ONLINE CLASS

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SUB- Chemistry SEM-I MJC-1

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Molecular orbital theory

Molecular orbital theory describes chemical bonding by assuming that atomic orbitals combines to form delocalized molecular orbitals, spread across the entire molecule.

It is developed by F-Hund and R.S. Mulliken. MOT successfully explains Molecular stability, Magnetic properties and bond characteristics that simpler valence bond theories cannot.

POSTULATES AND LCAO METHOD

(1) Delocalization:- Electrons in a Molecule don't belong to individual atoms, they reside in molecular orbitals (MOs) encompassing all Nuclei.

(2) Linear combination of Atomic orbitals. Molecular orbitals are formed Mathematically by adding or ~~subst~~ subtracting the wave functions (ψ) of combining atomic orbitals.

(3) Conservation of orbitals:- The total no. of Molecular orbitals formed always equals to the number of combining atomic orbitals.

P(-I)

(4) condition for ~~combining~~ combination:- Atomic orbitals must have comparable energy, proper orientation, and maximum overlap.

TYPES OF MOLECULAR ORBITALS

(1) Bonding molecular orbitals (BMO):- It is formed by constructive interference (in-phase addition $\psi_A + \psi_B$) of atomic waves. It has lower energy, higher stability and high electron density between the nuclei.

(2) Antibonding Molecular orbital (ABMO)- It formed by the destructive interference (out of phase subtraction $\psi_A - \psi_B$). It has high energy, lower stability, and features a nodal plane with zero electron density between the nuclei.

~~Denoted with an asterisk (*) sign~~

(3) Sigma (σ) MO:- cylindrically symmetrical around the internuclear axis, formed by head on - overlap.

(4) Pi (π) (MO):- Symmetrical with nodal planes formed by lateral (side-by-side) overlap of p - orbitals