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Date:
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For Deg II & Deg I Chemistry Hons
(Paper III) (Paper I)

The Molecular Orbital Theory

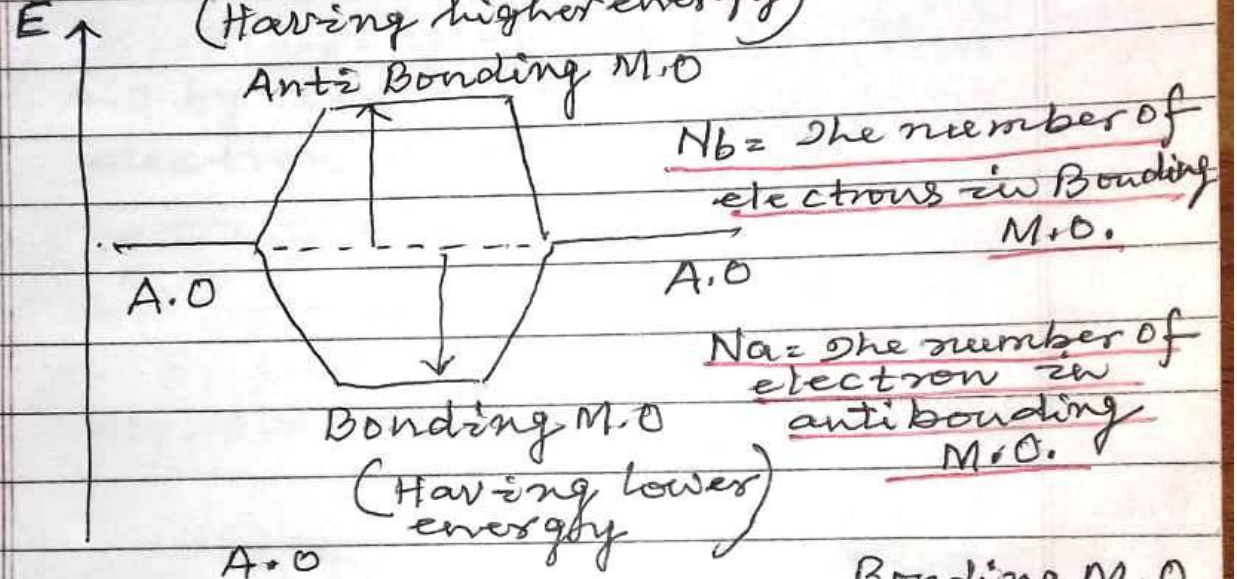
The High electron concentrations in between the two Possitive nuclei shield them from mutual repulsion and hold them together at the observed distance from each other such a molecular orbital is said to a Bonding molecular orbital.

The two electron waves being oriented in opposite direction will cancel out and thus the Probability of finding electrons in the region of overlap will be Practically nil. Thus there will be no shielding of the nuclei and on account of the mutual repulsion these will be pushed apart from each other. The molecular orbital obtained in this manner is called an antibonding molecular orbital.

The molecular orbital, equal in energy to Atomic orbital is called non-bonding M.O.

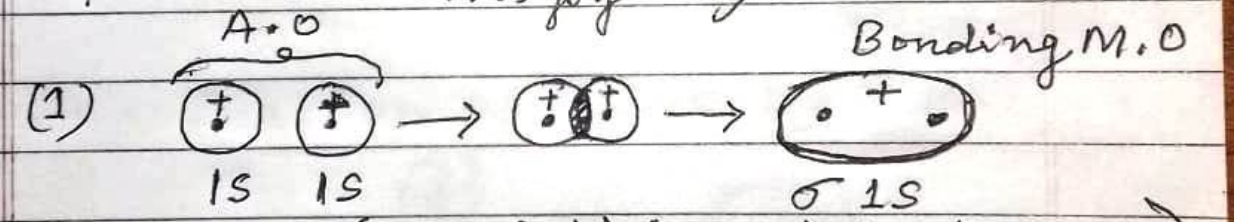
(1) If $N_b > N_a$ — the molecule will be stable.

(2) If $N_b = N_a$ or $N_b < N_a$ — the molecule will be unstable.

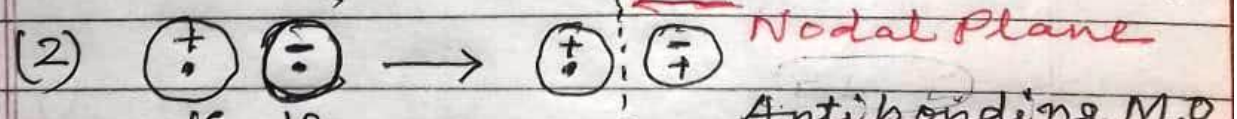


N_b = the number of electrons in Bonding M.O.

N_a = the number of electron in antibonding M.O.



(overlapping of A.O by addition of electron wave)

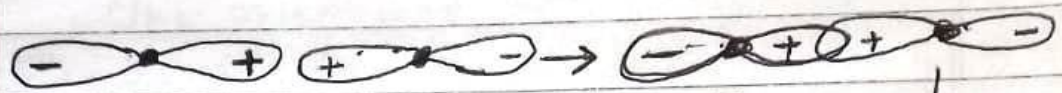


(Overlapping of A.O by subtraction of electron waves)

Note - * — Star mark or Asterisk mark denotes antibonding M.O.

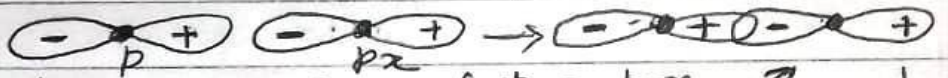
Higher the energy lower the stability & Vice-Versa.

Combination of two px orbitals

(1) 

(overlapping of two px A.O by addition of electron waves)

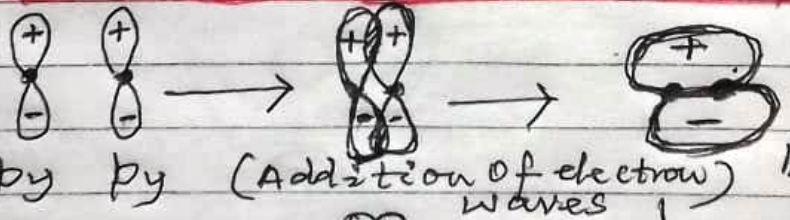
Bonding M.O (σ)

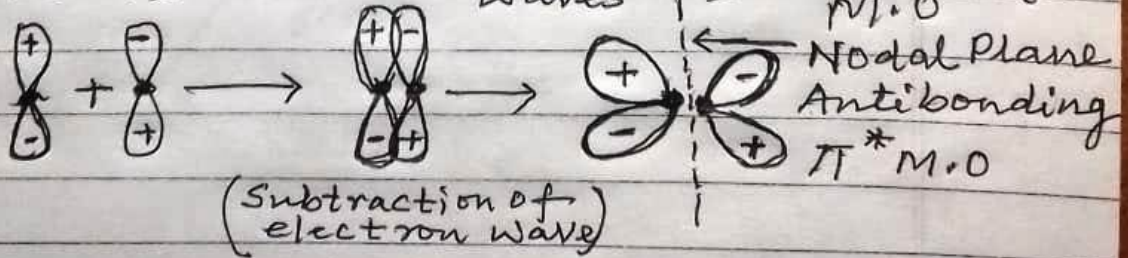
(2) 

(overlapping of two px A.O by subtraction of electron waves)

Anti Bonding M.O (σ^*)

Combination of two py orbitals

(1) 

(2) 

• → Thick dot represents atomic nuclei

Nodal Plane — A plane having zero electron density.

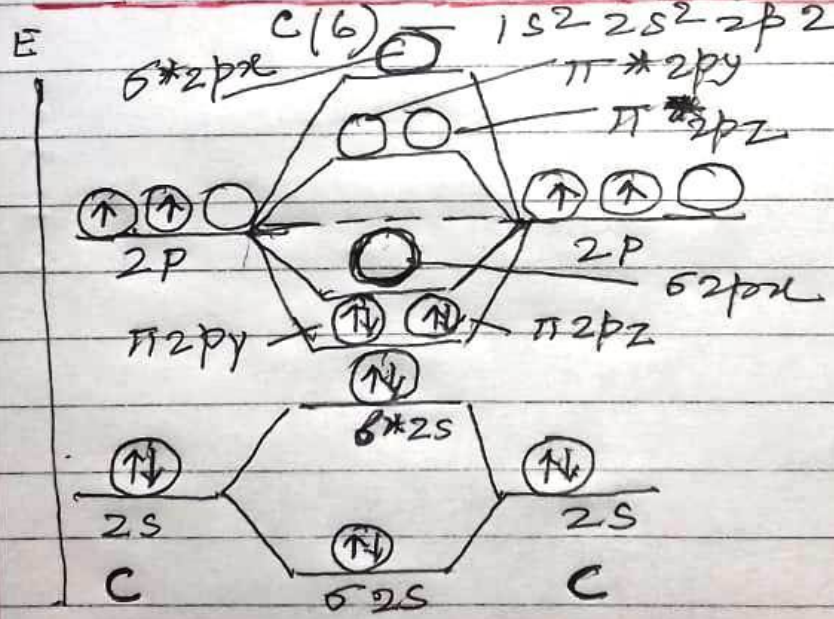
Bond order :—

The number of covalent bonds present in a molecule is called bond order.

It is equal to the half of the difference between the number of bonding electrons and anti bonding electrons.

$$\text{Bond order} = \frac{n_b - n_a}{2}$$

Molecular orbital diagram of C_2



$$\text{Bond order} = \frac{n_b - n_a}{2} = \frac{4-2}{2} = 1$$

As C_2 molecule has no unpaired electron hence it is diamagnetic.