Chapter Name: Atomic Structure, Chemical Bonding and Solution

Rutherford's Model of Atom

- Proposed by Ernest Rutherford in 1911 after his gold foil experiment.
- He bombarded thin gold foil with alpha particles and observed that most particles passed through, while a few were deflected.

Main postulates:

- The atom has a small, dense, positively charged nucleus at the center.
- Electrons revolve around the nucleus in circular orbits, similar to planets around the sun.
- Most of the atom's space is empty.

Limitations:

- Could not explain why negatively charged electrons don't fall into the positively charged nucleus (atomic stability problem).
- Failed to explain the line spectrum of hydrogen.

Bohr's Theory of Atom

- Proposed by Niels Bohr in 1913 to overcome Rutherford's limitations.

Main postulates:

- Electrons revolve around the nucleus in fixed orbits called energy levels (shells) without radiating energy.
- Each orbit has a fixed energy, and these are represented as K, L, M, N… or n = 1, 2, 3, 4…
- Energy is absorbed or emitted only when an electron jumps from one orbit to another.

1. If an electron jumps to a higher orbit → energy is absorbed.
2. If it jumps to a lower orbit → energy is emitted in the form of light.

(Expression for energy and radius are omitted as per instruction.)

Hydrogen Spectrum (Based on Bohr's Model)

- When an electron in a hydrogen atom returns from a higher energy level to a lower one, photons are emitted.
- Each transition gives a line in the emission spectrum.

Series of hydrogen spectrum:

- Lyman series – ultraviolet region (transitions to n=1)
- Balmer series – visible region (transitions to n=2)
- Paschen, Brackett, Pfund series – infrared region (transitions to n=3, 4, 5)

Each spectral line corresponds to a specific wavelength, confirming quantized energy levels.

Heisenberg's Uncertainty Principle

- Proposed by Werner Heisenberg (1927).
- It is impossible to determine simultaneously the exact position and momentum (velocity) of an electron.

$$\Delta x \times \Delta p \geq \frac{h}{4\pi}$$

where;
Δx = uncertainty in position,
Δp = uncertainty in momentum,
h = Planck's constant.

This principle shows that electrons cannot revolve in fixed paths as Bohr suggested. Instead, their position is described by probability clouds (orbitals).

Quantum Numbers

Quantum numbers describe the position and energy of electrons in an atom.

Quantum Number	Symbol	Meaning	Possible Values
Principal	n	Size and energy level	1, 2, 3, …
Azimuthal (Angular)	l	Shape of orbital	0 to n−1
Magnetic	m	Orientation of orbital	−l to +l
Spin	s	Direction of electron spin	+½ or −½

Orbitals and Their Shapes

- Orbitals are regions around the nucleus where there is a high probability of finding an electron.
- Each orbital corresponds to a particular energy level, shape, and orientation in space.
- The shape of an orbital depends on the azimuthal quantum number (l)

Types of Orbitals:

(a) s-Orbitals

- For l = 0.
- **Shape:** Perfectly spherical around the nucleus.
- The size of the s-orbital increases with increasing principal quantum number (n).
- **Example:** 1s < 2s < 3s
- Only one s-orbital exists in each energy level.

(b) p-Orbitals

- For l = 1.
- **Shape:** Dumbbell-shaped, having two lobes on opposite sides of the nucleus.
- There are three orientations along the x, y, and z axes: px, py, pz.
- All three p-orbitals are degenerate, i.e., they have the same energy in an isolated atom.

(c) d-Orbitals

- For l = 2.
- **Shape:** Mostly clover-leaf type (four lobes).
- There are five orientations – dxy, dyz, dzx, dx^2-y^2, and dz^2.
- d-orbitals appear first in the third energy level (n = 3).
- These orbitals are important in explaining transition elements and their magnetic properties.

Pauli's Exclusion Principle

- Proposed by Wolfgang Pauli (1925).
- It states that no two electrons in an atom can have the same set of four quantum numbers (n, l, m, s).

Key Points:

- Since there are only two possible spin quantum numbers (+½ and −½), each orbital can accommodate a maximum of two electrons.
- The two electrons in an orbital must have opposite spins (paired electrons).
- This principle explains why electrons occupy separate orbitals and how electronic configurations are arranged.

Example:

In a 1s orbital → $1s^2$
Here, one electron has spin +½, and the other has spin −½.

Hund’s Rule of Maximum Multiplicity

- Proposed by Friedrich Hund.
- It describes how electrons are filled into degenerate orbitals (orbitals with the same energy) within a subshell.

Hund’s Rule States:

- Electrons occupy all degenerate orbitals singly first before any pairing takes place.
- All the unpaired electrons in singly occupied orbitals have parallel spins to minimize repulsion and maximize total spin.

Reason:

- This arrangement results in the lowest energy configuration because parallel spins cause less electron–electron repulsion.

Example:

For a p^3 configuration (like in nitrogen, $1s^2\ 2s^2\ 2p^3$):
Each of the three p orbitals (px, py, pz) gets one electron with parallel spin.

Aufbau Principle

- The term Aufbau is a German word meaning **“building up.”**
- It explains the order in which electrons fill atomic orbitals as atomic number increases.

Key Rules:

- Electrons fill orbitals in increasing order of energy (from lowest to highest).
- The order of filling can be determined using the (n + l) rule, where
- n = principal quantum number
- l = azimuthal quantum number
- The orbital with lower (n + l) value has lower energy and is filled first.
- If two orbitals have the same (n + l) value, the orbital with lower n value fills first.

Filling Order of Orbitals:
1s → 2s → 2p → 3s → 3p → 4s → 3d → 4p → 5s → 4d → 5p → 6s → 4f → 5d → 6p → 7s ...

Example:
After 3p, 4s is filled before 3d because the (n + l) value for 4s (4+0=4) is less than that for 3d (3+2=5).

Electronic Configuration

- Electronic configuration represents the distribution of electrons among the orbitals of an atom.
- It follows the Pauli Exclusion Principle, Hund's Rule, and Aufbau Principle.

Representation:
Written as:

$$(\text{Energy level})(\text{Subshell})^{\text{Number of electrons}}$$

Example:
- Hydrogen (Z = 1): $1s^1$
- Helium (Z = 2): $1s^2$
- Oxygen (Z = 8): $1s^2\ 2s^2\ 2p^4$
- Sodium (Z = 11): $1s^2\ 2s^2\ 2p^6\ 3s^1$
- Iron (Fe, Z = 26): [Ar] $4s^2\ 3d^6$

General Rules:
- Each shell (n) can hold a maximum of $2n^2$ electrons. n=1 → 2 electrons, n=2 → 8 electrons, n=3 → 18 electrons, etc.
- Stable configurations occur when subshells are completely filled or half-filled (e.g., Cr, Cu show exceptions due to extra stability).
- Shorthand notation: Uses noble gas symbols to represent core electrons, e.g., Fe: [Ar] $4s^2\ 3d^6$

Types of Chemical Bonding

Atoms combine to form molecules or compounds by sharing or transferring electrons to attain stability (usually an octet in the outer shell).

The attractive force which holds two or more atoms together in a molecule is called a chemical bond.

1. Ionic Bond (Electrovalent Bond)

Definition:
A bond formed by the complete transfer of electrons from one atom to another, resulting in the formation of oppositely charged ions that attract each other electrostatically.

Conditions:
Formed between metal and non-metal.
Large difference in electronegativity between the two atoms.

Example:
Sodium chloride (NaCl)
$Na \rightarrow Na^+ + e^-$
$Cl + e^- \rightarrow Cl^-$
$\Rightarrow Na^+ + Cl^- \rightarrow NaCl$

Properties:
- High melting and boiling points.
- Conduct electricity in molten or aqueous state.
- Soluble in polar solvents (like water).

2. Covalent Bond

Definition:
A bond formed by the mutual sharing of electrons between two atoms to achieve stable electron configuration.

Conditions:

- Usually formed between non-metals.
- Small or no electronegativity difference.

Example:

- Chlorine molecule (Cl_2):
- Each Cl atom shares one electron forming a Cl–Cl single bond.

Properties:

- Low melting and boiling points.
- Poor conductors of electricity.
- Often insoluble in water but soluble in organic solvents.

3. Metallic Bond

Definition:

A bond is formed between metal atoms due to attraction between positively charged metal ions and the 'sea of delocalized electrons' around them.

Example:

Copper (Cu), Sodium (Na), and Iron (Fe) metals.

Properties:

- Good conductors of heat and electricity.
- Malleable and ductile.
- High tensile strength and metallic lustre.

4. Hydrogen Bond

Definition:

An electrostatic attraction between a hydrogen atom covalently bonded to a highly electronegative atom (like N, O, or F) and another electronegative atom having a lone pair of electrons.

Types:

- Intermolecular H-bonding: Between different molecules (e.g., H_2O, HF).
- Intramolecular H-bonding: Within the same molecule (e.g., o-nitrophenol).

Example:
Water (H_2O): Each H_2O molecule forms hydrogen bonds with four neighboring molecules.

Properties:

- Responsible for higher boiling point of water.
- Increases viscosity and surface tension.
- Plays an important role in biological molecules (like DNA).

Types of Hybridization and Examples

Type	Orbitals Involved	Example	Geometry	Bond Angle
sp	1 s + 1 p	**$BeCl_2$**	Linear	180°
sp^2	1 s + 2 p	**BF_3**	Trigonal planar	120°
sp^3	1 s + 3 p	**CH_4**	Tetrahedral	109.5°
sp^3 (with lone pair)	1 s + 3 p	NH_3, H_2O	NH_3 – Trigonal pyramidal (107°), H_2O – Bent or V-shaped (104.5°)	

Examples Explained

A. $BeCl_2$ (sp hybridization)

- Be: $1s^2\ 2s^2$ → one 2s electron excited to 2p.
- Two orbitals (2s, 2p) hybridize → 2 sp orbitals.
- Linear structure, bond angle = 180°.

B. BF_3 (sp^2 hybridization)

- B: $2s^2\ 2p^1$ → one 2s and two 2p orbitals hybridize → 3 sp^2 orbitals.
- Forms 3 sigma bonds with F atoms.
- Trigonal planar shape, 120°.

C. CH_4 (sp^3 hybridization)

- C: $2s^2\ 2p^2$ → four equivalent sp^3 orbitals.
- Forms four σ bonds with H atoms.
- Tetrahedral shape, 109.5°.

D. NH_3 (sp^3 hybridization)

- N: $2s^2\ 2p^3$ → four sp^3 orbitals (one with a lone pair).
- Pyramidal shape, bond angle ~107°.

E. H_2O (sp^3 hybridization)

- O: $2s^2\ 2p^4$ → four sp^3 orbitals (two with lone pairs).
- Bent or V-shaped structure, bond angle ~104.5°.

● Structure of Diamond and Graphite

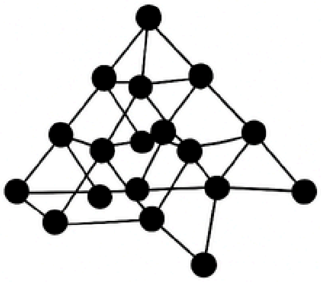
Diamond

Each carbon atom is sp^3 hybridised. Tetrahedrally bonded to four other carbon atoms by strong σ bonds. Forms a 3D rigid network.

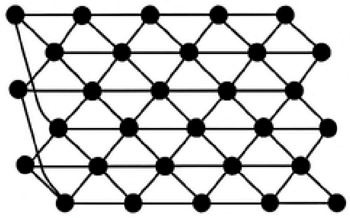
Properties:

- Hardest natural substance.
- High melting point.
- Poor conductor of electricity (no free electrons).

Structure of Diamond



Structure of Graphite



Graphite

- Each carbon atom is sp^2 hybridized.
- Forms three σ bonds with neighboring carbon atoms in a hexagonal planar layer; one electron remains delocalized.
- Layers are held together by weak van der Waals forces and can slide over each other.

Properties:

- Good conductor of electricity (delocalized electrons).
- Soft and slippery (used as lubricant and pencil lead).

Methods to Express Concentration of a Solution

1. Molarity (M)

- Number of **moles of solute** dissolved in **1 liter of solution**.

$$M = \frac{\text{Moles of solute}}{\text{Volume of solution (in liters)}}$$

2. Parts Per Million (ppm)

- Used for very dilute solutions.

$$\text{ppm} = \frac{\text{Mass of solute}}{\text{Mass of solution}} \times 10^6$$

3. Mass Percentage (% by mass)

- Mass of solute per 100 g of solution.

$$\%\ \text{by mass} = \frac{\text{Mass of solute}}{\text{Mass of solution}} \times 100$$

4. Volume Percentage (% by volume)

- Volume of solute per 100 mL of solution.

$$\%\ \text{by volume} = \frac{\text{Volume of solute}}{\text{Volume of solution}} \times 100$$

5. Mole Fraction (x)

- Ratio of moles of one component to the **total moles** of all components.

$$x_A = \frac{n_A}{n_A + n_B}$$

where n_A and n_B are moles of solute and solvent.