Code: 23BS1102

I B.Tech - I Semester – Regular Examinations - JANUARY 2024

CHEMISTRY
(Common for EEE, ECE, CSE)

Duration: 3 hours   Max. Marks: 70

Note: 1. This question paper contains two Parts A and B.
2. Part-A contains 10 short answer questions. Each Question carries 2 Marks.
3. Part-B contains 5 essay questions with an internal choice from each unit. Each Question carries 10 marks.
4. All parts of Question paper must be answered in one place.

BL – Blooms Level   CO – Course Outcome

PART – A

		BL	CO
1.a)	Write notes on molecular orbital theory.	L2	CO1
1.b)	Write the significance of Ψ and Ψ^2.	L2	CO1
1.c)	Explain superconductors with an example.	L2	CO2
1.d)	Write about the nanomaterials and give examples.	L2	CO2
1.e)	Write about the secondary batteries with an example.	L2	CO2
1.f)	Explain about the Potentiometric sensor.	L2	CO2
1.g)	Outline the applications of PVC.	L2	CO3
1.h)	Explain polymerization with an example.	L2	CO3
1.i)	Explain the electromagnetic radiation and interaction with matter.	L3	CO3
1.j)	Describe the basic principle of UV-visible spectroscopy.	L2	CO3

PART – B

			BL	CO	Max. Marks
		UNIT-I			
2	a)	Make use of neat diagram to explain the formation of pi molecular orbital in benzene.	L3	CO2	5 M
	b)	Derive the Schrodinger wave equation and explain the significance of the terms involved.	L4	CO4	5 M
		OR			
3	a)	Make use of neat diagram to explain energy level diagram of O_2 molecule.	L3	CO2	5 M
	b)	Analyze the significance of homo and hetero nuclear diatomic molecules in the field of chemistry.	L4	CO4	5 M
		UNIT-II			
4	a)	Classify super – capacitors based on their characteristics and explain them in detail.	L4	CO2	5 M
	b)	Describe the extrinsic semiconductor and its types. Explain the processes which are occurred during the formation of a P-N junction.	L3	CO4	5 M
		OR			
5	a)	Explain the preparation, structure and properties of high temperature super conductor-$CaTiO_3$.	L3	CO2	5 M

	b)	List out the properties and applications of carbon nanotubes.	L4	CO4	5 M

UNIT-III

6	a)	Describe the construction and working of Hydrogen-Oxygen Fuel cell with a neat diagram.	L3	CO2	6 M
	b)	What is the emf of the following cell at 25°C Zn (s) | Zn^{2+} (0.2M) || Ag^+ (0.002M) | Ag (s). The standard emf of the cell $E°$ is 1.54 V.	L4	CO4	4 M

OR

7	a)	Explain the construction and working of Zinc-air battery with a neat diagram and list out the advantages.	L3	CO2	6 M
	b)	Write the half-cell and net reactions of the following cell: Zn/Zn^{+2} (1M) || Cu^{+2} (1M)/Cu Find the EMF of the above cell given E^0 (Zn^{+2}/Zn) = - 0.76 V and $E^0(Cu^{+2}/Cu)$ = + 0.34 V.	L4	CO4	4 M

UNIT-IV

8	a)	Describe the properties, preparation and applications of Bakelite.	L3	CO5	5 M
	b)	Write a detailed step wise mechanism of cationic polymerization.	L4	CO3	5 M

OR

9	a)	Explain the properties, preparation and applications of nylon-6,6.	L3	CO3	5 M
	b)	Write about the mechanism of conducting polymers and its applications with suitable example.	L4	CO5	5 M

UNIT-V

10	a)	Describe the Instrumentation and applications of IR spectroscopy.	L3	CO3	5 M
	b)	Explain the principle and instrumentation of High-Performance Liquid Chromatography (HPLC) with a neat diagram.	L4	CO5	5 M

OR

11	a)	Explain the Beer-Lambert's law statement and limitations.	L3	CO3	5 M
	b)	List out the characteristics of electromagnetic spectrum.	L4	CO5	5 M

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PVP SIDDHARTHA INSTITUTE OF TECHNOLOGY
(Autonomous)
I B.Tech – I Semester Regular Examinations-JANUARY-2024
CHEMISTRY
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Duration: 3 Hours   **Max. Marks: 70**

KEY AND SCHEME OF VALUATION
PART-A

1. a) Write notes on molecular orbital theory – 2M
1. b) Write the Significance of ψ and $\psi2$ – 2M
1. c) Explain Superconductors with example – 2M
1. d) Write about the nanomaterial's and give examples – 2M
1. e) Write about the secondary batteries with an example – 2M
1. f) Explain about the Potentiometric sensor—2M
1. g) Outline the applications of PVC –2M
1. h) Explain polymerization with an example – 2M
1. i) Explain the electromagnetic radiation and interaction with matter—2M
1. j) Describe the basic principle of UV- visible spectroscopy—2M

PART – B
UNIT-I

2 a) Diagram of Pi molecular orbital in benzene – 5M
  b) Schrodinger Wave equation – 3M, Significance – 2M

OR

3 a) Energy level diagram of O_2 molecule – 5M
  b) Significance of homo -2.5 M, Significance of hetero diatomic molecule- 2.5 M

UNIT-II

4 a) Super capacitors Characteristics – 5 M
  b) Types of Extrinsic Semiconductor –3M, Formation of P-N junction   --2M

OR

5. a) Preparation – 2M , Structure and properties of $CaTiO_3$ – 3M
  b) Any five Properties and applications of Carbon nanotubes –5M

UNIT-III

6. a) Construction, Diagram- 3M, Working of hydrogen-oxygen fuel cell –3M
  b) emf calculation of the cell- 4M

OR

7. a) Construction, Diagram- 3M,Working of Zinc-air battery cell –2M, Advantages- 1M
  b) Half-cell and emf calculation of the cell – 4M

UNIT-IV

8 a) Preparation -2 M, Any three Properties and Application of Bakelite – 3M
  b) Step wise mechanism of cationic polymerization
     Initiation -2M, Propagation – 1M, Termination—2M

OR

9 a) Preparation – 2M
     Any three Properties and Application of nylon-6,6 – 3M
  b) Mechanism of conduction polymers-3M,   Applications –2M

UNIT-V

10 a) Instrumentation of IR Spectroscopy- 3M, Applications –2M
  b) Principle – 1M,   Explanation of Instrumentation with diagram – 4M

OR

11 a) Beer-Lambert's Law statement – 3 M, Limitations- 2M
  b) Any five points regarding Characteristics of electromagnetic spectrum – 5M

PART-A

1a) Molecular Orbital Theory, proposed by Mulliken, explains molecular bonding. Atomic orbitals overlap, losing identity to form molecular orbitals (MOs). MOs are polycentric regions in space, defined by shape and size, involving multiple atoms. The MO count equals overlapping atomic orbitals. Successful combinations require comparable energies and proper orientations of atomic orbitals.

1 b) In the context of the Schrödinger wave equation, Ψ represents the wave function's amplitude, while Ψ^2 holds physical significance as it indicates the probability of finding an electron in a specific space. Ψ^2 is linked to electronic charge density, offering valuable insights into the electron's distribution within a given region.

1 c) Superconductivity is a phenomenon where certain materials exhibit zero electrical resistance, allowing indefinite current flow without energy loss as heat. An example is the high-temperature superconductor $CaTiO_3$. These materials, unlike traditional superconductors, can operate at relatively higher temperatures, enhancing their practical applications in various technologies. The Meissner effect, the expulsion of magnetic fields, is also a characteristic of superconductors.

1d) nano-materials are substances engineered or naturally occurring with structures at the nanoscale, typically below 100 nanometers. Their unique properties, arising from their small size, make them versatile in diverse fields, including medicine, electronics, and materials science. Examples include carbon nanotubes, nanoparticles, and quantum dots.

1 e) Secondary batteries, also known as rechargeable batteries, can be repeatedly charged and discharged. They play a crucial role in portable electronic devices and electric vehicles.
 Common examples include: 1. Lithium-ion (Li-ion) Batteries 2. Lead-Acid Batteries

1f) Potentiometric sensors, a type of chemical sensor, assess the concentration of components in an analyte by measuring the electrical potential of an electrode without current. Functioning like fuel cells, they consist of noble metal electrodes immersed in an electrolyte, typically a strong inorganic acid aqueous solution, offering versatile applications in analytical chemistry.

1 g) PVC used for the preparation of
➤ Safety helmets   ➤ Light fittings   ➤ Tyres, cycles   ➤ Refrigerator components

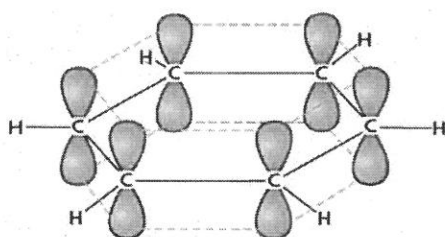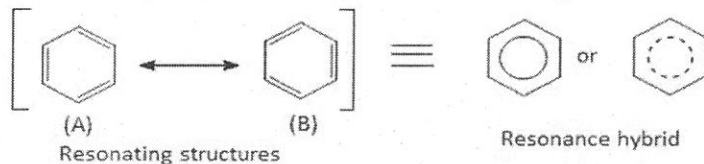1 h) **Polymerization** is the process of forming a polymer by using number of repeating units.
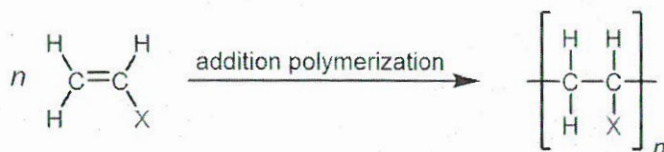
1 i) Electromagnetic radiation consists of waves or particles that propagate through space. When it interacts with matter, the energy is absorbed, transmitted, or reflected. This interaction can cause electronic transitions or vibrations within atoms or molecules. The absorption and emission patterns are characteristic, aiding applications such as spectroscopy and medical imaging in a diverse range of fields.
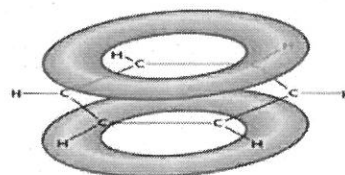
1j) The basic principle of UV (Ultraviolet) spectroscopy involves the absorption of ultraviolet light by molecules, leading to electronic transitions. Molecules absorb UV radiation, causing electrons to move to higher energy levels. The absorption pattern, examined in the UV spectrum, furnishes information about the compound's structure and concentration, facilitating applications in analytical chemistry and biochemistry.

# 2 a) Formation of pi molecular orbital in benzene

π-Molecular orbitals of Benzene: Benzene is an organic compound with planar hexagonal cyclic structure. Each carbon atom in benzene is sp^2 hybridised and contains one p_z orbital unhybridised. Each p_z orbital contains one unpaired electron. All the six carbon-carbon bonds are found to be identical and the molecule exhibits high stability. This is due to delocalization of π-electrons in the entire molecule. The six p_z orbitals oriented perpendicular to the plane of the molecule overlap to form six π-molecular orbitals denoted as Ψ_1, Ψ_2, Ψ_3, Ψ^*_4, Ψ^*_5 and Ψ^*_6. Here Ψ_1, Ψ_2 and Ψ_3 are bonding MO while Ψ^*_4, Ψ^*_5 and Ψ^*_6 are antibonding MO.

(A)   (B)
Resonating structures   Resonance hybrid

Sidewise overlap of unhybridised p orbitals to form π-bonds

π-electrons cloud lying above and below the plane of the molecule

Ground state   Excited state
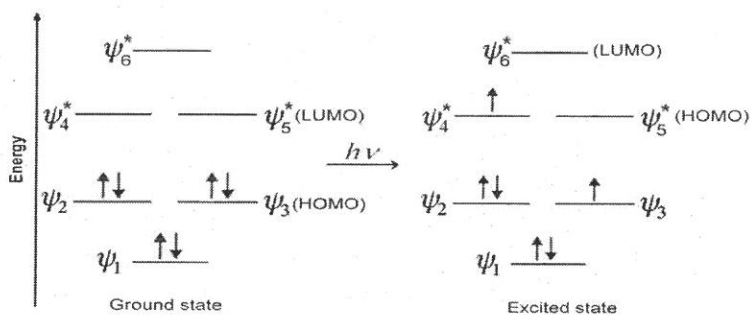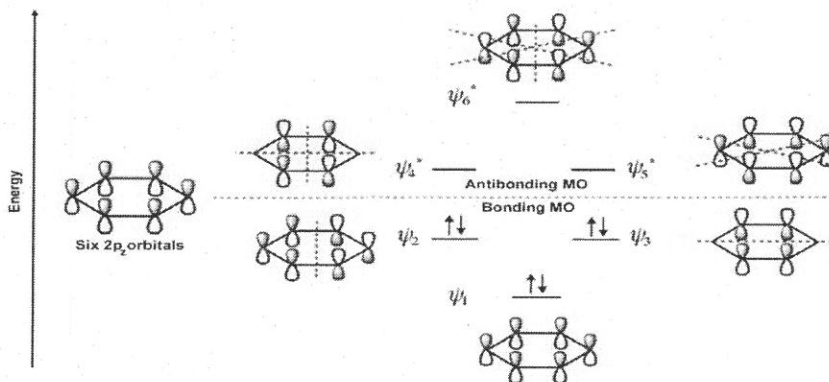
MO	Type	No. of bonding interactions	No. of vertical nodes
Ψ_1	Bonding	6	0
Ψ_2 and Ψ_3	Bonding-degenerate	4	1
Ψ^*_4 and Ψ^*_5	Antibonding-degenerate	2	2
Ψ^*_6	Antibonding	0	3

•After formation of molecular orbitals, the six electrons are filled in bonding MO as three
Pairs and antibonding MO do not contain any electrons. Vertical nodes are the planes indicating the
space where the possibility of finding of Electron is zero.
• The bonding MO $\Psi 1$ has the least energy and is formed by the interaction of the pz
Orbitals of all the six carbon atoms. The resulting MO has no nodal planes.
• The bonding MO $\Psi 2$ and $\Psi 3$ are degenerate orbitals. Each orbital has four bonding
Interactions and one nodal plane.
• The antibonding MO $\Psi *4$ and $\Psi *5$ are degenerate orbitals. Each orbital has two bonding
Interactions and two nodal planes.
• The antibonding MO $\Psi *6$ exhibits highest energy and has no bonding interactions. It has
Three nodal planes.

2 b) Schrodinger wave equation and significance

Schrodinger wave equation: The fundamental equation describing the behaviour of a small
particle in terms of wave motion is

$$\frac{d^2\psi}{dx^2} + \frac{4\pi^2\psi}{\lambda^2} = 0$$

$$\Rightarrow \frac{1}{\lambda^2} = -\frac{d^2\psi}{dx^2} \times \frac{1}{4\pi^2\psi} \qquad \text{-----(1)}$$

where ψ =amplitude of the wave, x =displacement in a given direction and λ =wavelength.
According to de Broglie equation,

$$\lambda = \frac{h}{mc}$$

$$\Rightarrow \frac{1}{\lambda^2} = \frac{m^2c^2}{h^2} \qquad \text{-----(2)}$$

where m =mass of the particle, c =velocity of the particle and h =Planck's constant.
From eqs.(1) and (2),

$$\frac{m^2c^2}{h^2} = -\frac{d^2\psi}{dx^2} \times \frac{1}{4\pi^2\psi}$$

$$\Rightarrow m^2c^2 = -\frac{h^2}{4\pi^2\psi} \times \frac{d^2\psi}{dx^2} \qquad \text{-----(3)}$$

For a particle of mass m moving with velocity c, the kinetic energy is given by,

$$K = \frac{1}{2}mc^2 \quad \text{or,} \quad K = \frac{m^2c^2}{2m}$$

$$\Rightarrow m^2c^2 = K \times 2m \qquad \text{-----(4)}$$

From eqs.(3) and (4),

$$K \times 2m = -\frac{h^2}{4\pi^2\psi} \times \frac{d^2\psi}{dx^2}$$

$$\Rightarrow K = -\frac{h^2}{8\pi^2 m\psi} \times \frac{d^2\psi}{dx^2}$$

As the total energy E is the sum of kinetic energy K and potential energy V,
$$E = K + V$$

$$\therefore E = -\frac{h^2}{8\pi^2 m\psi} \times \frac{d^2\psi}{dx^2} + V$$

$$\Rightarrow \frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2}(E-V)\psi = 0$$

This is the Schrodinger wave equation in one dimension, X. If the motion of the particle is in
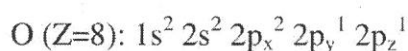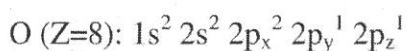three coordinates, X, Y and Z, then the equation becomes

$$\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2} + \frac{8\pi^2 m}{h^2}(E-V)\psi = 0$$

Significance of ψ and ψ^2: In Schrodinger wave equation, ψ is the amplitude of wave, called
wave function. $\frac{d^2\psi}{dx^2}$ represents the second derivative of ψ w.r.t. x and so on. Being a second
order differential equation, Schrodinger wave equation has several possible solutions. However,
only a few values of ψ have physical significance. Each permitted solution of ψ is called Eigen
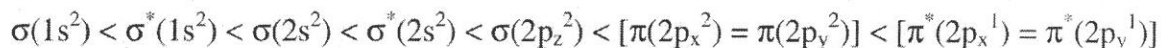function and it corresponds to a definite energy state of electron. The Eigen function for an

electron is called an atomic orbital. The wave function (ψ) has no physical significance except that it represents the amplitude of the wave. It may be positive, negative or imaginary. However, ψ^2 has a physical meaning and it is related to the probability of finding of electron (particle) with definite energy within a certain domain in space. ψ^2 provides the measure of electronic charge density at a point.

3a) Energy Level diagram of O_2 molecule.

Oxygen: Atomic number of oxygen is 8 and molecular formula of oxygen is O_2.

O (Z=8): $1s^2\, 2s^2\, 2p_x^2\, 2p_y^1\, 2p_z^1$ O (Z=8): $1s^2\, 2s^2\, 2p_x^2\, 2p_y^1\, 2p_z^1$

Its molecular orbital configuration is:

$$\sigma(1s^2) < \sigma^*(1s^2) < \sigma(2s^2) < \sigma^*(2s^2) < \sigma(2p_z^2) < [\pi(2p_x^2) = \pi(2p_y^2)] < [\pi^*(2p_x^1) = \pi^*(2p_y^1)]$$

$$\text{Bond order} = \frac{N_b - N_a}{2} = \frac{8 - 4}{2} = 2.0$$

Hence, oxygen molecule contains a double bond and it is highly stable. It is a paramagnetic molecule, since there are two unpaired electrons in its antibonding molecular orbitals.
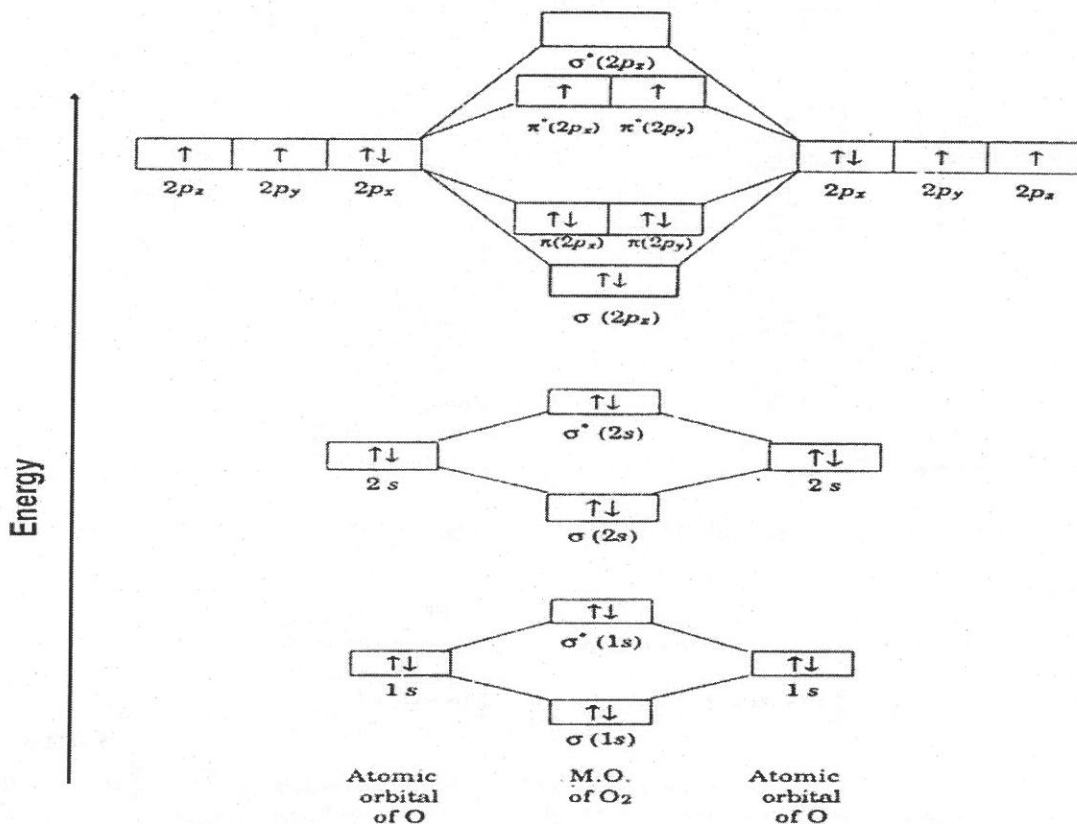
3b) Significance of Homo and hetero nuclear molecules in the field of chemistry

Homo and hetero nuclear molecules play significant roles in the field of chemistry, particularly in understanding molecular structure, bonding, and reactivity. The terms "homo" and "hetero" refer to the types of atoms involved in a molecule:

HOMONUCLEAR MOLECULES:

Definition: Homo nuclear molecules consist of identical atoms. For example, diatomic molecules like O_2 (oxygen gas) or N_2 (nitrogen gas) are homo nuclear.
Significance:
Bonding Studies: Homonuclear molecules help in studying the nature of chemical bonds, such as the covalent bond, as the atoms are of the same type.
Spectroscopy: They are frequently used in spectroscopy experiments to understand molecular properties and behaviours.
HETERONUCLEAR MOLECULES:

Definition: Heteronuclear molecules involve different types of atoms. For instance, water (H_2O) is a heteronuclear molecule because it contains hydrogen and oxygen.
Significance:
Chemical Diversity: Heteronuclear molecules are essential for understanding the vast chemical diversity found in compounds. They allow for the study of how different elements interact.
Reactivity and Bonding: The presence of different atoms in heteronuclear molecules influences their reactivity and bonding, providing insights into the principles of chemical reactions.
Applications:
Biological Molecules: Many biological molecules, such as proteins, DNA, and RNA, are heteronuclear. Understanding their structure and function is crucial for biochemistry and molecular biology.
Catalysis: Heteronuclear molecules are often involved in catalytic processes. For example, transition metal complexes with different ligands play a vital role in catalysis.
Material Science: Both homo and heteronuclear molecules are relevant in the development of materials with specific properties, such as polymers, catalysts, and electronic materials.
Technological Applications:
Magnetic Resonance Imaging (MRI): Heteronuclear molecules, especially those containing isotopes like 13C and 15N, are crucial in MRI, providing detailed images of internal structures in medical diagnostics.
Semiconductor Industry: The study of heteronuclear molecules is important in the development of materials for the semiconductor industry, influencing the properties of electronic components.

4a) Classify Super-capacitors based on their characteristics

A super capacitor, also known as an ultra-capacitor or electric double-layer capacitor (EDLC), is an energy storage device that stores and releases electrical energy much like traditional capacitors. However, it distinguishes itself by having a much higher energy density compared to conventional capacitors. Super-capacitors are designed to bridge the gap between traditional capacitors (which release energy rapidly but have low energy density) and batteries (which have higher energy density but release energy more slowly).

Super-capacitors can be classified into three main types based on their characteristics: Double-layer capacitors, Pseudo-capacitors, and Hybrid capacitors.

Double-layer capacitors:

These capacitors primarily store charge electrostatically in the electric double layer formed at the interface between the electrode and the electrolyte.
The electrodes are typically made of activated carbon, which provides a large surface area for the formation of the electric double layer.

The separation of charge in the electric double-layer capacitors is much smaller than in traditional capacitors, ranging from 0.3–0.8 nm.

Energy storage occurs through the physical separation of charges at the electrode-electrolyte interface.

Pseudo-capacitors:

Pseudo-capacitors store charge electrochemically, involving redox reactions at the electrode-electrolyte interface.

Metal oxide or conducting polymer electrodes are commonly used, providing a high amount of electrochemical pseudocapacitance.

Energy storage happens through reversible oxidation and reduction reactions, resulting in a faradaic charge transfer.

Pseudo-capacitors can offer higher energy densities compared to double-layer capacitors due to the additional electrochemical contributions.

Hybrid capacitors:

Hybrid capacitors combine the characteristics of both double-layer capacitors and pseudo-capacitors, utilizing electrodes with different properties.

One electrode exhibits electrostatic capacitance (double-layer capacitor behavior), while the other electrode displays electrochemical capacitance (pseudo-capacitor behavior).

These capacitors leverage the strengths of both types to achieve a balance between high power density (from double-layer capacitors) and high energy density (from pseudo-capacitors).

An example of a hybrid capacitor is the lithium-ion capacitor, which combines aspects of lithium-ion batteries and super-capacitors.

Each type of super-capacitor has distinct characteristics, making them suitable for different applications. Double-layer capacitors are known for their high power density, pseudo-capacitors for their higher energy density, and hybrid capacitors for a balance between the two. The choice of super-capacitor type depends on the specific requirements of the application, such as power demand, energy storage needs, and desired performance characteristics.

4 b) Extrinsic Semiconductor and its types; the processes which occurred during the formation of a P-N junction.

An extrinsic semiconductor is a semiconductor material that has been intentionally doped with impurities to modify its electrical properties. The intentional addition of impurities, known as doping, introduces charge carriers into the crystal lattice, thereby increasing the electrical conductivity of the semiconductor. There are two types of extrinsic semiconductors based on the type of impurity added:

N-Type Semiconductor:

Doping Material: Phosphorus, arsenic, or antimony (group V elements with five valence electrons).
Effect: The added impurity atoms have more valence electrons than the semiconductor atoms, creating excess electrons (negative charge carriers) in the crystal lattice.
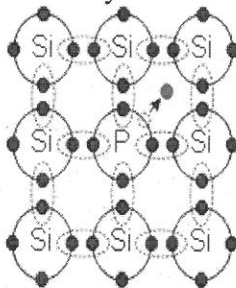

The phosphorus atom donates ist fifth valence electron. It acts as a free charge carrier.

P-Type Semiconductor:

Doping Material: Boron, aluminum, or gallium (group III elements with three valence electrons).
Effect: The added impurity atoms have fewer valence electrons than the semiconductor atoms, creating electron deficiencies or "holes" (positive charge carriers) in the crystal lattice.
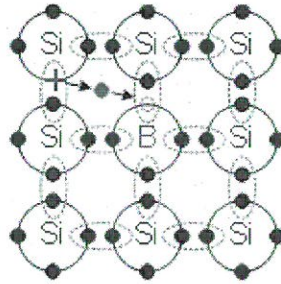
The free place on the boron atom is filled with an electron. Therefore a new hole ("defect electron") is generated. This holes move in the opposite direction to the electrons

P-N Junction Diode Formation:
The resulting structure is a P-N junction diode, a semiconductor device with distinct P-type and N-type regions separated by the depletion region. When a voltage is applied in the forward direction (P-side connected to the positive terminal), it reduces the barrier potential, allowing current flow.
When a voltage is applied in the reverse direction, it increases the barrier potential, preventing significant current flow. The P-N junction diode is a fundamental building block in semiconductor electronics, serving as the basis for various electronic devices like rectifiers, amplifiers, and semiconductor transistors. The controlled formation and manipulation of P-N junctions are crucial for the design and functionality of electronic circuits.

5 a) Preparation, structure and properties of high temperature super conductor- $CaTiO_3$

Superconductivity is a remarkable physical phenomenon where certain materials can conduct electric current with zero electrical resistance. This means that when a material becomes superconducting, it can carry electrical current indefinitely without any loss of energy as heat. Superconductors also have the property of expelling magnetic fields, a phenomenon known as the Meissner effect.

Preparation of High temperature Superconductor (CaTiO3):

1. Material Selection: Choose high-purity calcium carbonate (CaCO3) and titanium dioxide (TiO2) as starting materials.
2. Weighing: Measure the appropriate amounts of CaCO3 and TiO2.
3. Mixing: Thoroughly mix the powders to create a uniform mixture.
4. High-Temperature Furnace: Use a high-temperature furnace capable of reaching 1400-1600°C.
5. Crucible: Place the mixture in a crucible suitable for high-temperature reactions.
6. Heating: Heat the crucible in an oxygen-rich atmosphere within the furnace.
7. Reaction: Maintain the high temperature for several hours to allow the reaction to occur.
8. Cooling: Gradually cool the sample to room temperature to prevent defects.
9. Characterization: Analyze the sample using X-ray diffraction and microscopy to confirm CaTiO3 formation.
10. Superconductivity Testing: Verify superconducting properties through electrical and magnetic measurements.

These steps of the preparation process for CaTiO3 superconductors.

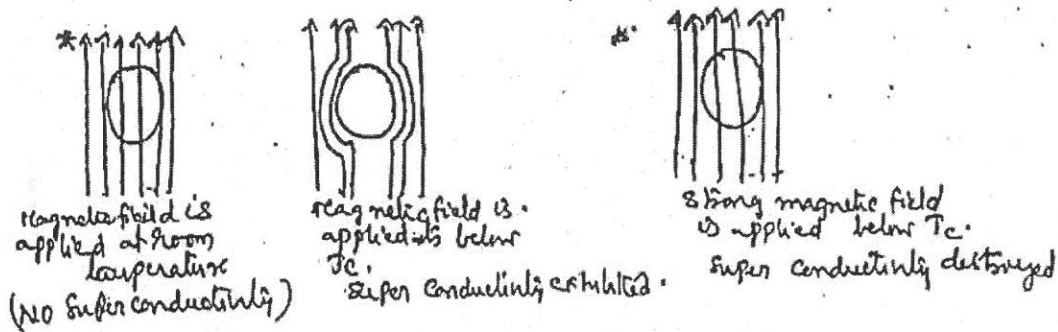<u>Structure:</u> Structure of high temperature superconductors : The structure of 1:2:3 compound is akin to that of ABO_3 structure of mineral perovskite ($CaTiO_3$). The A-type perovskite structure see figure 4.21) contains A atom in the centre, B atoms at the corners of the unit cell and O atoms occupy the mid-points of the edges. Composition of the unit cell can be deduced as follows:

Atom at the centre of unit cell = 1 A

$$\text{Effective atoms at the 8 corners} = \left(8 \times \frac{1}{8}\right) B = 1B$$

$$\text{Effective O atom at the mid-points} = \left(12 \times \frac{1}{4}\right) C = 3 \, O$$

Magnetic field is applied at Room temperature (No Super conductivity)

Magnetic field is applied its below Tc. Super conductivity exhibited.

Strong magnetic field is applied below Tc. Super conductivity destroyed

Properties of Superconductors:

1. Zero Electrical Resistance: Superconductors have no electrical resistance, meaning they can conduct electricity without any loss of energy due to heat. This makes them extremely efficient conductors.

2. Critical Temperature (Tc): Superconductivity is temperature-dependent. Each superconducting material has a critical temperature (Tc) which it becomes superconducting. At normal temperature, the material behaves like a normal conductor.

3. Meissner Effect: Superconductors expel magnetic fields from their interior when they enter the superconducting state. This leads to the complete exclusion of magnetic flux lines, making them ideal for

applications   involving   strong   magnetic   fields.
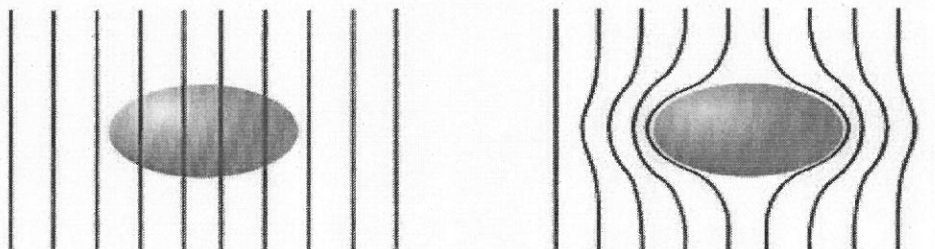
For normal conductor   For super conductor

4. Perfect Diamagnetism: Superconductors exhibit perfect diamagnetism, which means they repel magnetic fields. This property is a direct consequence of the Meissner effect.

5 b) Properties and applications of carbon nanotubes.

Properties of carbon nanotubes:

Mechanical properties: Carbon nanotubes possess amazing mechanical properties. They are the strongest and stiffest materials in terms of tensile strength and elastic modulus respectively. Their strength can be explained on the basis of sp^2 carbon-carbon bonds between the individual atoms. Carbon nanotubes are softer in the radial direction than along the tube axis. These properties together with the lightness make the carbon nanotubes useful for their application in aerospace. It has been suggested that nanotubes can be used in space elevator, on earth to space cable.

Hardness: A super hard material could be synthesized by compressing SWNTs to above 24Gpa at room temperature. The hardness of this material was measured by Nano indenter and was found to be 62-152 Gpa.

Electrical properties: Carbon nanotubes can be metallic or semiconducting depending upon their structure. For a given nanotube with n=m, the nanotube is metallic. If n-m is a multiple of 3 then a nanotube is semiconducting and possesses a very small band gap. Otherwise a Nano tube is a moderate semiconductor. Thus all arm chair nanotubes are metallic with conductivities higher than that of copper. Others behave more like silicon.

Vibration properties: Carbon nanotubes show two normal modes of vibration

A_1g mode: It involves in and out oscillation.

E_2g mode: It involves oscillation between sphere and an ellipse.

Engineering applications of carbon nanotubes:

Carbon nanotubes have high strength, small dimensions and remarkable physical properties.

Due to this they find application in different fields.

- They find application in conductive composites, high strength composites, energy storage devices energy conversion devices, energy storage media, sensors, nanometre sized semi conductor devices etc. They are used as Nano probes in biological and chemical investigations. They are the alternative and efficient tools for transporting and trans locating therapeutic molecules.

- CNT can be functionalized with bio active peptides, proteins, nucleic acids, and drugs and can be used to deliver them to cells and organs.

- Functionalized CNTs possess low toxicity. Hence they are used in the fields of Nano biotechnology, and Nano medicine.

6 a) Construction and working of Hydrogen-Oxygen Fuel cell

Anode electrode –Porous carbon electrode containing Ni.
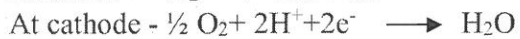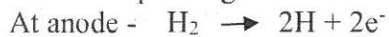**Cathode electrode**-- Porous carbon electrode containing CoO or Ni and NiO
Electrolyte -- NaOH or KOH

1. It has two electrodes where the reactions take place and an electrolyte i.e., molten KOH which carries the charged particles from one electrode to the other.
2. $E^O{}_{cell}$ Is positive, the cell reaction is spontaneous. The fuel cell produces power through redox reaction between hydrogen and oxygen.
3. At anode the hydrogen is oxidized through reaction with producing water and releasing two electrons.
4. The electrons flow through external circuit and returns to the cathode, reducing oxygen which consequently reacts with water to produce.
5. The fuel cell electrodes contain catalysts to speed up electrode reactions and the process is known electro catalysis. In the mixture of Ni and NiO embedded in porous carbon electrodes which serves electro catalysts in the cell.
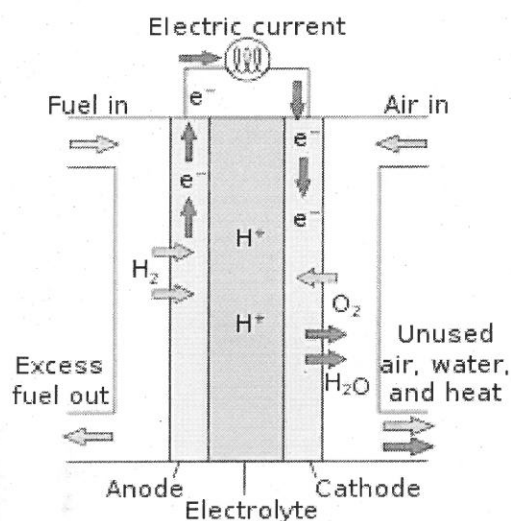
Hydrogen- Oxygen fuel cell

The corresponding reactions at anode cathode are;
At anode - $H_2 \longrightarrow 2H + 2e^-$
At cathode - $\frac{1}{2} O_2 + 2H^+ + 2e^- \longrightarrow H_2O$
The overall reaction $H_2 + \frac{1}{2} O_2 \longrightarrow H_2O$

6 b) emf calculation of the cell

Given cell: $Zn(s)|Zn^{2+}(0.2\,\text{M})||Ag^+(0.002\,\text{M})|Ag(s)$

Standard cell potential (E°): 1.54 V

Cell reaction: $Zn(s) + 2Ag^+ \rightarrow Zn^{2+} + 2Ag$

Number of moles of electrons transferred (n): 2

Calculate the reaction quotient (Q):
$$Q = \frac{[Zn^{2+}]}{[Ag^+]^2} = \frac{0.2}{(0.002)^2}$$

Now use the Nernst equation:
$$E = E^\circ - \frac{RT}{nF}\ln(Q)$$

$$E = 1.54\,\text{V} - \frac{(8.314\,\text{J mol}^{-1}\text{K}^{-1})(298\,\text{K})}{(2)(96485\,\text{C mol}^{-1})}\ln\left(\frac{0.2}{(0.002)^2}\right)$$

$$E = 1.54 - \frac{0.0591}{2}\log\left(\frac{0.2}{(0.002)^2}\right)$$

$$E = 1.54 - 0.02955\log\left(\frac{0.2}{0.000004}\right)$$

$$E = 1.54 - 0.02955\log(50000)$$

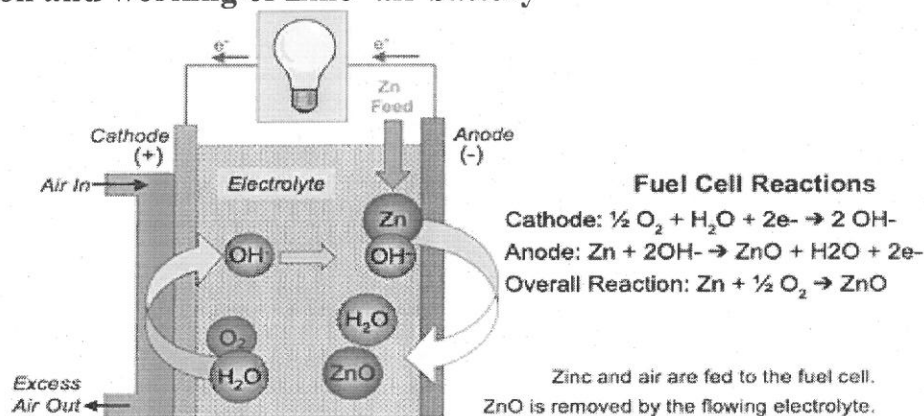Now, use a calculator to find the logarithm and complete the calculation:

$$E \approx 1.54 - 0.02955 \times 4.69897$$

$$E \approx 1.54 - 0.1386$$

$$E \approx 1.4014\,\text{V}$$

Therefore, the cell potential (E) at 25°C for the given cell is approximately 1.4014 V.

7 a) Construction and working of Zinc- air battery

Fuel Cell Reactions

Cathode: ½ O_2 + H_2O + 2e- → 2 OH-
Anode: Zn + 2OH- → ZnO + H_2O + 2e-
Overall Reaction: Zn + ½ O_2 → ZnO

Zinc and air are fed to the fuel cell.
ZnO is removed by the flowing electrolyte.

Anode - Amalgamated Zinc powder
Cathode – Air|C
Electrolyte - KOH 6M

Zinc – Air battery: Zn| KOH|| Air C

1. Zinc – Air battery is a primary battery i.e. non-rechargeable and the reaction is Irreversible.
2. It is also known as alkaline battery.
3. In this battery the cathode is made up of porous carbon plate which activated by Manganese oxide. Anode is made up of rectangular an pellets which are placed Between two cathodes.
4. Because it is alkaline battery we can use wither KOH or Noah as an electrolyte. But Use KOH only as the ionic conductance of KOH is higher than NoaH.
5. The electrodes are separated by gascade insulating material. The whole assembly is Enclosed in glass or ebonite container coated with Teflon, which is hydrophobic i.e. it Allows only oxygen but not moisture.
6. At cathode the electro active species air i.e. oxygen. During the cell reactions in Battery the electrolyte concentrations is remains constant.

The reactions occur are as follows:

At anode: At anode the Zn undergoes oxidation in presence of electrolyte to produce zinc Oxide and eater.

$$Zn + 2OH^- \longrightarrow ZnO + H_2O + 2e^-$$

At cathode, water undergoes reduction reaction in presence of oxygen and electrons to give Up hydroxyl ions, so the OH - ions consumed at anode and liberated at cathode, hence the Overall concentration of electrolyte is constant.

$$1/2\ O_2 + H_2O + 2e^- \longrightarrow 2OH^-$$
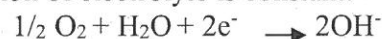
The overall reaction is $Zn + 1/2\ O_2 \longrightarrow ZnO$

The output of the Zn-air battery is 1.65V

Advantages:
1. High energy density.
2. Low cost
3. Capacity is independent of load and temperature.

Applications:
1. Power source for hearing aids
2. Used in electric pagers
3. Used in military radio receivers
4. Used in voice transmitters

## 7 b) Half-cell and emf calculation of the cell

1. Zinc half-cell: $Zn \mid Zn^{2+}(1\,M)$
2. Copper half-cell: $Cu^{2+}(1\,M) \mid Cu$

The overall (net) cell reaction can be obtained by combining these two half-reactions. The electrons on each side should be balanced to ensure charge conservation.

The balanced half-reactions are:

1. Oxidation half-reaction (Zinc electrode loses electrons):
$$Zn \rightarrow Zn^{2+} + 2e^-$$
2. Reduction half-reaction (Copper ions gain electrons):
$$Cu^{2+} + 2e^- \rightarrow Cu$$

Now, combine the half-reactions, ensuring that the electrons cancel out:

$$Zn + Cu^{2+} \rightarrow Zn^{2+} + Cu$$
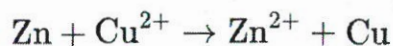
This is the net cell reaction for the given electrochemical cell.

To find the standard cell potential (E°) for the given electrochemical cell, you can use the standard reduction potentials (E°) for the half-reactions involved. The cell potential (E°_{cell}) is given by the formula:

$$E^\circ_{cell} = E^\circ_{cathode} - E^\circ_{anode}$$

Given:
$$E^\circ(Zn^{2+}/Zn) = -0.76\,V$$
$$E^\circ(Cu^{2+}/Cu) = +0.34\,V$$

Now, substitute these values into the formula:

$$E^\circ_{cell} = E^\circ_{cathode} - E^\circ_{anode}$$

$$E^\circ_{cell} = (+0.34) - (-0.76)$$
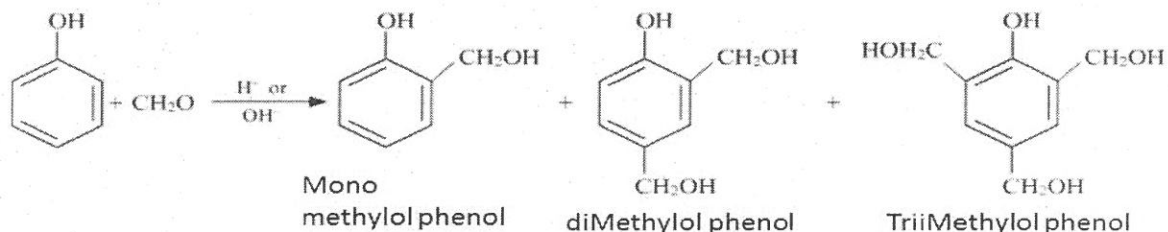
$$E^\circ_{cell} = 1.10\,V$$

So, the standard cell potential (E°_{cell}) for the given electrochemical cell is 1.10 V.

8a) Properties, preparation and applications of Bakelite
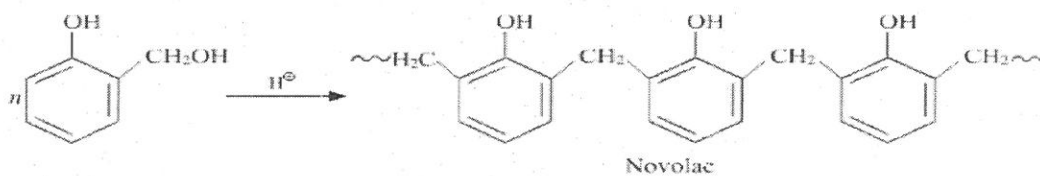
Preparation:

Step-1

The first step is reaction between phenol and formaldehyde to form mono, di and tri- methylol phenols.

Step-II

When methylol phenols are heated with excess of phenol in presence of acid catalyst, the methylol phenols condense with phenol through methylene linkages to **from linear product novolac** with the elimination of water molecule.

Step-III

Further heating novolac and phenol in the presence of a catalyst(hexamethylenetetramine) leads to formation of hard, rigid, infusible cross linked polymer called bakelite.
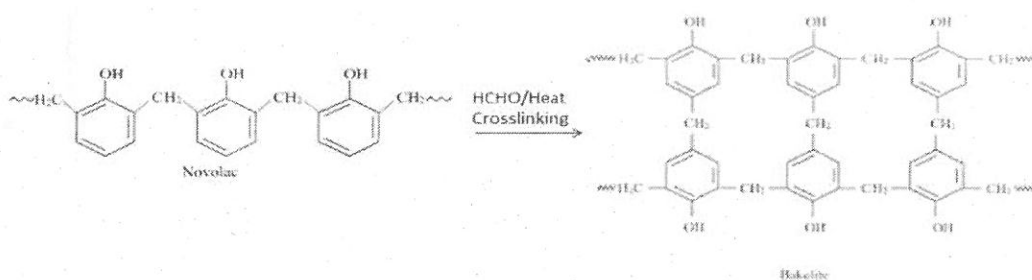
Properties: These are

Rigid
Hard, resistant to heat
With stand to high temperature
Good insulator
Applications : Used for the preparation of
Electrical insulator parts like Switches, Plugs &
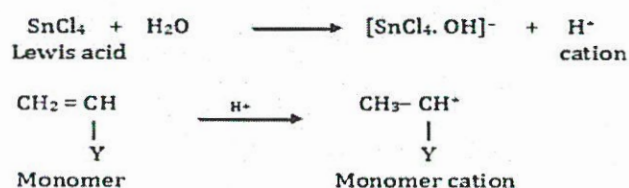Handles

8b) Step wise mechanism of cationic polymerization:

Cationic polymerization:- Monomers with electron releasing groups (-OCH3, -OC2H5 & - C6H5 etc) undergo cationic polymerization in the presence of Lewis acids like AlCl3, BF3, SnCl4 etc. Cationic polymerization takes place with higher rates even at low temperature.

Mechanism of cationic polymerization:-
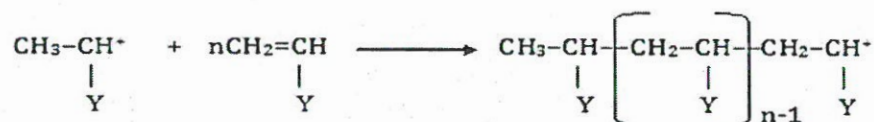
It involves three steps.

a) Initiation:-

H^+ ion is produced from Lewis acid and it forms cation with monomer.

$$SnCl_4 + H_2O \longrightarrow [SnCl_4.OH]^- + H^+$$
Lewis acid   cation

$$\underset{\substack{| \\ Y \\ Monomer}}{CH_2=CH} \xrightarrow{H+} \underset{\substack{| \\ Y \\ Monomer\ cation}}{CH_3-CH^+}$$
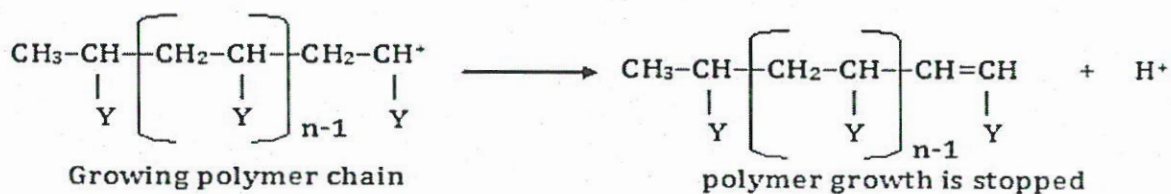
Where, Y is electron releasing group.

b) Propagation:-

Monomers are added to monomer cation in a sequence and length of polymer chain increases gradually.
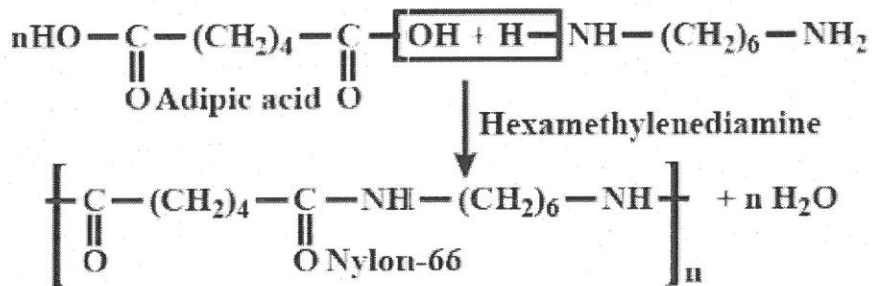
$$\underset{\substack{| \\ Y}}{CH_3-CH^+} + \underset{\substack{| \\ Y}}{nCH_2=CH} \longrightarrow \underset{\substack{| \\ Y}}{CH_3-CH} \left[\underset{\substack{| \\ Y}}{CH_2-CH} \right]_{n-1} \underset{\substack{| \\ Y}}{CH_2-CH^+}$$

c) Termination:-

Growing polymer chain is stopped by removing H+ ion from the chain.

$$\underset{\substack{| \\ Y}}{CH_3-CH} \left[\underset{\substack{| \\ Y}}{CH_2-CH} \right]_{n-1} \underset{\substack{| \\ Y}}{CH_2-CH^+} \longrightarrow \underset{\substack{| \\ Y}}{CH_3-CH} \left[\underset{\substack{| \\ Y}}{CH_2-CH} \right]_{n-1} \underset{\substack{| \\ Y}}{CH=CH} + H^+$$
Growing polymer chain   polymer growth is stopped

$$[SnCl_4 OH]^{(-)} + H^+ \longrightarrow SnCl_4 + H_2O$$

9 a) Preparation, properties and Applications of nylon 6,6

It is obtained by condensation polymerisation of hexamethylene diamine with adipic acid under high pressure and at high temperature.

$$nHO-\overset{O}{\underset{\parallel}{C}}-(CH_2)_4-\overset{O}{\underset{\parallel}{C}}-\boxed{OH + H}-NH-(CH_2)_6-NH_2$$

Adipic acid

↓ **Hexamethylenediamine**

$$\left[\overset{O}{\underset{\parallel}{C}}-(CH_2)_4-\overset{O}{\underset{\parallel}{C}}-NH-(CH_2)_6-NH\right]_n + n\ H_2O$$

Nylon-66

Properties: These are

Rigid
high mechanical strength
Hard , resistant to heat
With stand to high temperature

Applications: Used for the preparation of

fibers for textiles
carpets and molded parts
outdoor equipment, sports gear, and components exposed to moisture.
Nylon 6,6 exhibits excellent wear resistance properties, enabling it to withstand friction and abrasion. This makes it suitable for applications involving sliding or rotating components, such as bearings, gears, and conveyor belts.
It finds applications in automotive components, consumer goods, and aerospace industries.
Its high tensile strength and abrasion resistance make it ideal for applications that require durability, such as backpacks, luggage, and heavy-duty workwear.
Electrical and Electronics: The industry relies on Nylon 6,6 for its insulating properties and high dielectric strength.

9 b) Mechanism of conducting polymers and its applications

Conducting polymers: The polymers which can conduct electricity are called conducting polymers.

Ex. poly acetylene, polyaniline etc.

conducting polymers are also called as organic semiconductors.

Conducting polymers can be classified into following types:

➤ On the basis of their conduction properties conducting polymers are classified into two types
  ➤ Intrinsically Conducting Polymers
  ➤ Extrinsically Conducting Polymers

Intrinsically Conducting Polymers:
Conjugation:

These polymers contain conjugated or delocalized π - e⁻ pairs in the back bone responsible for conduction.

The orbital's of conjugated π - e⁻ form valency band as well as conduction band and they are extended over the entire polymer molecule.

When current is passed electrons enter conduction band due to shifting of π - e⁻.
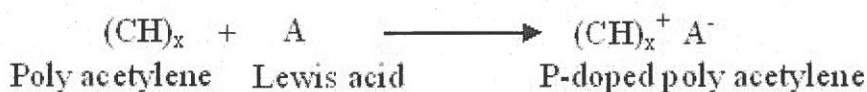
Ex; Conduction of poly acetylene due to conjugation.
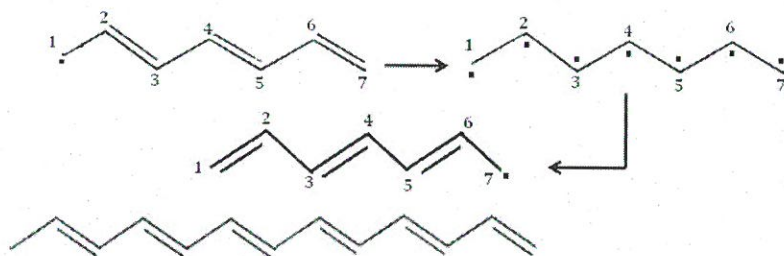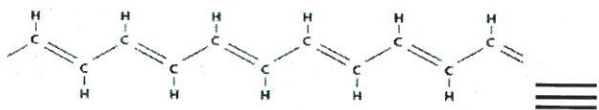
▪ When current is passed into poly acetylene, the electron enters the unhybridised P-orbital of carbon atom and moves through the C – C bonds.

➤ When the electron enters the chain, breakage of π - bond takes place and a new π -bond is formed.
➤ π -bond between 2&3 is broken and a new π - bond is formed between 1&2.
➤ Similarly π -bond between 4&5 is broken and anew π -bond is formed between 3&4.
➤ π -bond between 6&7 is broken and a new π - bond is formed between 5&6.

A long as current flows in to the polymer this process is continued and there by a conducting path is created in the polymer.

Doped conducting polymers:

> Polymers can conduct due to doping and by using doping agents or dopants.
> Doping of conducting polymers can be two different types.
>> o p-Doping (or) Oxidative Doping
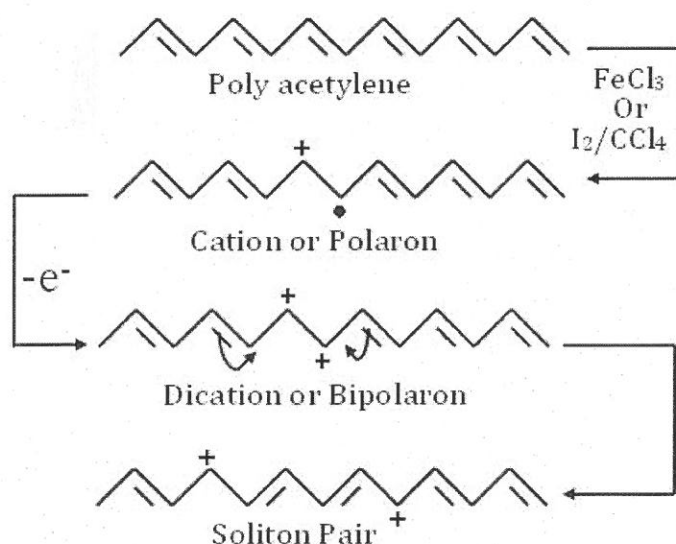>> o n-Doping (or) Reductive Doping

p- Doping (or) Oxidative Doping:

o In this method the polymer is treated with an oxidizing agent like Lewis acid which acts as a dopant.

o Examples of dopants used: $FeCl_3$, I_2 etc.

$$(CH)_x \ + \ A \ \longrightarrow \ (CH)_x^+ \ A^-$$
Poly acetylene   Lewis acid   P-doped poly acetylene

$$(CH)_x \ + \ 2FeCl_3 \ \longrightarrow \ (CH)_x^+ \ FeCl_4^- \ + \ FeCl_2$$

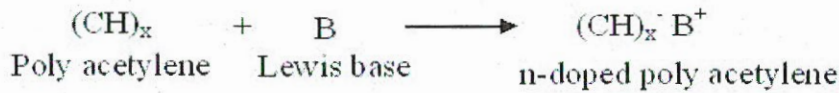$$2(CH)_x \ + \ 3I_2 \ \longrightarrow \ 2(CH)_x^+ \ I_3^-$$

Mechanism of p-Doping:

> During this process, oxidation of polymer takes place due to dopant and forms a cation called Polaron.
> On further oxidation of polymer results in the formation of a dication or bipolaron.
> The charges get separated by forming a soliton pair.
> The cation occupies the band gap between valency band and conduction band, thereby creating a conducting path.
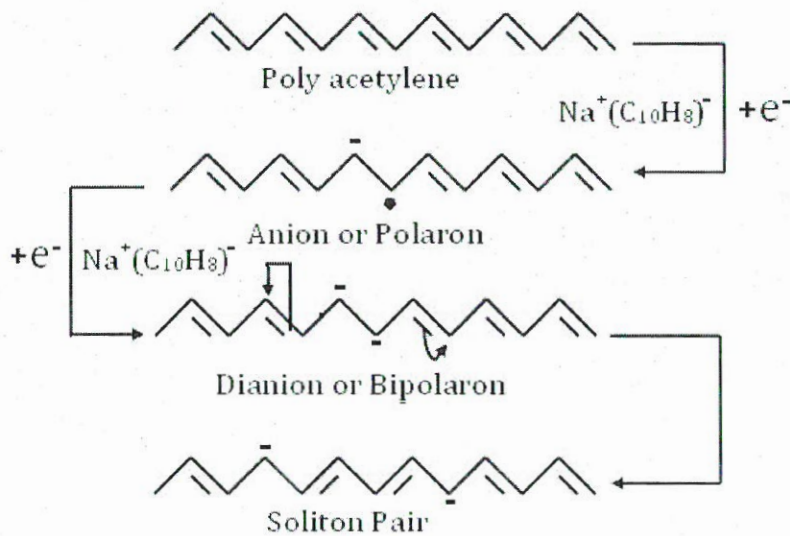> So electrons move through this path.

n- Doping (or) Reductive Doping:

In this method, the polymer is treated with a reducing agent like a Lewis base which acts as a dopant.

Ex; Sodium Naphthalide $Na^+ (C_{10}H_8)^-$

$$(CH)_x \quad + \quad B \quad \longrightarrow \quad (CH)_x^- B^+$$
Poly acetylene   Lewis base   n-doped poly acetylene

$$(CH)_x \quad + \quad Na^+ (C_{10}H_8)^- \longrightarrow Na^+ (CH)_x^- \quad + \quad C_{10}H_8$$

Mechanism of n-doping:

- During this process, reduction of polymer takes place due to dopant and forms an anion called Polaron.
- On further reduction of polymer results in the formation of a dianion or bipolaron.
- The charges get separated to form a soliton pair.
- The anions occupy the band gap between valency band and conduction band thereby creating a conducting path.
- So that electrons move through this path.

Applications of conducting polymers in electronics:
- They are used in rechargeable batteries.
- They are used in analytical sensors of p^H, O_2, NO_2, SO_2, NH_3 etc.
- Used in photo voltaic cells. Ex; Al/polymer/Au.
- Used in telecommunication systems.
- Used in transistors and diodes.
- Used in solar cells.
- Used as wiring in air crafts and aerospace parts.

10 a) Instrumentation and applications of IR Spectroscopy

It has the following components: two pairs of splitters, sample solution, a monochromator, an infrared light source, a digital reader, a reference or standard solution and a detector.
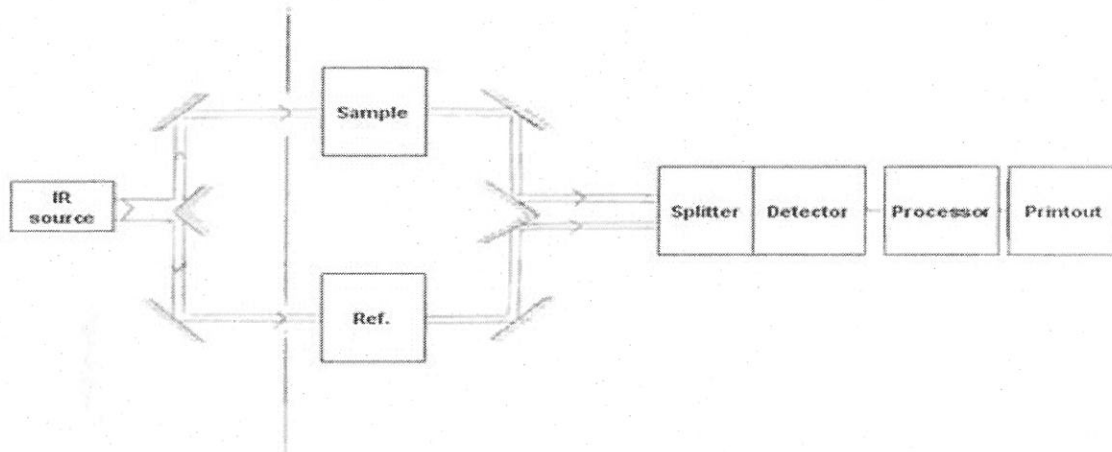
Frequency and Molecular Structure:
- The frequency at which a molecule vibrates and subsequently absorbs IR radiation offers direct insights into its structure.
- Factors affecting absorption frequency include bond strength (stronger bonds vibrate at higher frequencies) and the mass of the atoms involved (heavier atoms vibrate at lower frequencies).

IR Spectrometer Components

Source: Often a ceramic type, this generates the necessary infrared radiation.

Monochromator/Interferometer: This component segregates the wide-ranging IR radiation into individual frequencies, allowing for detailed spectral analysis.

Sample Holder:
- Samples can be in solid, liquid, or gaseous form.
- Common methods involve creating a pellet with potassium bromide or using a liquid cell with sodium chloride plates.

Detector:
- This crucial component measures the radiation passing through the sample.
- Any decrease in radiation intensity at a particular frequency suggests absorption at that frequency.

Computer System: In modern spectrometers, computers play an instrumental role in processing, plotting, and storing.

Applications in Chemistry

1)Qualitative and Structural Analysis
- The unique nature of IR spectra, akin to molecular fingerprints, allows chemists to identify unknown compounds by juxtaposing their spectra with reference spectra.
- Structural elucidation is further enhanced as the presence or absence of specific peaks can validate or debunk a proposed molecular formula.

2)Quantitative Insight
- While primarily qualitative, IR spectroscopy isn't limited to identifying compounds.

- The intensity of specific absorption peaks can be calibrated to quantify the concentration of the absorbing species in a sample.

3)Real-time Reaction Monitoring
- IR spectroscopy shines as a tool in research environments, especially when observing real-time chemical reactions.
- The emergence or disappearance of specific peaks enables chemists to track reactants turning into products, facilitating a better understanding of reaction dynamics.

4)Material and Environmental Science
- Beyond pure chemistry, IR spectroscopy finds relevance in material science to decipher the compositions of complex materials.
- In environmental studies, it helps in detecting pollutants or monitoring air quality.

Application of IR

1. Determination of Molecular Structure.
2. Studying the Progress of the Reactions.
3. Qualitative Analysis of Functional Groups.
4. Detection of Impurity in a Compound.
5. Shape of Symmetry of a molecule
6. Presence of Water in a Sample
7. Examination of Old Paintings and Artefacts.
8. Identification of Organic Compound.

10 b) Principle and Instrumentation of HPLC

A separation column separates the stationary and mobile phases during purification.

- In a separation column, the stationary phase is a granular substance with very small porous particles.
- The mobile phase is a solvent or solvent combination that is pushed through the separation column under high pressure.
- The sample is loaded into the mobile flow regime from the pump to the separation column using a syringe through a valve with a linked sample loop, i.e. a tiny tube or capillary made of stainless steel.
- A chromatogram is generated in the HPLC software at the conclusion of this operation/run.
- The chromatogram allows the various compounds to be identified and quantified.
- As a result, owing to interactions with the stationary phase, the constituent components of a mixture migrate through the column at different speeds.
- Individual compounds are identified by an appropriate detector after exiting the column and transmitted as a signal to the computer's HPLC software.
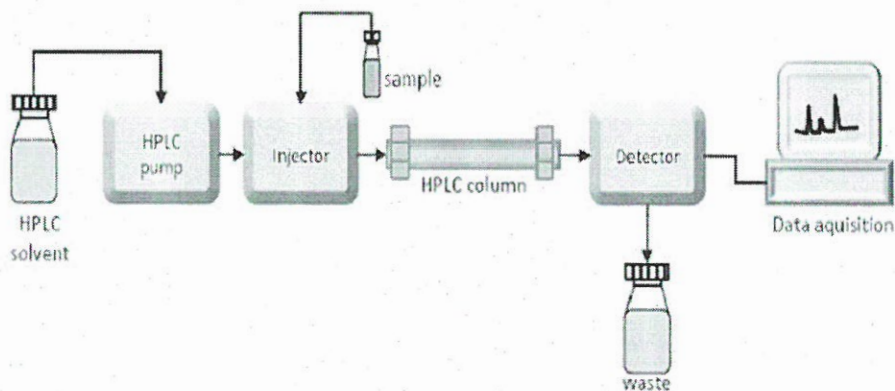
Solvent Reservoir

- A glass reservoir holds the mobile stage ingredient.
- In HPLC, the flexible stage, or dissolvable, is often a mixture of polar and non-polar liquid segments where specific fixations change depending on the specimen arrangement.

Pump

- The pump system was developed as a result of the development of HPLC.
- The pump is located in the upper stream of the liquid chromatographic column and pumps eluent into the system from the solvent reservoir.

Injector

- Next to the pump, there is an injector.
- The easiest way is to use a syringe to insert the sample into the eluent flow.
- Sampling loops are the most extensively utilised injection mechanism.

Column

- The separation takes place within the column.
- Instead of glass columns, contemporary columns are frequently manufactured in a stainless steel housing.
- In comparison to calcium carbonate, silica or polymer gels are commonly used as packing materials. (octadecylsilyl groups (ODS groups or C18 groups) chemically bonded to a silica gel carrier.)

Detector

- The separation of analytes takes place inside the column, and the separation is seen using a detector.
- When no analyte is present, the element has a constant composition.
- While the presence of analyte alters the eluent's composition.
- These differences are measured by the detector.
- This disparity is measured using an electrical signal.
- Different kinds of detectors are available.

Data Collection

- Signals from the indicator might be collected via outline recorders or electronic integrators with varying degrees of multi-sided fidelity and the ability to analyse, store, and reprocess chromatographic data.
- The PC coordinates the identifier's reaction with each component and records it in a chromatograph that is simple to read and understand.

11a) Beer-Lambert's law statement and limitations
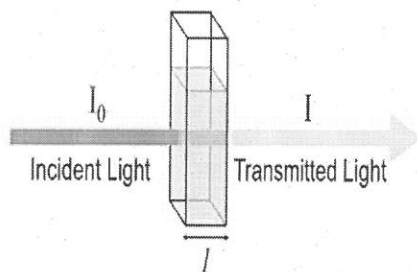
- The Beer-Lambert Law (also called Beer's Law) is a relationship between the attenuation of light through a substance and the properties of that substance.
- In this article, the definitions of transmittance and absorbance of light by a substance are first introduced followed by an explanation of the Beer-Lambert Law.
- Consider monochromatic light transmitted through a solution; with an incident intensity of I0 and a transmitted intensity of I
- The transmittance, T, of the solution is defined as the ratio of the transmitted intensity, I, over the incident intensity, I0 and takes values between 0 and 1.

However, it is more commonly expressed as a percentage transmittance:

$$T(\%) = 100\frac{I}{I_0} \qquad T = \frac{I}{I_0}$$

The absorbance, A, of the solution is related to the transmittance and incident and transmitted intensities through the following relations:

$$A = \log_{10}\frac{I_0}{I}$$
$$A = -\log_{10} T$$

The Beer-Lambert law is a linear relationship between the absorbance and the

Concentration, molar absorption coefficient and optical path length of a solution:

$$A = \varepsilon cl$$

A	Absorbance	
ε	Molar absorption coefficient	$M^{-1}cm^{-1}$
c	Molar concentration	M
l	optical path length	cm

- The molar absorption coefficient is a sample dependent property and is a measure of how strong an absorber the sample is at a particular wavelength of light.
- The concentration is simply the moles L-1 (M) of the sample dissolved in the solution, and the optical path length is the width of the cuvette used for the absorbance measurement and is typically 1 cm.
- The Beer-Lambert law states that there is a linear relationship between the concentration and the absorbance of the solution, which enables the concentration of a solution to be calculated by measuring its absorbance.

Limitations of Beer-Lambert law

- The linearity of the Beer-Lambert law is limited by chemical and instrumental factors. Causes of non-linearity of the law occur in the following conditions:

- deviations in absorptivity coefficients at high concentrations (>0.01M) due to electrostatic interactions between molecules in close proximity
- scattering of light due to particulates in the sample
- fluorescence or phosphorescence of the sample
- changes in refractive index at high analyte concentration
- shifts in chemical equilibria as a function of concentration
- non-monochromatic radiation, deviations can be minimised by using a relatively flat part of the absorption spectrum such as the maximum of an absorption band

11 b) Characteristics of electromagnetic spectrum

- A technique used to investigate a molecule's properties based on how it reacts to electromagnetic radiations is known as spectroscopy.
- The electromagnetic (EM) spectrum is the range of all types of EM radiation.
- Radiation is energy that travels and spreads out as it goes – the visible light that comes from a lamp in your house and the radio waves that come from a radio station are two types of electromagnetic radiation.
- The other types of EM radiation that make up the electromagnetic spectrum are microwaves, infrared light, ultraviolet light, X-rays and gamma-rays.
- The electromagnetic spectrum is a range of frequencies, wavelengths and photon energies covering frequencies from below 1 hertz to above 1025 Hz, corresponding to wavelengths which are a few kilometres to a fraction of the size of an atomic nucleus in the spectrum of electromagnetic waves.
- Generally, in a vacuum, electromagnetic waves tend to travel at speeds which are similar to that of light.
- However, they do so at a wide range of wavelengths, frequencies and photon energies.
- The electromagnetic spectrum consists of a span of all electromagnetic radiation which further contains many sub ranges, which are commonly referred to as portions.
- These can be further classified as infrared radiation, visible light or ultraviolet radiation.
- **Radio**: radio captures radio waves emitted by radio stations, bringing your favourite tunes. Radio waves are also emitted by stars and gases in space.
- **Microwave**: Microwave radiation will cook your popcorn in just a few minutes, but is also used by astronomers to learn about the structure of nearby galaxies.
- **Infrared:** Night vision goggles pick up the infrared light emitted by our skin and objects with heat. In space, infrared light helps us map the dust between stars.
- **Visible:** Our eyes detect visible light. Fireflies, light bulbs, and stars all emit visible light.
- **Ultraviolet:** Ultraviolet radiation is emitted by the Sun and are the reason skin tans and burns. "Hot" objects in space emit UV radiation as well.
- **X-ray:** A dentist uses X-rays to image your teeth, and airport security uses them to see through your bag. Hot gases in the Universe also emit X-rays.
- **Gamma ray:** Doctors use gamma-ray imaging to see inside your body. The biggest gamma-ray generator of all is the Universe

Electromagnetic radiation can be expressed in terms of energy, wavelength, or frequency. Frequency is measured in cycles per second, or Hertz. Wavelength is measured in metres. Energy is measured in electron volts.