

Molecular Orbitals

As to Hund and Mulliken molecular orbital theory, when nuclei of two atoms come close to each other, their atomic orbitals interact leading to the formation of molecular orbitals.

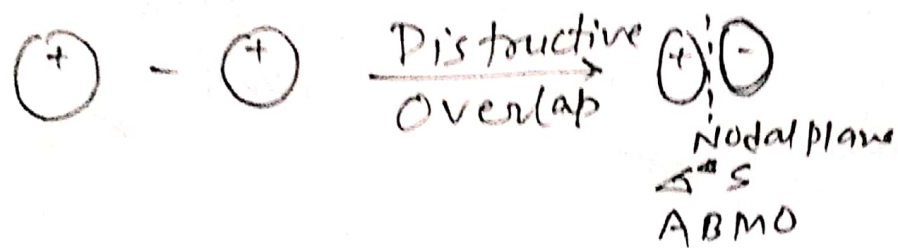
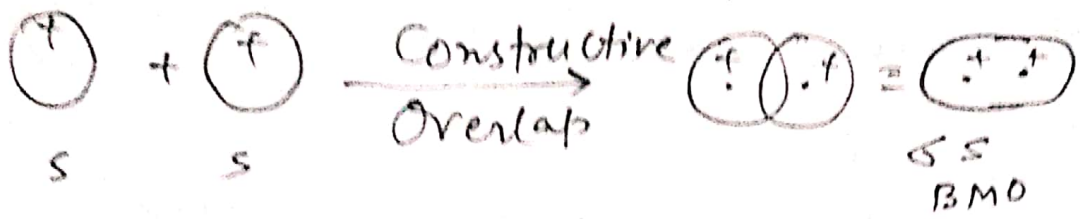
Thus molecular orbitals are formed by overlap (constructive & destructive) of atomic orbitals of atoms. Each molecular orbital is formed by linear combination of atomic orbitals.

- When two atomic orbitals undergo linear combination by constructive overlap then it leads to formation of bonding molecular orbitals (BMO).

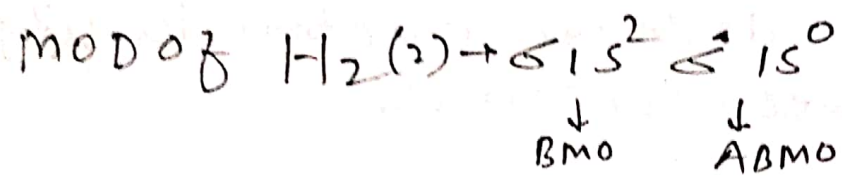
- BMO are denoted by σ , σ^* , π , π^* .

- When two atomic orbitals are undergoing LCAO by destructive overlap it leads to formation of antibonding molecular orbitals (ABMO).

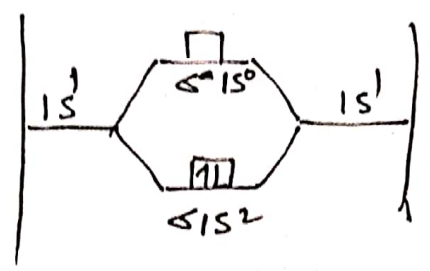
- ABMO are denoted by σ^* , σ , π^* , π .



In molecular orbital diagram
 The energy of BMO is less than
 that of A.O. and the energy of
 ABMO is more than that of A.O.

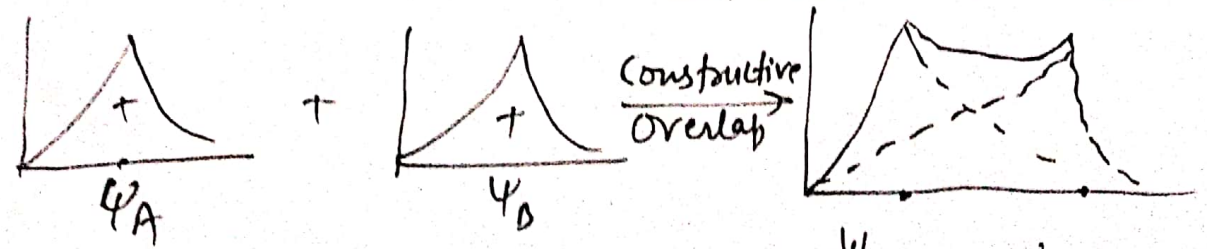


Bond order = $\frac{1}{2} (N_b - N_a)$
 $= \frac{1}{2} (2 - 0)$
 $= 1$



Since bond order is non zero hence
 H_2 exists and diamagnetic in nature

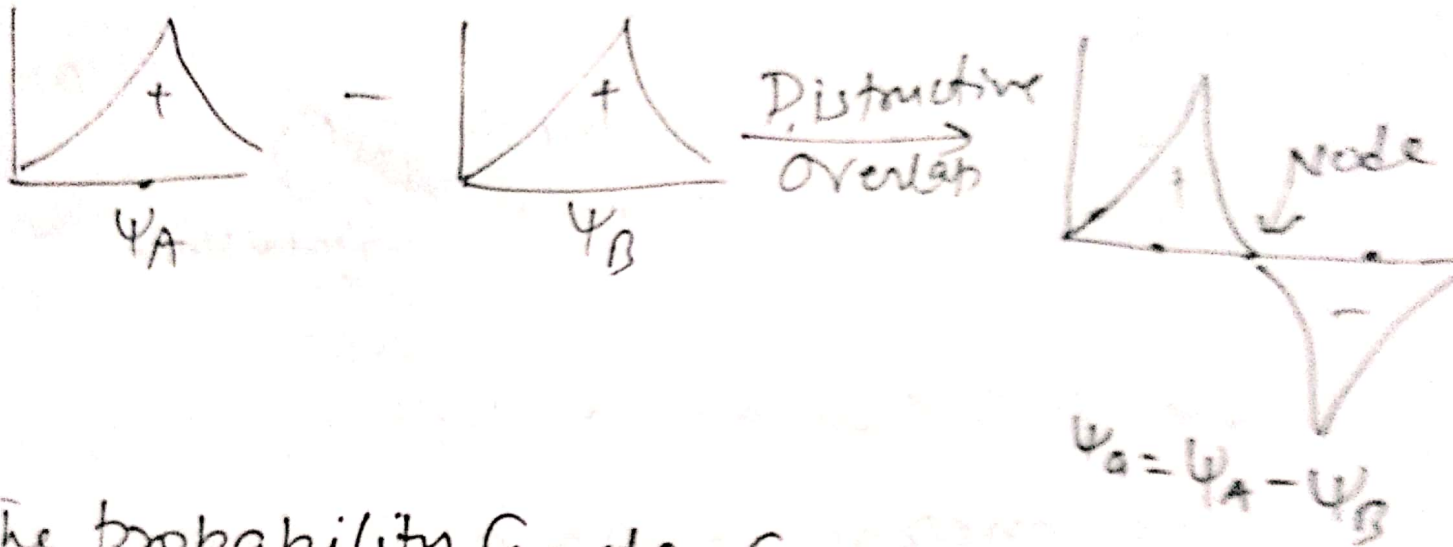
\rightarrow If ψ_A & ψ_B are wave function for 2 individual
 hydrogen atoms then $\psi_b = \text{BMO}$ increases e density
 between the nuclei



$\psi_b^2 = \text{Probability function} = \psi_A^2 + \psi_B^2 + 2\psi_A\psi_B$

$\psi_b = \psi_A + \psi_B$
 B.M.O.

Similar for ABMO

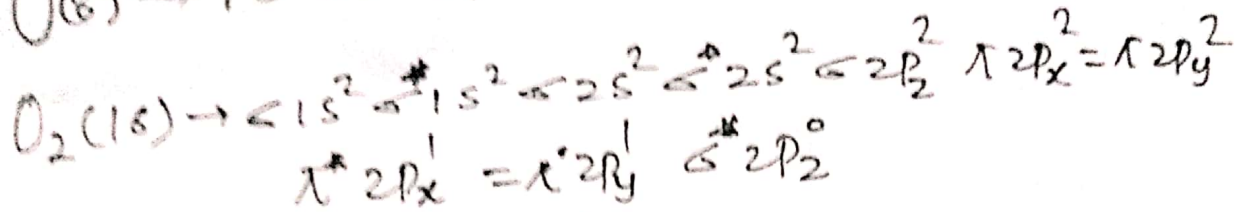


The probability function for ABMO

$$\psi_a^2 = \psi_A^2 - 2\psi_A\psi_B + \psi_B^2$$

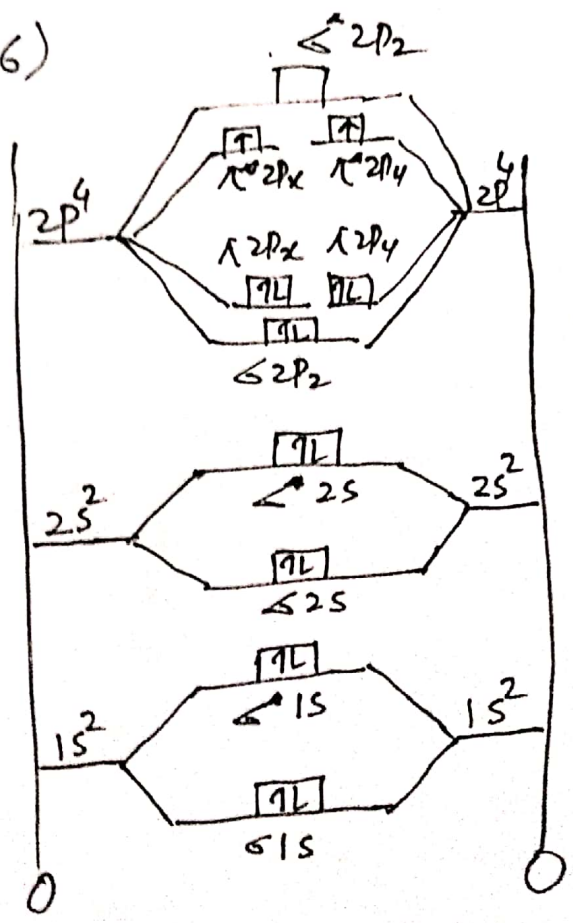
— ABMO decreases electron density between the nuclei

molecular orbital Diagram of O₂



HOMO = SOMO = singly occupied m.o.
 hence paramagnetic with two unpaired electrons in HOMO

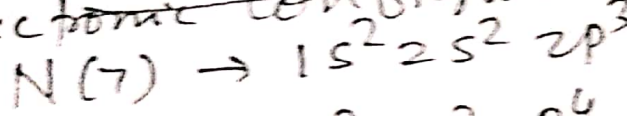
Bond Order = $\frac{1}{2}(N_b - N_a)$
 = $\frac{1}{2}(10 - 6)$
 = 2



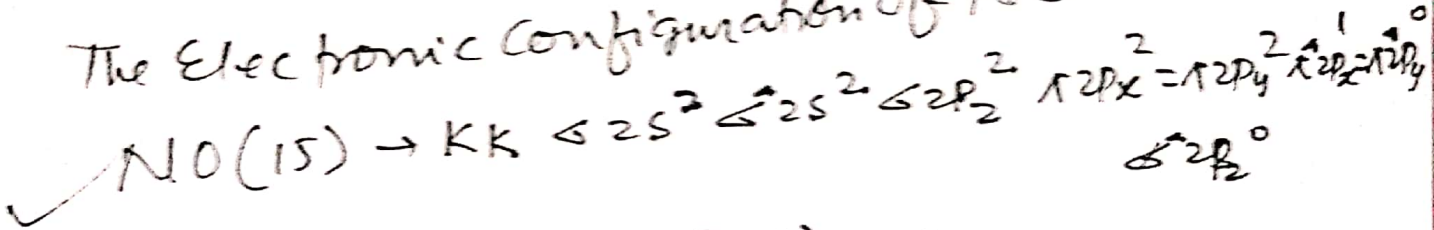
O₂ MO Diagram.

✓ Molecular Orbital Diagram of NO

The electronic configuration of components are



The Electronic Configuration of NO



$$\text{Bond order} = \frac{1}{2}(8-3) = 2.5$$

✓ NO is paramagnetic substance due to presence of one unpaired electron in H.O.M.O.

✓ The Molecular Orbital Diagram of NO

The presence of AB electron in NO makes it

less stable than N_2

As Bond Energy

of NO is 667.8 kJ/mol

while Bond Energy

of N_2 is 945.6 kJ/mol

