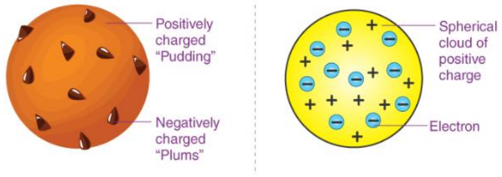
ATOMIC STRUCTURE

RUTHERFORD MODEL OF ATOM

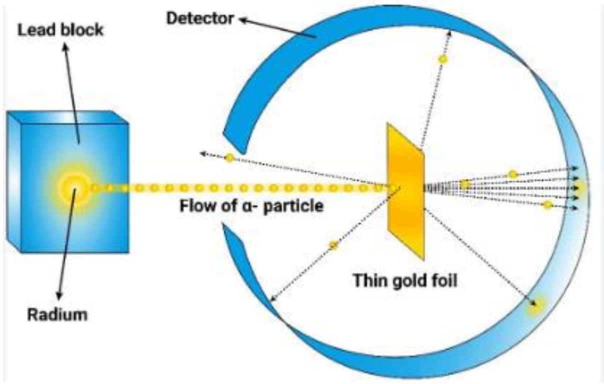
Before Rutherford's experiment, the best model of the atom that was known to us was the Thomson or "plum pudding" model. In this model, the atom was believed to consist of a positive material "pudding" with negative "plums" distributed throughout. Later, Rutherford's alpha-particle scattering experiment changed our perception of the atomic structure. Rutherford directed beams of alpha particles at thin gold foil to test this model and noted how the alpha particles scattered from the foil.



Thomson's model of an atom

The **Rutherford Model of the Atom** was proposed by **Ernest Rutherford in 1911** after his famous **gold foil experiment**.

In the experiment, Rutherford showed us that the atom was mainly empty space with the nucleus at the centre and electrons revolving around it. When alpha particles were fired towards the gold foil, Rutherford noticed that 1 in 20000 particles underwent a change in direction of motion of more than 90 degrees. The rest 19999 particles deviated from their trajectory by a very small margin. This led to the conclusion that the atom consisted of an empty space with most of the mass concentrated at the centre in tiny volumes. This volume at the centre was named 'the nucleus'; Latin for 'little nut'.



- Alpha particles (positively charged) were directed at a thin sheet of gold foil.
- Most particles passed through, but some were deflected at large angles.
- This led Rutherford to conclude the presence of a **tiny, dense, positively charged nucleus**.

Observations of Rutherford's Alpha Scattering Experiment

The observations made by Rutherford led him to conclude that:

1. A major fraction of the α-particles bombarded towards the gold sheet passed through the sheet without any deflection, and hence **most of the space in an atom is empty**.
2. Some of the α-particles were deflected by the gold sheet by very small angles, and hence the **positive charge** in an atom **is not uniformly distributed**. **The positive charge** in an atom **is concentrated in a very small volume**.
3. Very few of the α-particles were deflected back, that is only a few α-particles had nearly 180^{o} angle of deflection. So the **volume occupied by the positively charged particles in an atom is very small as compared to the total volume of an atom**.

Rutherford Atomic Model

Based on the above observations and conclusions, Rutherford proposed the atomic structure of elements. According to the Rutherford atomic model:

1. The positive charge and most of the mass of an atom is concentrated in an extremely small volume. He called this region of the atom as a nucleus.

2. Rutherford's model proposed that the negatively charged electrons surround the nucleus of an atom. He also claimed that the electrons surrounding the nucleus revolve around it with very high speed in circular paths. He named these circular paths as orbits.
3. Electrons being negatively charged and nucleus being a densely concentrated mass of positively charged particles are held together by a strong electrostatic force of attraction.

Limitations of Rutherford Atomic Model

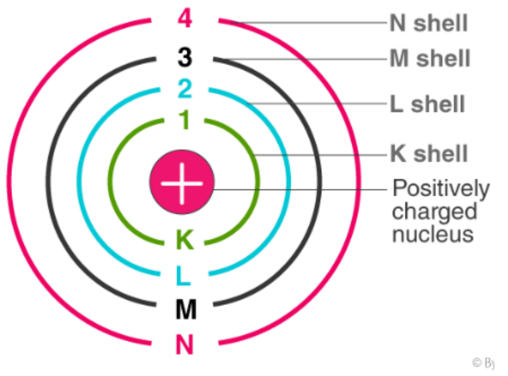
Although the Rutherford atomic model was based on experimental observations, it failed to explain certain things.

- Rutherford proposed that the electrons revolve around the nucleus in fixed paths called orbits. According to Maxwell, accelerated charged particles emit electromagnetic radiations and hence an electron revolving around the nucleus should emit electromagnetic radiation. This radiation would carry energy from the motion of the electron which would come at the cost of shrinking of orbits. Ultimately the electrons would collapse in the nucleus. Calculations have shown that as per the Rutherford model, an electron would collapse into the nucleus in less than 10^{-8} seconds. So, the Rutherford model was **not in accordance with Maxwell's theory and could not explain the stability of an atom**.
- One of the drawbacks of the Rutherford model was also that he **did not say anything about the arrangement of electrons in an atom** which made his theory incomplete.
- Although the early atomic models were inaccurate and failed to explain certain experimental results, **they formed the base for future developments in the world of quantum mechanics**.

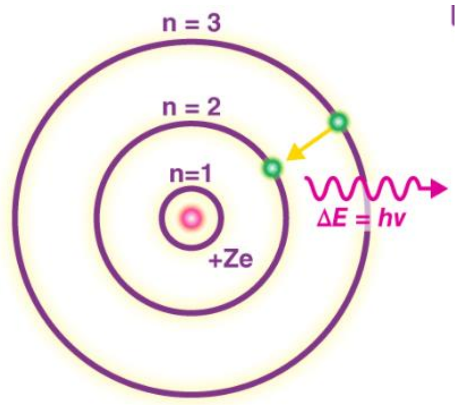
BOHR'S THEORY

The Bohr model of the atom was proposed by Neil Bohr in 1915. It came into existence with the modification of Rutherford's model of an atom. Rutherford's model introduced the nuclear model of an atom, in which he explained that a nucleus (positively charged) is surrounded by negatively charged electrons.

Bohr theory modified the atomic structure model by explaining that electrons move in fixed orbitals (shells) and not anywhere in between and he also explained that each orbit (shell) has a fixed energy. Bohr's model consists of a small nucleus (positively charged) surrounded by negative electrons moving around the nucleus in orbits. Bohr found that an electron located away from the nucleus has more energy, and the electron which is closer to nucleus has less energy.



Bohr's Model of an Atom



Postulates of Bohr's Model of an Atom

- In an atom, electrons (negatively charged) revolve around the positively charged nucleus in a definite circular path called orbits or shells.
- Each orbit or shell has a fixed energy and these circular orbits are known as orbital shells.
- The energy levels are represented by an integer (n=1, 2, 3…) known as the quantum number. This range of quantum number starts from nucleus side with n=1 having the lowest energy level. The orbits n=1, 2, 3, 4… are assigned as K, L, M, N…. shells and when an electron attains the lowest energy level, it is said to be in the ground state.
- An electron emits or absorbs energy when it jumps from one orbit or energy level to another. When it jumps from a higher energy level to lower energy level it emits energy while it absorbs energy when it jumps from a lower energy level to a higher energy level.

- The energy absorbed or emitted is equal to the difference between the energies of the two energy levels (E_1, E_2) and is determined by Plank's equation.

  $\Delta E = E_2 - E_1 = h\nu$

  Where,

  ΔE = energy absorbed or emitted

  h= Plank's constant

  ν= frequency of electromagnetic radiation emitted or absorbed

- The angular momentum of an electron revolving in energy shells is given by:

  $m_e vr = nh/2\pi$

  Where,

  n= number of corresponding energy shell; 1, 2, 3 …..

  m_e= mass of the electron

  v= velocity

  r=radius

  h= Plank's constant

Limitations of Bohr's Model of an Atom

- Bohr's model of an atom failed to explain the Zeeman Effect (effect of magnetic field on the spectra of atoms).
- It also failed to explain the Stark effect (effect of electric field on the spectra of atoms).
- It violates the Heisenberg Uncertainty Principle.
- It could not explain the spectra obtained from larger atoms.

Bohr–Bury rules of electronic configuration: Bohr and Bury simultaneously proposed the following rules for the distribution of electrons in different shells.

Rule 1: The maximum number of electrons that can be accommodated in a shell is equal to $2n^2$ where 'n' is the quantum number of the shell (i.e., the serial number of the shell from the nucleus).

Rule 2: Electrons may go into a new outer shell although the inner shells are incompletely filled.

Rule 3: The outermost shell cannot have more than 8 electrons and the next inner, i.e., the penultimate, shell cannot have more than 18 electrons.

Rule 4: Even if the capacity of the penultimate shell exceeds 8, it cannot have more than 8 electrons unless there are 2 electrons in the outermost shell. And it cannot have more than 9 electrons unless the anti–penultimate shell (i.e., the shell immediately preceding the penultimate shell) is completely filled. In such cases, the outermost shell can have more than 2 electrons only after there are 18 electrons in the penultimate shell.

Hydrogen Spectrum Explanation Based on Bohr's Model Of Atom

- In a hydrogen atom (which has **1 electron**), the electron can **jump between energy levels**.
- When it **jumps from a higher energy level to a lower one**, it emits a **photon**.
- The energy of this photon determines the **wavelength (or color)** of light emitted.
- These different wavelengths form the **hydrogen emission spectrum** – a series of **bright lines** on a dark background.

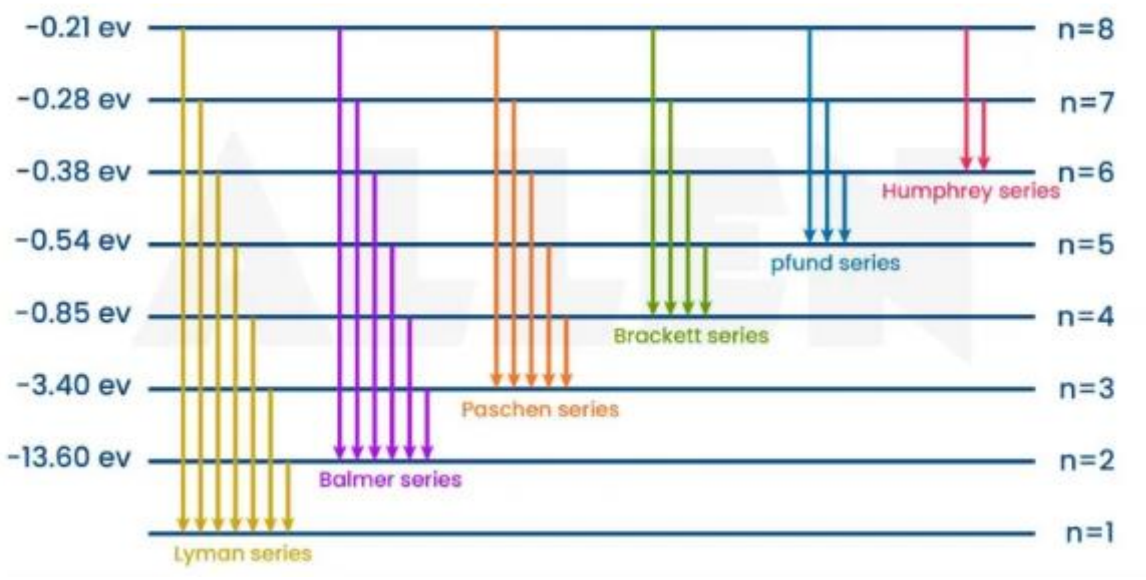
Energy of Emitted Light:

Bohr derived a formula:

$$E = h\nu = E_2 - E_1$$

Where:

- E = energy of photon emitted
- h = Planck's constant
- ν = frequency of emitted light
- E_2, E_1 = energy of higher and lower levels



HEISENBERG UNCERTAINTY PRINCIPLE (1927)

It is **impossible to measure both the position and momentum of a microscopic particle (like an electron) exactly at the same time**.

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

Where:

- Δx = uncertainty in position
- Δp = uncertainty in momentum
- h = Planck's constant = **6.626 × 10^{-34} Js**

Explanation:

- If we try to measure **position accurately**, the **momentum becomes uncertain**.
- If we measure **momentum accurately**, the **position becomes uncertain**.
- This is because **observing tiny particles disturbs them**.

Example:

- Trying to see an **electron** using light disturbs it.
- As a result, we cannot know exactly **where it is and how fast it's moving at the same time**.

Importance:

1. Applicable only to **small particles** like **electrons**.
2. Not noticeable for **big objects**.
3. Replaced the idea of **definite paths** of electrons with **probability clouds**.
4. Helped in developing the **quantum mechanical model of the atom**.

QUANTUM NUMBERS

1. Principal Quantum Number (n)

- Values: **1, 2, 3, 4…**
- Represents: **Shell** or **energy level** of electron.
- Determines: **Size and energy** of orbital.
- Example:
  n=1n = 1n=1 → K-shell,
  n=2n = 2n=2 → L-shell.

2. Azimuthal Quantum Number (l)

- Values: **0 to (n – 1)**
- Represents: **Subshell** and **shape of orbital**.
- Subshell Types:
  l =0 → **s** (spherical),
  l =1 → **p** (dumbbell),
  l =2 → **d**
  l =3 → **f**

3. Magnetic Quantum Number (m or m_l)

- Values: **–l to +l** (including 0)
- Represents: **Orientation** of orbital in space.
- Example: If l =1 → m=–1, 0, +1

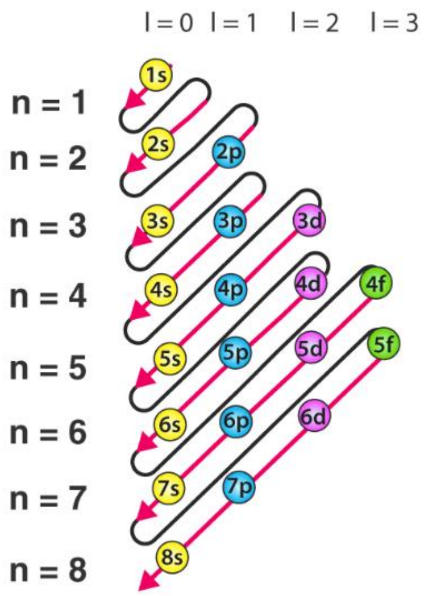
4. Spin Quantum Number (s or m_s)

- Values: **+½ or –½**
- Represents: **Spin** of electron (clockwise or anti-clockwise).
- Only **two electrons** can exist in one orbital with **opposite spins**.

AUFBAU PRINCIPLE

It states that electrons are filled into atomic orbitals in the increasing order of orbital energy level. According to the Aufbau principle, the available atomic orbitals with the lowest energy levels are occupied before those with higher energy levels.

The word 'Aufbau' has German roots and can be roughly translated as 'construct' or 'build up'. A diagram illustrating the order in which atomic orbitals are filled is provided below. Here, 'n' refers to the principal quantum number and 'l' is the azimuthal quantum number.



Salient Features of the Aufbau Principle

- According to the Aufbau principle, electrons first occupy those orbitals whose energy is the lowest. This implies that the electrons enter the orbitals having higher energies only when orbitals with lower energies have been completely filled.
- The order in which the energy of orbitals increases can be determined with the help of the (n+l) rule, where the sum of the principal and azimuthal quantum numbers determines the energy level of the orbital.
- Lower (n+l) values correspond to lower orbital energies. If two orbitals share equal (n+l) values, the orbital with the lower n value is said to have lower energy associated with it.
- The order in which the orbitals are filled with electrons is: 1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s, 5f, 6d, 7p, and so on.

Writing the Electron Configuration of Nitrogen

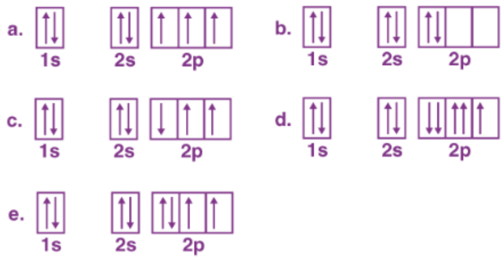
- *The element nitrogen has 7 electrons (since its atomic number is 7).*
- *The electrons are filled into the 1s, 2s, and 2p orbitals.*
- *The electron configuration of nitrogen can be written as $1s^2 2s^2 2p^3$*

HUND'S RULE

Aufbau principle tells us that the lowest energy orbitals get filled by electrons first. After the lower energy orbitals are filled, the electrons move on to higher energy orbitals.

According to Hund's rule:

- *Before the double occupation of any orbital, every orbital in the sub level is singly occupied.*
- *For the maximization of total spin, all electrons in a single occupancy orbital have the same spin*



Hund's Rule

This rule was discovered in the year 1925 by Friedrich Hund

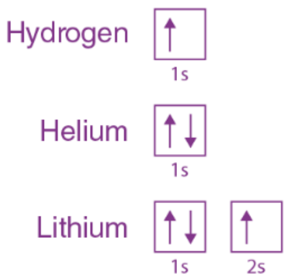
<u>Hund's rule of maximum multiplicity</u>

The rule states that, for a stated electron configuration, the greatest value of spin multiplicity has the lowest energy term. It says if two or more than two orbitals having the same amount of energy are unoccupied then the electrons will start occupying them individually before they fill them in pairs. It is a rule which depends on the observation of atomic spectra, which is helpful in predicting the ground state of a molecule or an atom with one or more than one open electronic shells.

PAULI'S EXCLUSION PRINCIPLE

The Pauli exclusion principle states that in a single atom, no two electrons will have an identical set or the same quantum numbers (n, l, m_l, and m_s). To put it in simple terms, every electron should have or be in its own unique state (singlet state). There are two salient rules that the Pauli exclusion principle follows:

- Only two electrons can occupy the same orbital.
- The two electrons that are present in the same orbital must have opposite spins, or they should be antiparallel.



Formulation of the Pauli Exclusion Principle

CHEMICAL BONDING

Concept of Chemical Bonding

Chemical bonding is the force of attraction that holds atoms together in compounds. It allows atoms to combine and form stable molecules or crystals.

Cause of Chemical Bonding

Atoms bond with each other mainly to achieve stability, which means having low energy and a full outermost shell (octet or duet), like noble gases.

Main Causes of Chemical Bonding:

1. ***Octet Rule (Stability Factor):***
   - *Atoms tend to gain, lose, or share electrons to get **8 electrons in their outer shell** (2 for hydrogen, helium – duet rule).*
   - *Example: Oxygen (O) needs 2 electrons to complete its octet → forms bonds.*
2. ***Decrease in Potential Energy:***
   - *When atoms bond, their total **potential energy decreases**, making the system **more stable**.*
   - *Bonded atoms are at a **lower energy level** than free atoms.*
3. ***Electrostatic Forces:***
   - *Attractive forces between **positive nuclei and negative electrons** or between **oppositely charged ions** lead to bonding.*
   - *Example: Na^+ and Cl^- attract each other → form NaCl.*
4. ***Incomplete Outer Shell:***
   - *Atoms with **incomplete valence shells** are **unstable** and tend to **react** to achieve stability by bonding.*

Types of Chemical Bonds:

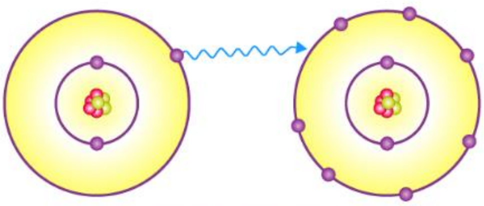
1. ***Ionic Bond** – Transfer of electrons (e.g., NaCl)*
2. ***Covalent Bond** – Sharing of electrons (e.g., H_2O)*
3. ***Metallic Bond** – Free-flowing electrons among metal atoms (e.g., Fe, Cu)*

IONIC BOND OR ELECTROVALENT BOND

A chemical bond is formed between two atoms by the complete transfer of one or more electrons from one atom to the other as a result of which the atoms attain their nearest inert gas configuration.

*There are primarily three ways in which two atoms combine to lose energy and to become stable. One of the ways is by donating or accepting electrons to complete their octet configuration. The bond formed by this kind of combination is known as an **ionic bond** or **electrovalent bond**. This kind of bond is formed when one atom gains electrons while the other atom loses electrons from its outermost level or orbit.*

Electrovalent bonds are produced when electrons are transferred from atoms of one element to atoms of another element, producing positive and negative ions. The bond which is formed by the transfer of electrons between the atoms is called electrovalent bond or ionic bond. Electrovalent bonds are only formed between metals and non-metals. Electrovalent bonds are not formed between two non-metals.



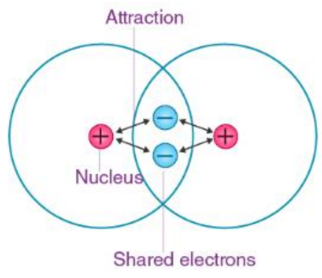
Ionic Bond (Electrovalent Bond)

- *An Ionic bond is the bond formed by the complete transfer of valence electron to attain stability.*
- *This type of bonding leads to the formation of two oppositely charged ions – positive ions known as **cations** and negative ions known as **anions**.*
- *The presence of two oppositely charged ions results in a strong attractive force between them. This force is an ionic or electrovalent bond.*
- *Ionic bonds form between atoms with large differences in electronegativity, whereas covalent bonds formed between atoms with smaller differences in electronegativity.*
- *The compound formed by the electrostatic attraction of positive and negative ions is called an ionic compound.*

COVALENT BOND

*A **covalent bond** is formed by the equal sharing of electrons from both participating atoms. The pair of electrons participating in this type of bonding is called a shared pair or bonding pair. Covalent bonds are also called molecular bonds. Sharing of bonding pairs will ensure that the atoms achieve stability in their outer shell, which is similar to the atoms of noble gas.*

Elements having very high ionisation energies are incapable of transferring electrons, and elements having very low electron affinity cannot take up electrons. The atoms of such elements tend to share their electrons with the atoms of other elements or with other atoms of the same element in a way that both the atoms obtain octet configuration in their respective valence shells, and thus achieve stability. Such association through sharing of electron pairs among different or same kinds is known as Covalent Bond.



Formation of Covalent Bond

- *Sharing of electrons between atoms of the same kind, for example, formation of H_2, Cl_2, O_2, etc.*
- *Sharing of electrons between atoms of different kinds, for example, formation of CH_4, H_2O, NH_3, etc.*

Types of Covalent Bonds

Depending upon the number of shared electron pairs, the covalent bond can be classified into:

- *Single Covalent Bond: A single bond is formed when only one pair of electrons is shared between the two participating atoms. It is represented by one dash (-).*
- *Double Covalent Bond: A double bond is formed when two pairs of electrons are shared between the two participating atoms. It is represented by two dashes (=).*
- *Triple Covalent Bond: A triple bond is formed when three pairs of electrons are shared between the two participating atoms. Triple covalent bonds are represented by three dashes (≡)*

CO-ORDINATE BOND

*A **Co-ordinate bond** is a type of alternate covalent bond that is formed by sharing of an electron pair from a single atom. Both shared electrons are donated by the same atom. It is also called a dative bond or dipolar bond.*

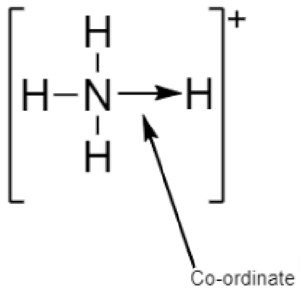
Co-ordinate covalent bonds are usually formed in reactions that involve two non-metals, such as a hydrogen atom or during bond formation between metal ions and ligands.

Characteristics of Coordinate Covalent Bond

1. *In this type of bonding, the atom that shares an electron pair from itself is termed as the donor.*
2. *The other atom which accepts these shared pair of electrons is known as a receptor or acceptor.*
3. *The bond is represented with an arrow →, pointing towards the acceptor from the donor atom.*
4. *After sharing of electron pairs, each atom gets stability.*
5. *This type of bonding is central to the Lewis theory.*
6. *Getting a good understanding of co-ordinate covalent bonds can help in properly designing complex organic molecules.*

Coordination bond in NH4+

In NH4+the fourth hydrogen containing a vacant orbital is attached to the nitrogen atom containing a lone pair of electrons by a dative covalent bond or coordinate bond, thereby making nitrogen atom a donor and hydrogen atom an acceptor. Thus, satisfying the condition for the formation of a coordinate bond. contains three single covalent N−H bonds where one electron is shared by both nitrogen atom and hydrogen atom.



Anomalous Properties of NH_3 and H_2O Due to Hydrogen Bonding

*Hydrogen bonding gives **NH_3 (ammonia)** and **H_2O (water)** several **unique (anomalous) properties** compared to other hydrides in their respective groups (Group 15 and Group 16).*

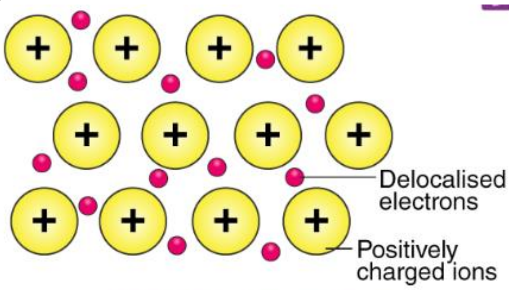
- **High Boiling and Melting Points**: *NH_3 and H_2O have higher boiling/melting points than other hydrides (like PH_3, H_2S) because of strong hydrogen bonds between molecules.*
- **High Solubility**: *NH_3 dissolves well in water due to hydrogen bonding.*
- **H_2O – Ice Floats**: *Ice is less dense than water because of hydrogen bonding, so ice floats*.
- **H_2O – High Surface Tension & Heat Capacity**: *Water has high surface tension and absorbs heat slowly due to hydrogen bonding.*

METALLIC BONDING

'Metallic bond' is a term used to describe the collective sharing of a sea of valence electrons between several positively charged metal ions.

Metallic bonding is a type of chemical bonding and is responsible for several characteristic properties of metals such as their shiny lustre, their malleability, and their conductivities for heat and electricity.

Metallic bond, force that holds atoms together in a metallic substance. Such a solid consists of closely packed atoms. In most cases, the outermost electron shell of each of the metal atoms overlaps with a large number of neighbouring atoms. As a consequence, the valence electrons continually move from one atom to another and are not associated with any specific pair of atoms. In short, the valence electrons in metals, unlike those in covalently bonded substances, are nonlocalized, capable of wandering relatively freely throughout the entire crystal. The atoms that the electrons leave behind become positive ions, and the interaction between such ions and valence electrons gives rise to the cohesive or binding force that holds the metallic crystal together.



Metallic Bonding in Sodium

IONIC BOND	COVALENT BOND	METALLIC BOND
Occurs during the transfer of electrons	Occurs when 2 atoms share their valence electrons	The attraction of metal cations/atoms and delocalized electrons
Binding energy is higher than the metallic bond	Binding energy is higher than the metallic bond	Binding energy is less than covalent and ionic bond
Low conductivity	Very low conductivity	Has high electrical conductivity
Non-directional bond	Directional bond	Non-directional bond
Present only in one state: solid-state	Present only in all 3 states: solid, liquid, gases	Present only in one state: solid-state
Non-malleable	Non-malleable	Malleable
Higher melting point	Lower melting point	High melting point
Non-ductile	Non-ductile	Ductile
Higher boiling point	Lower boiling point	High boiling point

SOLUTIONS

SOLUTE, SOLVENT, AND SOLUTION – BASIC IDEA

1. Solution

A **homogeneous mixture** of two or more substances.

Example: Salt water, sugar in tea.

2. Solute

The substance that is **dissolved** in a solution.

- Present in **smaller amount**.
- Example: **Salt** in salt water, **sugar** in tea.

3. Solvent

The substance that **dissolves the solute**.

- Present in **larger amount**.
- Example: **Water** in salt water, **tea** in sugar tea.

Example Table: **Solution = Solute + Solvent**

Solution	*Solute*	*Solvent*
Salt water	Salt (NaCl)	Water (H_2O)
Sugar tea	Sugar	Tea
Air (mixture)	Oxygen, etc.	Nitrogen

Methods to Express Concentration of Solution

1. Molarity (M)

M = Moles of solute / Volume of solution (in liters)

- Unit: **mol/L or M**
- Example: 1 M NaCl means 1 mole NaCl in 1 liter solution.

2. Parts Per Million (ppm)

ppm = (Mass of solute / Mass of solution) × 10^6

- Used for **very small concentrations** (e.g., pollutants in water/air).
- No units (dimensionless).

3. Mass Percentage (%)

Mass % = (Mass of solute / Mass of solution) × 100

- Both solute and solution mass in **grams**.

4. Volume Percentage (%)

Volume % = (Volume of solute / Volume of solution) × 100

- Used in **liquid-liquid mixtures** (e.g., alcohol in water).

5. Mole Fraction (χ)

χ = Moles of component / Total moles of all components

- No units.
- **χ(solute) + χ(solvent) = 1**

Summary Table:

Method	**Formula**	**Units**
Molarity (M)	M = moles / liters	mol/L or M
ppm	(Mass solute / Mass solution) × 10^6	ppm
Mass %	(Mass solute / Mass solution) × 100	%
Volume %	(Volume solute / Volume solution) × 100	%
Mole Fraction (χ)	moles of one / total moles	No units