CHEMISTRY GRADE 11

CHAPTER THREE PART 3

Valence Bond Theory (VBT)

The Molecular Orbital Theory(MOT).

HYBRIDIZATION

CHEMICAL BONDING THEORIES

- The two modern chemical bonding theories which use quantum mechanics are the

Valence Bond Theory (VBT)

The Molecular Orbital Theory(MOT).

Cont....

Valence Bond Theory (VBT)

- The valence-bond approach is the most useful approach to answer questions like:
- What is a covalent bond?
- How can we explain molecular shapes from the interaction of atomic orbitals?
- The basic principle of valence bond theory is that a covalent bond forms when orbitals of two atoms overlap and the overlap region, which is between the nuclei, is occupied by a pair of electrons.

Cont.....

- ❖ According to the VBT two atoms form a bond when both of the following conditions occur

i. There is orbital overlap between two atoms. Half filled orbitals overlaps to form covalent bond

ii. A maximum of two electron of opposite spin , can be present in the overlapping orbitals

- ❖ According to the VBT the greater the overlap the stronger is the bond

Cont.....

- **Sigma bond** is formed when orbitals overlap in head or end to end or linear overlap
- The electron density of sigma bond is greatest along the axis
- s-s and s-p will always overlap along the nuclear axis and result only sigma bond

Cont..

- A side - to - side or parallel overlap forms another type of covalent bond called a **pi(π) bond**.
- It has two regions of electron density. One above and one below the sigma bond axis.
- One π-bond holds two electrons that occupy both regions of the bond.
- A double-bond always consists of one σ and one π bond.
- The double-bond increases electron density between the nuclei.
- A triple bond consists of one σ and two π bonds.

Hybridization of Orbitals

- **Hybridization** is a process of replacing pure atomic orbitals with reformulated atomic orbitals for bonded atoms.
- When different atomic orbital of same or nearly same energy combined together to form new hybrid orbitals is called hybridization
- The new orbitals formed are called **hybrid orbitals**
- study hybridization teach us two important concept

i. it shows us molecular geometry or shape of molecules

ii. it shows as bonding of orbitals

- Hybridization of atomic orbitals doesn't take place in every molecule

Hybridization of Orbitals

Why orbitals are hybridized?

Cont.....

sp hybrid orbitals

- The combination of one s and one p orbitals is called sp hybridization
- The resultant orbitals are known as sp hybrid orbitals
- sp hybrid orbitals posses 50% s-character and 50% p-character
- Sp hybrid orbitals result linear molecular shape

Example -$BeCl_2$

Cont....

Sp2 hybrid orbitals

- The combination (mixing) of one s and two p orbitals is called sp2 hybridization
- The orbitals formed during this process are termed as sp2 hybrid orbitals
- Sp2 hybrid have 33% s-character and 67% p-character
- Sp2 hybrid result trigonal planar electron arrangement

Example-BH_3

Cont....

Sp3 hybrid orbitals

- **Combination of one s and three p orbitals**
- The orbitals formed during this process are termed as sp3 hybrid orbitals
- Sp3 hybrid have 25% s-character and 75% p-character
- Sp3 hybrid result tetrahedral electron arrangement

Example-CF4

Cont....

Sp3d hybrid orbitals

- The combination (mixing) of one s ,three p and one d orbitals called sp3d hybridization
- The orbitals formed during this process are termed as sp3d hybrid orbitals
- Sp3d hybrid have 20% s-character, 60% p-character and 20%d-character
- Sp3d hybrid result trigonal bipyramid electron arrangement

Example-PCl5

Cont.....

Sp3d2 hybrid orbitals

- The combination (mixing) of one s ,three p and two d orbitals called sp3d2hybridization
- The orbitals formed during this process are termed as sp3d2 hybrid orbitals
- Sp3d2hybrid have 16.7% s-character, 50% p-character and 33.3%d-character
- Sp3d2 hybrid result octahedral electron arrangement

Example-SF6

Cont....

Hybridization in multiple bond

- Sigma bond and pi bonds are present in molecules having two atoms connected by double or triple bonds

Example C2H4

Cont....

Hybridization in multiple bond

Example C2H2

Cont….

For each of the following species propose the hybridization scheme for the central atom?

a.SF_4 b. SO_3 c. CO_2 d. SO_2 e. N_2

Molecular orbital theory

Why we study molecular orbitals?

Dues to the defect of Lewis structure, VSEPR theory and valance bond theory failed explain these question

- Doesn’t explain the molecular orbitals of the molecules
- Doesn’t explain the stability of the molecules
- Doesn’t explain the paramagnetic or diamagnetic effect of molecules
- these question is answered by MOT

Note! This theory doesn’t explain the formation of molecules. studies how molecules behave after its formation? I mean Teach us BDSP

Cont....

- Atomic orbitals combine to form new orbitals known as molecular orbitals
- The molecular orbital that results from the addition of the atomic orbitals that overlap is called bonding molecular orbital. is denoted by $\delta \; or \; \pi$
- Places high electron charge density between the two nuclei
- The molecular orbital that results from the subtraction of the atomic orbital that overlap is known as anti bonding molecular orbital. is denoted by $\delta^{*} \; or \; \pi^{*}$
- Places low electron charge density between the two nuclei

Cont....

Basic ideas concerning molecular orbitals

- The number of molecular orbitals formed is equal to the number of atomic orbitals combined
- Of the two MOs formed when two atomic orbitals are combined, one is bonding MO at a lower energy than the original atomic orbitals. The other is an anti bonding M0 at higher energy
- In ground- state configuration electrons enter the lowest energy Mos available (building up principle)

$\delta 1s$, $\delta 1s^*$, $\delta 2s$, $\delta 2s^*$, $\delta 2px$ $\pi 2py$ $\pi 2py$

Cont..

- The maximum number of electrons in a given MO is two(pauli exclusion principle
- In ground state electron configuration elections enter MOs of identical energies singly before they pair up (hunds rule)
- When two atomic orbitals overlap end to end they form δMOs
- When atomic orbital overlap side to side they form π.

Cont....

Molecular orbital diagram

- It shows the relative energy and number of electrons in each MO and the atomic orbitals from which they form.
- Note! A stable molecular species has more electrons in bonding MOs than in anti bonding MOs

The stability of molecular species is determined by bond order(BO)

$$BO=1/2(n_b- na)$$

i. If BO=0, such types of molecules are unstable i.e doesn't exist

ii. If BO>0, such types of molecules are stable

iii. As BO increases the stability of the molecules are also increase

Cont....

Molecular orbital diagram

- It shows the relative energy and number of electrons in each MO and the atomic orbitals from which they form.
- The expected order of filling MOs for element whose atomic number is ≤ 7 is

  $\delta 1s, \delta^{*}1s, \delta 2s, \delta * 2s, \{\pi 2px, \pi 2py\}, \delta 2pz, \{\pi * 2px, \pi * 2py\}, \delta^{*} 2pz$
- The expected order of filling MOs for element whose atomic number is ≥ 8 is

  δ 1s, δ *1s, $\delta 2$ s, $\delta * 2$ s, $\delta 2pz, \{\pi 2px$, $\pi 2py$ $\}$, $\{\pi * 2px, \pi * 2py\}, \delta^{*} 2pz$
- Note! A stable molecular species has more electrons in bonding MOs than in anti bonding MOs

Cont.....

Paramagnetic vs diamagnetic

- A species with unpaired electrons exhibits paramagnetic property(attracted by external magnet)
- A species with paired electrons exhibits diamagnetic property(repeld by magnetic field)

Cont.....

Identify those which exist and doesn't exist, stability or not paramagnetic or diamagnetic by using molecular orbitals diagram

a.C_2 b. Ne_2 c. C_2^- D. NO^+ e.CN^+

THE END

THANK YOU

WE ARE FATHER STUDENT!