp^3 Hybridization.

Atomic number of carbon = 6

Ground state configuration = $2s^2 2p^2$

Excited state configuration = $\boxed{\uparrow\downarrow} \boxed{\uparrow\downarrow} \boxed{\uparrow} \boxed{\uparrow}$

According to sp^3 hybridization, the process of mixing of 1, $2s$ orbital, & 3, $2p$ orbitals leads to formation of 4, sp^3 hybrid orbitals. These hybrid orbitals on two carbon atoms arranged in such a way such that at which all the repulsions are minimised. 2, sp^3 hybrid orbitals of 2, carbon atoms overlaps along the inter nuclear axis to give a Sigma bond known to be $\overline{sp^3-sp^3}$. The remaining overlaps with 6, $1s$ orbitals of two carbon atoms to give 6, $\overline{sp^3-s}$. The ideal geometry of the molecule is "Bi-tetra hydral" and the bond angle is " $109^\circ 28'$ ".

2)
✱

Ethelene -



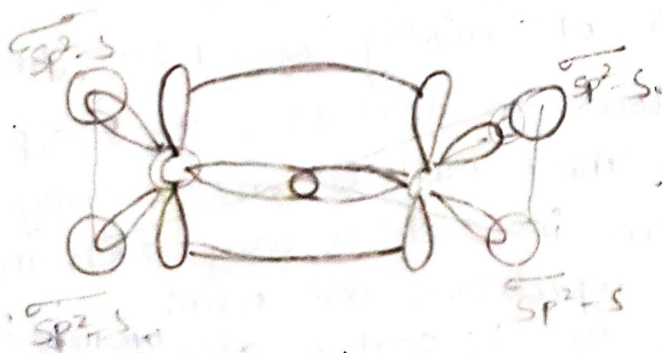
In Ethelene two carbon atoms are undergoes sp^2 Hybridization.

Atomic no. of carbon = 6

Ground state confi. = $2s^2 2p^2$

Excited state confi. = $\boxed{\uparrow\downarrow} \boxed{\uparrow} \boxed{\uparrow} \boxed{}$ } 2 vacant orbital.

Excited state confi. = $\boxed{\uparrow\downarrow} \boxed{\uparrow\uparrow} \boxed{\uparrow}$



Total Bonds
↓
4
↓
✓ 3σ
↓
3 hybrid orbitals.
 sp^2
1π
X

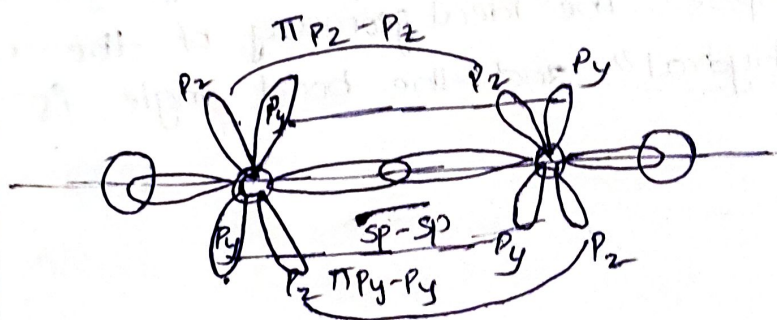
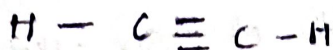
Bi-triangular with Bond angle 120° ,

According to sp^2 Hybridization the process of

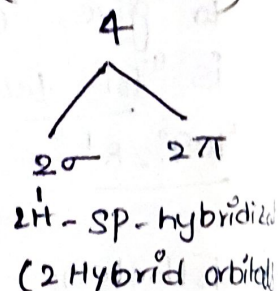
mixing of 1, 2s orbital and 2, 2p orbitals to give 3, sp^2 hybrid orbitals in which one sp^2 hybrid orbital of 1 carbon atom overlaps along internuclear axis towards another sp^2 hybrid orbital of carbon atom to give a sigma bond ($\sigma_{sp^2-sp^2}$). The remaining 4, sp^2 hybrid orbitals overlaps with the 4, 1s orbitals of 4, Hydrogen atoms to give 4, sigma bonds (σ_{sp^2-s}). The ideal geometry of the molecule is Triangular with bond angle 120° .

④ AE ACETYLENE: (C_2H_2)

(3)



(Total Bond)



In Acetylene two carbon atoms undergo 'sp' hybridization.

Atomic number of carbon = 6

Excited state configuration = $2s^1 2p_x^2 2p_y^1 2p_z^1$



The process of mixing of 1, 2s orbital, 1, 2p orbital leads to formation of 2, sp hybrid orbitals. These orbitals are arranged on central atom in such a way such that all the repulsions are minimised. 2, sp hybrid orbitals of 2, carbon atom overlap along the internuclear axis to give a sigma bond (σ_{sp-sp}). The remaining 2, sp hybrid orbitals overlap

with 2, hydrogen atoms to give 2, sigma bonds (σ_{sp-s}). The remaining two unhybridized p-orbitals lateral overlaps to give two- π bonds ($\pi_{p_y-p_y}$, $\pi_{p_z-p_z}$). And the ideal geometry of the molecule is 180° (Linear)

④ PCl_5 :- (Phosphorus penta chloride)

(4) In PCl_5 the center atom phosphorus undergoes sp^3d hybridization.

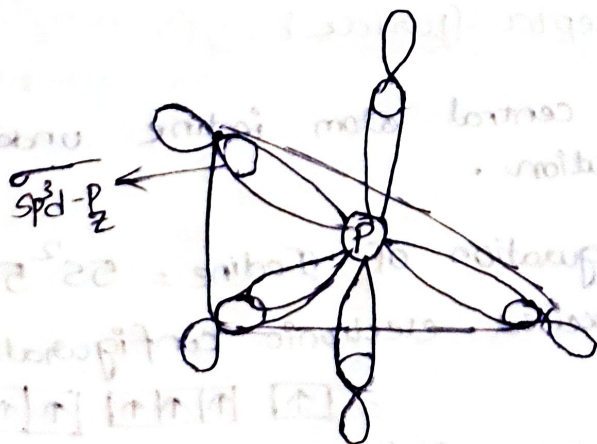
Phosphorus atomic no = 15

Ground State configuration = $3s^2 3p^3$

Excited State configuration = $3s^1 3p^3 3d^1$

= $\uparrow \uparrow \uparrow \uparrow \uparrow$

According to sp^3d hybridization the process of mixing of 1, 3s & 3, 3p orbitals, 1, 3d orbitals to give 5, sp^3d Hybrid orbitals these are arranged on central atom at which repulsions are minimised. Then, all these 5, sp^3d orbitals (hybrid) overlaps with the 5, p_z orbitals of 5 chlorine atoms to give 5 $\sigma_{sp^3d-p_z}$. The ideal geometry of the molecule is "Trigonal bi-pyramid".



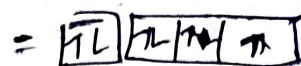
The ideal geometry of the molecule is Trigonal Bi-pyramid with the bond angles 120° , 180° .

⑥ SF₆ :- Sulphur hexachloride

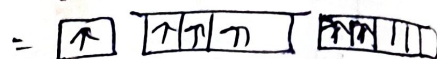
In SF₆ the central atom Sulphur undergoes sp³d² hybridization.

Atomic no. of Sulphur = 16

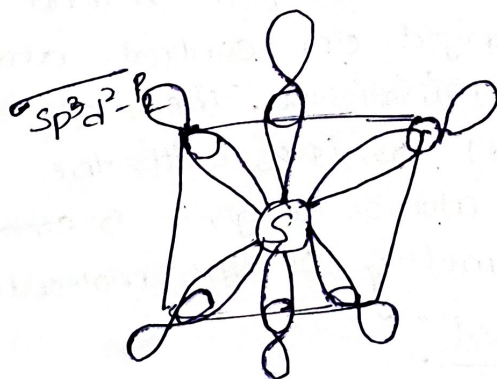
Ground State configuration = 3s²3p⁴



Double excited state configuration



According to sp³d² hybridization, 6, sp³d² hybrid orbitals. These are arranged on central atom at which all repulsions get minimum. These 6 hybrid orbitals overlaps with 6, p_z orbitals of 6 Fluorine atoms to give 6, sp³d²-p_z bonds. Ideal geometry of the molecule is 'Octahedral' and the bond angles are 90°, 180°.

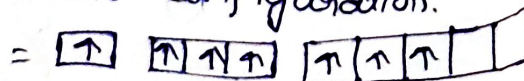


⑦ IF₇ :- Iodine hepta fluoride

In IF₇ the central atom iodine undergoes sp³d³ hybridization.

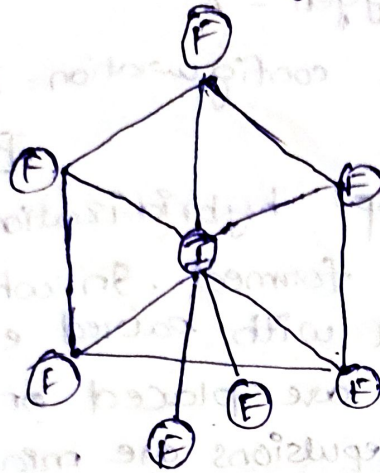
Electronic configuration of Iodine = 5s²5p⁵

The triple excited electronic configuration.



According to sp³d³ hybridization, 7, sp³d³ hybrid orbitals are formed. These are arranged on central atom at which repulsions are

minimised. then, 7, p_z orbitals of 7, Fluorine atoms overlaps with the 7, sp^3d^3 hybrid orbitals to give 7, Sigma bonds. ($sp^3d^3 - p_z$). The ideal geometry of the molecule is "Pentagonal bi-Pyramid" with the bond angles " $110^\circ, 180^\circ$ ".



$sp^3d^3 - p_z$

⑧ AlH_3 :- (Ammonia)

1

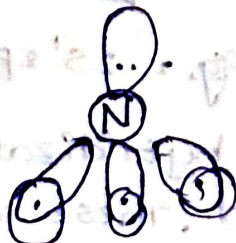
In ammonia the central atom Nitrogen undergoes sp^3 hybridization.

Atomic no. of Nitrogen = 7

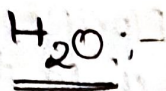
Electronic configuration: $2s^2 2p^3$



According to sp^3 hybridization 4, sp^3 hybrid orbitals are formed. In which 1, sp^3 hybrid orbital is placed with 1, lone pair of electrons. The remaining 3, sp^3 hybrid orbitals overlaps with the s-orbitals of 3, hydrogen atoms to give 3, Sigma sp^3-s (sp^3-s) bonds. The ideal geometry of the molecule is 'Pyramidal' with the bond angle 107° .



8

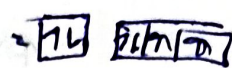


9

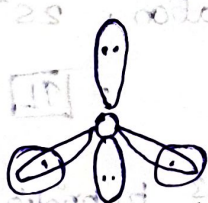
In H₂O the central atom oxygen undergoes sp³ hybridization.

Atomic no. of oxygen = 8.

Electronic configuration = 2s²2p⁴



According to sp³ hybridization 4, sp³ hybrid orbitals are formed. In which 2, sp³ orbitals are filled with paired electrons. All these orbitals are placed on central atom at which repulsions are minimised. 2, sp³ hybrid orbitals overlaps with the s-orbital of two hydrogen atoms to give 2, (sp³-s bonds). The ideal geometry of the molecule is angular (V-shaped). The bond angle is 104°30'.



104°30'

10

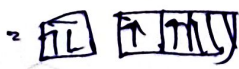
Methane CH₄

In methane the central atom carbon undergoes sp³ hybridization.

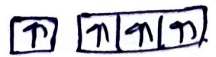
Atomic no. of [C] = 6

= 2s²2p²

Ground state

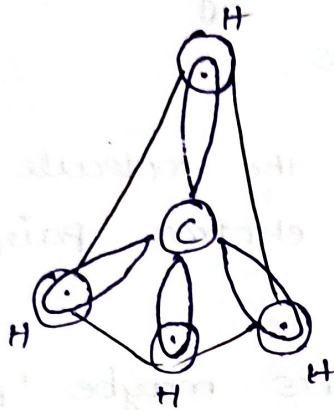


Excited state config. = 2s¹2p³



According to sp³ hybridization 4, sp³ hybrid orbitals are formed. These are arranged on central atom at which repulsions are minimised. These overlaps with the s-orbitals of 4, hydrog

atoms to give 4, (sp^3-s). The Ideal geometry of the molecule is "Tetra hedral" and the bond angle is $109^\circ 28'$.



Q) BCl_3 :- (Boron tri-chloride)

In BCl_3 the central atom Boron undergoes sp^2 hybridization.

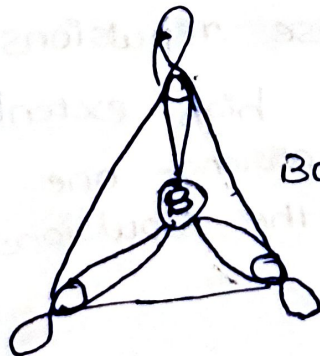
Atomic number of Boron = 5

Electronic configuration = $2s^2 2p^1$

Ground state: $\uparrow\downarrow \uparrow \uparrow$

Excited electronic configuration = $\uparrow \uparrow \uparrow$

According to sp^2 Hybridization 3, sp^2 hybrid orbitals are formed. These are overlaps with 3, p_z orbitals of 3, chlorine atoms to give 3, σ bonds. The Ideal geometry of the molecule is planar triangle with the bond angle 120° .



Bond angle 120°

sp^2-p_z

8M
★
★
★
Valency shell. Electron pair repulsion theory
VSEPR:-

1. According to this theory, electrons are considered as point charges.
2. The structure of the molecule mainly depends upon total no. of electron pairs on central atom.
3. These electron pairs may be 'bond pairs or lone pairs.'
4. Bond pairs always placed between two centers of two atoms where as, lone pairs always placed on 'apex' of central atom.
5. Since, bond pairs always placed between two atoms. They always occupy less space provided by the molecule. where as, lone pair of electrons occupies much more space provided by the molecule. which leads to the following repulsions in the molecule.
 - (i) Lone pair - Bond pair
 - (ii) Bond pair - Bond pair
 - (iii) Lone pair - lone pair
6. Among all these repulsions lone pair-lone pair is having high extent. That's why the molecule itself arrange one particular structure at which all the repulsions are minimised.

SNO	Total no. of electron Pairs	Bond Pairs	lone Pairs	Structure	Bond angle
01.	2	2	0	BeCl_2 linear	180°
02.	3	3	0	BeCl_3 Triangular	120°
03.	4	4	0	CH_4 Tetrahedral	$109^\circ 28'$
04.	4	3	1	NH_3 Pyramidal	107°
05.	4	2	2	H_2O Angular	$104^\circ 30'$

4m
*

Hydrogen bond :-

If hydrogen atom is placed between two highly electro-negative elements by strong electrostatic attraction force, then, this type of attraction force is known to be hydrogen bond.

Conditions for hydrogen bond :-

1. High electronegativity.
2. Less atomic radii, are the conditions to show hydrogen bond.

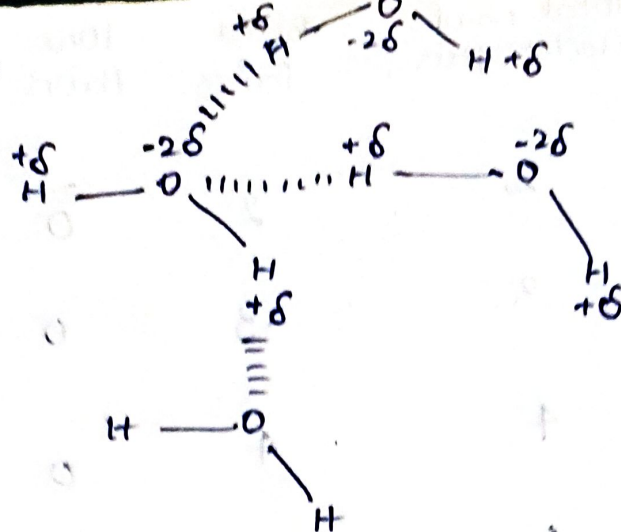
Hydrogen bond is 2 types :-

1. Inter hydrogen bonding
2. Intra hydrogen bonding

* Inter hydrogen bonding :-

If hydrogen bond is formed between similar molecules, then, it is known to be Inter hydrogen bonding.

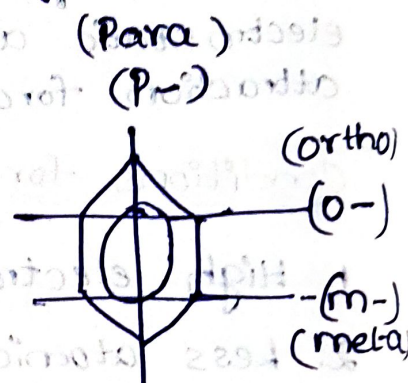
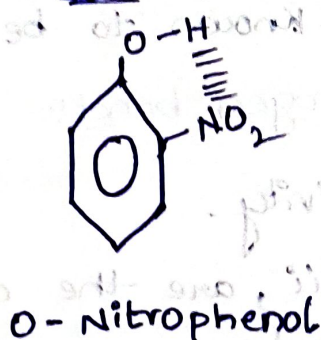
Eg:- H_2O



② Intra hydrogen bonding:-

If hydrogen bond is formed between the molecule (within the molecule) is known to be Intra hydrogen bonding.

Ex:- Nitrophenol



Applications for Hydrogen bond:-

1. Due to the existence of Hydrogen bond the Boiling points, of the liquids increases.
2. Due to the existence of Inter Hydrogen bonding (H_2O) is in liquid state whereas, (H_2S) is in gaseous state.

REASON:- Since Sulphur atom has got high atomic radius with low electronegativity. It doesn't form Inter hydrogen bonding.

3. H_2O is having high boiling point ($100^\circ C$) while 'HF' is $20^\circ C$.

Reason:- In the case of H_2O the extent of hydrogen bonds towards one water molecule is four (4). whereas, in the case of 'HF' the extent of hydrogen bonds are '2'. That's why H_2O has got high boiling point.

4. HCl molecules doesn't form inter hydrogen bond.

Reason Chlorine is having high electronegativity (3.1 units). But, due to high atomic radii it is incapable to form inter hydrogen bonding.

5. ' NH_3 ' is having high boiling point.

Reason Due to less atomic radii, high electronegativity (3.1 units). It can form inter hydrogen bonding. That's why it is having inter hydrogen bonding.

801

Molecular orbital theory:- (M.O. theory)

1. linear combination of atomic orbitals leads to formation of same number of molecular orbitals (M.O's) in which half of the M.O's are having less energy than individual A.O's. Similarly, the remaining half of M.O's are having high energy than individual A.O's.

A.O's - Atomic orbitals

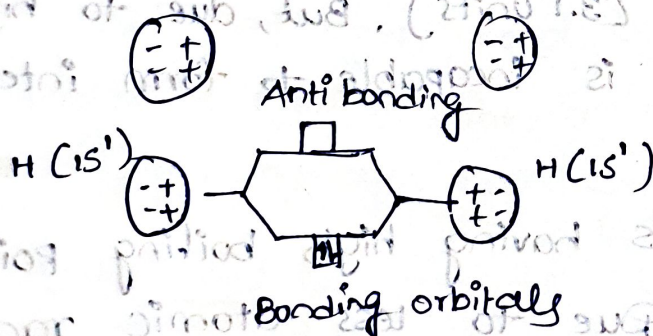
2. The lowest energy molecular orbitals are known to be bonding orbitals and high energy molecular orbitals known to be Anti bonding orbitals

3. According to M.O Theory ~~bond order~~

$$\text{Bond order} = \frac{1}{2} \left[\begin{array}{l} \text{Total no. of } e^{-} \text{ in Bonding orbital} \\ - \text{Total no. of electrons in Anti bonding orbital} \end{array} \right]$$

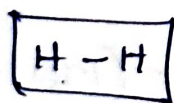
MOED :- (Molecular orbital energy diagrams) :-

① H₂ Molecule :-

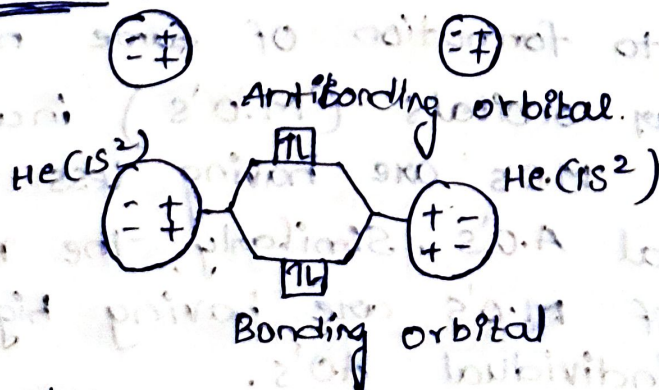


$$\text{Bond order} = \frac{1}{2} (2 - 0)$$

$$B.O = 1$$



② He₂ molecule :-



$$\begin{aligned} \text{Bond order} &= \frac{1}{2} (2 - 2) \\ &= \frac{1}{2} (0) \end{aligned}$$

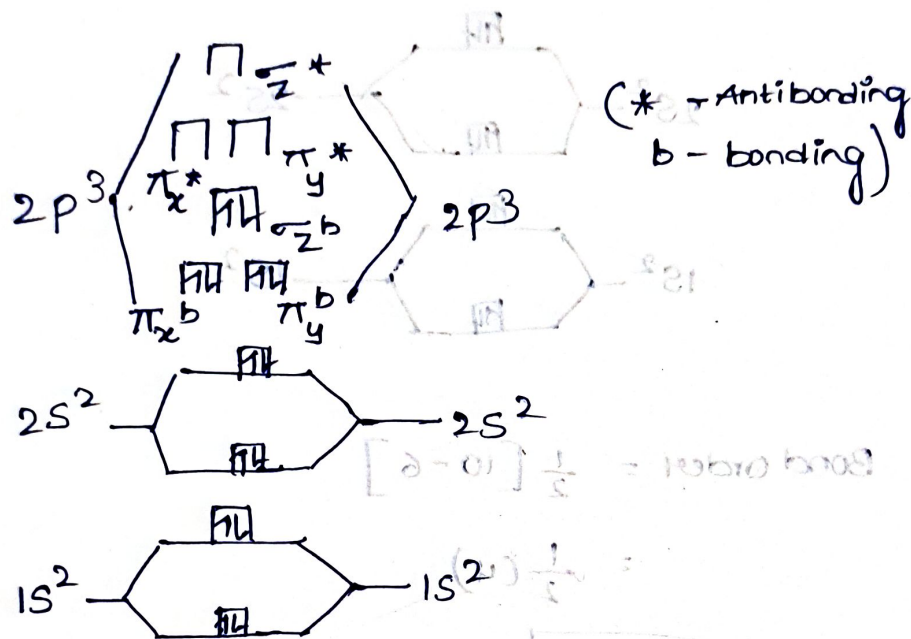
$$\Rightarrow \text{Bond order} = \frac{0}{2}$$

$$\therefore \text{B.O} = 0$$

According to M.O-theory bond order of He_2 is '0'. That's why Helium never forms a chemical bond. because of completely filled configuration (Inert gas configuration).

③ Atomic number = Z , ($Z \leq 7$)

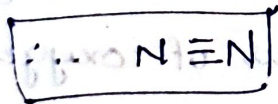
✱



here, Bond order = $\frac{1}{2} [10 - 4]$

$$= \frac{6}{2}$$

$$\text{B.O} = 3$$



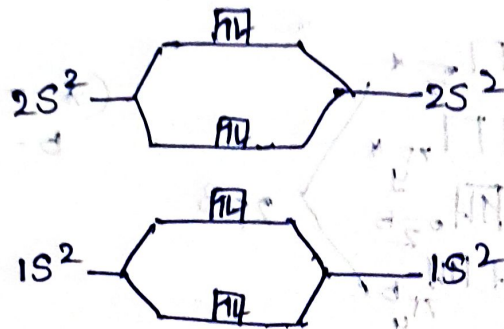
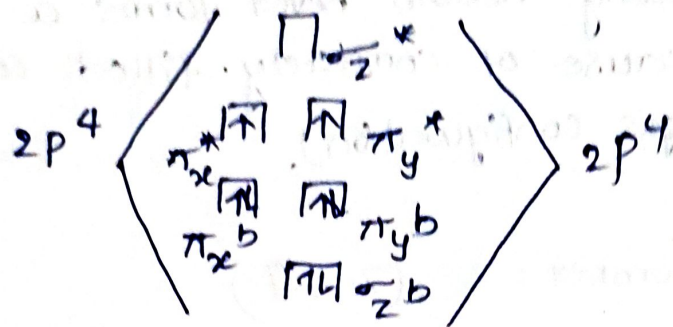
③

Atomic

④ Atomic number = Z , $Z \geq 8$, $Z \leq 20$

Oxygen molecule

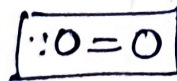
O₂



$$\text{Bond order} = \frac{1}{2} [10 - 6]$$

$$= \frac{1}{2} (4)$$

$$\therefore \text{B.O} = 2$$



The existence of two unpaired electrons in antibonding orbitals towards π -bond shows "Para-magnetic" behaviour of oxygen molecule