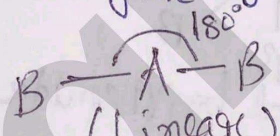
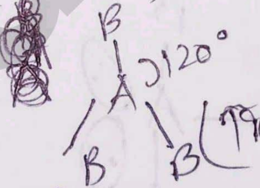
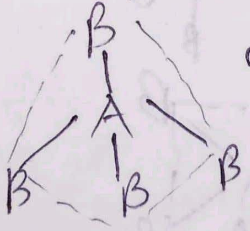
Valence Shell Electron paire repulsion Theory: (VSEPR)

i. This theory based on the repulsive interactions of the electron pairs in the valence shell of the atoms.

ii. This theory suggest that the shapes of molecule can be determined by the no. of electron pairs. (Bonding as well as non-bonding)

iii. This theory predict the shapes of covalent molecules.

Table 4.6:

Molecule type	no. of e^- pair	Molecular geometry	Bond angle	example
AB_2	2	 (Linear)	180°	Cl—Be—Cl $BeCl_2$ $HgCl_2$
AB_3	3	 (Trigonal planar)	120°	BF_3
AB_4	4	 Tetrahedral	109.5°	CH_4, NH_4^+

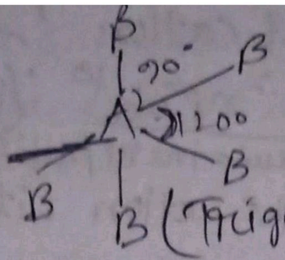
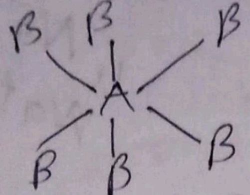
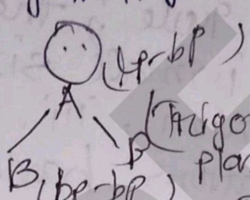
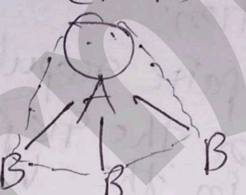
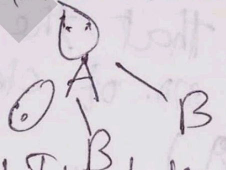
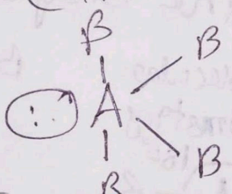
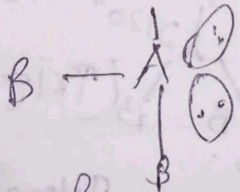
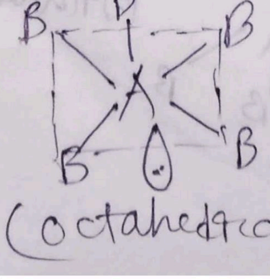
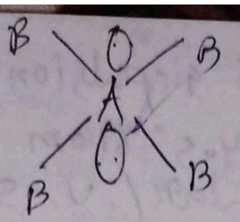
AB_5	5	 (Trigonal bipyramidal)	120°, 90°	PCl_5
AB_6	6	 (octahedral)	90°	SF_6

Table 4.7 :—

Molecular type	No. of é pairs	Molecular geometry	shape	example
AB_2L	B.P (2) LP (1) (3)	 (Trigonal planar)	bent, V-shape	SO^2O_3
AB_3L	B.P (3) LP (1) (4)	 Tetrahedral	Trigonal pyramidal	NH_3
AB_2L_2	BP (2) LP (2) (4)	 (Tetrahedral)	bent, V-shape	H_2O
AB_4L	BP (4) LP (1) (5)	 Trigonal bypyramidal	see-saw	SF_4
AB_3L_2	BP (3) LP (2) (5)		T-shape	ClF_3
AB_5L	BP (5) LP (1) (6)	 (octahedral)	Square pyramid	BrF_5

AB_4L_2 BP ④ LP ②
⑥

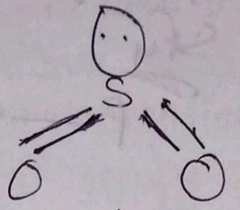


square planar XeF_4

Table 4.8

i. AB_2L BP ② LP ①
Total – ③

SO_2



In SO_2, we have 3 e^- pairs (i.e, 2bp & 1lp) which acquire trigonal planar geometry.

But shape is bent/angular/V-shape since one position is occupied by a lone pair (lp).

Since, lp-bp repulsion > bp-bp repulsion

∴ Bond angle reduces to 119.5° to 120°

ii. AB_3L bp ③ lp ①
Total ④

NH_3

In NH_3, we have 4 e^- pairs (i.e, 3bp & 1lp) which acquire tetrahedral geometry.

But, all 4 e^- pairs are not equivalent and therefore NH_3 has distorted tetrahedral geometry which is due to 1 lp.

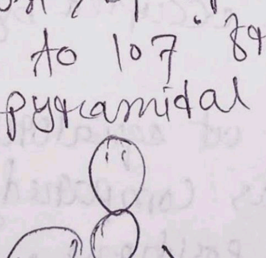
Since, lp-bp repulsion > bp-bp repulsion

∴ Bond angle reduces to 107° from 109.5°

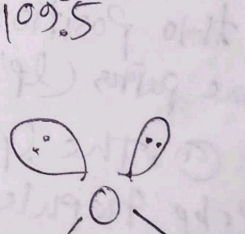
Shape is trigonal pyramidal

iii. AB_2L_2 bp ② lp ②
Total – ④

H_2O



or



In H_2O, we have 4 e^- pairs (i.e, 2bp & 2lp) which acquire tetrahedral,

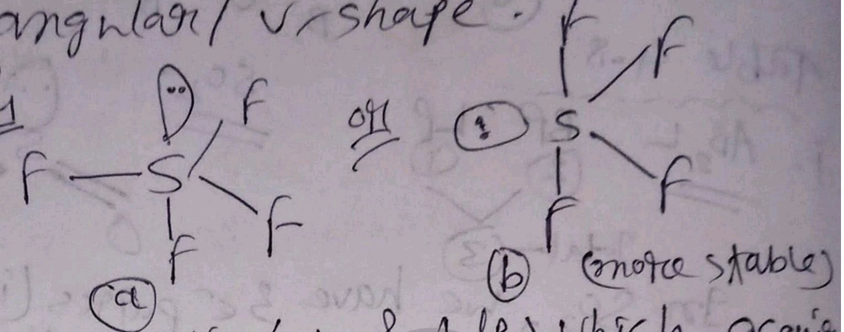
But, all 4 e^- pairs are not equivalent and therefore H_2O has distorted tetrahedral geometry which is due to 2 lp's.

Since, lp-lp repulsion > lp-bp repulsion > bp-bp repulsion
∴ Bond angle reduces to 104.5° from 109.5°
shape is bent / angular / v-shape.

iv. AB_4L

bp lp
④ ①
Total - ⑤

SF_4



In SF_4, we have 5 e⁻ pairs (i.e, 4 bp & 1 lp) which acquire trigonal bipyramidal geometry in which one position is occupied by a lone pair (lp).

SF_4 can have structure ⓐ or ⓑ –

ⓐ lp on axial, 3 lp-bp repulsions at 90°

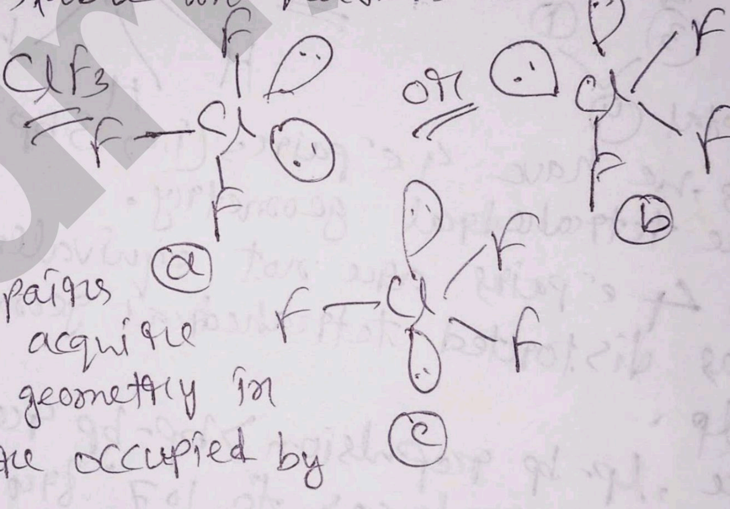
ⓑ lp on equatorial, 2 lp-bp repulsions at 90°

∴ ⓑ is more stable and have see-saw shape

v. AB_3L_2

bp lp
③ ②
Total - ⑤

ClF_3



In ClF_3, we have 5 e⁻ pairs (i.e, 3bp & 2 lp) which acquire trigonal bipyramidal geometry in which two positions are occupied by lone pairs (lp's)

In ⓐ, the lp are at equatorial position so there are less lp-bp repulsions as compared to others in which the lp are at axial positions. So, structure ⓐ is most stable and have T-shape structure.

~~Valence Bond Theory:~~

— x —

Main postulates of valence shell electron pair repulsion theory :-

i. The shape of a molecule depends upon the no. of valence shell electron pairs around the central atom.

ii. Pairs of electrons in the valence shell repel one another since there electron clouds are negatively charged.

iii. These pairs of electrons tend to occupy such positions in space that minimise repulsion and thus maximise distance between them.

iv. The valence shell is taken as a sphere with the electron pairs localising on the spherical surface at maximum distance from one another.

v. A multiple bond is treated as if it a single electron pair and the two or three electron pairs of a multiple bond are treated as a single super pair.

vi. The repulsive interaction of electron pairs decreases in the order :

lone pair - lone pair > lone pair - bond pair > bond pair - bond pair

Valence Bond Theory :- (VBT)

Consider two hydrogen atoms A and B approaching each other having nuclei N_A and N_B and electrons present in them are represented by e_A and e_B. When the two atoms are at large distance from each other, there is no interaction between them. As these two atoms approach each other, new attractive and repulsive forces begin to operate.

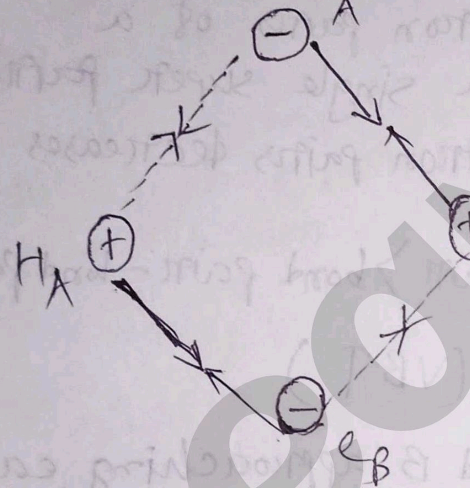
Attractive forces arise between :-

i. nucleus of one atom and its own electron that is $N_A - e_A$ and $N_B - e_B$.

ii. nucleus of one atom and electron of other atom i.e, $N_A - e_B$, $N_B - e_A$

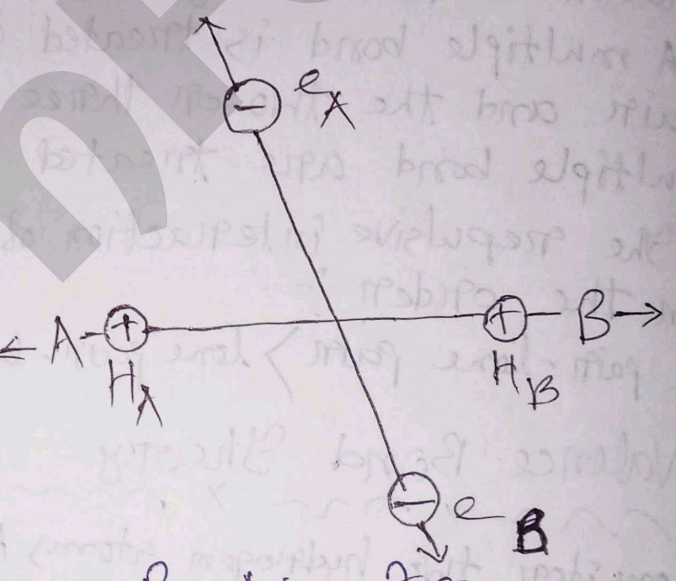
Similarly repulsive forces arise between:-
i. electrons of two atoms like $e_A - e_B$,
ii. nuclei of two atoms $N_A - N_B$.

Experimentally it has been found that the magnitude of new attractive force is more than the new repulsive forces. As two atoms approach each other and potential energy decreases. A stage is reached where the net force of attraction balances the force of repulsion and system acquires minimum energy. And thus two hydrogen atoms are said to be bonded together to form a stable molecule having the bond length of 74 pm.

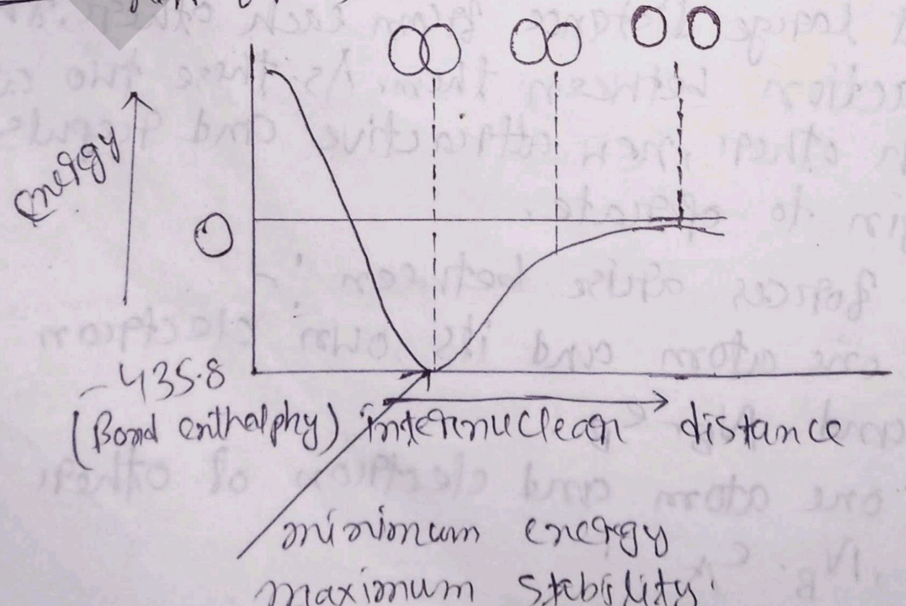


Attractive forces

---- old forces
—— new forces



Repulsive forces

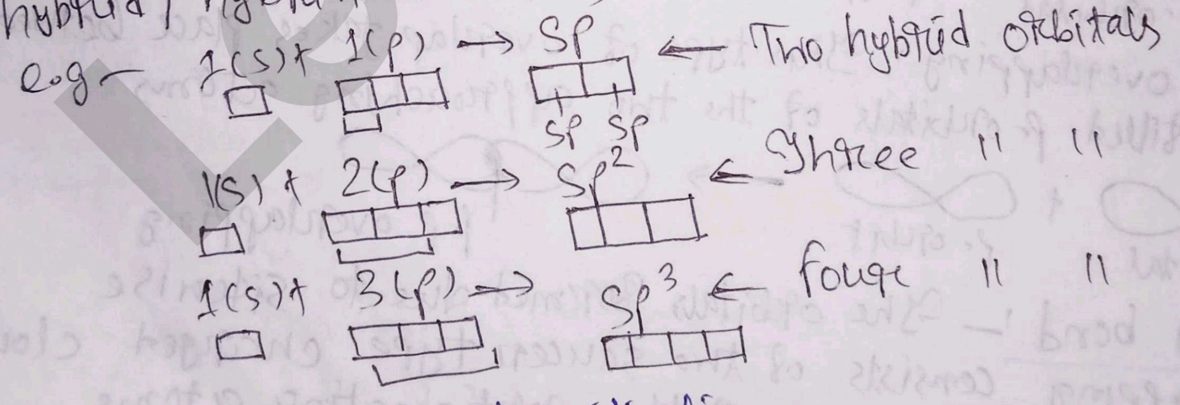


Differences between Sigma bond & Pi-bond :-

σ-bond	π-bond
i. formed by the end to end (head on) overlap of bonding orbitals along the internuclear axis. i.e; s-s overlapping, s-p overlapping, p-p overlapping	i. formed by the sidewise overlap of two half filled p-orbitals. i.e; p-p overlapping, p-d overlapping
ii. Overlapping takes place to a larger extent and therefore σ-bond is a strong bond.	ii. overlapping occurs to a lesser extent and therefore π-bond is **weak bond**.
iii. Free rotation of atoms around the σ-bond is allowed.	iii. Free rotation of atoms around π-bond is not possible.
iv. σ-bond may be present either alone or along with π-bond.	iv. π-bond is always present in addition to σ-bond.
v. S-orbitals can participate in the formation of σ-bond.	v. S-orbitals can't participate in the formation of π-bond.

Hybridisation :-

Hybridisation can be defined as the process of intermixing of the orbitals of slightly different energies so as to redistribute their energies, resulting in the formation of new set of orbitals of equivalent energies and shape. The new orbitals formed due to hybridisation are called hybrid / hybridised orbitals.



e.g - 1(s) + 1(p) → sp ← Two hybrid orbitals
sp sp

1(s) + 2(p) → sp^2 ← Three " "

1(s) + 3(p) → sp^3 ← four " "

Salient features of hybridisation :-

1. The number of hybrid orbitals is equal to the number of the atomic orbitals that get hybridised.
2. The hybridised orbitals are always equivalent in energy and shape.

3. The hybrid orbitals are more effective in forming stable bonds than the pure atomic orbitals.

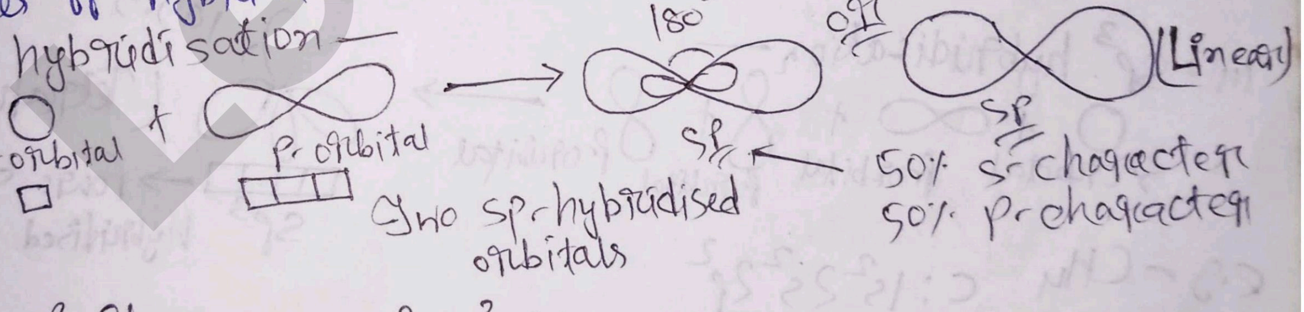
4. These hybrid orbitals are directed in space in some preferred direction to have minimum repulsion between electron pairs and thus a stable arrangement. Therefore, the type of hybridisation indicates the geometry of the molecules.

Important conditions for hybridisation —

1. The orbitals present in the valence shell of the atom are hybridised.
2. The orbitals undergoing hybridisation should have almost equal energy.
3. Promotion of electron is not essential condition prior to hybridisation.
4. It is not necessary that only half filled orbitals participate in hybridisation. In some cases, even filled orbitals of valence shell take part in hybridisation.

Types of hybridisation —

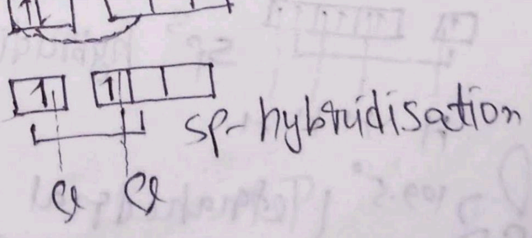
1. SP-hybridisation —

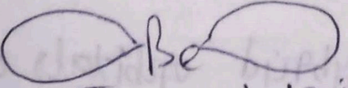


e.g – $BeCl_2$ Be : $1s^2 2s^2 2p$

Ground state → (G.S)

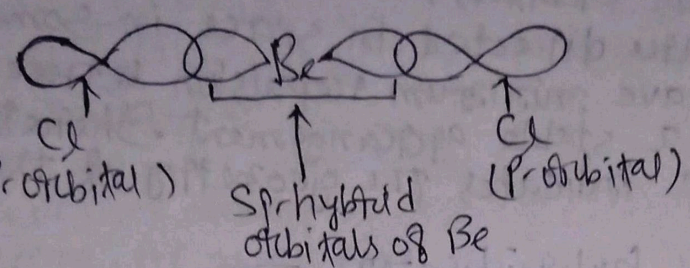
excited state → (E.S)



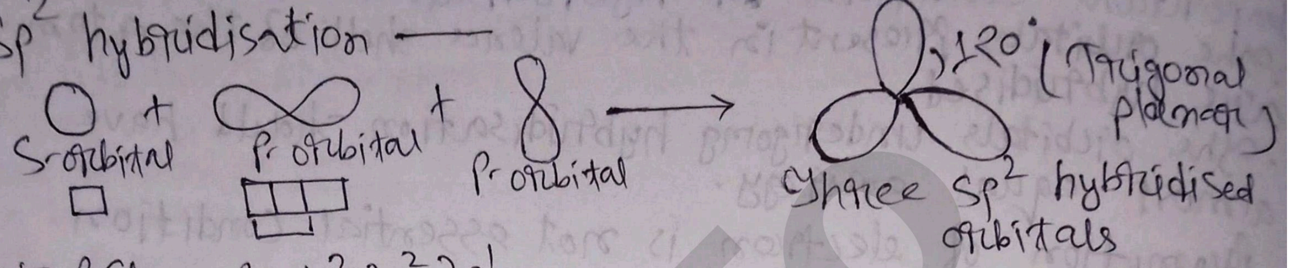


Two sp-hybrid orbitals of Be

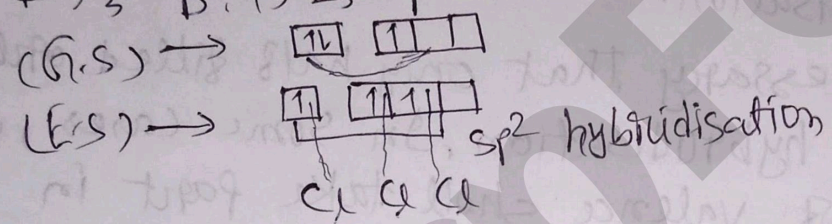
In $BeCl_2$ molecule,



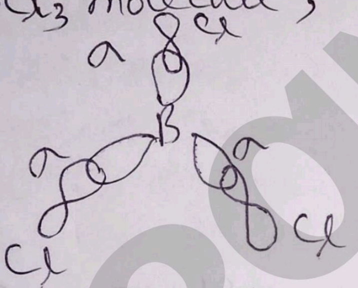
ii. Sp^2 hybridisation —



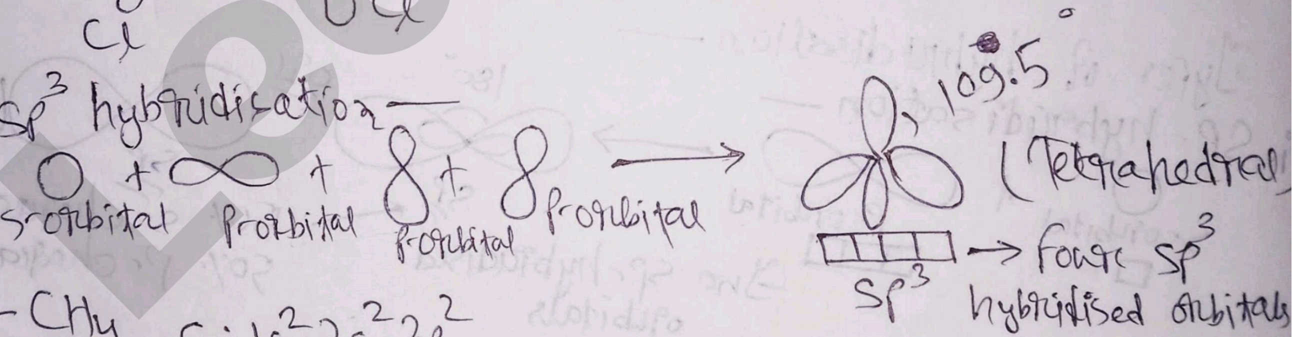
e.g:- BCl_3 B: $1s^2 2s^2 2p^1$



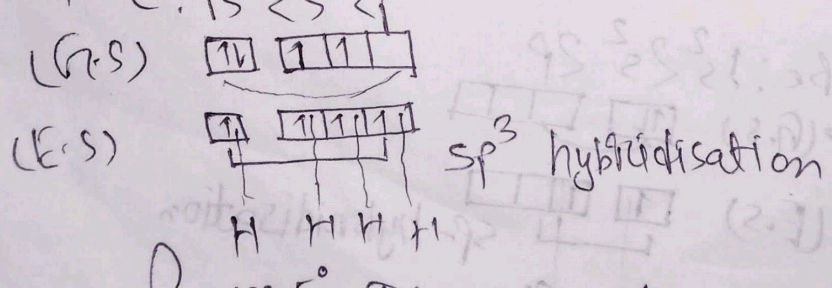
In BCl_3 molecule,

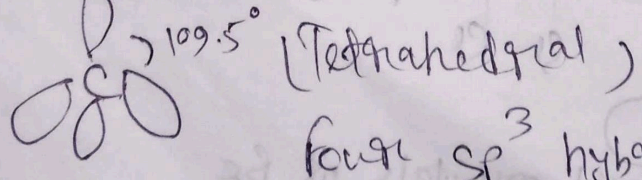


iii. Sp^3 hybridisation —



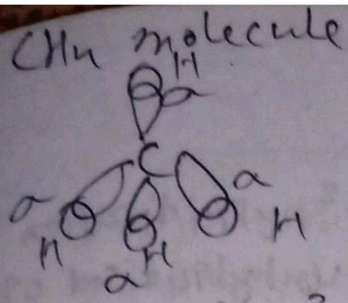
e.g - CH_4 C: $1s^2 2s^2 2p^2$





four sp^3 hybrid orbitals of carbon

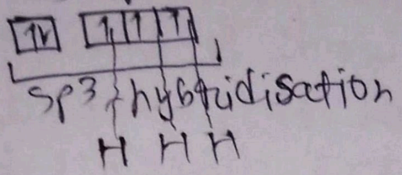
In CH_4 molecule,



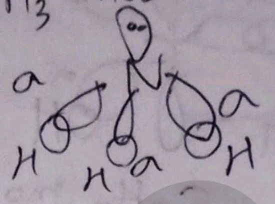
NH_3

N: $1s^2 2s^2 2p^3$

(G.S)



In NH_3 molecule,



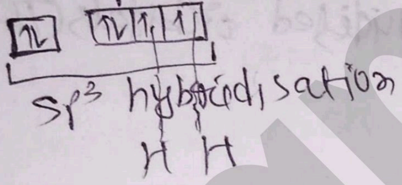
Here, 3 bp's & 1 lp

∵ lp-bp repulsion > bp-bp repulsion
Thus NH_3 molecules gets distorted and the bond angle reduces to 107° from 109.5°. Shape is trigonal pyramidal.

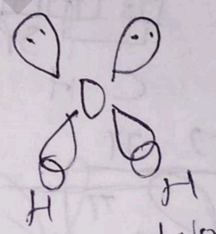
H_2O

O: $1s^2 2s^2 2p^4$

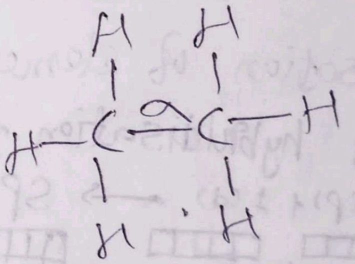
(G.S)



In H_2O molecule,



∵ lp-lp repulsion > lp-bp repulsion > bp-bp repulsion
Thus H_2O molecule gets distorted and bond angle reduces to 104.5° from 109.5°. Shape is bent/angular shape.

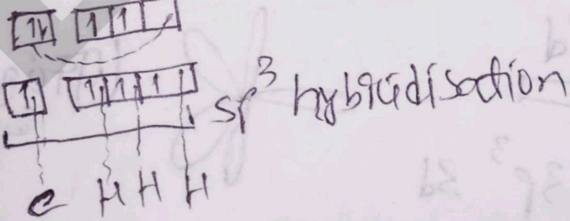


C_2H_6

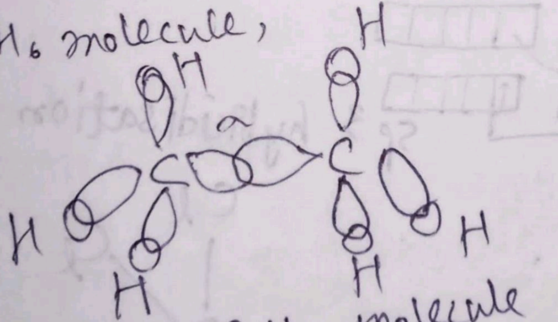
C: $1s^2 2s^2 2p^2$

(G.S):

(E.S):

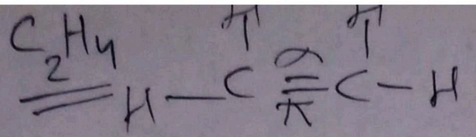


In C_2H_6 molecule,



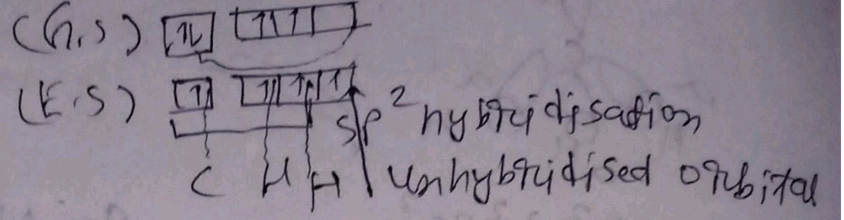
C_2H_6 molecule

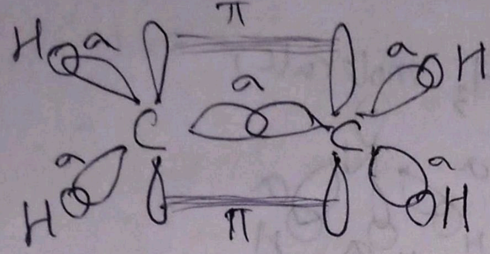
C_2H_4



C: $1s^2 2s^2 2p^2$

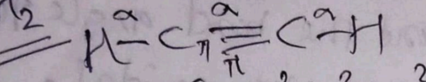
In C_2H_4 molecule,





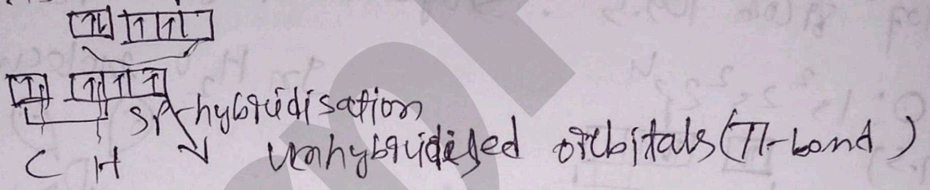
C_2H_2 molecule

C_2H_2

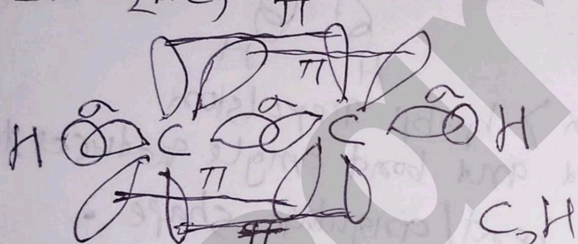


(G.S) :- C: $1s^2 2s^2 2p^2$

(E.S) :-



In C_2H_2,

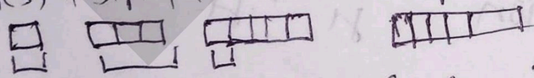


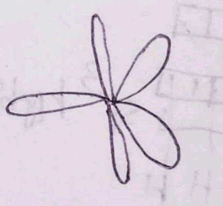
C_2H_2 molecule

Hybridisation of elements involving d-orbitals :-

i. sp^3d hybridisation :-

1(s) + 3(p) + 1(d) ⟶ sp^3d



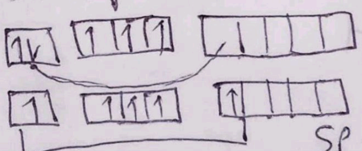


(Trigonal bypyramidal)

PCl_5 P: $1s^2 2s^2 2p^6 3s^2 3p^3$ 3d

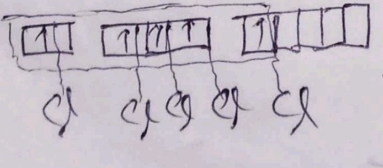
(G.S) :-

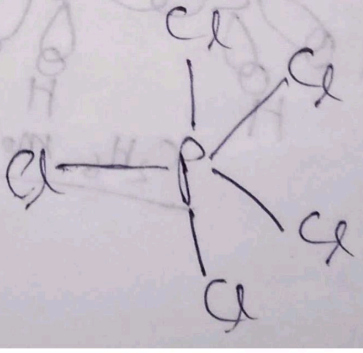
(E.S) :-



sp^3 hybridisation

PCl_5 :

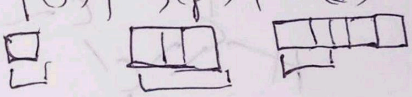




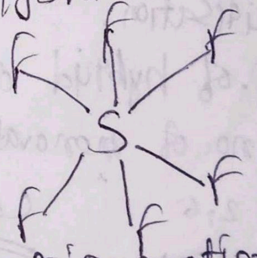
~~In PCl$_5$~~, In PCl$_5$ five orbitals (i.e, 1(s), 3(p) & 1(d)) hybridised to form five sp^{3}d hybridised orbitals which adopt ~~which~~ with trigonal bipyramidal geometry.

It should be noted that all the bond angles in trigonal bipyramidal geometry are not equivalent. In PCl$_5$ the five sp^{3}d orbitals of phosphorus overlap with the singly occupied p orbitals of chlorine atoms to form five P-Cl sigma bonds. Three P-Cl bond lie in one plane and make an angle of 120° with each other; these bonds are termed as equatorial bonds. The remaining two P-Cl bonds - one lying above and the other lying below the equatorial plane, make an ~~a~~ angle of 90° with the plane. These bonds are called axial bonds. As the axial bond pairs suffer more repulsive interaction from the equatorial bond pairs, therefore axial bonds have been found to be slightly longer and hence slightly weaker than the equatorial bonds; which makes PCl$_5$ molecule more reactive.

ii. sp^{3}d^2 hybridisation :- $1(s) + 3(p) + 2(d) \rightarrow sp^3d^2$



SF$_6$ S: $1s^2 2s^2 2p^6 3s^2 3p^4$ 3d

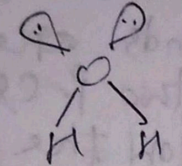


In SF$_6$ the central sulphur atom has the ground state outer electronic configuration $3s^2 3p^4$. In the exited state the available six orbitals i.e; one s, three p and two d are singly occupied by electrons. These orbitals hybridise to form six new sp^{3}d^2 hybrid orbitals, which are projected towards the six corners of a regular octahedron in SF$_6$. These six sp^{3}d^2 hybrid orbitals overlap with singly occupied orbitals of fluorine atoms to form six S-F sigma bonds. Thus SF_6 molecule has a ~~bo~~ regular octahedral geometry.

Prediction of hybridisation of central atom from structure :-

No. of hybrid orbitals (x) = no. of σ bond + l.p on central atom
↙
hybridisation

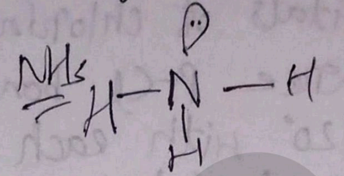
H_2O



$x = 2+2$
$= 4 (sp^3)$

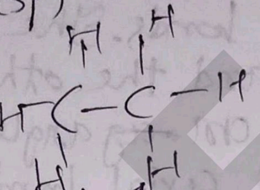
CO_2 $O=C=O$
$x = 2 (sp)$

NH_3



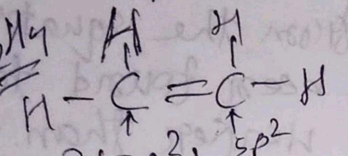
$x = 3+1$
$= 4 (sp^3)$

C_2H_6



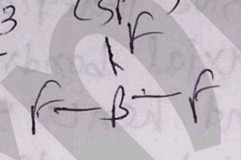
$x =$ 4 (sp^3)

C_2H_4



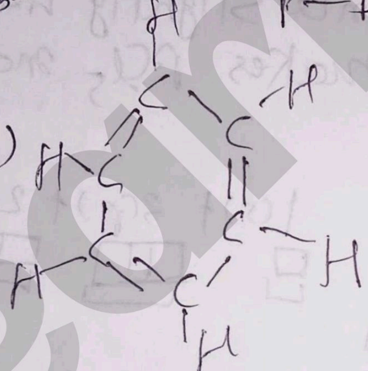
$x = 3 (sp^2)$

BF_3

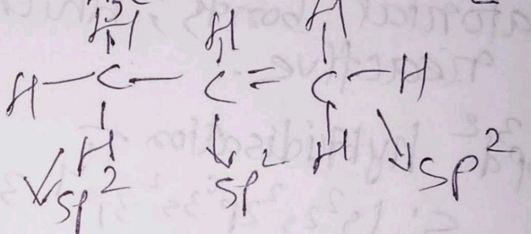


$x = 3 (sp^2)$

C_6H_6 $x = 3 (sp^2)$



$H_3C-HC=CH_2$



***... Hybridisation,

no. of hybrid orbitals on C.A $(x) = \frac{1}{2}$[valence e⁻s on C.A + no. of monovalent atom + (-ve) charge − (+ve) charge]

1. $H_2O \rightarrow 2,6$
$x = \frac{1}{2}(6+2)$
$= \frac{1}{2} \times 6$
$= 4 (sp^3)$

CO_2
$x = \frac{1}{2} \times 4$
$= 2 (sp)$

BF_3
$x = \frac{1}{2}(3+3)$
$= \frac{1}{2} \times 6$
$= 3 (sp^2)$

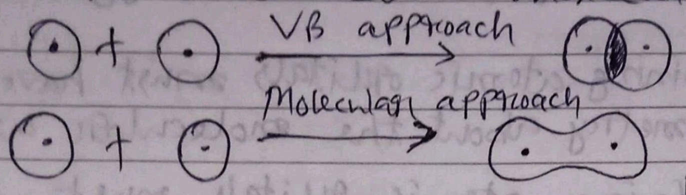
IF_5
$x = \frac{1}{2}(7+5)$
$= \frac{1}{2} \times 12$
$= 6 (sp^3d^2)$

NH_4^+
$x = \frac{1}{2}(5+4-1)$
$= \frac{1}{2} \times 8$
$= 4 (sp^3)$

CO_3^{2-}
$x = \frac{1}{2}(4+2)$
$= \frac{1}{2} \times 6$
$= 3 (sp^2)$

Molecular orbital Theory (MOT) :-

When two atomic orbitals combine, they lose their identity and form new orbitals. The new orbitals thus formed are called molecular orbitals.



new orbitals not formed

New orbital form

Linear combination of atomic orbitals (LCAO) :-

H_A (Hydrogen) H_B

$\downarrow \qquad \downarrow$

$\underbrace{\psi_A \qquad \psi_B}$

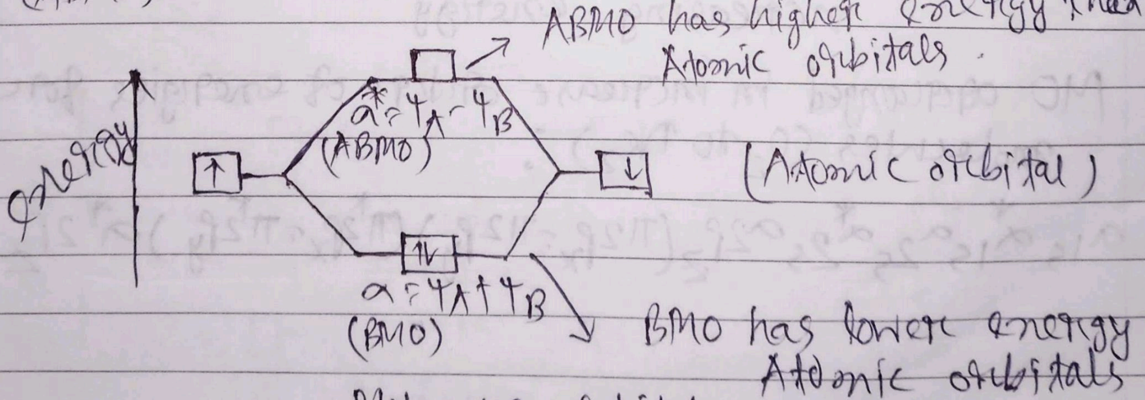
wave function of atomic orbitals

$\therefore \psi_{(MO)} = \psi_A \pm \psi_B$ (MO = molecular orbital)

Addition of wave fn	Subtraction of wave fn
$\psi(MO) = \psi_A + \psi_B$	$\psi(MO) = \psi_A - \psi_B$
$\boxed{\sigma = \psi_A + \psi_B}$	$\boxed{\sigma^* = \psi_A - \psi_B}$
↓ Bonding molecular orbital (BMO)	↓ Anti-bonding molecular orbital (ABMO)

$\therefore \underset{(BMO)}{\sigma} = \psi_A + \psi_B$ Lower energy, higher stability.

$\underset{(ABMO)}{\sigma^*} = \psi_A - \psi_B$, higher energy & lower stability



ABMO has higher energy than Atomic orbitals.

BMO has lower energy than Atomic orbitals

Molecular orbital (MO)

Conditions for the combination of Atomic orbitals -

1. The combining atomic orbitals must have the same or nearly the same energy.

2. The combining atomic orbitals must have the same symmetry about the molecular axis.

3. The combining atomic orbitals must overlap to the maximum extent.

Types of molecular orbitals (MO) :-

σ-MO : If two atomic orbitals overlap along the internuclear axis, the MO formed is called σ-MO. Such molecular orbitals are designated as σ (bonding) and σ^* (anti-bonding).

π-MO : If two atomic orbitals overlap sideways, the MO formed is called π-molecular orbital. Such molecular orbitals are designated as π (bonding) and π^* (anti-bonding).

Energy level diagram for molecular orbitals :-

MO arranged in increase order of energies for molecules (upto N_2) :

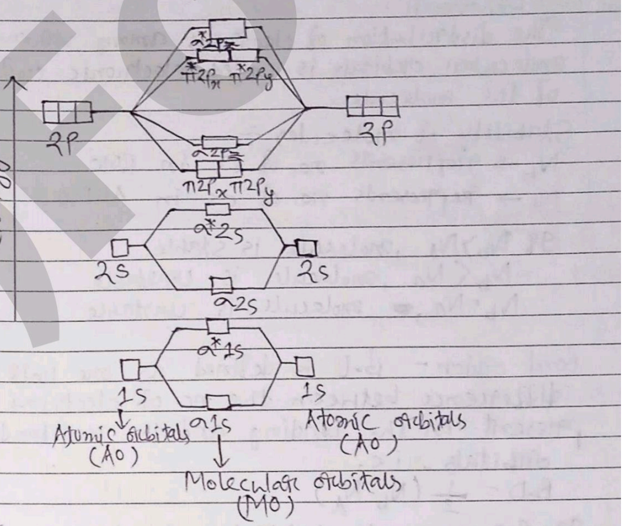
$$\sigma_{1s}\ \sigma^*_{1s}\ \sigma_{2s}\ \sigma^*_{2s}\ (\pi 2p_x = \pi 2p_y)\ \sigma 2p_z\ (\pi^* 2p_x = \pi^* 2p_y)\ \sigma^* 2p_z$$

$$\xrightarrow[\text{increasing energy}]{}$$

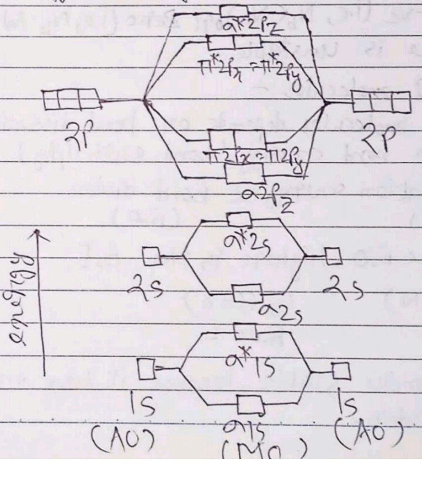
MO arranged in increase order of energies for molecules (O_2 to Ne_2) :

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

Energy level diagrams for molecules (upto N_2) :



Energy level diagram for molecules (O_2 to Ne_2) :-



Electronic configuration and molecular behaviour –

The distribution of electrons among various molecular orbitals is called electronic configuration of the molecule.

Stability of molecules :-

N_b → represents no. of e's in BMO

N_A → represents no. of e's in ABMO

If $N_b > N_A$, molecule is stable

$N_b < N_a$, molecule is unstable

$N_b = N_a$, molecule is unstable

Bond order – B.O is defined as one half the difference between the no. of electrons present in the bonding and the antibonding orbitals. i.e,

$B.O = \frac{1}{2}(N_b - N_A)$

If B.O is +ve (i.e, $N_b > N_a$), molecule is stable

If B.O is –ve (i.e, $N_b < N_a$) or zero (i.e, $N_b = N_a$), molecule is unstable.

Stability of molecules :-

Stability of molecules depends on bond dissociation energy (or bond energy / bond enthalphy)

∴ Bond dissociation energy (B.E) ∝ Bond order (B.O)

i.e, greater the B.O, higher is the B.E

e.g:- $N_2 (N \equiv N)$ $O_2 (O = O)$

B.O = 3 B.O = 2

∴ N_2 is more stable because it has more Bond order.

Bond length –

Bond length is inversely proportional to Bond order

$\therefore B.L \propto \frac{1}{B.O}$

i.e, higher the B.O, shorter is the B.L.

eg: $N_2 (N \equiv N)$ $O_2 (O = O)$

∴ N_2 will have shorter Bond ~~order~~ length.

Magnetic nature –

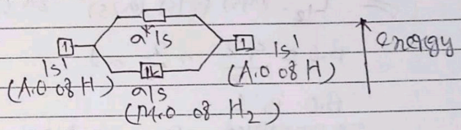
All e's paired → Diamagnetic (repelled by magnetic field)

Unpaired e's → Paramagnetic (attracted by magnetic field)

Bonding in some Homonuclear diatomic molecules :-

H_2 → 2e's

$H_2 = (\sigma 1s)^2$

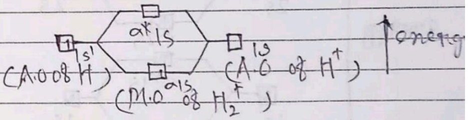


$B.O = \frac{N_b - N_a}{2} = \frac{2-0}{2} = \frac{2}{2} = 1$

No unpaired e's ∴ Diamagnetic

H_2^+ → 1 e's

$H_2^+ = (\sigma 1s)^1$



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

∴ Unpaired e's present ∴ paramagnetic

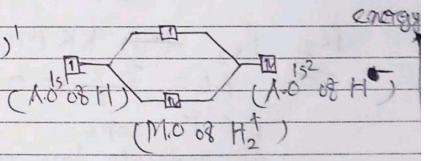
H_2^- → 3 e's

$H_2^- = (\sigma 1s)^2 (\sigma^* 1s)^1$

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

∴ unpaired e's

∴ paramagnetic



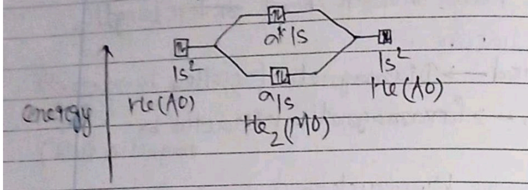
He₂ $He_2 : (\sigma 1s)^2 (\sigma^* 1s)^2$

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

∵ B.O is zero

∴ He_2 molecule does not exist

No unpaired e's, ∴ Diamagnetic



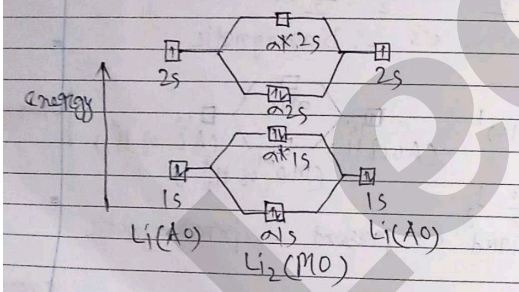
He: 1s²

Li₂ $Li_2 : (\sigma 1s)^2 (\sigma^* 1s)^2 (\sigma 2s)^2$ or $Li_2 = \underbrace{KK}_{\text{completely/filled inner cell}} (\sigma 2s)^2$

$B.O = \frac{4-2}{2} = \frac{2}{2} = 1$ $\qquad$ $B.O = \frac{2-0}{2} = 1$

∵ B.O is 1

no unpaired e's, ∴ Diamagnetic



Li: 1s² 2s¹

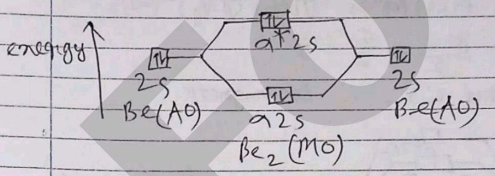
Be₂ $Be_2 :$ ~~(σ1s)~~ $KK (\sigma 2s)^2 (\sigma^* 2s)^2$

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

∵ B.O is zero

∴ Be_2 molecule does not exist

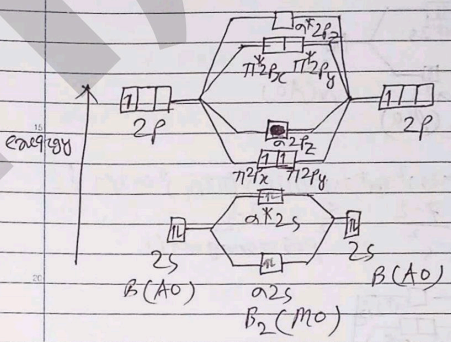
no unpaired e's, ∴ Diamagnetic



B₂ $B_2 : KK (\sigma 2s)^2 (\sigma^* 2s)^2 (\pi 2p_x)^1 (\pi 2p_y)^1$

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

∴ ~~no~~ unpaired e's ∴ paramagnetic

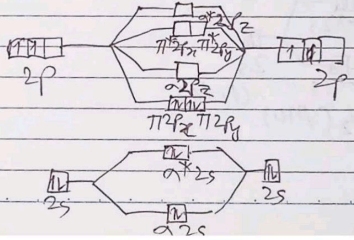


B: 1s² 2s² 2p¹

C₂ $C_2 : KK (\sigma 2s)^2 (\sigma^* 2s)^2 (\pi 2p_x)^2 (\pi 2p_y)^2$

$B.O = \frac{6-2}{2} = \frac{4}{2} = 2$

∴ no unpaired electrons ∴ Diamagnetic



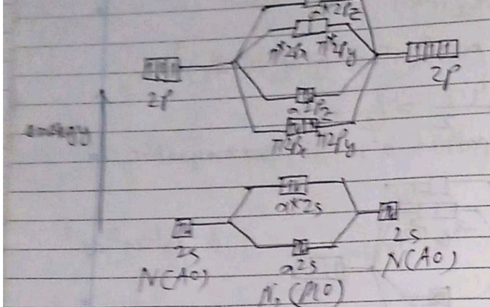
C: 1s² 2s² 2p²

N_2

$N_2 : KK(\sigma 2s)^2(\sigma^* 2s)^2(\pi 2p_x)^2(\pi 2p_y)^2(\sigma 2p_z)^2$

$B.O = \frac{8-2}{2} = \frac{6}{2} = 3$

no unpaired e⁻s, ∴ Diamagnetic



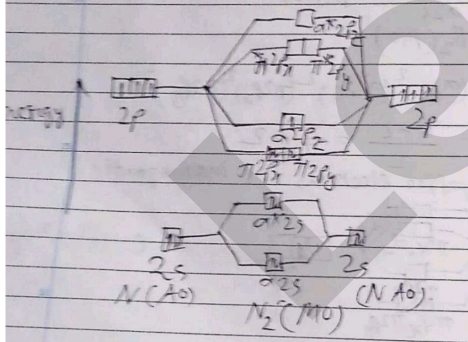
$N : 1s^2 2s^2 2p^3$

N_2^+

$N_2^+ : KK(\sigma 2s)^2(\sigma^* 2s)^2(\pi 2p_x)^2(\pi 2p_y)^2(\sigma 2p_z)^1$

$B.O = \frac{7-2}{2} = \frac{5}{2} = 2\frac{1}{2}$

∴ unpaired e⁻s, ∴ paramagnetic



$N : 1s^2 2s^2 2p^3$

N_2^-

$N_2^- : KK(\sigma 2s)^2(\sigma^* 2s)^2(\pi 2p_x)^2(\pi 2p_y)^2(\sigma 2p_z)^2(\pi^* 2p_z)^1$

∴ paramagnetic

$B.O = \frac{8-3}{2} = \frac{5}{2} = 2\frac{1}{2}$

N_2^{2-}

$N_2^{2-} : KK(\sigma 2s)^2(\sigma^* 2s)^2(\pi 2p_x)^2(\pi 2p_y)^2(\sigma 2p_z)^2(\pi^* 2p_x)(\pi^* 2p_y$

∴ paramagnetic

∴ $B.O = \frac{8-4}{2} = \frac{4}{2} = 2$

	N_2	N_2^-	N_2^+	N_2^{2-}
B.O :-	3	$2\frac{1}{2}$	$2\frac{1}{2}$	2

B.E order : $N_2 > N_2^+ = N_2^- > N_2^{2-}$

← Bond dessociation energy increase

Stability order : $N_2 > N_2^+ = N_2^- > N_2^{2-}$ (∵ $B.E \propto B.O$)

← stability increase)

Bond length order : $N_2^{2-} > N_2^+ = N_2^- > N_2$ (∵ $B.L \propto \frac{1}{B.O}$)

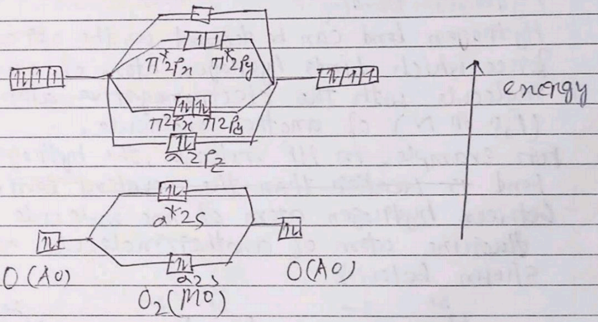
O_2

~~$O_2 : KK(\sigma 2s)^2(\sigma^* 2s)^2(\pi 2p_x)^2 \pi 2$~~

$O_2 : KK(\sigma 2s)^2(\sigma^* 2s)^2(\sigma 2p_z)^2(\pi 2p_x)^2(\pi 2p_y)^2(\pi^* 2p_x)^1(\pi^* 2p_y)^1$

$B.O = \frac{8-4}{2} = \frac{4}{2} = 2$

∵ unpaired e⁻s, ∴ paramagnetic



O_2^+ O_2^+: $KK(\sigma 2s)^2(\sigma^* 2s)^2(\sigma 2p_z)^2(\pi 2p_x)^2(\pi 2p_y)^2(\pi^* 2p_x)^1(\pi^* 2p_y)$

$B.O = \frac{8-3}{2} = \frac{5}{2} = 2\frac{1}{2}$

unpaired e's, ∴ paramagnetic

O_2^- O_2^-: $KK(\sigma 2s)^2(\sigma^* 2s)^2(\sigma 2p_z)^2(\pi 2p_x)^2(\pi 2p_y)^2(\pi^* 2p_x)^2(\pi^* 2p_y)$

$B.O = \frac{8-5}{2} = \frac{3}{2} = 1\frac{1}{2}$

∵ unpaired e's, ∴ paramagnetic

O_2^{2-} O_2^{2-}: $KK(\sigma 2s)^2(\sigma^* 2s)^2(\sigma 2p_z)^2(\pi 2p_x)^2(\pi 2p_y)^2(\pi^* 2p_x)^2(\pi^* 2p_y)^2$

$B.O = \frac{8-6}{2} = \frac{2}{2} = 1$

∵ no unpaired e's, ∴ Diamagnetic

	O_2	O_2^+	O_2^-	O_2^{2-}
B.O −	2	$2\frac{1}{2}$	$1\frac{1}{2}$	1

B.E order − $O_2^+ > O_2 > O_2^- > O_2^{2-}$

Stability order − $O_2^+ > O_2 > O_2^- > O_2^{2-}$

Bond length order − $O_2^{2-} > O_2^- > O_2 > O_2^+$

Hydrogen Bonding :-

Hydrogen bond can be defined as the attractive force which binds hydrogen atom of one molecule with the electronegative atom (F, O or N) of another molecule.

For example, in HF molecule, the hydrogen bond ~~is weaker than the covalent bond~~ exists between hydrogen atom of one molecule and fluorine atom of another molecule as shown below :-

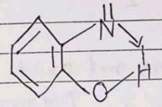
$$\cdots H^{\delta+} - F^{\delta-} \cdots H^{\delta+} - F^{\delta-} \cdots H^{\delta+} - F^{\delta-}$$

Types of H-Bonds :-

i. Intermolecular hydrogen bond − It is formed between two different molecules of the same or different compounds. For example,

$$^{\delta+}H - F^{\delta-} \underset{\text{Inter molecular}}{\underset{\downarrow}{\cdots\cdots}} H^{\delta+} - F^{\delta-}$$

ii. Intramolecular hydrogen bond − It is formed when hydrogen atom is in between the two highly electronegative (F, O, N) atoms present within the same molecule. For example, in O-nitrophenol the hydrogen is in between the two oxygen atoms.



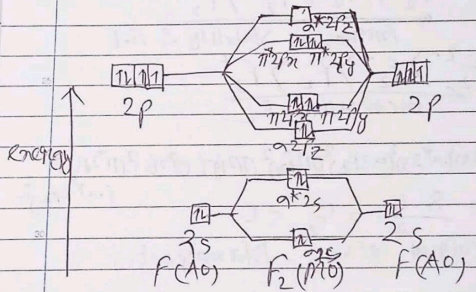
— × —

Homework

F_2 F_2: $KK(\sigma 2s)^2(\sigma^* 2s)^2(\sigma 2p_z)^2(\pi 2p_x)^2(\pi 2p_y)^2(\pi^* 2p_x)^2(\pi^* 2p_y)^2$

18e's $B.O = \frac{8-6}{2} = \frac{2}{2} = 1$

∵ no unpaired e's, ∴ Diamagnetic



F : $1s^2 2s^2 2p^5$

F_2^+: $KK(\sigma 2s)^2(\sigma^* 2s)^2(\sigma 2p_z)^2(\pi 2p_x)^2(\pi 2p_y)^2(\pi^* 2p_x)^2(\pi^* 2p_y)^1$

$B.O = \frac{8-5}{2} = \frac{3}{2} = 1\frac{1}{2}$

∵ unpaired e⁻s, ∴ paramagnetic

F_2^-: $KK(\sigma 2s)^2(\sigma^* 2s)^2(\sigma 2p_z)^2(\pi 2p_x)^2(\pi 2p_y)^2(\pi^* 2p_x)^2(\pi^* 2p_y)^2(\sigma^* 2p_z)$

$B.O = \frac{8-7}{2} = \frac{1}{2}$

∵ unpaired e⁻s, ∴ paramagnetic

F_2^{2-}: $KK(\sigma 2s)^2(\sigma^* 2s)^2(\sigma 2p_z)^2(\pi 2p_x)^2(\pi 2p_y)^2(\pi^* 2p_x)^2(\pi^* 2p_y)^2(\sigma^* 2p_z)$

$B.O = \frac{8-8}{2} = \frac{0}{2} = 0$

∵ B.O is zero.

∴ F_2^{2-} molecule does not exist

∵ no unpaired e⁻s, ∴ Diamagnetic

F_2 F_2^+ F_2^- F_2^{2-}

B.O - 1 $1\frac{1}{2}$ $\frac{1}{2}$ 0

B.E order → $F_2^+ > F_2 > F_2^- > F_2^{2-}$

stability order → $\underleftarrow{F_2^+ > F_2 > F_2^- > F_2^{2-}}$

increasing stability & B.E

B.L order → $\underleftarrow{F_2^{2-} > F_2^- > F_2 > F_2^+}$

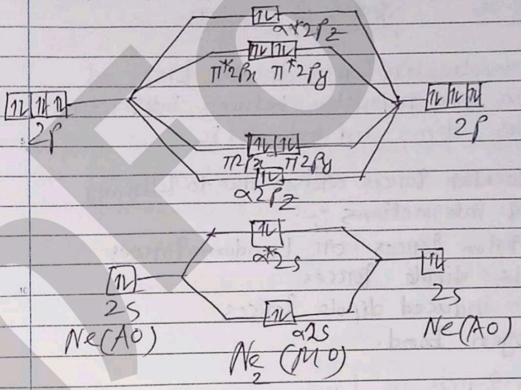
increasing B.L

Ne₂

Ne_2: $KK(\sigma 2s)^2(\sigma^* 2s)^2(\sigma 2p_z)^2(\pi 2p_x)^2(\pi 2p_y)^2(\pi^* 2p_x)^2(\pi^* 2p_y)^2(\sigma^* 2p_z)^2$

$B.O = \frac{8-8}{2} = \frac{0}{2} = 0$

∵ no unpaired e⁻s, ∴ Diamagnetic



Ne: $1s^2 2s^2 2p^6$

——×——