CONCEPT MAP

CHEMICAL BONDING AND MOLECULAR STRUCTURE

The attractive force which holds together the constituent atoms or ions of a chemical species is known as chemical bond and different types of bonds formed between various elements govern the molecular structure and properties of compound formed.

CHEMICAL BONDING

Modern theory

- Atoms form bonds since it leads to decrease in energy.
- Whenever atoms come close, both attractive and repulsive forces operate and if the magnitude of attractive forces is more than those of repulsive forces, a chemical bond is formed.

Important Terms/Formulae

- **Formal charge of an atom in a Lewis structure**

$$= V - L - \frac{1}{2}S$$

- **Bond length :** Equilibrium distance between the nuclei of two bonded atoms in a molecule.
  - Bond length $\propto$ size of atoms, bond length $\propto \frac{1}{\text{bond order}}$
- **Bond angle :** Angle between the orbitals containing bonding electron pairs around the central atom in a molecule/complex ion.
- **Bond enthalpy :** Amount of energy required to break one mole of bonds of a particular type between two atoms in a gaseous state.
- **Bond order :** Number of bonds formed between two atoms in a covalent compound.

Theories of Chemical Bonding

Kossel-Lewis approach

Atoms can combine either by transfer of valence electrons from one atom to another or by sharing of valence electrons in order to have an octet in their valence shell (octet rule).

- **Resonance :** The phenomenon of existence of a molecule in different structural forms each of which can explain most of the properties of the molecule but none can explain all the properties of the molecule.
- **Dipole moment (μ) =** Charge $\times$ Distance of separation
- **Stability of molecule :** If $N_b > N_a$, molecule is stable and if $N_b < N_a$, molecule is unstable.
- **Polar covalent Bond :** Covalent bond formed between two dissimilar atoms.
- **Hybridisation :** Phenomenon of intermixing of orbitals of slightly different energies and shapes to generate orbitals of same energy and shape.

Types of Bonds

- **Ionic or Electrovalent :** Strong electrostatic force of attraction between positive and negative ions.
- **Covalent Bond :** Bond formed by mutual sharing of electrons.
- **Coordinate Bond :** Bond formed by one sided sharing of electrons i.e., one atom donates a pair of electrons while other simply shares it.
- **Hydrogen Bond :** Attractive force that binds H-atom directly attached with electronegative atom of one molecule with electronegative atom of other molecule.

Theories of Covalent Bonding

VSEPR Theory (*Nyholm and Gillespie*)

- The shape of a molecule depends upon the number of valence shell electron pairs (bonded or non bonded) surrounding the central atom.
- Electron pairs tend to occupy such positions in space which minimise repulsions.
- The repulsive interactions of electron pairs decrease in the order:

$$lp - lp > lp - bp > bp - bp$$

Valence Bond Theory (*Pauling*)

- A bond is formed between two atoms when the new forces of attraction are greater than forces of repulsion.
- A covalent bond is formed between two atoms by pairing of electrons present in the valence shell having opposite spins.

Molecular Orbital Theory (*F. Hund and R.S. Mulliken*)

- Molecular orbitals are formed by the linear combination of atomic orbitals.
- The number of molecular orbitals formed is equal to the number of atomic orbitals combined.
- When two atomic orbitals combine they form one bonding molecular orbital of lower energy and one anti bonding molecular orbital of higher energy.
- The molecular orbitals are filled in accordance with Aufbau principle obeying Pauli's exclusion principle and Hund's rule.

HYBRIDISATION AND MOLECULAR STRUCTURES

Molecules having bond pairs only

Type of hybridisation	No. of hybrid orbitals	Shape of molecule	Bond angle
sp	2	Linear	180°
sp^2	3	Trigonal planar	120°
sp^3	4	Tetrahedral	109.5°
dsp^2	4	Square planar	90°
dsp^3 or sp^3d	5	Trigonal bipyramidal	120° and 90°
d^2sp^3 or sp^3d^2	6	Octahedral	90°
d^3sp^3 or sp^3d^3	7	Pentagonal bipyramidal	72° and 90°

Molecules having bond pairs and lone pairs

Type of molecule	Hybridisation	Bond angle	Actual shape
AB_2L	sp^2	<120°	V-shape or Bent
AB_2L_2	sp^3	<109°28'	V-shape or Bent
AB_2L_3	sp^3d	180°	Linear
AB_3L_2	sp^3d	90°	T-shape
AB_3L_1	sp^3	<109°28'	Trigonal pyramidal
AB_4L_1	sp^3d	120°, 90°	see saw or Distorted tetrahedron
AB_4L_2	sp^3d^2	90°	Square planar
AB_5L_1	sp^3d^2	<90°	Square pyramidal
AB_6L_1	sp^3d^3		Distorted octahedron