# **UNIT-1 Structure and Bonding Models**

### 1. What is quantum mechanics?

### **Answer:**

Quantum mechanics is the branch of physics that deals with the behavior of matter and energy at microscopic scales (atomic and subatomic levels), where the classical laws of mechanics fail.

### 2. What is the Schrödinger wave equation?

### **Answer:**

It is a fundamental equation of quantum mechanics that describes how the wave function  $(\psi)$  of a particle evolves in space and time.

$$H^{\psi}=E_{\psi}$$

where  $H^{\wedge}$  is the Hamiltonian operator and  $E^{\wedge}$  is the energy of the system.

### 3. What is the significance of $\psi$ (psi)?

### **Answer:**

 $\psi$  represents the wave function of a particle and contains all the information about the system's quantum state.

### 4. What is the significance of $\psi^2$ ?

### **Answer:**

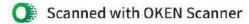
 $\psi^2$  (or  $|\psi|^2$ ) represents the **probability density** of finding a particle at a given point in space.

### 5. What are the boundary conditions for a particle in a 1-D box?

#### Answers

For a particle confined between x = 0 and x = L,

$$\psi(0)=\psi(L)=0$$



6. What is the expression for energy of a particle in a one-dimensional box?

Answer:

Where n is the quantum number, h is Planck's constant, m is mass, and L is the length of the box.

7. What does the quantum number 'n' signify in the 1D box model?

### **Answer:**

'n' denotes the energy level or the number of half wavelengths fitting inside the box.

8. What is molecular orbital theory (MOT)?

### Answer:

MOT explains bonding by considering the combination of atomic orbitals to form molecular orbitals that extend over the entire molecule.

9. What is bond order and how is it calculated?

### **Answer:**

Bond order =  $\frac{1}{2}$  (Number of bonding electrons – Number of ant bonding electrons) It indicates bond strength and stability.

10. What is the bond order of O2 molecule?

### **Answer:**

Molecular configuration of O<sub>2</sub>:

$$(\sigma 1s)^2(\sigma * 1s)^2(\sigma 2s)^2(\sigma * 2s)^2(\sigma 2pz)^2(\pi 2px)^2(\pi 2py)^2(\pi * 2px)^1(\pi * 2py)^1$$

Bond order =  $\frac{1}{2}(10-6) = 2$ .

### 11. Why is O<sub>2</sub> paramagnetic?

### **Answer:**

 $O_2$  has two unpaired electrons in  $\pi^*2p$  orbitals, making it paramagnetic.

### 12. What is the bond order of CO molecule?

### Answer:

Electronic configuration of CO:

$$(\sigma 1s)^2 (\sigma * 1s)^2 (\sigma 2s)^2 (\sigma * 2s)^2 (\sigma 2pz)^2 (\pi 2px)^2 (\pi 2py)^2$$

Bond order =  $\frac{1}{2}(10-4) = 3$ .

### 13. Why is CO a stable molecule?

### **Answer:**

Because it has a high bond order (3), indicating a strong triple bond.

### 14. What are $\pi$ molecular orbitals?

### **Answer:**

 $\pi$ -Molecular orbitals form by lateral (sidewise) overlap of p-orbitals, resulting in electron density above and below the internuclear axis.

### 15. How many $\pi$ molecular orbitals are present in 1,3-butadiene?

### **Answer:**

1,3-butadiene (C<sub>4</sub>H<sub>6</sub>) has  $4\pi$  molecular orbitals formed from 4 p-orbitals.

### 16. What is the delocalization in benzene?

### Answer:

In benzene, 6 p-orbitals combine to form 6  $\pi$  molecular orbitals with delocalized electrons spread over the ring.

### 17. What is the bond order in benzene?

### **Answer:**

Each C–C bond has a bond order of 1.5 due to delocalization of  $\pi$  electrons.

## 18. What is the energy order of molecular orbitals for homonuclear diatomic molecules (Z < 8)?

### **Answer:**

$$\sigma1s < \sigma*1s < \sigma2s < \sigma*2s < (\pi2px = \pi2py) < \sigma2pz < (\pi*2px = \pi*2py) < \sigma*2pz$$

### 19. What changes in energy order occur for $O_2$ and $F_2$ (Z > 8)?

### **Answer:**

For heavier atoms (O<sub>2</sub>, F<sub>2</sub>):

$$\sigma1s < \sigma*1s < \sigma2s < \sigma*2s < \sigma2pz < (\pi2px = \pi2py) < (\pi*2px = \pi*2py) < \sigma*2pz$$

### 20. What is normalization of a wave function?

### **Answer:**

It means the total probability of finding a particle in all space is

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1$$

### **EASSAY QUESTIONS**

1. Derive the Schrodinger Time-Independent wave equation?

schrodingers wave Schrödinger time-independent wave equation Classical mechanics failed to provide a comect explanation to the properties of the physical system of particles. According to de-Broglie theby, a material particle is associated with a wave. A wave motion can be described effectively if we have paremeter related to that wave which varies space and time. According to De-Broglie-theory, a partitle of mass cm' is always associated with a wave whose wavelength consider a System of Stationary waves associated with the particle—let x, y, z be the co-sidinates & be the displacement of the matter at any time t.

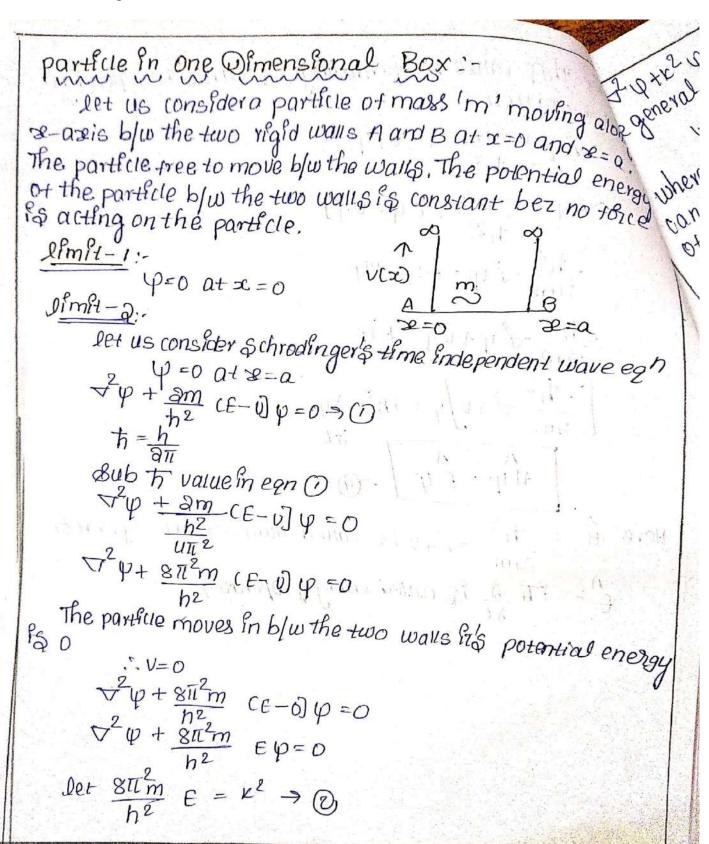
fromth The differential equation of a wave-function is given  $\frac{\partial^2 \psi}{\partial t^2} = v^2 \left[ \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right] = v^2 \neq \psi \rightarrow 0$ where,  $=\frac{8^2 + 8^2}{3x^2} + \frac{8^2}{3y^2} + \frac{8^2}{3z^2}$ , is a laplacean operate,  $=\frac{8^2 + 8^2}{3x^2} + \frac{8^2}{3y^2} + \frac{8^2}{3z^2}$ V = wave velocity. The Solution of equation (1) is given by  $\Psi = \Psi_0 \, s \, lm \, w \, t$ Ψ = Ψο sin str »t →@ [: w = all ) w is Angular
-frequency where visthe frequency of the stationary wave associated with the particle. Differentiating eqn @ twice with respect to t, we get <u>δΨ</u> = Ψο (2πν) cos 2π 2+ and 8 p = - 40 (att 2) sin att 2+  $\frac{1}{\lambda t^2} = -u \pi^2 \vartheta^2 \psi = -u \pi^2 \vartheta^2 \Rightarrow 3$ &ub the values of [ 3 4] from eq 2 3 line 2 m) we get -ull x2 y = x2 2 y  $\nabla^2 \varphi + \underline{u} \underline{u}^2 \varphi = 0 \rightarrow (\underline{\varphi})$ 

from the Debroglie relation,  $\lambda = \frac{h}{mi}$ lence eqn Q becomes  $\sqrt{\psi + u \bar{u}^2} m^2 v^2 \psi = 0 - \sqrt{5}$ If V and E are the potential and total energy of the partfile respectively, then it's kinetic energy is given by Total energy E=K.E+P.E E= 1-mv2+v E-V= 1 mu2 a(E-V)=mV2 muHplyIng 'm' on both sides

am(E-v) = m2v2 -> B

Sub eqn B in eqn B  $\sqrt{2}\psi + \frac{u\overline{u}^2}{h^2} \partial m(E-v) \psi = 0$ √ 4 + 8 [[ m (E-v] φ = 0 → f) let ti=h => h=trate &ub hi value in eqn (7) 2 y +2 8 1 m (E-V) ψ = 0 V + 2m (E-v) φ=0 ... This is the Schrodinger time independent wave egn

2. Derive the Energy equation for particle in one dimensional box and write significance of  $\Psi$  and  $\Psi^2$ ?

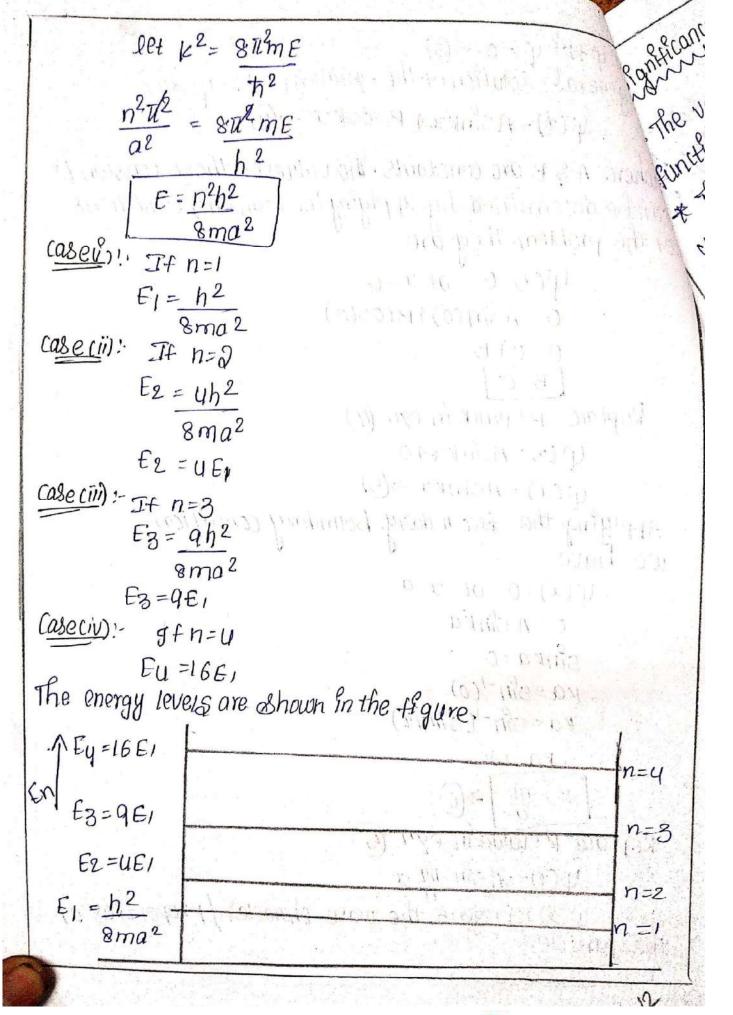


Figeral Solution of the equation (3) is +φcx):

ψ(x) = Asinkx+ B coskx > (4)

where A & B are constants. The values of these constants

where he was a constants and the boundary conditions of the problem. They are. (x)=0 at x=0 0 = ASM(0)+B(05(0) 0 = 0+B B=0 Replace B' value in egn (4) (p(2) = ASInk =+0 w(x) =ASPARIAS Applying the Secon dary boundary condition. we have ψ(x) =0 at x=0 0 = A Sinka Sinka =0 12=58n-1(0) Ka = Sin-1(Sinna) ka =nii K=n[1 /2)(6) Replace (k' value in egn (5) 4(1) = A5m mil 2 Here Wish represents the wave character/ properties of the particle.



# Ranticance of 4 & 42:

The value of wis called wave function (8) Eigen function of the Schrodinger's wave equation

\* The wave function  $\psi$  contains an the information we want to know about system

If I wave function.

\* The wave function is in the schrodinger's eq n represents the amplitude of the et wave

\* The probablility of finding an electron of a given point in the 3d space is proportional to  $\phi^2$ 

\* Hence  $\varphi^2$  gives the problity of finding an electron with energy in a given region around the nucleus

those places around the nucleus can be detected where the probability of finding the electron is highest

3. Draw the molecular diagrams of O<sub>2</sub> and CO?

```
Oz mole cule:-

NO. Of et in 02 = 16e (Heavier molecule)

Oz [ 0 = 8; 162 262 2p4

Configuration of 02 molecule:-

162 962 962 262 8pz 2 112p==112py 112px=112py)

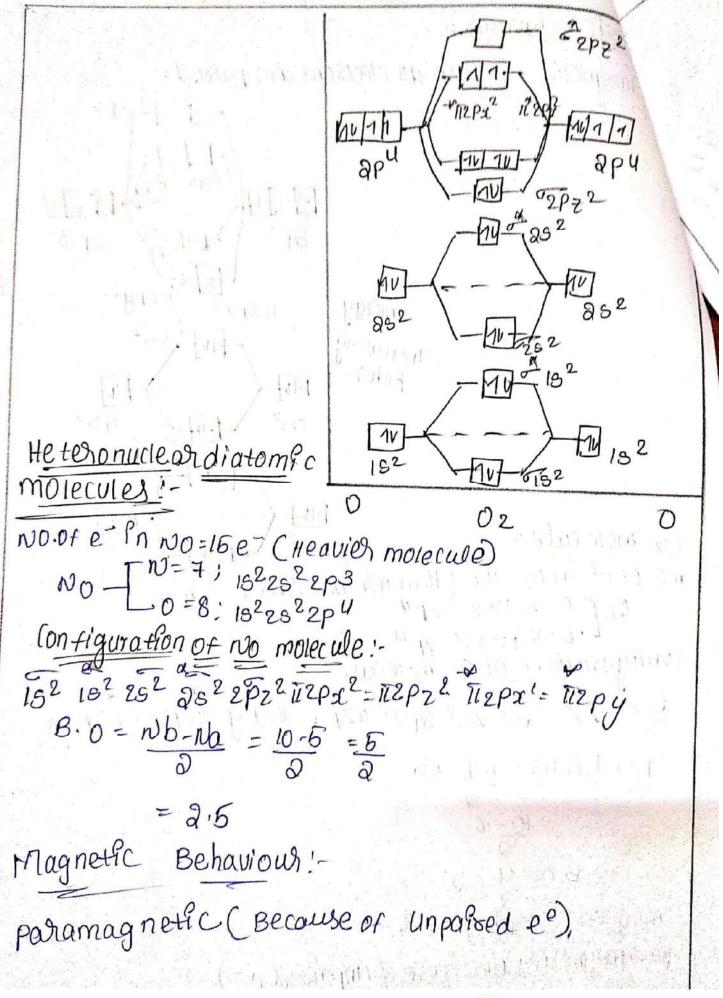
Bond & do = Nb-Na

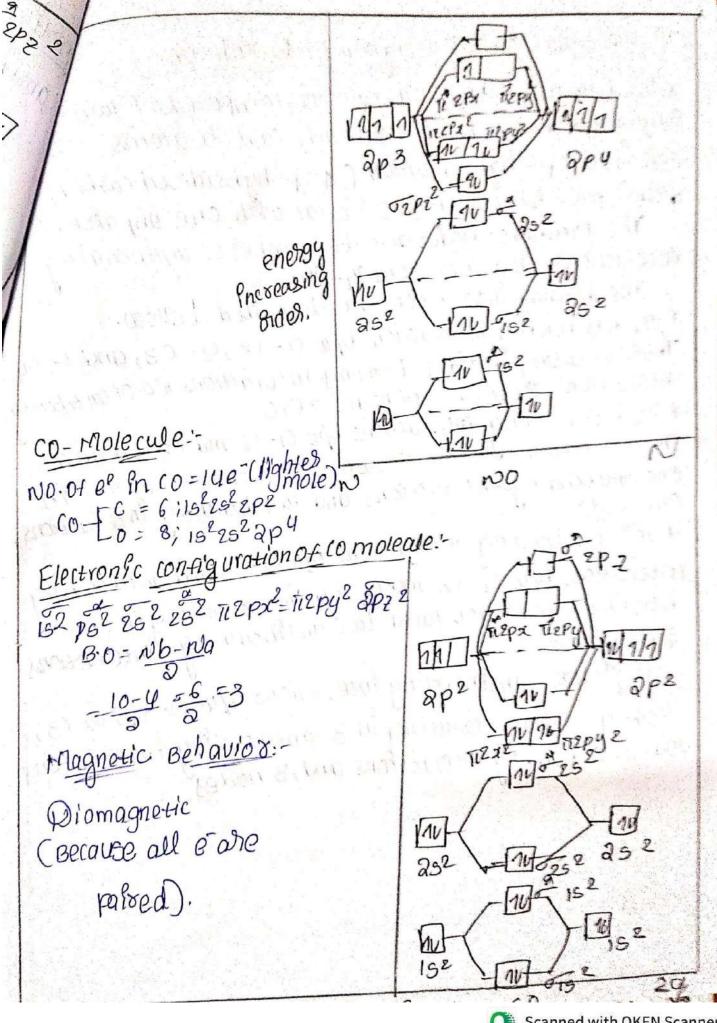
= 10-6

B. O = 4 = 2

magnetic Behavio uh:-

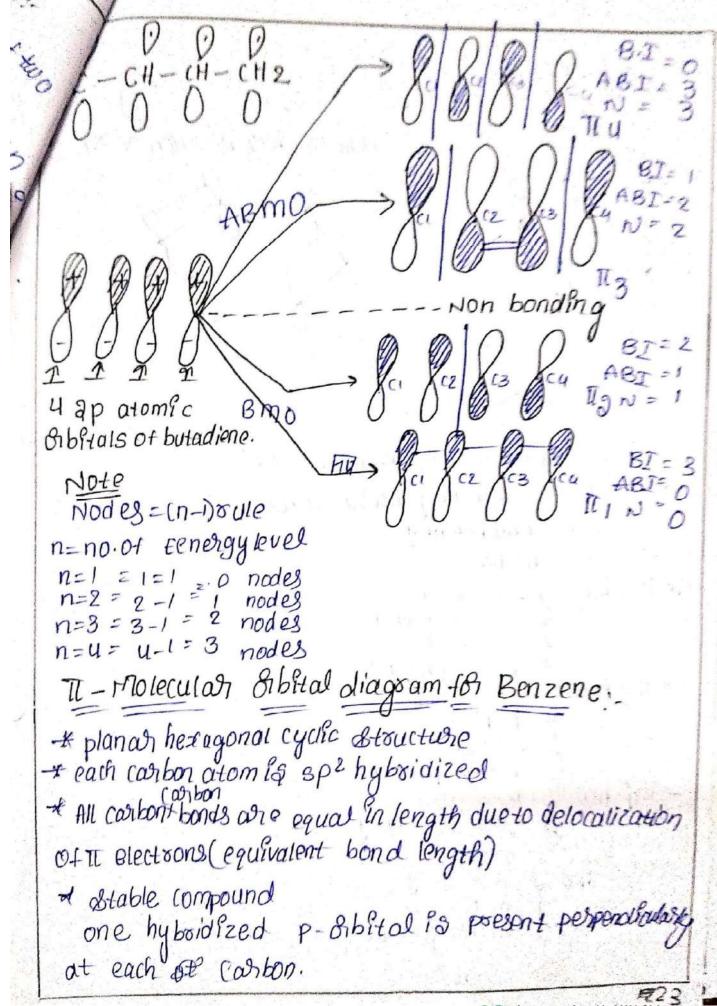
por omagnetic (Because of unpassed e-)
```

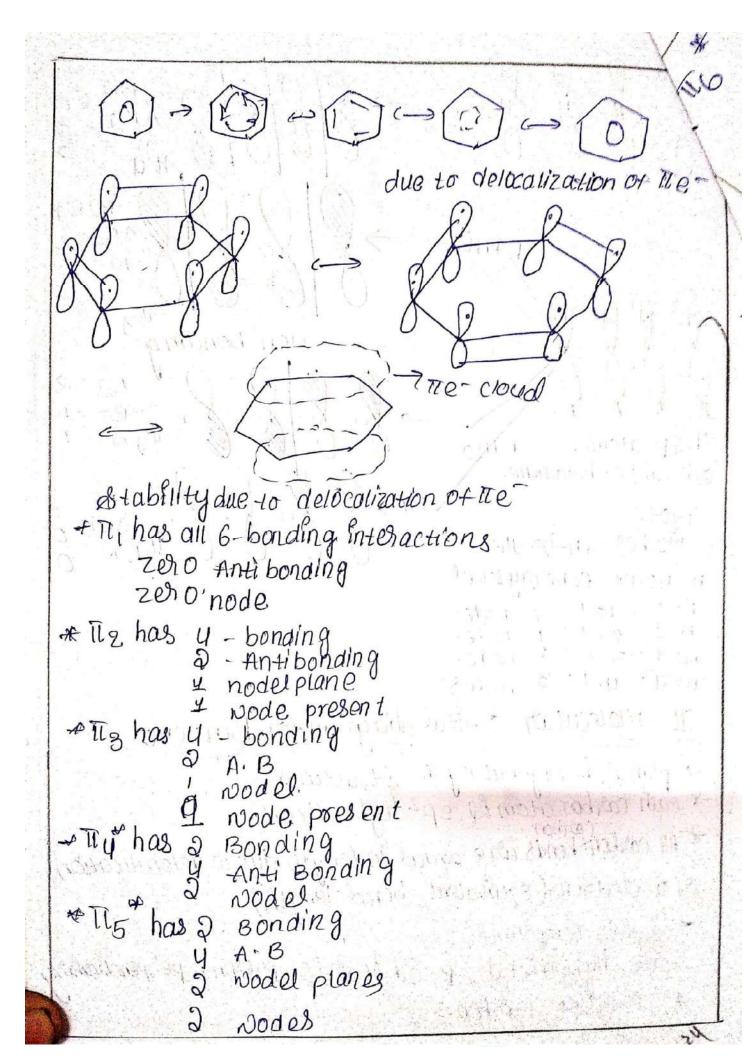




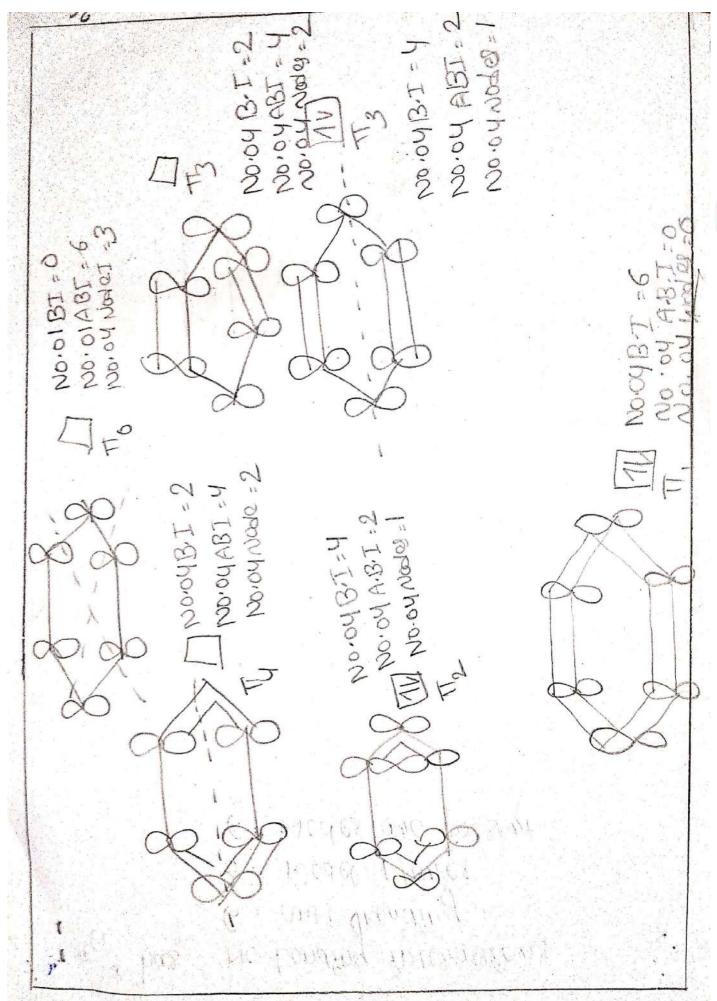
4. Write the molecular orbital diagrams for 1-3 butadiene and benzene?

# II molecular Sibital Diagram of Butadienes \* 113 butadiene is H2C = CH -CH = CH2 · Composed of two C Conjugated double bonds Here each carbon atoms undergoes sp2 hybridisation (4sp2hybridised carbon atoms) and It has one atomic dibital with one unparted e The number of nodes and the number of antibonaing Priteractions Pricreases from II, - II4 The bonding interactions are described bellow. \* It, has bonding interaction b/w ci-cz, cz-c3, and ez-e Thus resulting in three bonding interactions No of antibons Enteractions Lero, No. of nodes zero -\* The has bonding interactions b/w ci-ce and ca-cu and an antibonding linteractions b/w cz-cz thus resulting interactions and two bonding interactions \* Its has bon ding interactions b/wcz-cz and antibonating Protestactions blu ci-ce and cz-cy thus resulting in one bonding interaction land two antibonarny interactions Trut has antibonding interactions b/w c1-co, c2-c3, C35C4 - Thus, resulting in 3-antibonding interaction and zero bonding interactions and, 3 nodes





No bonding interactions
6 = Anti Bonding
3 = Nodel planes
6 = Nodes are present. \* has



### **MCQs**

1. Schrödinger wave equation is a fundamental equation in:
A) Classical mechanics
B) Quantum mechanics
C) Nuclear physics
D) Relativity theory
Answer: B) Quantum mechanics
☐ It describes the behavior of particles at atomic and subatomic levels.
2. In the Schrödinger wave equation, the symbol $\psi$ (psi) represents:
A) Energy of the system
B) Wave function of the particle
C) Momentum of the particle
D) Potential energy
Answer: B) Wave function of the particle
3. The term $\psi^2$ (psi squared) represents:
A) Kinetic energy
B) Probability of finding the electron
C) Charge density
D) Wave amplitude
Answer: B) Probability of finding the electron
$\Box \psi^2$ gives the probability density function.
4. For a particle in a one-dimensional box, the allowed energy levels are proportional to:
A) n
B) $n^2$
C) 1/n
D) $1/n^2$
Answer: B) n <sup>2</sup>
$\Box E_n = n^2h^2/(8mL^2)$

### 5. The lowest energy state of a particle in a box is called the:

- A) Excited state
- B) Zero energy state
- C) Ground state
- D) Forbidden state

**Answer:** C) Ground state

### 6. In Molecular Orbital (MO) theory, atomic orbitals combine to form:

- A) Hybrid orbitals
- B) Molecular orbitals
- C) Crystal orbitals
- D) Nodal planes

Answer: B) Molecular orbitals

### 7. The number of molecular orbitals formed equals:

- A) Number of electrons
- B) Number of nuclei
- C) Number of atomic orbitals combined
- D) Twice the number of atomic orbitals

Answer: C) Number of atomic orbitals combined

### 8. In MO theory, bonding molecular orbitals have:

- A) Higher energy than atomic orbitals
- B) Lower energy than atomic orbitals
- C) Same energy as atomic orbitals
- D) Zero energy

**Answer:** B) Lower energy than atomic orbitals

### 9. In O<sub>2</sub> molecule, according to molecular orbital theory, the bond order is:

- A) 1
- B) 2
- C) 3
- D) 2.5

Answer: B) 2

□ Bond order = $\frac{1}{2}$ (Nb – Na) = $\frac{1}{2}$ (10 – 6) = 2
10. The magnetic nature of O <sub>2</sub> molecule is:
A) Diamagnetic
B) Paramagnetic
C) Ferromagnetic
D) None of these
Answer: B) Paramagnetic
$\Box$ Due to two unpaired electrons in $\pi_2$ p orbitals.*
11. In CO molecule, the bond order is:
A) 1
B) 2
C) 3
D) 2.5
Answer: C) 3
□ Bond order = $\frac{1}{2}$ (Nb – Na) = $\frac{1}{2}$ (10 – 4) = 3
12. The correct filling order of molecular orbitals up to O <sub>2</sub> is:
A) $\sigma$ 1s, $\sigma$ 2s, $\sigma$ 2s, $\sigma$ 2p, $\sigma$ 2p, $\sigma$ 2p
B) $\sigma$ 1s, $\sigma$ 2s, $\sigma$ 2s, $\pi$ 2p, $\sigma$ 2p
C) $\sigma$ 1s, $\sigma$ 2s, $\pi$ 2p, $\sigma$ 2s

### 13. In 1,3-butadiene, $\pi$ molecular orbitals are formed by the combination of:

- A) 2 p-orbitals
- B) 3 p-orbitals
- C) 4 p-orbitals
- D) 6 p-orbitals

**Answer:** C) 4 p-orbitals

D)  $\pi$ 2p,  $\sigma$ 1s,  $\sigma$ 2p,  $\sigma$ 2s

 $\square$  *Each carbon contributes one p-orbital*  $\rightarrow$  4 total  $\pi$ -MOs.

Answer: A)  $\sigma ls$ ,  $\sigma ls$ ,  $\sigma 2s$ ,  $\sigma 2s$ ,  $\pi 2p$ ,  $\sigma 2p$ ,  $\pi 2p$ ,  $\sigma *2p$ 

14. The number of $\pi$ molecular orbitals in benzene is:
A) 3
B) 6
C) 12
D) 2
Answer: B) 6
$\Box$ One from each of the six $sp^2$ carbons.
15. The delocalized $\pi$ -electron system in benzene contributes to:
A) Its instability
B) Its high reactivity
C) Its aromatic stability
D) Its ionic character
Answer: C) Its aromatic stability
16. The bond order between two atoms can be calculated using the formula:
A) $(Nb + Na)/2$
B) $(Nb - Na)/2$
C) $(Nb \times Na)/2$
D) (Nb / Na)
Answer: B) $(Nb - Na)/2$
$\square$ Nb = number of electrons in bonding MOs, Na = in antibonding MOs.
17. In the O <sub>2</sub> <sup>-</sup> ion, the bond order is:
2.0 2.0 0.0 0.2 20.0, 0.10 20.10 0.10 0.10 0.10 0.10 0.10 0.1
A) 1.5
B) 2
C) 2.5
D) 3
<b>Answer:</b> C) 2.5
□ Extra electron enters $\pi$ 2p → bond order = ½ (10–5) = 2.5.*

### UNIT-II MODERN ENGINEERING MATERIALS

### **SEMICONDUCTORS**

### 1. What is a semiconductor?

A semiconductor is a substance whose electrical conductivity lies between that of a conductor and an insulator.

Example: Silicon (Si), Germanium (Ge).

### 2. What are the types of semiconductors?

- Intrinsic semiconductor: Pure semiconductor (e.g., Si, Ge).
- Extrinsic semiconductor: Doped with impurities to increase conductivity.
  - o **n-type:** Doped with pentavalent element (P, As).
  - o **p-type:** Doped with trivalent element (B, Al).

### **3.** What is the band gap in semiconductors?

It is the small energy gap (about 1 eV) between the valence band and conduction band.

### **4.** Give two applications of semiconductors.

- Used in diodes, transistors, and integrated circuits (ICs).
- Used in solar cells and LEDs.

### **4**SUPERCONDUCTORS

### 1. What is superconductivity?

It is the phenomenon in which a material shows zero electrical resistance and expulsion of magnetic field (Meissner effect) below a critical temperature.

### **2.** What is the critical temperature (Tc)?

The temperature below which a material becomes superconducting.

### **3.** Give examples of superconductors.

- Mercury (Hg)
- Niobium (Nb)
- YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> (Yttrium barium copper oxide high-Tc superconductor)

- **4.** Mention two applications of superconductors.
  - Magnetic Resonance Imaging (MRI) machines.
  - Maglev (magnetic levitation) trains.
  - Superconducting power cables.

### □□ SUPERCAPACITORS

### **1.** What is a supercapacitor?

A supercapacitor (ultracapacitor) is an energy storage device that stores electrical energy between a capacitor and a battery, with higher energy density than conventional capacitors.

### **2.** What is the basic concept?

Supercapacitors store charge either by electrostatic double-layer formation or fast surface redox reactions.

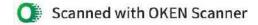
- **3.** What are the types (classification) of supercapacitors?
  - Electrochemical Double Layer Capacitors (EDLCs) charge stored electrostatically.
  - **Pseudocapacitors** charge stored by redox reactions.
  - **Hybrid supercapacitors** combination of both.
- **4.** Give two applications of supercapacitors.
  - Energy storage in electric vehicles (EVs).
  - Power backup in electronic devices and renewable energy systems.

### NANOMATERIALS

### 1. What are nanomaterials?

Materials having at least one dimension in the nanometer range (1-100 nm).

- 2. What are the classifications of nanomaterials?
  - **Zero-dimensional (0D):** Nanoparticles, quantum dots.
  - One-dimensional (1D): Nanowires, nanotubes.
  - Two-dimensional (2D): Graphene sheets.
  - Three-dimensional (3D): Nanocomposites.



### **3.** What are the important properties of nanomaterials?

- High surface area to volume ratio.
- Enhanced mechanical strength.
- Improved electrical and optical properties.

### **4.** What are Fullerenes?

Fullerenes are spherical carbon molecules (C<sub>60</sub>, buckyballs) composed of pentagons and hexagons.

### **5.** What are Carbon Nanotubes (CNTs)?

CNTs are cylindrical fullerenes with high tensile strength and conductivity. **Types:** Single-walled (SWCNT) and multi-walled (MWCNT).

### **6.** What is Graphene?

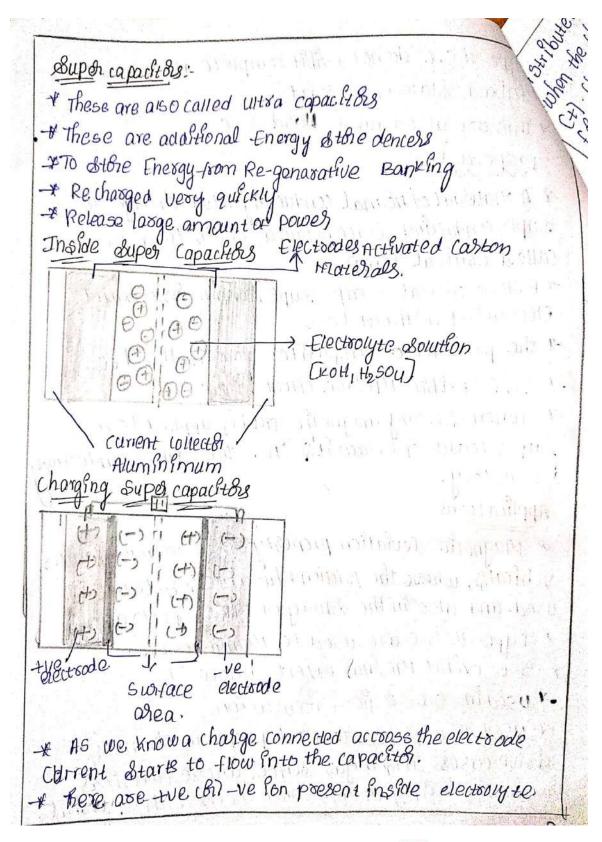
Graphene is a single layer of carbon atoms arranged in a hexagonal lattice; it has excellent electrical, thermal, and mechanical properties.

### 7. Mention applications of nanomaterials.

- Drug delivery and biosensors.
- Nanoelectronics and solar cells.
- Strengthening materials (nanocomposites).
- Catalysts and coatings.

### **EASSAY QUESTIONS**

1. Write about super capacitors and classification applications of super capacitors?



stributed randomly occross ft. when the charger about 13 to charges the (+) electrode with (+) charge it Starts to attract (-) lons from electrolyte. forming layer + Simplary the (-) electrook for charge with (-) fors and aware the (+) long from electrolyte forming another layer accoss &. Electrostatic loice do the Alignment of (+) & (-) charges accoss the boundary of Electrode Soln couse Electric double layer. \* And this is Responsible for Stores Electrical charges \* Then capacito known as Double layer capacitos - The capacito CGD formed along with the another apaches (C) which alt as they are connected as serves => A=high Swrface whea electrode Electroode \* 100d connected to accoss the electoficity and the Electrode &tank to 100e the charge and charge flows the external

# and then lig ht atter 1000 to complete the changes & Hence & Both the electrodes (+) & (-) 1008e the changes & Hence & They can not attract the sons and lons set are distoshured accross the electrolyte as it way be tope it being change. Applications + Luper capacition is used to as an additional power source for regenerating Banking.

\* And also it is used not of power is needed in less time like quick accieration's Tused in electronic's like laptopicomputer, Gips, portable media player, hand held divisers and photo volatic system \*70 provide back up, shud down i RAM, &com.

2. Write about Nano materials classification properties and applications of Carbon nano tubes and Fullerenes?

Nano Materials
The materials like metals, ceramion, polymetic materials tompostic materials with dimensions and tolerance in the range of Inm to loon mare called movements in the one billionth (10-9) of a meter.

\* Im = 39 inches

\* Inm = 10-9 m

Inm = 10-9 m

Inm = 10-9 nm

Eq: Aster = H = 0. Inm, llgoz Inm

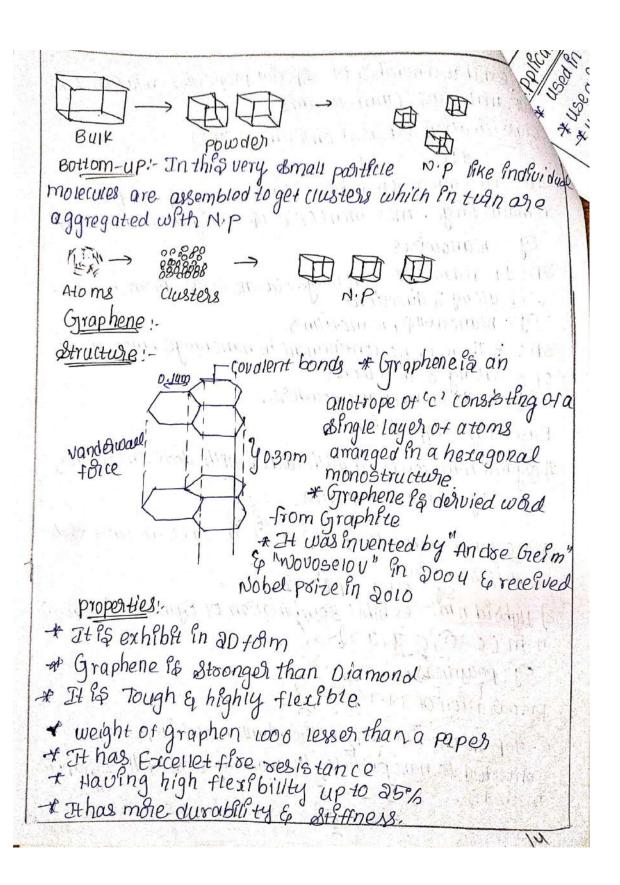
& gniftcance

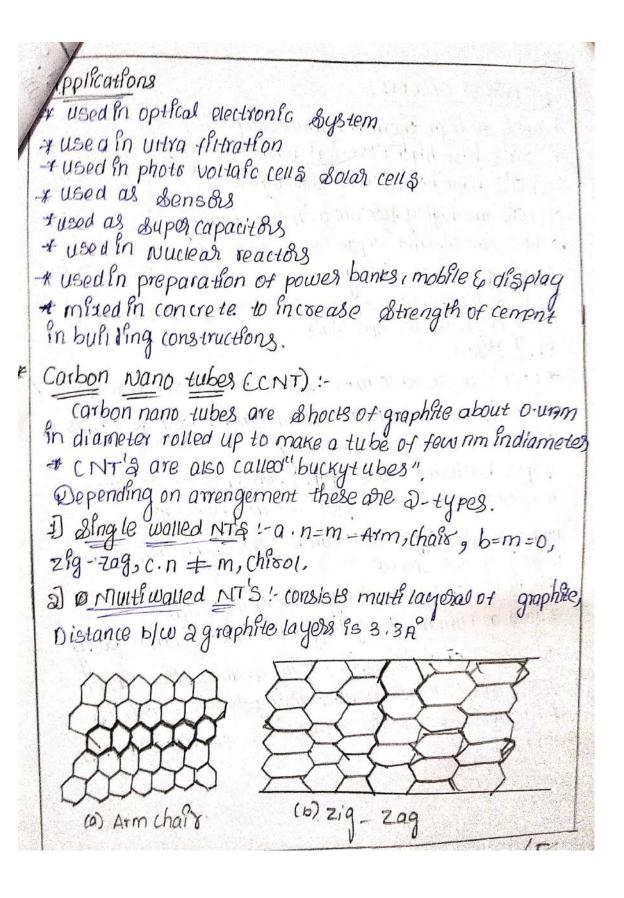
\* Due to their & mail size

\* M. P. reaction rates, conductivity, wow

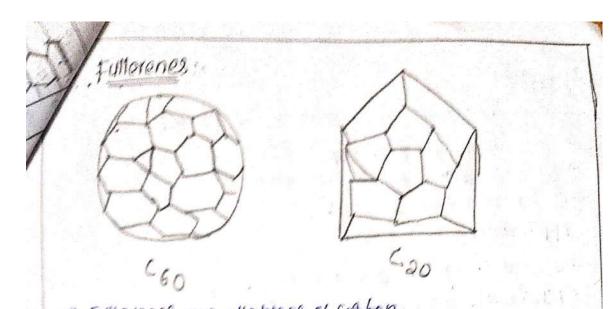
A nanoparticle is defined as a & may object that behaves as a whole unit interms of its transport

d exhibit a number of special properties relative to bulk materfais. (Inm-100nm). Classification (Based on Plmens fons) 20 m 16 30 the fill all the mostly YD: Two dimension reduced to nanorange & one Dia remains large. movement of e-is along these direction Eg: Nanowises aD: 10 reduced to nanorange, an are large, momement of Eg: Nanowell & Nanoflims 30: 8 There is no confinement in nanorange, movement of e along 3 directions Eg: Bulk N:m, wano powders. Based on composition !-. I Biganicnim: composed with carbon with different forme Eg: CNT, fullerenes of In organic n.m: - composed with metal Emetal oxido Endifferent torms Eg - AUIFO, PtiAl 3) Hyboid nm: exhibit combination of Eganic & in Ergonic n·m (0-0,0-1,1-1) Eg!- polymers was was supported to the second preparation of N.M: 4. Top-down: - In this method bulk materials are converted to nanopasticles by making use of lithing raphic method &





## properties of CNT: \* CNTS are high thermal conductivity \* CNTS have high Electrical conductivity \* CNT's have high tensile strength or cnip are highly flexible with out damage or Have eaw thermal expansion coefficien t or CMT posses To sicity A CNT'S have unfque optical Obsorption properties and differ from in bulk materials Applications \* CNT'S are used to make space elevates, Stab-Proof \* CNTS are recently used its making electrical cables & curses bez of high conductivity paper batteries: use a paper the sheet of cellulose Physica with CNT-Here CNT act as electrode. Hydrogen Storage: - CNT can be Store hydrogen to be used as a tue source Medical: -xused as doug delivery material \* used as tumaur targeting material in human body Textile: - CTIS used to coating & absorption on the abuliface of fibre 18 manufactualing fabolic which is antibocterial electronic conductive, flame retaildant etc .



\* Fullerenes are allotrops of conton \* It can be prepared by vaporasing rod in the Atmosphere & carbon atoms in fullesenes are connected by isingle and double bonds and forms closed mesh network.

+ the shape of fullesene may be a hallow sphere.

C60 fullerenes

\* As attrect us like about both t each coabon atom is spe hybridised and tolgonally linked (each coabon atom is linked with other 3 Cotibon atoms)

\* It has polyhedral Network

a It has 60 vertices & 32 faces

out of 32 faces 12 de pentagonal & 20 are hexagonal sings.

# properties

- \* It can be compressed up 30% of 81's volume.
- \* It is thermally Stable up to 60°C \* It is soluble in Borzene Solution.
- # It has good tens? Strength. Applications
- \* used as charge carries in Battriey.
- \* Alkali metal fullerences are used as super conductors
- \* It is used as lubricant due to spherical shape.

  \* used to controlgrowth of HN-I visus
- \* used to make hydrogen fuel
- \* used to making cosmetic related materials

3. Define super conductor and discuss about their classification and applications? Super conductors: \*A solld which ofers no resistance to the passage Electoficity through it it is caused super conduct ors \* The phenomeno was Discovered by Dutch scientist " one " in 1911, He was measuring the resistivity of Mecury below 4.2 K. Super conductivity! The phenomeno of disapperance of electrical energ resistance of a material below a certain temperature is known as Super conductivity, Critical temperature: \* The temperature below which the electorical resistance becomes zero la called costiscal temperature (Tc) \* At this temperature a material changes to puper conducting state. Types of Super conductors Classification - 4 ( magnetization) Type-I Temp

classification's super conducting transition the super conductors are following to two types 4) law temperature a) tilgh temperature law Tem:-\* Super conductors with law To are known as law temperature super conductos \* useually the Teof law Temp S. Cisless than Jok \* The other name is Elemental S.C. High temperature! \* & upen conductors with high temperature are known as High temperation S.C \* usually the To Pa Zaok Eg:- Metalic alloys. Misinal Effect !-An Explusion of a magnetic fletal from a s. c during PLS to the super conducting state is cared misinar effect. Below the transfition temperature the super conductors concre nearly on the magnetic field inside Classification - I

are divided into two-types

4. Type-I &. C

Y. Type. I super conductos!

\* Example pure metals, conductors, Hg, Pb

\* In type-I super conductors the magnetic tierd is totally experd from the interes of the material below a certain magnitization field (Hc)

Aft Hc the material losses his magnification sudenly

This type of dupen conductors exhibits misland effect.

2. Type-II S. C. - June 1/19

\* Examples allays, metals

-\* In type-II super conductors the magnitization is.

\* there are two magnetic field.

A PART TO THE STATE OF THE

A lower costical magnetic field (Hc] & upper costical

The Below Ho the Super conductor excludes all magnetic field lines in between (Hci) & (Hcz) the field becomes to enter.

\* type-II s. c. do not exibit complete tylisinal effect

\* This are also called Hord S.C.

# proporties

- \* A Material of normal conducting state changes to super conducting state below a certain temp is called critical temp
- + Below critical temp super conductors conduct electricity without loss.
- \* The presence of Impurites lower's the To
- + S.C exhit Missinal effect below To
- when strong magnetic field is applied to a super conductivity of distry.

  Applications
- Magnetic leviation property of 5.c to make trains, vehicals, where the friction b/w wheels & tracks is used and also in the Study of MRI spector
- \* Type-Il S.C are used to manufactures

  \* S.C exibit Mislan effect below To
- \* used in s.c logic calculation
- of used as a sence to find people in dounk & dolve cases. It is a gas dence whose flectofcal oesistance sharply changes when meets with Alkohal.

4. Define semi conductor and discuss various types and applications of semi conductor?

Demi Conductors Between the valence band and the conduction band in a Demiconductor, there is a slight energy difference of around \* This band gap is also known as Foi bidden energy gap temperature but an Increasing the temperature it conduct electricity called Semiconductors". Eg: 58/Gp. En Insulators, so they have law conductivity. To Encrease, conductivity of S. c we are adding impurities to it eg: siffere Then s.c are classified into 9-5-1-1-3-5-3-5-6- - Shulmanin Se Extrinsic Story Intrinsic S.C p-type N-type s.c At 'O' ke win temperature: There is no free electron as all the valence electron are Envolved en bonding so that zero Keluin temp sic behave as an Insulation.

At temperature above then zero: on increasing temperature Crystal Start ulbrating due to which same of the covalent bond break and some free e ore generated so there s.c acts as conductors Class Hication: 4. on the basis of chemical composition. a) flement type semiconductors: Those s.c are available in natura tom. Eg: - sticon & Grermantum b) compound type semiconductors: Those s.c which are formed by the combination of metals Eg! cdTe, Znse etc. a) on the Basi's of Charger carrier

Intrinsic Semiconductos

Expure form of s.c are called I.s.c

Eg: - 58,678.

\* Impurities do not effect it's electrical behaviour hence are also called undopped /s.c.

\* It has equal no of e-& holes(+ve).

\* This s.c pentavalent impurities are added that acts as N-typesc & Torvalent are added.

wBring:-

twict Electronic configuration of both the elements siffer have 4e- in its valence cell.

50 (10) = 2,8,4 - 159 252 2p6 362 3p2

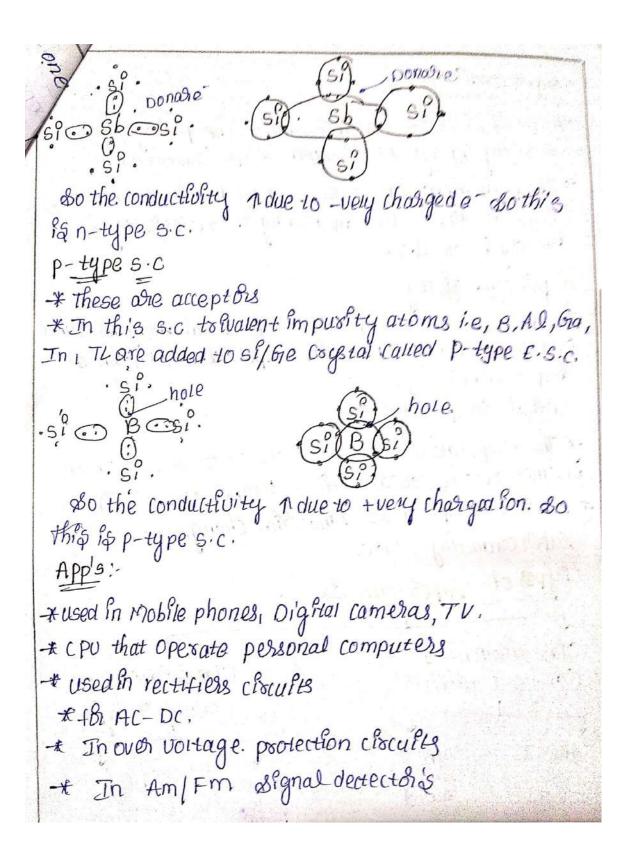
Temp it behaves like an insulation at zero k 71 temp above zero, act as conductor.

\* further of Temp the covalent band is broken and the e for free. The position from which the e gets discodged has a hole.

The hore is occupied by a free e as a result of which vaccant position becomes a hore

\* This way the hole / +ve charge is transferred from one position to another. To a Temp to coeate hole Estrinisic s.c: + E.s.c are + 8 med by the doping of pure s.c with cestain specific impurity atom. \* So It is also known as impure & Dopped s. c \* NO. Of e-# + NI-0. of holes \* Electore conductivity is high Depending on Doping E.S. Care a types. 1 N-type E.S.C a) p-type E.S.C \* It is also called Donas group

\* In this s. c pentavalent impusity atoms i.e., PI AS, Sb, BP etc are added to pure sf/Gie crystal % called , N-type E.S.C. \* The conductivity of silfae is 1 by the process of Dopling.



#### **MCQs**

- 1. Substances whose conductivity lies between conductors and insulators are called:
- A) Conductors
- B) Semiconductors
- C) Superconductors
- D) Insulators

**Answer:** B) Semiconductors

- 2. In an intrinsic semiconductor, conduction is due to:
- A) Electrons only
- B) Holes only
- C) Electrons and holes both
- D) Impurities

Answer: C) Electrons and holes both

- 3. Example of an intrinsic semiconductor:
- A) Silicon (Si)
- B) Copper (Cu)
- C) Germanium (Ge)
- D) Both A and C

**Answer:** D) Both A and C

- 4. In *n-type* semiconductors, the majority charge carriers are:
- A) Holes
- B) Electrons
- C) Protons
- D) Neutrons

**Answer:** B) Electrons

- 5. In *p-type* semiconductors, the majority carriers are:
- A) Holes
- B) Electrons
- C) Ions
- D) Protons

**Answer:** A) Holes

#### 6. The process of adding impurities to increase conductivity is called:

- A) Polarization
- B) Doping
- C) Deionization
- D) Magnetization

Answer: B) Doping

#### 7. A common application of semiconductors is:

- A) Transformers
- B) Diodes and Transistors
- C) Heating elements
- D) Capacitors

Answer: B) Diodes and Transistors

#### 8. Band gap of silicon at room temperature is approximately:

- A) 1.1 eV
- B) 2.2 eV
- C) 0.7 eV
- D) 3.2 eV

Answer: A) 1.1 eV

# 42 Superconductors – Concepts and Applications

#### 9. A superconductor is a material which shows:

- A) Infinite resistance
- B) Zero resistance
- C) High resistance
- D) Variable resistance

**Answer:** B) Zero resistance

#### 10. The temperature below which a material becomes superconducting is called:

- A) Transition temperature (Tc)
- B) Critical temperature
- C) Both A and B
- D) Melting temperature

Answer: C) Both A and B

#### 11. The Meissner effect is related to:

- A) Thermal expansion
- B) Magnetic field expulsion
- C) Photoelectric emission
- D) Electrolysis

Answer: B) Magnetic field expulsion

□ Superconductors expel magnetic flux below Tc.

#### 12. Which of the following is a high-temperature superconductor?

- A) Mercury
- B) YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> (Yttrium barium copper oxide)
- C) Tin
- D) Lead

Answer: B) YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub>

#### 13. One major application of superconductors is in:

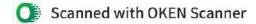
- A) Transformers
- B) Magnetic levitation (Maglev) trains
- C) Electric irons
- D) LEDs

**Answer:** B) Magnetic levitation (Maglev) trains

#### 14. The property lost by a superconductor above Tc is:

- A) Conductivity
- B) Diamagnetism
- C) Luster
- D) Elasticity

**Answer:** B) Diamagnetism



43 Supercapacitors – Concepts, Classification & Uses

#### 15. Supercapacitors are also called:

- A) Chemical capacitors
- B) Ultracapacitors
- C) Quantum capacitors
- D) Power capacitors

**Answer:** B) Ultracapacitors

#### 16. Supercapacitors store energy mainly by:

- A) Chemical reaction
- B) Electrostatic charge separation
- C) Magnetic induction
- D) Nuclear reaction

Answer: B) Electrostatic charge separation

#### 17. Supercapacitors are classified mainly as:

- A) Electrochemical double-layer capacitors (EDLCs)
- B) Pseudocapacitors
- C) Hybrid capacitors
- D) All of the above

**Answer:** D) All of the above

#### 18. Which of the following is used as electrode material in supercapacitors?

- A) Graphite
- B) Activated carbon
- C) Silicon
- D) Copper

**Answer:** B) Activated carbon

19. An important application of supercapacitors is in:
A) Long-term energy storage B) Fast charge/discharge backup systems C) Food preservation D) Light emission Answer: B) Fast charge/discharge backup systems
2 4 Nanomaterials – Concepts, Types, Properties, and Applications
20. Nanomaterials have at least one dimension in the range of:
A) 1–100 μm B) 1–100 nm C) 1–10 cm D) 0.1–1 mm <b>Answer:</b> B) 1–100 nm
21. Fullerenes are:
A) Allotropes of sulfur B) Allotropes of carbon C) Allotropes of silicon D) None of these Answer: B) Allotropes of carbon
22. The most famous fullerene molecule is:
A) C <sub>60</sub> B) C <sub>70</sub> C) C <sub>80</sub> D) C <sub>120</sub> Answer: A) C <sub>60</sub>

#### 23. Carbon nanotubes (CNTs) are formed by:

- A) Folding graphite sheets into cylinders
- B) Melting diamond
- C) Polymerizing carbon monoxide
- D) Heating hydrocarbons in air

Answer: A) Folding graphite sheets into cylinders

#### 24. Graphene is a:

- A) 0D nanomaterial
- B) 1D nanomaterial
- C) 2D nanomaterial
- D) 3D nanomaterial

Answer: C) 2D nanomaterial

#### 25. The electrical conductivity of graphene is due to:

- A) Localized  $\pi$ -electrons
- B) Delocalized  $\pi$ -electrons
- C) σ-bonds
- D) Ionic bonds

**Answer:** B) Delocalized  $\pi$ -electrons

#### 26. Nanoparticles have unique properties mainly due to:

- A) High surface-to-volume ratio
- B) High temperature
- C) Bulk density
- D) Crystal defects only

**Answer:** A) High surface-to-volume ratio

#### 27. An important application of carbon nanotubes is in:

- A) Bulletproof vests
- B) Nanoelectronics and sensors
- C) Cement manufacture
- D) Paints

**Answer:** B) Nanoelectronics and sensors

#### 28. Fullerenes are used in:

- A) Drug delivery and lubricants
- B) Nuclear reactors
- C) Fertilizers
- D) None of these

Answer: A) Drug delivery and lubricants

#### 29. Graphene is used in:

- A) Transparent conductive displays
- B) Electrical insulators
- C) X-ray tubes
- D) Glass polishing

**Answer:** A) Transparent conductive displays

#### 30. Nanomaterials are widely used in:

- A) Medicine
- B) Electronics
- C) Energy storage
- D) All of the above

Answer: D) All of the above

#### UNIT III ELECTROCHEMISTRY AND APPLICATIONS

#### 1. Electrochemical Cell

#### Q1. What is an electrochemical cell?

**A:** An electrochemical cell converts chemical energy into electrical energy or vice versa through redox reactions. It consists of two electrodes (anode and cathode) and an electrolyte.

#### Q2. Differentiate between galvanic and electrolytic cells.

A:

- Galvanic cell: Spontaneous redox reaction, generates electricity.
- **Electrolytic cell:** Non-spontaneous reaction, electricity is supplied to drive the reaction.

#### 2. Nernst Equation

#### Q3. What is the Nernst equation?

**A:** It relates the cell potential to the concentration of ions:

$$E=E0-0.0591/n \log Q$$

Where E = cell potential,  $E_0 = \text{standard potential}$ , n = electrons, Q = reaction quotient.

#### Q4. Numerical example:

For the cell: Zn|Zn2+||Cu2+|Cu, [Cu2+]=0.01M, E0=1.10 V

$$E=1.10-0.0591\log[Cu2+]/[Zn2+]$$

 $=1.10-0.0591\log 0.1/0.01$ 

$$=1.10-0.0591(1)\approx1.041V$$

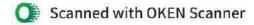
#### 3. Potentiometry & Titrations

#### Q5. What is potentiometry?

**A:** Measurement of the voltage of an electrochemical cell without current to determine analyte concentration.

#### Q6. What is a potentiometric titration?

**A:** A titration in which the potential of the solution is measured as a function of titrant volume. Example: redox titration of  $Fe^{2+}$  with  $Ce^{4+}$ .



#### 4. Conductivity & Conductometric Titrations

#### Q7. What is conductivity?

**A:** The ability of a solution to conduct electric current due to the presence of ions.

#### Q8. Conductivity cell:

A device with electrodes immersed in solution to measure conductivity.

#### **Q9.** Conductometric titration:

Titration based on changes in conductivity.

• **Example:** Strong acid vs. strong base (HCl vs. NaOH). Conductivity decreases till equivalence point, then increases.

#### 5. Electrochemical Sensors

#### Q10. Potentiometric sensor example:

• **P**<sup>H</sup> **meter** using glass electrode, measures potential due to H<sup>+</sup> concentration.

#### Q11. Amperometric sensor example:

• **Glucose biosensor**, current proportional to glucose concentration via enzymatic reaction.

#### 6. Primary Cells

#### Q12. Example of primary cell:

• Zinc-air battery

**Reaction:** 

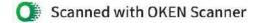
• Anode:  $Zn \rightarrow Zn^{2+} + 2e^{-}$ 

• Cathode:  $O_2+2H_2O+4e^-\rightarrow 4OH^-$ 

• Characteristics: Non-rechargeable, high energy density.

#### 7. Secondary Cells

#### Q13. Example of secondary cell:



• Lithium-ion battery

**Reaction:** 

- Charging:  $LiCoO_2 + C \rightarrow Li_{1-x}CoO_2 + LiC_6$
- Discharging: Reverse reaction.
- Characteristics: Rechargeable, high energy density, long cycle life.

#### 8. Fuel Cells

#### Q14. Hydrogen-Oxygen Fuel Cell:

• Anode:  $H_2 \rightarrow 2H^+ + 2e^-$ 

• Cathode:  $O_2+4H^++4e^-\rightarrow 2H_2O$ 

• Converts chemical energy directly to electrical energy, clean.

#### Q15. Polymer Electrolyte Membrane Fuel Cell (PEMFC):

- Uses **proton-conducting polymer membrane** as electrolyte.
- Working:  $H_2$  at anode  $\rightarrow H^+$  moves through membrane, electrons via circuit;  $O_2$  at cathode reacts with  $H^+ \rightarrow$  water.

#### **EASSAY QUESTIONS**

1. Write about Potentiometric titrations and discuss various types and write about conductometric titrations?

#### **Potentiometric titrations:**

The potential of electrode depends upon the concentration of the ions to which it is reversible in accordance with Nernst equation. Thus in a titration, the potential of an electrode is measured by the change in ionic concentration.

The potentiometric titrations are those titrations which involve the measurement of electrode potentials with the addition of the titrant. The end point is detected by measuring the changes in the potential of a suitable electrode during the course of reaction. No indicator is used in this titrations. The end point of the reaction is indicated by a sharp change in the potential of the system.

#### (i) ACID BASE TITRATIONS:

The acid solution whose strength has to be determined is taken in a beaker and the hydrogen electrode and calomel electrode were dipped in the solution. The electrodes were connected to the potentiometer and the E.M.F is measured. A known volume of standard alkali solution is added from a burette and stirred and the EMF of the cell is recorded. Like this 10-15 readings are recorded by repeating the procedure of the addition of standard alkali. On adding alkali solution (NaOH) from the burette, the H<sup>+</sup> concentration goes on decreases, i.e. pH of the solution goes on increases and hence the EMF of the cell goes on

increases gradually, but at the end point the rate of change of potential will be suddenly quite large. After the end point, further addition of NaOH produces very little change in the H<sup>+</sup> ion concentration and hence there is very little change in the EMF of the cell.

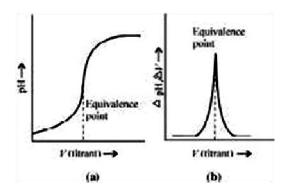
The complete cell may be represented as

Pt, 
$$H_2$$
 (1atm) /  $H^+$  (unknown) //KCl (sat. sol<sup>n</sup>) /  $Hg_2Cl_2.Hg$ 

The emf of the indicator electrode (hydrogen

Exectrode) is given as 
$$E_{H2/H^+} = E^o$$
  
+ 0.0591 log  $[H^+]$ 

A graph is plotted by taking volume of alkali added against EMF observed. A sigmoid curve is obtained and the steepest portion of the curve indicates the equivalence point of the titration



From the graph, we draw the conclusion that the EMF increases with the decrease in concentration of hydrogen ions because electrode potential of indicator electrode depends on the concentration of H<sup>+</sup> ions.

#### (ii) OXIDATION- REDUCTION TITRATIONS:

The procedure adopted for oxidation titration is the same as in acid-base titration; the only difference is that the electrode reversible to hydrogen ions is replaced by a bright platinum electrode. The EMF of the electrode is determined by the activity of ratio of the substance being oxidized or reduced. For E.g.; Fe<sup>2+</sup> titrated against K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>. The Fe<sup>2+</sup> solution is taken in the beaker, treated with dil.H<sub>2</sub>SO<sub>4</sub> and Pt electrode and calomel electrodes are dipped. The electrodes are connected to the potentiometer and EMF of the solution after the addition of K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> is recorded. On addition of K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> from the burette, EMF of the cell increase first slowly, but at the equivalence point there will be sudden jump in potential, since change in ratio of Fe<sup>2+</sup>/Fe<sup>3+</sup> ion concentration. A graph is plotted with EMF and volume of K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>. A sigmoid curve is obtained and the steepest portion of the curve indicates the end point of the titration.

#### (iii) PRECIPITATION REACTION:

In precipitation reaction also an electrode reversible to one of the ions involved is made use of, for **e.g:** titration of AgNO<sub>3</sub> with NaCl, where AgCl precipitates out, Ag- electrode is used along with calomel electrode. The silver nitrate is placed in the micro burette and added to sodium chloride taken in the beaker, containing electrodes. The EMF of the cell is measured and plotted against volume of silver nitrate added. The steep rise in the curve shows the end point of the titration.

### 1. Real life applications

Potentiometry represents a powerful technique with a myriad of different applications in biology, physics as well as chemistry. It was also used for the respiratory gas analysis in the hospitals consisting of respired gas samples from the patients undergoing anesthesia. It can also be used for the genomic studies with potential applications for clinical medicine. Due to its speed and sensitivity, potentiometry has played a pivotal role in space related applications, drug discovery, for geologic research petroleum composition measurements,



carbon dating and some other research endeavors. Three most interesting uses of potentiometry in real life are as follows:

- Food industry: Titration is a method or the process of determining
  the concentration of a dissolved substance in terms of the
  smallest amount of a reagent of known concentration required to
  bring about a given effect in reaction with a known volume of the
  test solution.
- Paper manufacturing: Atmospheric emissions from the pulp and paper manufacturing industry can be determined by the potentiometric measurements.
- Pharmaceutical industry: To determine the pH of given chemical

agents and also in the detection of end point in potentiometry titration of certain drugs like amoxicillin, propranolol.

**Example:** Determination of pH of blood for diagnosis of acidosis or alkalosis

**Example:** Determination of NO<sub>3</sub>, NO<sub>2</sub> in meat preservatives.

**Example:** To determine the NaCl content in meat, fish, dairy products

and fruit juice **Example:** To determine the Ca content in dairy products,

beer, wines and brewing solutions **Example:** To determine the K content in fruit juices, beer and wines.

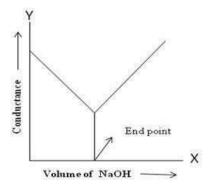
**CONDUTOMETRIC TITRATIONS:** Titrations involving conductivity measurements of electrolytes to get endpoint are called conductometric titrations. The end point is generally found out by plotting the conductance values on y-axis against the volume of electrolyte on x-axis. The electrical conductance of an aqueous solution depends up on:

- 1. The number of free ions in the solution containing an electrolyte.
- 2. The charge on the free ions.
- 3. The mobility of the ions.

### 1. Strong acid Vs Strong base titrations:

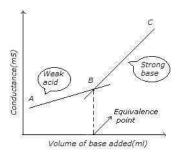
In an acid-base titration, acid is taken in the conical flask and base is added through the burette. Consider the titration of strong acid (HCl) with strong base (NaOH). Before the addition of NaOH, the conductivity is mainly due to the H<sup>+</sup> ions; hence the conductivity is high. On the gradual addition of NaOH from the burette, the fast moving H<sup>+</sup> ions of acid are replaced by OH<sup>-</sup> ions. The conductivity of the solution decreases progressively by the addition of NaOH till the equivalence point is reached. The conductance again increases after the equivalence point.

$$HCl + NaOH \rightarrow NaCl + H_2O$$



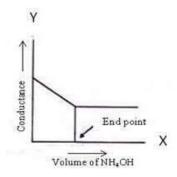
## 2. Weak acid Vs Strong base titration:

When weak acid is titrated with strong base, the conductance of the solution is low in the beginning, since the dissociation of weak acid is very low. On addition of base, highly dissociated sodium acetate is formed. Due to the common ion effect, the acetate ion tends to suppress the ionization of acetic acid. Later the conductivity begins to increase due to the conductivity power of the highly ionized salt exceeds that of weak acid. After end point, the addition of NaOH contributes sharp increase in the conductivity of the solution. The point of intersection of the two cures gives the end point of the titration.



**3. Strong acid Vs weak base titrations:** When strong acid is titrated against a weak base, the conductance of the solution first decrease due to the replacement of fast moving H<sup>+</sup> ions with slow moving NH<sub>4</sub><sup>+</sup> ions. After the end point, the addition of excess of NH<sub>4</sub>OH will not result in any appreciable change in the conductivity.

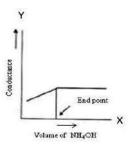
$$HC1 + NH_4OH \rightarrow NH_4C1 + H_2O$$



#### 4. Weak acid Vs weak base Titration:

Consider the titration of acetic acid against ammonium hydroxide. The titration of weak acid with weak base does not give sharp end point by volumetric titrations. The initial conductance of the solution is low due to the poor dissociation of weak acid, but starts raising as CH<sub>3</sub>COONH<sub>4</sub> is formed. After the equivalent point, the conductivity remains almost constant because the free base NH<sub>4</sub>OH is weak electrolyte. The end point is quite sharp by conductometric titrations

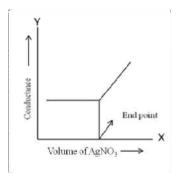
$$CH_3COOH + NH_4OH \rightarrow CH_3COONH_4 + H_2O$$



# 5. Precipitation titrations:

In precipitation titrations, sharp endpoint is obtained, e.g. The titration of KCl against AgNO<sub>3</sub>. There is no sharp increase in conductance after the addition of AgNO<sub>3</sub>, because the mobility of K<sup>+</sup> and Ag <sup>+</sup> is one and the same. After the end point, there is a sharp increase in conductance due to an increase in the number of free ions in the solution.

$$KCl + AgNO_3 \rightarrow KNO_3 + AgCl (ppt)$$



# Advantages of conductometric titrations:

- 1. The results obtained by conductometric titrations are more accurate because the end point is obtained graphically.
- 2. The titrations of a weak acid with a weak base do not give a sharp end point with indicator in volumetric titrations. Accurate results are

- obtained in conductometric titrations.
- 3. Colored solutions where no indicator is found to work satisfactorily can be successfully titrated.
- 4. Conductometric titrations can be used even in case of polybasic acids.

#### **Precautions:**

- 1. The temperature must be kept constant throughout the experiment.
- 2. In acid—base titration, the titrant should be about 10 times stronger than the solution to be titrated so that the volume change is as little as possible.

# 2. Define primary and secondary cells? Write about construction and working of lithium-ion battery with neat diagram?

Primary cells are the ones which cannot be recharged and have to be discarded after the expiration of the lifetime.

Secondary cells need to be recharged when the charge gets over.

Both the types of battery are used extensively in various appliances and these cells differ in size and material used in them.

Difference between Primary Cell and Secondary Cell		
Primary Cell	Secondary Cell	
Have high energy density and slow in discharge and easy to use	They have smaller energy density	
There are no fluids in the cells hence	These are made up of wet cells (flooded and liquid cells) and molten salt (liquid cells with different composition)	
it is also called as dry cells		
It has high internal resistance	It has a low internal resistance	
It has an irreversible chemical	It has a reversible chemical reaction	
reaction		
Its design is smaller and lighter	Its design is more complex and heavier	
Its initial cost is cheap	Its initial cost is high	

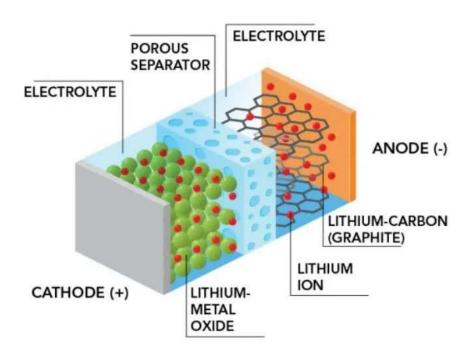
A lithium-ion (Li-ion) battery is a type of **rechargeable battery** that uses lithium ions as the main component of its electrochemical cells. It is **characterised** by **high energy density**, fast charge, long cycle life, and wide temperature range operation. Lithium-ion batteries have been **credited** for revolutionising communications and transportation, enabling the rise of super-slim smartphones and electric cars with a practical range such as portable electronics and electrified transportation.

M. Stanley Whittingham, John B. Goodenough, and Akira Yoshino received the **Nobel Prize in Chemistry** for their contributions to the development of the **modern Li-ion battery in 2019.** 

#### **Lithium-ion Battery Structure**

A lithium-ion battery consists of an **anode** (negative electrode), **cathode** (positive electrode), separator, electrolyte, and two current collectors (positive and negative).

# PARTS OF A LITHIUM-ION BATTERY



Cathode: The cathode of a lithium-ion battery is typically made of a lithium metal oxide, such as lithium cobalt oxide (LiCoO2), lithium manganese oxide (LiMn2O4), or lithium iron phosphate (LiFePO4).

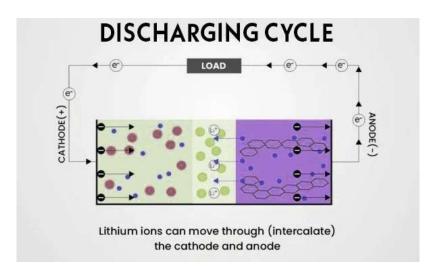
The choice of cathode material influences the performance characteristics of the battery.

- Anode: The anode is usually composed of graphite. During discharge, lithium ions move from the anode to the cathode through the electrolyte, and during charging, they move back to the anode.
- **Electrolyte:** The electrolyte is a **conductive medium** that allows the flow of lithium ions between the cathode and anode.
  - o It is typically a **lithium salt** dissolved in a solvent.
- **Separator:** The separator is a **permeable membrane** that keeps the cathode and anode apart to prevent a short circuit while allowing the passage of lithium ions.
- Rechargeability: One of the key advantages of lithium-ion batteries is their rechargeability.

 They can be recharged hundreds to thousands of times, depending on the specific chemistry and use conditions such as overcharging or undercharging.

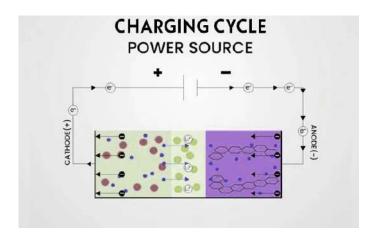
#### **Working of Lithium-ion Battery**

Working principle of Lithium-ion Battery based on **electrochemical reaction**. Inside a lithium-ion battery, **oxidation-reduction (Redox)** reactions take place which sustain the charging and discharging cycle.



#### • Discharging:

- o During this cycle, **lithium ions** form from the ionization of lithium atoms in the anode.
  - Oxidation reaction takes place:  $LiC6 \rightarrow C6 + Li + e$
- The lithium ions move from the anode and pass through the electrolyte until they reach the cathode, where they recombine with their electrons and electrically neutralise.
- The lithium ions are small enough to be able to move through a micropermeable separator between the anode and cathode.
- Li-ion batteries are capable of having a very high voltage and charge storage per unit mass and unit volume owing to the small size of lithium.



#### Charging cycle:

- o **During the charging cycle**, the process is exactly the opposite of the discharging cycle. The lithium ions return to the anode from the cathode and electrons are transferred from the anode to the cathode.
- o Lithium ions flow from the cathode to the anode, and electrons flow from the **anode to the cathode**, as the battery is charging.
- o There is a **steady flow of electrons** as long as lithium ions are making their way from one electrode to the next.
- o **Reduction** takes place at the cathode  $-CoO2 + Li + e \rightarrow LiCoO2$  (Cobalt oxide combines with lithium ions to form lithium-cobalt oxide (LiCoO2).

#### Lithium-ion Battery Significance

The excellent electrochemical properties of lithium such as highly reactive properties give Lithium the potential for high-density batteries, enhanced standby power, complacent design, etc.

- **High charge density**: Since lithium is the most electropositive element, it has a high charge density, and can give a lot of energy without being very heavy. This means they can store a significant amount of energy for their size and weight.
  - o **Electropositivity** is a measure of how easily an element can produce positive ions or how easily an element can produce energy.
- Compact design: They can store a large amount of energy in a relatively small and lightweight package.
- Low self-discharge rate: They also exhibit a relatively low self-discharge rate when compared to other rechargeable batteries, allowing them to hold their charge for extended periods.
- **High-scale current:** Lithium-ion batteries can deliver large amounts of current for high-power applications.
  - o For example- Lithium-ion battery cells can deliver up to 3.6 Volts, 3 times greater than any present technology.
- No memory effect: Lithium-ion batteries have no memory effect, a detrimental process where repeated partial discharge/charge cycles can cause a battery to 'remember' a lower capacity.
- Free-form toxic materials: These batteries do not contain toxic cadmium, which makes them easier to dispose of than Ni-Cd batteries.
- Fossil Fuel-free society: Modern society is completely dependent on fossil fuels, and lithium-ion batteries have great potential to replace the internal combustion engine and store solar energy, and wind energy, which will reduce dependency on fossil fuels by providing sustainable renewable energy.

#### **Lithium-ion Battery Application**

The versatility and performance characteristics of lithium-ion batteries make them a preferred choice in a wide range of applications, such as aerospace, electric vehicles, electronics industries, etc.

- **Portable electronic devices:** Lithium-ion batteries are predominantly used in various portable electronic devices such as **smartphones** and **laptops** etc.
- **High-end application:** It can also be employed to power electrical systems for aerospace applications and submarines.
  - o For Example, Aircraft-Boeing 787, where weight is a significant cost factor.
- Hybrid electric vehicles: Lithium-ion technology so far has the best option for
  potential applications in battery-powered vehicles with a practical range thereby
  reducing dependency on fossil fuels.
- Example- Tesla's Model S cars are using a P85 battery consisting of 18,650 Liion cells, with an energy output of 80-90 kWh.
- **Defence:** Various submarines are using lithium-ion batteries as a source of power back in emergency and enhanced stealth operation.
- **Medical devices:** They are used in cardiac pacemakers and other implantable devices.

#### **Lithium-ion Battery Disadvantages**

Despite several promising applications of lithium-ion batteries, they have certain limitations:

- **Highly Inflammable:** The batteries tend to overheat and can face insulation failure at high voltages.
  - o In some cases, this can lead to thermal runaway and combustion.
- **Performance constraints:** Lithium-ion batteries face the situation of increased weight and **limited performance** in some cases due to the requirement of safety mechanisms to limit voltage and internal pressures.
- Low self-life: Lithium-ion batteries are also subject to ageing, meaning that they can lose capacity and frequently fail after some years.
- Heavily dependent on imports: Another factor limiting their widespread adoption is their uneven geographical distribution of lithium leading to higher cost, which is around 40% higher than Ni-Cd.
  - 3. Define Fuel cells? Write about construction and working of H<sub>2</sub>-O<sub>2</sub> fuel cell and polymeric electrolyte membrane fuel cell with neat diagram?

#### **FUEL CELLS**

**Definition:** A fuel cell is an electrochemical which converts chemical energy contained in readily available fuel oxidant system into electrical energy.

**Principle:** The basic principle of fuel cell is as same as that of an electrochemical cell. The fuel cell operates like a galvanic cell. The only difference is that the fuel and the oxidant are stored outside the cell. Fuel

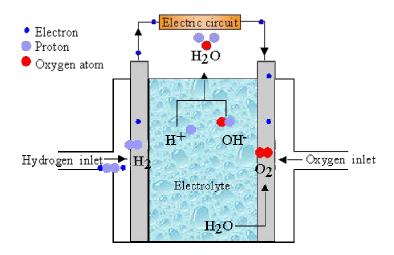
and oxidant are supplied continuously and separately to the electrodes at which they undergo redox reaction. Fuel cells are capable of supplying current as long as reactants are replenished.

Examples: 1. H<sub>2</sub>-O<sub>2</sub> fuel cell

2. CH<sub>3</sub>OH-O<sub>2</sub> fuel cell

#### Hydrogen oxygen fuel cell:

This cell is a common type of fuel cell. Similar to a galvanic cell, fuel cell also have two half cells. Both half cells have porous graphite electrode with a catalyst (platinum, silver or a metal oxide). The electrodes are placed in the aqueous solution of NaOH or KOH which acts as an electrolyte. Hydrogen and oxygen are supplied at anode and cathode respectively at about 50 atmospheric pressure, the gases diffuse at respective electrodes. The two half-cell reactions are as follows;



**At anode:**  $2H_2$  (g) +  $4OH^-$  (aq)

 $\rightarrow$  4H<sub>2</sub>O (I) + 4e<sup>-</sup> At cathode: O<sub>2</sub>

(g) +  $2H_2O$  (l) +  $4e^- \rightarrow 4OH^-$ 

(aq) The net reaction:  $2H_2(g) +$ 

 $O_2(g) \rightarrow 2H_2O(I)$ 

The EMF of this cell is measured to be 1.23V. A number of such fuel cell are stacked together in series to make a battery.

#### **Advantages:**

- 1. The energy conversion is very high (75-82%).
- 2. Fuel cell minimizes expensive transmission lines and transmission losses.
- 3. It has high reliability in electricity generation.
- 4. The byproducts are environmentally acceptable.
- 5. Maintenance cost is low for these fuels.
- 6. They save fossil fuels.
- 7. Noise and thermal pollution are very low.
- 8. They have low maintenance cost.
- 9. They have quick start system.

#### **Disadvantages:**

- 1. The major disadvantage of the fuel cell is the high cost and the problems of durability and storage of large amount of hydrogen.
- 2. The accurate life time is also not known.

### **APPLICATIONS:**

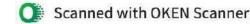
- 1. The most important application of a fuel cell is its use in space vehicles, submarine or military vehicles.
- 2. The product H<sub>2</sub>O is valuable source of fresh water by the astronauts.
- 3. It is hoped that fuel cell technology will bring a revolution in the area of energy production.
- 4. Fuel cell batteries for automotive will be a great boom for the future.

#### **Limitations:**

- 1. The life time of fuel cells is not accurately known
- 2. It cannot store electricity
- 3. Electrodes are expensive ad short lived.
- 4. Storage and handling of H<sub>2</sub> gas is dangerous because it is inflammable.
- 4. Derive Nernest equation and numerical problems?

**Derivation of Nernst equation:** Nernst found that the single electrode potential varies with the change in concentration of ions and temperature and hence the EMF of the cell also varies. He derived a mathematical relationship between the standard electrode potential, temperature and the concentration of ions. This relationship is known as the Nernst equation.

Consider the redox reaction:  $M^{n+} + ne^{-} \rightleftharpoons M$ 



In the above reversible reaction the free energy change (G) and its equilibrium constant (K) are related by the following equation which is popularly known as Van't Hoff reaction isotherm.

$$\Delta G = RT \ln K + RT \ln \frac{product}{reactant}$$

$$\Delta G = \Delta G^0 + R \frac{\text{product}}{\text{reactant}}$$

When  $\Delta$  G<sup>0</sup> is the standard free energy change

The free energy change is equivalent to the electrical

energy 
$$-nFE$$
 Where  $n = valency$ 

F = Faraday

(96500

coloumbs)

E =

Electrode

potential

$$R = 8.314 \text{ Joules K}^{-1}$$

mole<sup>-1</sup>(Gas constant) T

= Temperature (K)

$$-nFE = -nFE^0 + RTln([M])/([M^{n+}])$$
 (Concentration of M is unity)

-nFE = - 
$$nFE^0 - RTln [M^{n+}]$$

$$= - nFE^0 - RT2.303 \log_{10} [M^{n+}]$$

Dividing the equation by -nF

$$E = E^{0+} + \frac{2.303RT}{nF} \log_{10} [M^{n+}]$$

$$E = E^{0} + \frac{0.0591}{n} \log_{10} [M^{n+}]$$

# **APPLICATIONS OF NERNST EQUATION:**

- 4. It can be used to study the effect of electrolyte concentration on electrode potential.  $E = E^{\circ} RT/nF \ln[1/M^{n+}]$
- 5. It can also be used for the calculation of the potential of a cell under non-standard conditions.

#### **MCQs**

- **1.** In a galvanic cell, which of the following statements is correct?
- A) Oxidation occurs at the cathode
- B) Reduction occurs at the anode
- C) Electrons flow from cathode to anode
- D) Oxidation occurs at the anode

✓Answer: D

**Explanation:** In a galvanic cell, oxidation takes place at the anode and reduction at the cathode.

- **2.** The standard electrode potential of  $Zn^{2+}/Zn$  and  $Cu^{2+}/Cu$  are -0.76 V and +0.34 V respectively. The EMF of the cell  $Zn \mid Zn^{2+} \mid Cu^{2+} \mid Cu$  is:
- A) 0.10 V
- B) 0.42 V
- C) 1.10 V
- D) 1.50 V

✓Answer: C

**Explanation:** Ecell=E <sub>cathode</sub>-E<sub>anode</sub>=0.34-(-0.76)=1.10V

# □ NERNST EQUATION & CELL POTENTIAL

- **3.** The Nernst equation for a half-cell reaction is given by:
- A)  $E=E^{\circ}+RTnF lnQ$
- B) E=E°-RT/nF lnQ
- C)  $E=E^{\circ}+nF \ln Q$
- D)  $E=E^{\circ}-RT/NfQ$

✓Answer: B

**4.** For the cell reaction:

 $Zn + Cu^{2+} \rightarrow Zn^{2+} + Cu,$ 

if  $[Zn^{2+}] = 0.1$  M and  $[Cu^{2+}] = 1$  M, the EMF at 25°C is approximately:

- A) 1.10 V
- B) 1.12 V
- C) 1.08 V
- D) 1.00 V

✓Answer: C

#### **Explanation:**

 $E_{cell}\!\!=\!\!E_{cathode}\!\!-\!\!E_{anode}$ 

- $E_{Cu2+/Cu} = +0.34 \text{ V}$
- $E_{Zn2+/Zn} = -0.76 \text{ V}$
- Ecell =0.34-(-0.76)=1.10 V

 $E=1.10-20.0591 \log(0.1)$ 

log(0.1)=-1

 $E=1.10-20.0591\times(-1)$ 

E=1.10+0.02955

E≈1.1295 V≈1.13 V

#### □ □ POTENTIOMETRY

- **5.** Potentiometry is based on the measurement of:
- A) Current at constant potential
- B) Potential at zero current
- C) Resistance at constant current
- D) Conductance at constant potential

✓Answer: B

**Explanation:** Potentiometric measurements involve determining potential differences under zero current flow conditions.

- **6.** Which electrode is commonly used as a reference electrode in potentiometry?
- A) Glass electrode
- B) Calomel electrode
- C) Silver electrode
- D) Platinum electrode

✓Answer: B

**Explanation:** The saturated calomel electrode (SCE) is a common reference electrode.

- 7. In potentiometric **redox titration**, the potential change is due to:
- A) pH variation
- B) Change in ion concentration
- C) Electron transfer between oxidant and reductant
- D) Change in temperature

✓Answer: C

### □ CONDUCTIVITY & CONDUCTOMETRIC TITRATIONS

- **8.** The unit of specific conductivity ( $\kappa$ ) is:
- A)  $\Omega$  cm
- B)  $\Omega^{-1}$  cm<sup>-1</sup>
- C) S m
- D) mho cm

✓Answer: B

**Explanation:** Conductivity ( $\kappa$ ) has the unit Siemens per centimetre (S cm<sup>-1</sup> or  $\Omega^{-1}$  cm<sup>-1</sup>).

- **9.** Molar conductivity ( $\Lambda$ m) increases with dilution because:
- A) Ion concentration increases
- B) Ion mobility increases
- C) Ion-pair formation increases
- D) Temperature decreases

✓Answer: B

**Explanation:** On dilution, interionic attraction decreases  $\rightarrow$  ion mobility increases  $\rightarrow$   $\Delta$ m increases.

- **10.** In conductometric acid–base titration, the end point is determined by:
- A) Sharp potential change
- B) Minimum conductance
- C) Maximum conductance
- D) Constant temperature

✓Answer: B

**Explanation:** Conductance decreases, then increases — the minimum point corresponds to the equivalence point.

### □ □ ELECTROCHEMICAL SENSORS

- **11.** A glass electrode is an example of a:
- A) Amperometric sensor
- B) Conductometric sensor
- C) Potentiometric sensor
- D) Optical sensor

✓Answer: C

**Explanation:** Glass electrode measures pH via potential difference  $\rightarrow$  a potentiometric sensor.

### 12. The Clark oxygen electrode is an example of:

- A) Potentiometric sensor
- B) Amperometric sensor
- C) Conductometric sensor
- D) Optical biosensor

✓Answer: B

**Explanation:** Clark electrode measures current produced by oxygen reduction at a cathode (amperometric principle).

- **13.** Amperometric sensors operate at:
- A) Constant voltage, measuring current
- B) Constant current, measuring voltage
- C) Variable resistance
- D) Constant power

✓Answer: A

**Explanation:** They maintain a fixed potential and measure the resulting current due to redox reactions.

- **14.** Which of the following is used in glucose biosensors?
- A) Glass electrode
- B) Clark oxygen electrode
- C) pH electrode
- D) Silver-silver chloride electrode

✓Answer: B

**Explanation:** Glucose oxidase enzyme reacts with glucose producing oxygen changes detected by Clark electrode.

- **15.** Conductivity cell constant depends on:
- A) Concentration of electrolyte
- B) Geometry of electrodes
- C) Nature of solvent
- D) Applied voltage
- ✓Answer: B

**Explanation:** Cell constant = distance between electrodes / area of electrodes.

## Electrochemical Cells MCQs

- 1. Primary Cells Zinc–Air Battery
- 1. Zinc—air battery is a type of:
- A) Primary cell
- B) Secondary cell
- C) Fuel cell
- D) Electrolytic cell
- ✓ Answer: A) Primary cell
- **2.** In a zinc–air cell, the **anode** is made of:
- A) Carbon
- B) Zinc
- C) Nickel
- D) Platinum
- ✓Answer: B) Zinc
- **3.** The **cathode reaction** in a zinc—air cell involves:
- A) Reduction of Zn<sup>2+</sup> ions
- B) Oxidation of O<sub>2</sub> gas
- C) Reduction of O2 gas
- D) Oxidation of H<sub>2</sub>O
- Answer: C) Reduction of O<sub>2</sub> gas
- **4.** The **overall reaction** in a zinc—air battery is:
- A)  $Zn + \frac{1}{2}O_2 \rightarrow ZnO$
- B)  $Zn + O_2 \rightarrow ZnO_2$
- C)  $Zn + O_2 \rightarrow ZnO$
- D)  $Zn \rightarrow Zn^{2+} + 2e^{-}$
- ✓ Answer: C)  $Zn + O_2 \rightarrow ZnO$
- **5.** Zinc—air batteries are **non-rechargeable** because:
- A) Zinc electrode gets corroded
- B) Electrolyte dries up
- C) Reaction is irreversible

D) All of the above

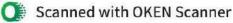
✓ **Answer:** D) All of the above

### 2. Secondary Cells – Lithium-Ion Batteries

- **6.** Lithium-ion batteries are:
- A) Primary cells
- B) Secondary cells
- C) Fuel cells
- D) Voltaic cells
- Answer: B) Secondary cells
- 7. The anode in a Li-ion cell is usually made of:
- A) Lithium metal
- B) Graphite
- C) Nickel
- D) Zinc
- ✓ **Answer:** B) Graphite
- **8.** The **cathode** in a Li-ion battery is commonly made of:
- A) Lithium cobalt oxide (LiCoO<sub>2</sub>)
- B) Zinc oxide
- C) Manganese dioxide
- D) Nickel-cadmium
- Answer: A) Lithium cobalt oxide (LiCoO<sub>2</sub>)
- **9.** The **overall cell reaction** during discharge of Li-ion battery:
- A) Li<sup>+</sup> moves from cathode  $\rightarrow$  anode
- B)  $Li^+$  moves from anode  $\rightarrow$  cathode
- C) Electrons move through electrolyte
- D) Lithium ions are not involved
- ✓ **Answer:** B) Li<sup>+</sup> moves from anode  $\rightarrow$  cathode
- 10. The electrolyte in lithium-ion cells is usually:
- A) KOH solution
- B) H<sub>2</sub>SO<sub>4</sub>
- C) LiPF<sub>6</sub> in organic solvent
- D) NaCl aqueous solution
- ✓ **Answer:** C) LiPF<sub>6</sub> in organic solvent

### 3. Fuel Cells - Hydrogen-Oxygen Fuel Cell

- 11. Hydrogen–oxygen fuel cell is an example of:
- A) Primary cell
- B) Secondary cell



- C) Fuel cell
- D) Dry cell
- Answer: C) Fuel cell
- 12. In a hydrogen-oxygen fuel cell, electrolyte used is:
- A) Concentrated H<sub>2</sub>SO<sub>4</sub>
- B) KOH solution
- C) NaCl solution
- D) HCl solution
- ✓ **Answer:** B) KOH solution
- 13. The anode reaction in hydrogen—oxygen fuel cell:
- A)  $O_2 + 4H^+ + 4e^- \rightarrow 2H_2O$
- B)  $2H_2 \rightarrow 4H^+ + 4e^-$
- C)  $H_2 + O_2 \rightarrow H_2O$
- D)  $O_2 \rightarrow 2O^{2-}$
- Answer: B)  $2H_2 \rightarrow 4H^+ + 4e^-$
- **14.** The **cathode reaction** in hydrogen—oxygen fuel cell:
- A)  $4H^+ + O_2 + 4e^- \rightarrow 2H_2O$
- B)  $2H_2 \rightarrow 4H^+ + 4e^-$
- C)  $O_2 + 2H_2O \rightarrow 4OH^-$
- D)  $O_2 \rightarrow 2O^{2-}$
- **Answer:** A)  $4H^+ + O_2 + 4e^- \rightarrow 2H_2O$
- 15. The overall cell reaction is:
- A)  $H_2 + \frac{1}{2}O_2 \rightarrow H_2O$
- $\stackrel{\frown}{B}$   $H_2 + O_2 \rightarrow 2H_2O$
- C)  $2H_2 + O_2 \rightarrow 2H_2O$
- D)  $H_2O \rightarrow H_2 + \frac{1}{2}O_2$
- Answer: C)  $2H_2 + O_2 \rightarrow 2H_2O$
- 4. Polymer Electrolyte Membrane Fuel Cell (PEMFC)
- **16.** The **electrolyte** in a PEM fuel cell is:
- A) Aqueous KOH
- B) Phosphoric acid
- C) Solid polymer membrane (Nafion)
- D) Molten carbonate
- Answer: C) Solid polymer membrane (Nafion)
- **17.** The **working temperature** of PEM fuel cell is typically:
- A) 1000°C
- B) 600°C
- C) 80°C
- D) 25°C
- Answer: C) 80°C

18. The anode reaction in a PEMFC is:

A) 
$$H_2 \rightarrow 2H^+ + 2e^-$$

B) 
$$O_2 + 4H^+ + 4e^- \rightarrow 2H_2O$$

C) 
$$2H_2 + O_2 \rightarrow 2H_2O$$

D) 
$$H_2O \to H_2 + \frac{1}{2}O_2$$

Answer: A) 
$$H_2 \rightarrow 2H^+ + 2e^-$$

19. The cathode reaction in a PEMFC is:

A) 
$$O_2 + 4H^+ + 4e^- \rightarrow 2H_2O$$

B) 
$$2H_2 \rightarrow 4H^+ + 4e^-$$

C) 
$$H_2 + \frac{1}{2}O_2 \rightarrow H_2O$$

D) 
$$H_2O \rightarrow H_2 + \frac{1}{2}O_2$$

**✓Answer:** A) 
$$O_2 + 4H^+ + 4e^- \rightarrow 2H_2O$$

20. The main advantage of PEM fuel cells is:

- A) High operating temperature
- B) Fast start-up, compact design
- C) Use of molten electrolytes
- D) Low efficiency

✓ Answer: B) Fast start-up, compact design

### 5. Conceptual & Application-Based

**21.** Which cell is rechargeable?

- A) Zinc-air cell
- B) Lithium-ion cell
- C) Dry cell
- D) Fuel cell

✓ **Answer:** B) Lithium-ion cell

**22.** Which of the following directly converts chemical energy to electrical energy **continuously** as fuel is supplied?

- A) Primary cell
- B) Secondary cell
- C) Fuel cell
- D) Electrolytic cell

✓ Answer: C) Fuel cell

23. In fuel cells, electrodes are:

- A) Consumed in reaction
- B) Permanent catalysts
- C) Made of zinc only
- D) Replaced after each use

✓ **Answer:** B) Permanent catalysts

**24.** The byproduct of hydrogen–oxygen fuel cell is:

A) CO<sub>2</sub>

- B) SO<sub>2</sub>
- C) H<sub>2</sub>O
- D) H<sub>2</sub>S

✓Answer: C) H<sub>2</sub>O

- **25.** The **efficiency** of a hydrogen–oxygen fuel cell is approximately:
- A) 10–20%
- B) 25–35%
- C) 50–60%
- D) 90-100%
- ✓**Answer:** C) 50–60%

#### **UNIT IV**

### **POLYMER CHEMISTRY**

### 1. Introduction to Polymers

**Q:** What is a polymer?

**A:** A polymer is a large molecule composed of repeating structural units called monomers, linked by covalent bonds.

**Q:** Give examples of natural and synthetic polymers.

**A**:

• Natural: Cellulose, rubber, proteins

• Synthetic: Polyethylene (PE), Nylon-6,6, Polystyrene (PS)

### 2. Functionality of Monomers

**Q:** What is the functionality of a monomer?

**A:** Functionality is the number of reactive sites on a monomer molecule that can form bonds during polymerization.

**Q:** Give an example.

**A:** Ethylene (C<sub>2</sub>H<sub>4</sub>) has a functionality of 2 (one double bond), allowing it to form polyethylene.

### 3. Polymerization Methods

### A. Chain Growth Polymerization

**Q:** What is chain growth polymerization?

**A:** Polymerization where monomers add to an active site on a growing chain, e.g., free radical polymerization.

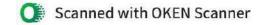
**Q:** Example and mechanism.

A: Polyethylene (PE)

- Initiation: Formation of radical by decomposing initiator (e.g., benzoyl peroxide)
- Propagation: Radical reacts with monomer → chain grows
- Termination: Two radicals combine → polymer chain ends

### **B. Step Growth Polymerization**

**Q:** What is step growth polymerization?



**A:** Polymerization where monomers with two or more reactive groups react stepwise to form dimers, trimers, and eventually high molecular weight polymer.

**Q:** Example and mechanism.

### **A:** Nylon-6,6

- Monomers: Hexamethylenediamine + Adipic acid
- Mechanism: Condensation reaction with release of water → amide bond formation

### C. Coordination Polymerization

**Q:** What is coordination polymerization?

**A:** Polymerization using metal catalysts (e.g., Ziegler–Natta catalyst) to control polymer structure and stereochemistry.

**Q:** Example.

**A: Polypropylene** – isotactic polypropylene produced via Ziegler-Natta catalysis.

#### 4. Plastics

**Q:** Differentiate thermoplastics and thermosetting plastics.

A:

- Thermoplastics: Soften on heating, can be reshaped (e.g., PVC, Teflon)
- **Thermosetting:** Harden permanently on heating, cannot be reshaped (e.g., Bakelite, epoxy)

Q: Examples, preparation, and uses:\*\*

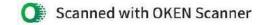
- PVC (Polyvinyl Chloride): Chain growth polymerization; pipes, flooring
- **Teflon (PTFE):** Free radical polymerization of tetrafluoroethylene; non-stick coatings
- **Bakelite:** Phenol + formaldehyde; thermosetting; electrical insulators
- Nylon-6,6: Step growth condensation; fibers, textiles
- Carbon fibers: Pyrolysis of polyacrylonitrile; high strength, aerospace

#### 5. Elastomers

**Q:** What are elastomers?\*\*

**A:** Polymers that can stretch and recover their original shape.

O: Examples:\*\*



- **Buna-S:** Copolymer of butadiene and styrene; tires, shoes
- Buna-N: Copolymer of butadiene and acrylonitrile; oil-resistant gaskets

### 6. Conducting Polymers

**Q:** What are conducting polymers?\*\*

**A:** Polymers that conduct electricity due to conjugated double bonds.

Q: Examples and conduction mechanism:\*\*

• Polyacetylene: Doping with halogens increases conductivity

• **Polyaniline:** Protonation/doping enhances conductivity **Applications:** Flexible electronics, sensors, batteries

### 7. Biodegradable Polymers

Q: Examples of biodegradable polymers:\*\*

A:

- Poly Glycolic Acid (PGA): Sutures, tissue engineering
- Poly Lactic Acid (PLA): Packaging, biomedical devices

**Q:** Why are they biodegradable?

**A:** They can hydrolyze or be metabolized into non-toxic products in the environment.

### **EASSAY QUESTIONS**

1. Write the addition polymerization and condensation polymerization? Write specific examples with mechanisms?

2) Chain Polymerisation:

This is also called addition polymerisation.

In this polymerisation, the functionality of monomer is double bond.

No biproducts like 11:0, cH3011 etc., one formed.

The molecular weight of the polymer is the exact multiple of the polymer is the exact multiple.

The polymers is the exact multiple of the polymers is the exact multiple of the polymers.

chain polynamical containing double bonds undergo chain polynamication.

For example: i) oletins ii) viril iii) ally and iv) dieres.

ACH\_1 = CH\_2 - Blumaticaling - (CIII\_2)\_1

Polyellylene

In CH\_2 = CH - Blumaticaling - (CIII\_2 - CIII\_2)\_1

Viryl chloride - Bly viryl chloride

In CH\_2 = CH - CII\_2 - CI - Blumaticaling - (CII\_2 - CII)\_1

CI - CII\_2 - CI - CII\_2 - CI - Blumaticaling - (CII\_2 - CII)\_1

CI - CII\_2 - CII - CII\_2 - CI - Blumaticaling - (CII\_2 - CII\_2 -

(in) Condensation Bymesiscones. Alicentario of hopimerivation takes blace ph congenishing inchanal groups of the monoments. Hence known as condensation polymerisation. .comple! 1) Formation of Byrster: riacid 4. DIOI - Pobjester + water Poly eligiblene texe phthalate Temphilic acid . eligiene gycol (8) PET Polyester Enthurs Fagos ii) Formition of Nylon 6:6: n 8000-{cH2+ cooH + n HN-{cH2+ NH2-Napou e:e . hoxa methylene diamine . Adepic ocid Characteristics of condensation <u>Polymerisation</u>; a) The monomous contain functional groups like -OH, -COOH, -6 -NH etc. b) This polymerisation is accompanied by the elimination of: 3 biproducks. like Hcl, HLO, NH3, CHOOH etc. 10 c) The functionality. As the monomer must be two or more: 16 than two. 10 d) The molecular weight of the polymer is not the sum the molecular weights & the monomous. 6 0 0

Mirro moleal

mechanism involves the following steps: o) Propagation slep 3) Texmination slep 1) Initiation slep

by two reactions. 1) soiliation slep: This step takes place The first is the production of tree radicals, the second addition of this radical to the first monomeric molec chain initiating species Mi. produce 1Re

> Free radicals initialor

'chain initiating species monomex

example: R+ CH2 = CH2 - R-CH2-CH2.

a) Propogation step: This step involves successive addition of large number of monomer molecules

3) chain Termination: chain termination takes place either by coupling reaction & dispropostionation reaction.

Disproportionation:

ii) Ionic Mechanism:

Conic mechanism is again classified into

à types.

A) Cationic mechanism . B) Anionic mechanism

A) Caltonie <u>Mechanism</u>:

# क्षेत्रिक्ष्यकींका

## 3) Termination

$$Z \leftarrow CH_2 - CH_$$

- 2. Write the coordination polymerization? Write specific examples with mechanisms?
- iii) Co-ordination polymerisation mechanism:

This mechanism is suggested by Zeiglez and Natto. In IRIS mechanism, a cambination of transition metal. halide and trialkyl aluminium is used as aid This catalyst is called zeiglar Natta catalyst. So, IRIS mechanism is also called zeiglar Natta catalysis.

one example for the zeighor- Noths cotalyst

Thonium Tetro chloride + Tri ethyl aluminium

Ti clu + (e,115) and

These two compounds react with each offered. Page a citabell compounds

This complex of cologs to active cologs in the mechanism.

mechanism & polymexication 1/1 given below:

## a) Initiation:

The catalyst form monomer calolyst complexes of will monomer molecule.

Cat-R + CHz=CH-

The !! mornomer catalyst complex reacts with fresh resulting the chain growth.

Cat- $cH_2$ -cH-R +  $cH_3$ =cH  $\longrightarrow$  Cat- $cH_2$ -cH- $cH_3$ -cH-R

Termination 1. carried out with an active halogen compound.

Cat-cil\_cil-cil-cil-cil-cil-R +HX --- Cat-X+ cil3-cil-(cil\_-cil)-R growing polymer

- 3. Write the Preparations of following Polymers
  - a) BUNA-S b) BUNA-N c) Bakelite d) Nylon 6,6 e) Teflon

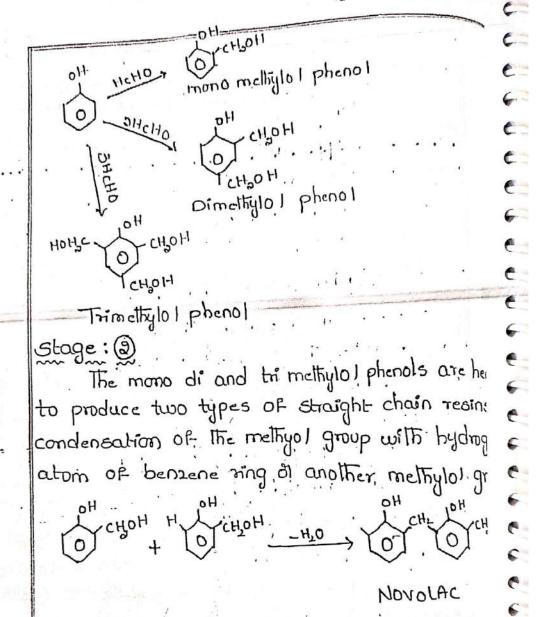
# \* Bakelite: (01) phenol-formaldehyde resin:

Bakelile is an important thermoset resin-It Preparation:

Bakelile is prepared by the slep polymerisation

of phenol with formaldehyde in presence of acid of alkali as a catalyst this polymensation takes place in 3 stages.

phenol is made to react with formal dehyde in presence of acid/alkali to produce nonpolymenic mono, di and tri methyol phenolo, depending on the phenol - formaldehyde ratio.



Stage: 3

this stage of preparation includes heating of Novolac, to produce Bakel

· CHO H CIPOII + CHIOH

Toperties:

)

1. It is hard, rigid and strong

2. Starch and water resistant

Good chemical resistant.

Excellent electrical insulator

5. Very good adhesive ;

Good comosion and atmospheric resistance

Engineering Applications:

Bakelite has wide range of applications,

1- Used to make electrical insulator parts like Switches, switch boards, heater hardles

2. Used to make telephone parls, radio & Tv cabinels.

Good anion éxechange resin.

Preparation: It is prepared by co-polymerisation

OF 715% 1,3 butadienc and 215%. Styrene in prese of peroxide catalyst at 50.c. Buna-S 1,3 butadiene i. High abrasion resistant High toading capacity. iii. poor resilience property IV. It swells in oils and solvents v. Low oxidation resistant, specially with traces of Uses: Used for motor pipes, shoe sols, foot wear, gaskets, adhesives, insulating cable wires, tank lin carpet backing, electrical insulation etc--

Cie 1 Buna - N: (Nitrile Rubber) Bieparation: It is prepared by polymerisation of ocry nitrile with 1,3-butadiene in presence of 1,0; catalyst.  $CH_{2}=CH+CH_{2}=CH-CH=CH_{2}\longrightarrow -\left\{ CH_{2}-CH-CH_{2}-CH=CH-CH_{2}\right\}$ 1,3 buladiene acylatrile Buna-N i). Excellent : Desistance to oils ii) High abrasion, nesistance and good tensile strength 111) Excellent: resistance to heat, sunlight and acids -iv) It is less resistant to alkalies because of CN group. -. Gaskets, adhesives, convoyor bulls -> used in oil aesistant toams - Tank Unings Aircraft components

n moc (chrt coon + n HN-(chrt NH= ) { (Chrt C-NH-(Chr) NH) } ii) Formation of Mylon 6:6: Adepte acid hexamethylene diamine

() C

> 0 0

### Polytetrafluoroethylene (Teflon)

Teflon is manufactured by free-radical polymerization of tetrafluoroethylene. The catalyst used is per sulphate at high pressure. The reaction is given as:

$$n F_2C=CF_2 \rightarrow -(F_2C-CF_2)_n$$

Teflon is hydrophobic and is inert in nature. It is used in making a non-stick coating for cookware and also as a lubricant in machinery to reduce friction.

4. What are Conducting Polymers and discuss various examples and mechanism of conduction?

Conducting polymers:

The polymers which conduct electricity as called conducting polymers. The conductivity of polymers may be due to unsaturation of due to the presence of externally added ingredients in them.

The conducting polymers can be classified.

Conducting polymers Intrinsic Extrinsic' conducting polymers. · conducting . polymer > conductive element conjugated Doped filled polymers conducting Polymers Es: - carbon black in. Polymers Blended Eg:- Poly acetylene conducting polymens p-doped n-doped boshbase) Conducting polymers: These polymers having conjugation in the backbone of the polymer. Again these are two types. · conjugated conducting polymers: these polymers have conjugated double bonds in the backbone the polymer. Their conductivity 3, is due to II - electrons. 0, -Geamples :-1) acetylene: n CH = CH Polymenisation poly acetylene.

n (ND Hollancisalius - (N) boly bhalle. Bilmol c

Doped conducting polymers.

The conductivity of conjugated polyrnors can be enhanced by introducing a positive charge of negative charge on polymer backbone by Oseidation or reduction. This process is caucal doping.

Doping is again two types.

a) P-doping b) n-doping.

a) p-doping: p-doping is done by oxidation of a conjugated polymer with a Lewis aud. During this process, removal of The electron from Polymer backbone leads to the formation of a radical cation (1) polaron. The second Oxeidation of polaron forms bipolaron.

/// + lewis Acid ==>/ Poly acetylone ( ladical cation)

Bi polaro

b) n-doping: n-doping is done by reduction of a conjugated polymer with a Lewis base. During This pracess, addition of @ to The polymer. backbone leads to the formation of a radical anion (1) polaron. The second reduction of Polaron forms bipolaron.

V lewis base, Poly acetylene + e (Radical anion) Bi pol aron polaron.

11) Extrinsic conducting polymers: The conductivity of these polymer's is due to the presence of externally added ingredients in them.

3- conductive element filled polymers:

The polymer acts as a brinder to hold the conducting element such as metallic fibre carbon

Animum amount of conducting filler is added so that the polymer starts conducting. This minimum amount is called percolation threshold.

Normal paymer- conductional paymer

69

Advantages

- ii) These are light weight and mechanically durable
- iii) Those are strong
- iv) They can be fabricated very easily.
- 4- Blended conducting polymers

The conventional polymer is blended with a conducting polymer to improve physical, chemical,

electrical and mechanical properties. Exi-polypyrrole is a conducting polyroner ax if it is present 40% in a conventional polym Then The impact strength increases. These bland polymers are used in electromagnetic shielding Applications of conducting polymers.

- 1. conducting polymers are Used in rechargable batteries.
- 2. In analytical sensors for pt, o, No, so, NH, and glucose.
- 3. The conducting polymers are Used for making ron exchangers.
- 4. In electronic displays and optical fibres
- 5. In photovoltaic devices.

### **MCQs**

1. Which of the following statements about polymers is 7	IKUE?
----------------------------------------------------------	-------

A)	Poly	ymers	are	alway	/S	natural	l.
----	------	-------	-----	-------	----	---------	----

- B) Polymers are made up of repeating structural units called monomers.
- C) All polymers are biodegradable.
- D) Polymers cannot be synthesized artificially.

### ✓Answer: B

**Explanation:** Polymers are large molecules formed by repeating monomer units through polymerization.

### $\square$ 2. The functionality of a monomer refers to:

- A) Its ability to conduct electricity
- B) The number of reactive sites present in the monomer
- C) Its molecular weight
- D) Its chemical stability

### ✓Answer: B

**Explanation:** Functionality = number of bonding sites that can form covalent links during polymerization.

Example: Ethylene (CH<sub>2</sub>=CH<sub>2</sub>) has functionality 2.

# $\ \square$ 3. Which of the following polymerization reactions involves free radicals, cations, or anions?

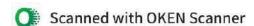
- A) Step-growth polymerization
- B) Chain-growth polymerization
- C) Condensation polymerization
- D) Coordination polymerization

### ✓ Answer: B

**Explanation:** Chain-growth polymerization proceeds via active centers like free radicals, cations, or anions.

### ☐ 4. Nylon-6,6 is prepared by condensation of:

- A) Adipic acid and hexamethylene diamine
- B) Caprolactam
- C) Maleic acid and ethylene glycol



✓ Answer: A Explanation: Nylon-6,6 = condensation polymer of adipic acid + hexamethylendiamine → amide linkages.	e
☐ 5. Which of the following is an example of coordination polymerization?	
A) Polymerization of ethylene using Ziegler–Natta catalyst B) Condensation of glycerol with phthalic acid C) Polymerization of formaldehyde D) Vulcanization of rubber	
Answer: A Explanation: Coordination polymerization uses transition metal catalysts (e.g., YAl(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> ).	ΓiCl4 +
C DVC (Delevined Chloride) is formed by the polymerization of	
☐ 6. PVC (Polyvinyl Chloride) is formed by the polymerization of:	
A) Vinyl chloride B) Ethylene C) Tetrafluoroethylene D) Styrene	
A) Vinyl chloride B) Ethylene C) Tetrafluoroethylene	
A) Vinyl chloride B) Ethylene C) Tetrafluoroethylene D) Styrene  Answer: A  Explanation: PVC is obtained by addition polymerization of vinyl chloride	
A) Vinyl chloride B) Ethylene C) Tetrafluoroethylene D) Styrene  Answer: A  Explanation: PVC is obtained by addition polymerization of vinyl chloride (CH <sub>2</sub> =CHCl).	

A) Phenol and formaldehyde B) Ethylene and benzene C) Styrene and butadiene D) Adipic acid and glycerol ✓Answer: A **Explanation:** Bakelite = phenol + formaldehyde  $\rightarrow$  cross-linked phenol-formaldehyde resin. □ 9. Which of the following is a thermoplastic polymer? A) Bakelite B) Melamine C) Teflon D) Urea-formaldehyde resin ✓ Answer: C **Explanation:** Teflon (PTFE) softens on heating  $\rightarrow$  thermoplastic. Bakelite & urea-formaldehyde → thermosetting. □ 10. Buna-S rubber is obtained by copolymerization of: A) Styrene and butadiene B) Styrene and acrylonitrile C) Butadiene and acrylonitrile D) Isoprene and butadiene ✓ Answer: A **Explanation:** Buna-S = butadiene + styrene  $\rightarrow$  synthetic rubber. □ 11. Buna-N is prepared by copolymerization of: A) Butadiene and acrylonitrile B) Styrene and butadiene C) Ethylene and propylene D) Isoprene and butadiene ✓ Answer: A **Explanation:** Buna-N = butadiene + acrylonitrile  $\rightarrow$  oil-resistant rubber.

$\square$ 12. Conducting polymer among the following is:
A) Polyethylene
B) Polyaniline
C) PVC
D) Nylon-6,6
All Answer: B Explanation: Polyaniline and polyacetylene conduct electricity due to delocalized π-electrons.
☐ 13. Mechanism of conduction in polyacetylene involves:
A) Ionic conduction
B) Electron delocalization through conjugated double bonds
C) Proton conduction
D) Hole conduction only
All Answer: B Explanation: Polyacetylene conducts through delocalized π-electrons along conjugated C=C bonds.
$\Box$ 14. Which of the following polymers is biodegradable?
A) PVC
B) Polythene
C) Poly(lactic acid) (PLA)
D) Nylon-6,6
Answer: C Explanation: PLA and PGA are biodegradable polyesters used in medical sutures.
☐ 15. Poly Glycolic Acid (PGA) is used mainly for:
A) Electrical insulation
B) Biodegradable surgical sutures
C) Textile fibers
D) Rubber materials
Answer: B Explanation: PGA is a biodegradable polymer used for absorbable sutures and implants.

$\Box$ 16. Thermoplastics differ from thermosetting plastics in that:							
A) They soften on heating and harden on cooling							
B) They are cross-linked							
C) They cannot be reshaped after molding							
D) They have high rigidity permanently							
Answer: A							
Explanation: Thermoplastics can be remolded; thermosets cannot due to cross-linking							
□ 17. Carbon fibers are made from:							
A) Polyacrylonitrile (PAN)							
B) Polystyrene							
C) Polyethylene							
D) Nylon							
Answer: A Explanation: PAN is pyrolyzed to form carbon fibers—lightweight, strong materials.							
18. Step-growth polymerization is also called:							
A) Addition polymerization							
3) Condensation polymerization							
C) Radical polymerization							
O) Ionic polymerization							
Answer: B Explanation: Step-growth involves condensation with elimination of small molecules e.g., H <sub>2</sub> O, HCl).							
19. In chain-growth polymerization, molecular weight increases:							
A) Gradually throughout							
B) Only at the end							
C) Rapidly at the beginning and then levels off							
O) After all monomers react							
Answer: C							

Explanation: Chain-growth polymerization forms high molecular weight early in the

	. •		
rea	Ct1	on	

### $\hfill\Box$ 20. The monomer of Teflon is:

- A)  $CF_2=CF_2$
- B) CH<sub>2</sub>=CHCl
- C)  $CH_2=CH_2$
- D) C<sub>6</sub>H<sub>5</sub>CH=CH<sub>2</sub>

✓Answer: A

 $\overline{\text{Explanation:}}$  CF<sub>2</sub>=CF<sub>2</sub>  $\rightarrow$  polytetrafluoroethylene (Teflon).

# UNIT V INSTRUMENTAL METHODS AND APPLICATIONS

### **Electromagnetic Spectrum**

### Q1. What is the electromagnetic spectrum?

**A1.** It is the range of all types of electromagnetic radiation, ordered by wavelength or frequency, including gamma rays, X-rays, UV, visible light, IR, microwaves, and radio waves.

# Q2. Which region of the electromagnetic spectrum is used in UV-Visible spectroscopy?

**A2.** The UV (200–400 nm) and visible (400–800 nm) regions.

### Absorption of Radiation & Beer-Lambert Law

### Q3. What is absorption of radiation?

**A3.** It is the process where molecules absorb specific wavelengths of radiation, causing electronic or vibrational transitions.

### O4. State the Beer-Lambert law.

**A4.**  $A=\varepsilon c lA = \forall c lA = \forall c lA = \varepsilon l$ 

Where AAA = absorbance,  $\varepsilon$ \varepsilon $\varepsilon$  = molar absorptivity, ccc = concentration, lll = path length.

### Q5. What is the significance of the Beer-Lambert law?

**A5.** It allows determination of concentration of a solution by measuring absorbance.

### **UV-Visible Spectroscopy**

### Q6. What is UV-Visible spectroscopy?

**A6.** It is a technique that measures absorption of UV or visible light by molecules, causing electronic transitions from ground to excited states.

### Q7. What are common electronic transitions in UV-Vis spectroscopy?

A7.  $\pi \to \pi^*$ ,  $n \to \pi^*$ , and  $d \to d$  transitions.

### Q8. Name main components of a UV-Vis spectrophotometer.

**A8.** Light source, monochromator, sample holder (cuvette), and detector.

### **IR Spectroscopy**

### Q9. What is IR spectroscopy used for?

**A9.** To identify functional groups in molecules by measuring vibrational transitions.

### Q10. What are fundamental vibrational modes?

**A10.** Stretching and bending (scissoring, rocking, wagging, twisting).

### Q11. State the selection rule for IR absorption.

**A11.** A vibration is IR active if it causes a change in the dipole moment of the molecule.

### Q12. Components of an IR spectrometer?

**A12.** IR source, sample holder, monochromator or interferometer, detector.

### Chromatography

### Q13. What is chromatography?

**A13.** A technique for separating components of a mixture based on differential partitioning between stationary and mobile phases.

### Q14. Name types of chromatography.

**A14.** Paper, thin-layer (TLC), column, gas (GC), and high-performance liquid chromatography (HPLC).

### Q15. What is the basic principle of chromatography?

**A15.** Components move at different rates due to differences in adsorption or solubility between stationary and mobile phases, leading to separation.

### **EASSAY QUESTIONS**

### 1. Write about the UV Spectroscopy with applications?

Absorption laws:-

There are two laws which are the absorption of light by the molecules they are lambert's law, beer's law.

Lambert's law:

It is applied to solids.

I Substance

when a beam of monochromatic radiation pass through a nomogenous absorbing medium the rate of decrease of intensity of the incident light.

Mathematically the law is expressed as

$$-\frac{dI}{dx} = KI_0$$

Where. I = Intensity of radiation after passing through a thicknessor fat the medium.

dI = Small decrease in the intensity

-dt = rate of decrease of intensity of radiation with thickness of the absorbing medium.

K = proportionality constant. Its value depends upon the mature of absorbing medium.

Let To be the intensity of rodiation entering the absorbing medium x=0.

Then I' is the Intensity of radiation after passing through any thickness x ( ) of the medium can be calculated as

$$\int_{T_0}^{T} \frac{dT}{T_0} = \int_{T=0}^{T-K} -Kdx$$

$$\log \frac{T_k}{T_0} = -kx + C \quad [i, c = constant]$$

$$\frac{T}{T_0} = e^{-KX+C} \Rightarrow \boxed{I = I_0 e^{-KX+C}}$$

The intensity of radiation absorbed Jabs is given by

Beer's law: It is applied to liquids. when a beam of monothromatic radiations passed the solution of absorbing medium substance the rate a decrease of intensity of radiation with thickness of absorbing solute is proportional to the incident radiance as well as the concentration of the Solution. Mathen it is represented as

$$-\frac{dI}{dx} = k'CI_0$$

where c= concentration of the solution in moles per liter k= molar absorption coefficient.

Suppose To be the intensity of radiation before entering medium (x=0) then the intensity of the radiation I aft Passing through the thickness of the medium can be a

as 
$$\frac{T}{dx} = -\int_{-\infty}^{\infty} K' c dx$$

$$I_0 = -K' c x$$

$$\frac{T}{T_0} = -K' c x$$

$$\frac{T}{T_0} = e^{-K' c x}$$

$$\therefore T = T_0 e^{-K' c x}$$

$$\frac{\mathbf{T}}{\mathbf{T}_0} = e^{-\mathbf{K}CA}$$

$$\therefore \mathbf{T} = \mathbf{T}_0 e^{-\mathbf{K}CA}$$

3

The intensity of radiation absorbed is given by

$$T_{abs} = T_0 - T$$

$$= T_0 - T_0^{-k'cx}$$

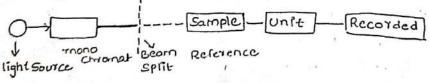
$$= T_0 \left[ 1 - e^{-k'cx} \right]$$

The above been's law can also be written by changing the natural logarithm to base

$$I = I_0 - 10^{-\alpha'} C_{\pi}$$
 [  $\frac{1}{2}$   $\alpha' = \frac{|K|}{2 \cdot 803}$ ]

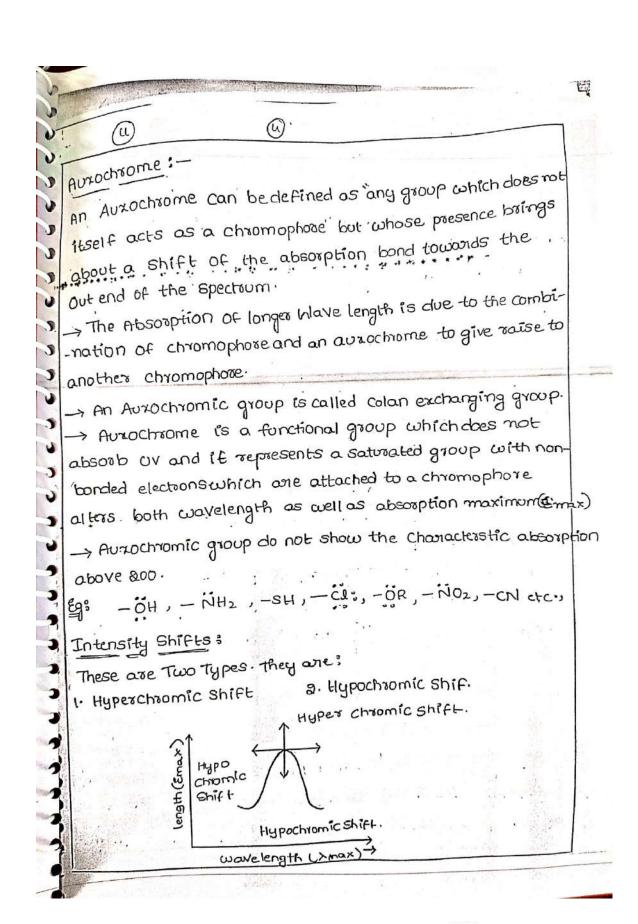
## Instrumentation:

In visible-UV spectrometer, a beam of light is split into two equal half. One-half of the beam (the sample beam) is directed through a transparent cell containing a solution of the compound being analyzed and one-half (The reference bear is directed through an identical cell that contains only the Solvent. The instrument is so-designed that it can compare the intensities of the two beams at each above length of the region



If the Compound absorbs, light at a particular wave length, the intensity of the sample beam (I) will be less than that if the references beam (Jo). The instrument gives output graph-a Plot the wavelength of the entire region Versus the absorbance (A) of the light at each wavelength, where absorbance (유)=18 (구)·

e Such a graph is known as an absorption spectrum. 6 Example of Visible-UV spectroscopy ?-(is <u>Spectoum of arenes</u>: Arenes are Organic Compounts y Contain one or more benzene rings. The electrons in Per C are spread around the hexagonal rings of carbon atom. fig a&b. shows UV spectro of benzene and napthalene. 6006. 1000% Absorption 200 250 250 wakelength (nm) inlave length com) Chromophore: All those compounds which absorbs light of wave length between 400-800 mu appears coloured to the humaneyer exact colour depends upon the wavelength of light absorb by the compound. " A chromophore was considered by substance which is the - sible for inporting colour to the compound ". Eg: Nitro Compounds are generally yellow in colour. YELLOW



It is an effect due to which the interior of the observation real is Hyperchromic shifts-· mum Increases (Eimx). This is called Elyper chromicsh The introduction of an auxochramic usually increases Eq: The board for pyridine of 857 nm [Ermx = 8750] (3 Shifted to 868 nm [Emax - 3650] - for 8-methyl pyridine. 7max-2629m >max = 2570m [Errax = 3650] [Emax = 2150] ciis Hypochromic Shift: It is an effect due to which the two Intensity of absorption maximum decreases. \* i.e., extinction coefficient [Emax] decreases. \* The Introduction of group which distorts the geometry of the molecule causes" Hypochromic Shif". Eg: &-methyl Biphen Bi phenyl mn FEB= xam K Amax = 250nm [Emax=19000] [Emax=10,250] 6 Bi-phenyl absorbs at 250nm [Emax=191000]. where as 2-methy BI-phenyl absorbs of 373nm [FMax=10,250]. It isdue to the distortion caused by the methyl group in a-methyl Bi-phergl

## 2. Write about the IR Spectroscopy with applications?

" VOLT Infrared Vibrations - active and forbidden (selection in \*In-Rased light is absorbed when a charge in the dipole charge of the molecule takes place. \* Total symmetry about a bond will eliminate Certain absorption bands so that the number of absorption bands does not coincide exactly the number of fundamental Vibrations on molecules display somewhat simplified spectra. Thus, some of the fundamental Vibrations are infrared or While the Others are not. This is governed by the selection rules which may be stipulated as follows: is In a molecule with a centre of symmetry, the vibrations symmetrical about the centre of symmetry one inactive in the inframed but active in the Raman. (ii) The Vibiations, without a centre of symmetry, areachi in infrared but in active in the Raman. Type of Vibrations Raman 2.40. Inflored active In active Centrosymmetric 1active Non-centrosymmetric Inactiv a. It means that the two types of spectra are complement and the more easily obtained the inflamed, is most informative for Organic Chemists because most of the ME I functional groups are not centrosymmetric · Conbondiox ide, C Eq: we have the following vibrations.

GE AMPLIFIER PLIETER (1) Asymmetrical Bercling Vibrations symmetrical identical motions Stretching Vmax = 667cm Shetching Umax = 2350 (IR-inactive) Fundamentals Vibration of Carbondioxide. \* These four vibrations (a-d) are the fundamental vibrations ) of Carbondioxide. The Symmetric C=0 strecting vibration (a) of carbon dioxide does not give rise to a change in the dipole moment of the molecule and consequently remains inactive. However, in the Asymmetric Stretching (b) the two C=0 bonds one of different length and hence the molecule has a net change in the dipole character (infrared active) and consequently absorbs at 2350m. \*The Bending of 0=c=0 bonds(candd) are identical motions but they occur in perpendicular, planes such vibrations and 3 called degenerate and appear in the same position in the spectrum. Thus, the two bands at 2350 cm-1 and 667 cm-1 pertaining to asymmetric stretching (b) and bending vibrations (cold) constitute the fundamental spectrum of Cambondioxide. Intensity and position of Infrared absorption bands 2 The intensity of a particular fundamental absorption 1 depends upon the difference between the dipole moments of the molecule in the ground Stale and the Vibrational

excited state. The greater the difference in the sedipole moments, the more intense the absorption . If no change in the dipole moment accompanies the vibrations then by The intensity of absorption bands in infrared spectroscopy Cannot be measured with the same accuracy as inultarion, Spectroscopy. It is usually sufficient for an organic chemist, to know that a bond is of strong, medium, weak or Variable intensity. This may be classified lestimated by assigning the , 6 most intense peak in the infrared spectrum , a relative intensity of 100%. Functional Group and Fingerprint regions: The Region of the infrared spectrum from 4800 cm-1 to 1400 cm exhibits absorption bonds assignable to a number of functional groups and called functional group region. \* These bonds are useful diagnestically but more usually they 10 Supplement the region below 1400cm-1: \* The region from 1400 cm-1 to 900 cm 1 is complex because it 10 16 Contains aposit from fundamental Streeting and bending Vibrations, many bonds resulting from the sum or difference of their vibrational flequencies. \* Specific Vibrational assignments in these region conetherables very difficult. Thus, this part of the spectrum is characterstic of a compound is called fingerpoint region. Similar comp -ounds may show very similar spectra in-functional group region but certainly exhibit discrible difference in fingerpoint

TAGE AMPLIFIER AMPLIFIER Infrared radiation & molecular for absorption of Inflavored readiation: \* The absorption of Infrared radiation corressponds to energy changes in the range from a to lo keal/mol. me Radiation in this energy range, corresponds to the range enco -mpassing the Streeting and bending vibrational frequencies of the bands in most Covalent modecules. \* Infrared light is absorbed when oscillating dipole moment interacts with the oscillating electric vector of infrared beam \* These vibrations absorb light at , certain quantized frequer given vise to characteristics bands when infrared light of that frequency is incident on the molecule, energy is absorbed and the amplitude of that vibration is increased. iii. Molecular Vibrations:... A molecule may be regarded as a system of balls (atoms) and springs Chords when it absorbs infrared radiation. It is Set into vibrations resulting in exclation of bond defo-> -rmations, streething and bending. -> Streching Vibrations: During streching Vibrations the distance between a atoms increases or decreases but the atoms remain in the same bond axis. Types of streching vibrations: strecking vibrations require high energy and occur at higher frequency. They one two types. (1) Symmetrical stretching: In this Stretching made both the atoms move in and out simultaneously.  Eg: for example, symmetrical, streeting of = CH2 giroup In Asymmetrical Streening one alom moves in while theoh moves out Bending Vibration: During bending vibrations, the dish b/w the atoms remains constant but the position of the atoms changes relative to the Original bond axis. \* Bending Vibrations require lower energy and occur at law frequency. They are divided into two types. a) In plane bending (b) Out-of plane bending. (a) In-plane Bending Vibrations: A bending vibrational mode in which the atoms remain the same plane as the modal plane of the system, is a in-plane bending vibration. The in-plane bending vibral in olefin & aromotic ring as shown. -H out of plane

Types of in-plane bending Vibrations:—
They are of two types (i) In-plane scissoring deformation.

(i) In plane rocking deformation.

(i) In-plane scissoring deformation.

In the seissoring deformation, mode, the atoms swing inconcert toward opposite directions as represented for yethefrap

\* Imagine Carbon as the pivot and the hydrogens as the points

of a scissors, then there is a plane passing all the atoms

and the motion is in-plane.

In-plane bending (scissoning).

1)

1

in this deformation made, both theatoms swing to the same side then both to the other side. This is shown for the CHZ group.

Imagine a person (c) sitting on a rocking chair of Hydren(H) as tips of the rockers. Then there is a plane passing through all the atoms. This is apport group frequency as all the atoms move

cos Out-of plane bending?

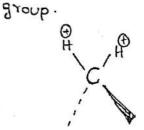
when the atoms bond out of the noch plane, the bending is called out-of-plane bending. The Out-of-plane bending vibrations in olefin or anomalic ring.

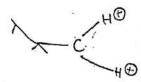
Types of out-of-plane bending Vibrations:

Out-of plane bending vibrations are of two types in Wlagging deformations with Twisting deformations.

Cisout-of-plane wagging deformation:

In this deformation made both the atoms swing up and out of the paper in Unison. This is illustrated for their





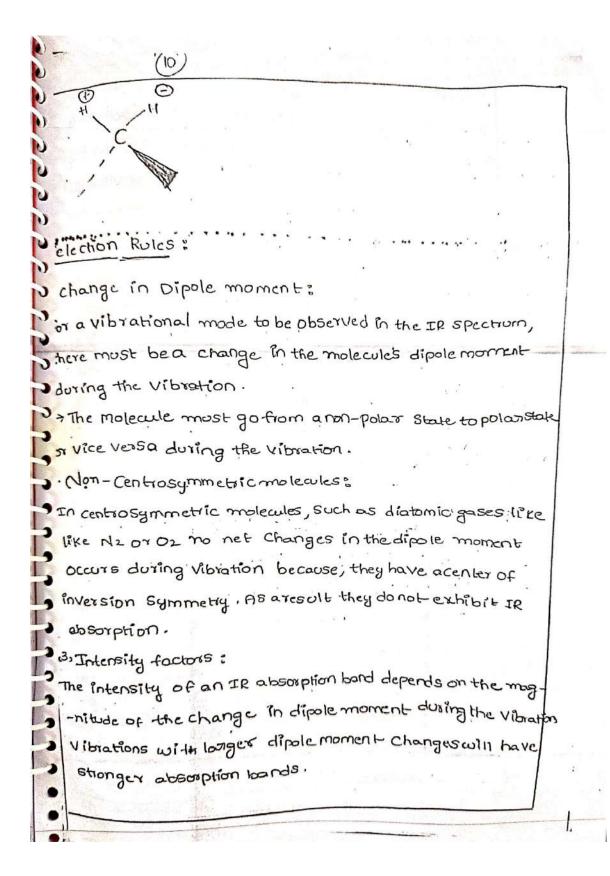
Expresse(c) represents the body of a dog and Hydrogen (4); tail, when the dogs wags its tail, the motion is form to side and out of the plane of the dog.

(ii) Out-of-plane Twisting Deformation:

In twisting deformation one atom swings up and the of swings down related to the plane of paper. The Par signs signify the movement of hydrogens in a direction I dicular to the plane of paper.

6

6



U) Quantization of Energy:

Vibrational Transitions in molecules one quantized and the energy difference ble Vibration level determines the frequency difference ble Vibrations ble quantized Vibration of absorption only transitions ble quantized Vibration energy levels are allowed.

These selection rules help explain why certain Vibration modes are observed in the TR spectrum while others not. It's Important to note that IR spectroscopy is as full tool for identifying functional groups and molecular structures in organic and inorganic Compounds by analy the pattern of absorption bands in the spectrum.

## **MCQs**

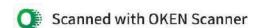
Electromagnetic Spectrum & Absorption of Radiation

- 1. Which of the following has the shortest wavelength?
- A) Infrared
- B) Ultraviolet
- C) Visible
- D) Microwave

✓ Answer: B) Ultraviolet

*Explanation:* Wavelength decreases from IR  $\rightarrow$  Visible  $\rightarrow$  UV  $\rightarrow$  X-ray  $\rightarrow$  Gamma.

- **2.** The relationship between energy and wavelength is given by:
- A) E=hc\*λ
- B)  $E=hc/\lambda$
- C) E=hcλ
- D)  $E=h\lambda c^2$
- Answer: B)



- **3.** Beer-Lambert's law is represented as:
- A) A=εcl
- B)  $A=c\varepsilon/1$
- C)  $A=\varepsilon+c1$
- D)  $A=1/\varepsilon c1$
- ✓Answer: A) A=εcl

 $\overline{Explanation}$ : Absorbance (A) is directly proportional to molar absorptivity ( $\epsilon$ ), concentration (c), and path length (l).

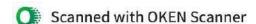
- **4.** Deviation from Beer-Lambert's law occurs due to:
- A) High concentration of solute
- B) Monochromatic radiation
- C) Constant temperature
- D) Dilute solution
- ✓ Answer: A) High concentration of solute

Explanation: At high concentration, molecular interactions alter linearity.

- **☀**□ UV-Visible Spectroscopy
- **5.** In UV-Visible spectroscopy, transitions involve:
- A) Rotational energy levels
- B) Vibrational energy levels
- C) Electronic energy levels
- D) Nuclear energy levels
- ✓ **Answer:** C) Electronic energy levels
- **6.**  $\pi \to \pi^*$  transitions are observed in:
- A) Alkanes
- B) Alkenes
- C) Alkynes
- D) Alkanols
- ✓ **Answer:** B) Alkenes

Explanation:  $\pi \to \pi^*$  transitions occur in compounds with C=C bonds.

- 7. Which component is used for wavelength selection in a UV-Vis spectrophotometer?
- A) Detector
- B) Grating or prism
- C) Lamp



D) Sample holder

✓ **Answer:** B) Grating or prism

Explanation: Monochromators (grating/prism) select specific wavelengths.

- **8.** A common light source for UV spectroscopy is:
- A) Tungsten lamp
- B) Deuterium lamp
- C) Sodium lamp
- D) Mercury lamp
- Answer: B) Deuterium lamp
- □ IR Spectroscopy
- **9.** IR spectroscopy deals with transitions between:
- A) Electronic energy levels
- B) Vibrational energy levels
- C) Nuclear spin levels
- D) Translational energy levels
- ✓ **Answer:** B) Vibrational energy levels
- **10.** The stretching vibration involves:
- A) Change in bond angle
- B) Change in bond length
- C) Both
- D) None
- ✓ **Answer:** B) Change in bond length
- 11. A molecule will show IR absorption only if:
- A) It has a change in dipole moment
- B) It has a change in mass
- C) It has  $\pi$  electrons
- D) It contains hydrogen
- ✓ **Answer:** A) It has a change in dipole moment
- **12.** The fundamental region in IR spectroscopy is:
- A) 400-4000 cm<sup>-1</sup>
- B) 4000-10000 cm<sup>-1</sup>
- C) 40-400 cm<sup>-1</sup>

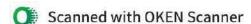
D) 10000-40000 cm<sup>-1</sup>

✓ Answer: A) 400–4000 cm<sup>-1</sup>

- **13.** The IR spectrometer uses which radiation source?
- A) Tungsten lamp
- B) Nernst glower or Globar
- C) Mercury vapor lamp
- D) Sodium lamp
- ✓ Answer: B) Nernst glower or Globar
- ☑ Chromatography Basic Principle
- **14.** Chromatography is based on:
- A) Difference in solubility
- B) Difference in adsorption
- C) Difference in partition
- D) All of the above
- ✓ **Answer:** D) All of the above

Explanation: Depending on the type—adsorption, partition, or ion exchange—different principles apply.

- **15.** The stationary phase in paper chromatography is:
- A) Paper itself
- B) Water trapped in paper
- C) Mobile solvent
- D) Ink
- Answer: B) Water trapped in paper
- **16.** The term *Rf value* represents:
- A) Ratio of distance moved by solute to solvent front
- B) Distance moved by solvent
- C) Ratio of solvent to solute concentrations
- D) Retardation factor
- Answer: A) Ratio of distance moved by solute to solvent front
- 17. In gas chromatography, the mobile phase is:
- A) Gas
- B) Liquid



- C) Solid
- D) Supercritical fluid
- ✓Answer: A) Gas
- **18.** The main use of chromatography is:
- A) Quantitative analysis
- B) Qualitative analysis
- C) Both
- D) None
- ✓Answer: C) Both
- 19. In thin layer chromatography (TLC), the stationary phase is often:
- A) Silica gel or alumina
- B) Paper
- C) Mercury
- D) Glass beads
- Answer: A) Silica gel or alumina
- **20.** The main principle behind HPLC is:
- A) Partition
- B) Adsorption
- C) Both A and B
- D) Electrophoresis
- Answer: C) Both A and B