

Ch03: Chemical Bond

Electronegativity: Chemical property that describes the tendency of an atom to attract electrons towards to itself.

Relations:

- Size of atom (inverse)
- Nuclear charge (Direct)
- Screening of electrons (inverse)

Trends:

- Group → Decrease
- Period → Increase

Dipole moment: Product of magnitude between the distance of positive and negative charges.

Unit: debye (1 debye is equal to $3.335 \times 10^{-30} \text{ Cm}$)

Polar Covalent: Type in which electrons aren't equally shared.

Non-Polar: Equal sharing of electrons

★ Only those molecules that have non-polar covalent bond have shapes. (Tetrahedral, Linear, Trigonal etc.).

Theories To explain Bonds

- ① Octet rule
- ② VSEPR (Valence Shell Electron pair Repulsion Theory)
- ③ VBT (Valence Bond Theory)
- ④ MOT (Molecular Orbital Theory)

Bond length: Distance between the nuclei of two atoms. ($\text{\AA}$)

VSEPR: Determine the shape and bond angle in the molecule. (Depends on lone and bond pair).

Shapes: A = Central atom

X = Bond pair E = lone pair

→ AX_2 → Linear Shape (180° - Bond angle) (BF_2)

→ AX_3 → Trigonal shape (120° - Bond angle) (BCl_3)

→ AX_4 → Tetrahedral (109.5° - Bond angle) (CH_4)

→ AX_2E_2 → Angular (104.5° - Bond angle) (H_2O)

→ AX_3E_1 → Trigonal (109.5° - Bond angle) (NH_3)

→ AX_5 → Trigonal bipyramidal shape (90° - 120° - Bond angle) (PCl_5)

→ AX_6 → Octahedral (90° - Bond angle) (SF_6)

Importance:

→ VSEPR helps to identify the 3D shape of drugs.

→ VSEPR guides the design of drugs with shapes that precisely fit into enzymes active site.

Octet hypervalency: 2nd row of the periodic, where a full valence shell include 8 electrons with an electronic configuration.

VBT: Describes that covalent bonds are formed by the overlapping of partially filled atomic orbital with another partially filled atomic orbital.

Proposed by Hestler and London (1927)

→ Bond is formed by the overlapping of atomic orbitals.

↳ Electrons of overlapping orbitals has opposite spin.

↳ Number of bonds formed = Unpaired electrons in the outermost shell.

↳ More overlapping result in stronger bond.
Overlapping of s

Head to head → Sigma bond (σ)

s-s



s-orbital
s-orbital

p-p



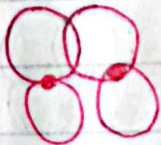
p-orbital
p-orbital

s-p



s-orbital
p-orbital

Lateral → Pi bond (π)



Sigma bond is stronger than pi bond.

MOTs Describe that atomic orbitals combine to form molecular orbitals.

Proposed by Hund and Mullikan in 1932.

Paramagnetic: Unpaired electrons attracted by external magnetic field.

Diamagnetic: Not attracted by external magnetic field that have no unpaired electrons.

Molecular Orbital

Bonding (B.M.O)

Constructive
High energy
No nodal plane

Anti-bonding (A.B.M.O)

Destructive
Low energy
Have nodal plane

Bond order: Total number of bonds formed when atomic orbitals overlap.

(If B.O is 0 then molecule is unstable).

↳ MOT tells the nature of atom/molecule (Para or diamagnetic).

↳ Molecular orbitals have different shape and energy a.c.t atomic orbitals.

Hybridization: Mixing of two orbitals.

(Hybrid = mix)

↳ ground state electrons are transported to excited state (lower to higher).

Types:

sp hybridization:

50% s, 50% p orbital

↳ Can form only sigma bonds.

Ex: BeCl₂, Acetylene,

sp² hybridization:

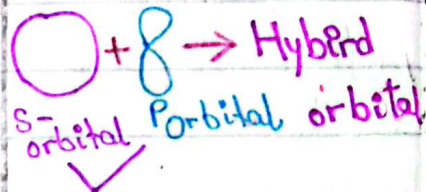
33.3% s, 66.6% p

Ex: BCl₃, Ethylene

sp³ hybridization:

25% s, 75% p

Ex: Ethane, NH₃, H₂O



Hybridization

(This resultant orbital will have energy equal to the atomic orbitals combined)

There is no sp⁴ or sp⁵ orbitals because it's only p_x, p_y, p_z.

σ bond → Hybridized
π bond → unhybridized