Engineering Chemistry

(KAS - 102)

UNIT - I

Lecture No - 1

(Molecular Orbital Theory.)

Introduction - This theory was given by Hund and Mulliken in 1932.

This theory explains → the formation of chemical bond.
→ relative bond strength
→ paramagnetic or diamagnetic nature. etc.

Postulates of Molecular orbital Theory -

The main postulates of molecular orbital theory are as follows -

1 ⇒ Molecular orbitals are formed by the linear combination of atomic orbitals, as a result atomic orbitals lose their individual identity.

2 ⇒ Only those atomic orbitals can combine to form molecular orbitals, which have almost same energy.

3 ⇒ Total no. of molecular orbitals formed is equal to the no. of overlapping atomic orbitals.

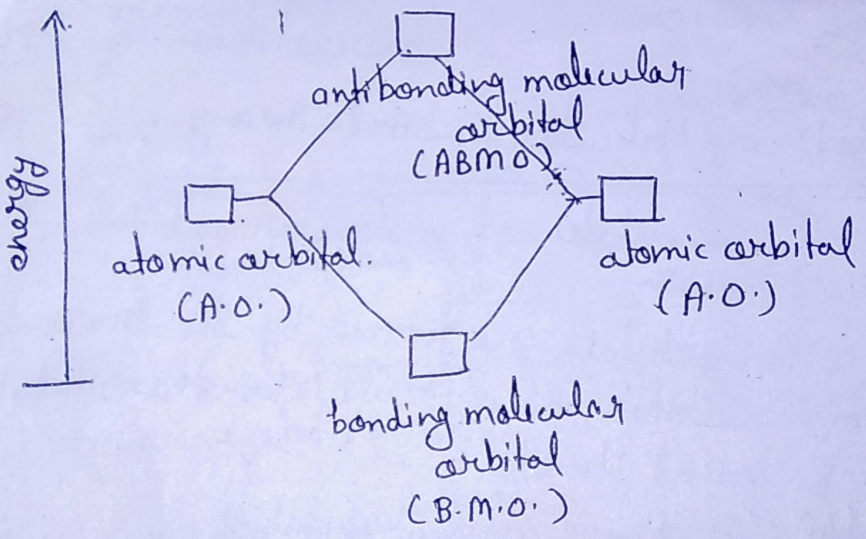
Thus the combination of two atomic orbitals gives rise to two molecular orbitals. out of these, one orbital is lower in energy than combining atom, is known as bonding molecular orbital, whereas

other is higher in energy & known as antibonding molecular orbital.

⇒ The energy of bonding molecular orbital is less than that of the constituent overlapping atomic orbitals

⇒ The difference in energy between the combining atomic orbitals and the bonding molecular orbitals formed is called the stabilization energy

4. Representation of orbitals-



⇒ Energy level sequence of orbitals are as follows-

B.M.O. < A.O. < A.B.M.O.

Magnetic Behaviour

5 ⇒ If there is any unpaired electron present in molecular orbitals, molecule will be paramagnetic, and if all electrons are paired, molecule will be diamagnetic

6. Configuration (Molecular orbital Theory)

The relative energies of first ten molecular orbitals increasing order have been found to be as follows-

for H_2 to N_2 (atomic no. 2 to 14)

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

(* indicates antibonding molecular orbital)

for O_2 to Ne_2 (atomic no. more than 14)

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

7. Bond Order

It is a measure of the stability or strength of the bond between two atoms.

$$\text{Bond order (B.O.)} = \frac{N_b - N_a}{2}$$

N_b – No. of electrons in bonding molecular orbitals.

N_a – No. of electrons in ~~anti~~ antibonding molecular orbitals

$$\text{Bond order} \propto \frac{1}{\text{Bond length}}$$

Bond order $\propto$ Dissociation energy

Bond order $\propto$ Stability

If B.O. is negative or zero – molecule is unstable and does not exist.

If B.O. is positive – molecule is stable and exist