Q1. The principal quantum number (n) describes which of the following?
 c) The energy level of the electron

Q2. The Aufbau principle states that electrons will fill:
 b) Orbitals in order of increasing energy

Q3. The magnetic quantum number (m) gives information about:
 d) The orientation of the orbital in space

Q4. The Pauli Exclusion Principle states that:
 b) Electrons in the same orbital must have opposite spins

Q5. In the IR spectrum, the C=O stretching vibration typically appears around:
 b) 1700–1750 cm^1

Q6. Which of the following bonds would absorb IR radiation at the highest frequency?
 a) C≡C
(Triple bonds absorb at higher frequencies than double and single bonds.)

Q7. Which of the following nuclei is commonly used in carbon-13 NMR spectroscopy?
 c) ^{13}C

Q8. The region of the electromagnetic spectrum used in UV-Vis spectroscopy typically ranges from:
 b) 200–800 nm

Q9. In UV-Vis spectroscopy, the intensity of absorption is proportional to:
 a) The concentration of the absorbing species

Q10. Which of the following trends is observed as you move across a period in the periodic table?
 b) Atomic size decreases

Q11. Which of the following elements has the highest first ionization energy?
 c) Neon (Ne)
(Noble gases have the highest ionization energies in their periods.)

Q12. Which of the following elements has the highest electronegativity?
 b) Fluorine (F)
(Fluorine is the most electronegative element.)

Q13. Electronegativity generally increases as you move:
 d) From left to right in a group (This is likely a typo in the options; it should be "From left to right in a period")
Most correct based on logic: b) Across a period from left to right

Q14. Which of the following is the strongest type of intermolecular force?
 c) Hydrogen bonding

Q15. Which of the following is true about entropy (S)?
a) Entropy is a measure of the disorder of a system.

Q16. Explain the forms of hydrogen atom wave functions and their plots.

The hydrogen atom wave functions are solutions to the Schrödinger equation. These are called orbitals and are defined by three quantum numbers:

Principal quantum number (n) – defines energy level and size

Azimuthal quantum number (l) – defines shape (s, p, d, f)

Magnetic quantum number (m) – defines orientation

The wave function ψ depends on both radial and angular parts. For example:

1s orbital is spherical and non-directional.

2p orbital has a dumbbell shape and is directional.

The radial distribution function shows the probability of finding an electron at a particular distance from the nucleus. Plots of ψ² give us visual representations of electron clouds.

Q17. Explain the π-molecular orbitals of butadiene.

Butadiene (CH=CH–CH=CH) is a conjugated diene with four π electrons. According to Molecular Orbital Theory:

The 4 p-orbitals (from the 4 carbon atoms) combine to form 4 π molecular orbitals: Ψ, Ψ (bonding), Ψ*, Ψ* (antibonding).

Electrons fill the lowest energy orbitals first (Ψ and Ψ).

Key points:

Delocalization: The π electrons are spread across the molecule, increasing stability.

HOMO and LUMO: Highest Occupied Molecular Orbital (Ψ), Lowest Unoccupied (Ψ*) are critical in reactivity and UV-Vis absorption.

The energy diagram and phase diagrams illustrate constructive and destructive overlaps.

Q18. Explain bending vibrations in IR spectroscopy.

Bending vibrations (also called deformation vibrations) occur when bond angles change. There are two main types:

In-plane bending:

Scissoring – atoms move toward each other like scissors.

Rocking – atoms move in the same direction.

Out-of-plane bending:

Wagging – atoms move up and down together.

Twisting – one atom moves up while the other moves down.

These vibrations usually occur at lower frequencies than stretching vibrations. They are useful in identifying functional groups in IR spectroscopy.

Q19. Explain applications of IR Spectroscopy.

IR spectroscopy is widely used in both qualitative and quantitative analysis:

Identification of functional groups (e.g., OH, C=O, NH):

Each bond has a characteristic absorption frequency.

Structure determination:

Helps confirm the presence of specific linkages.

Quality control in pharmaceuticals and polymer industries.

Environmental monitoring:

Detects pollutants like CO, SO.

Forensic analysis:

Fiber and drug identification.

Food industry:

Tests adulterants, moisture content.

Q20. Discuss in detail electronegativity.

Electronegativity is the ability of an atom to attract shared electrons in a bond.

Pauling scale is the most common, where fluorine is assigned 4.0.

Other scales: Mulliken, Allred-Rochow.

Trends in the periodic table:

Increases across a period (more nuclear charge)

Decreases down a group (more shielding)

Applications:

Predicting bond polarity

Determining ionic or covalent character

Influences acid/base behavior and reactivity

Example: In HCl, Cl is more electronegative and pulls the electron density, making the bond polar.
Q21. Discuss in detail ionization energy and electron affinity.

Ionization Energy (IE):

The energy required to remove an electron from a gaseous atom.

First IE < Second IE < Third IE (due to increasing nuclear attraction)

Electron Affinity (EA):

Energy released when an atom gains an electron.

High EA: Halogens

Low or negative EA: Noble gases, some alkaline earth metals

Trends:

IE increases across a period and decreases down a group.

EA becomes more negative across a period.

Applications:

Determines reactivity (e.g., alkali metals vs. halogens)

Helps explain formation of cations and anions.

Q22. Write a short note on entropy and how we can estimate it.

Entropy (S) is a measure of randomness or disorder in a system.

Higher entropy → more disorder

Gases have more entropy than liquids, which have more than solids.

Mathematically,
$\Delta S = q_{rev}T$
$\Delta S = Tq_{rev}$

where q_{rev} is reversible heat and T is temperature.

Standard molar entropy (S) is tabulated for various substances at 298 K.

Estimation:

From calorimetry data

Using statistical mechanics: $S = k\ln W$

Entropy increases in spontaneous processes (Second Law of Thermodynamics).
Q23. Write a short note on Nernst equation and applications.

Q.23: Write a short note on Nernst Equation and Applications.
Nernst Equation:

The Nernst Equation gives the relationship between the electrode potential of a half-cell in an electrochemical cell and the concentration (or partial pressure) of the species involved.
General Form:
$E = E^\circ - \frac{RT}{nF} \ln Q$
$E = E^\circ - \frac{RT}{nF} \ln Q$

Where:

  E = electrode potential under non-standard conditions

  E° = standard electrode potential

  R = universal gas constant = 8.314 J·mol^{-1}·K^{-1}

  T = temperature in Kelvin

  n = number of electrons transferred in the redox reaction

  F = Faraday's constant = 96485 C·mol^{-1}

  Q = reaction quotient

At 25°C (298 K), the equation becomes:
$E = E^\circ - \frac{0.0591}{n} \log Q$
$E = E^\circ - \frac{0.0591}{n} \log Q$
Applications of the Nernst Equation:

  Calculation of Cell Potential:

    Used to calculate the EMF of electrochemical cells under non-standard conditions.

  Determination of Ion Concentrations:

    Helps in calculating unknown ion concentrations (e.g., $[H+]$, $[Ag+]$, etc.) in redox systems.

  pH Measurement:

    Basis of the glass electrode used in pH meters.

    In this case, the Nernst equation relates pH and electrode potential.

  Predicting Direction of Redox Reactions:

    Helps determine whether a redox reaction is spontaneous based on the sign of cell potential.

  Electrochemical Sensors:

    Used in sensors like oxygen sensors, ion-selective electrodes, and biosensors.

  Corrosion Studies:

Useful in analyzing the conditions under which corrosion occurs, especially for metals.

Q.24: What is Schrödinger Equation? Derive it and explain the significance and their wave functions.

Schrödinger Equation:
It is a fundamental equation in quantum mechanics that describes how the quantum state of a physical system changes with time.
Time-independent Schrödinger Equation (TISE):
$\hat{H}\psi = E\psi$
$\hat{H}\psi = E\psi$

Where:

$\hat{H}$ $\hat{H}$ = Hamiltonian operator

$\psi\psi$ = wave function

EE = total energy of the system

For a single particle in one dimension:
$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$
$-\frac{\hbar}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$

Derivation Outline:

Start from the wave nature of particles (de Broglie hypothesis).

Use the classical total energy equation:
$E = K.E. + P.E. = \frac{p^2}{2m} + V(x)$
$E = K.E. + P.E. = \frac{p^2}{2m} + V(x)$

Replace classical momentum pp with quantum operator:
$\hat{p} = -i\hbar\frac{d}{dx}$
$\hat{p} = -i\hbar\frac{d}{dx}$

Construct the Hamiltonian operator and apply it to the wave function.

Significance:

Determines the allowed energy levels of quantum systems (e.g., electrons in atoms).

$\psi(x)\psi(x)$ gives the probability amplitude; $|\psi(x)|^2$ $|\psi(x)|^2$ gives the probability density.

Foundation for atomic orbitals, quantum tunneling, etc.

Q.25: Explain the principle and instrumentation of IR Spectroscopy.

Principle:
Infrared (IR) spectroscopy is based on the absorption of infrared light by molecules, causing vibrational transitions. Different bonds absorb different frequencies, producing a spectrum unique to each compound.

Instrumentation:

IR Source – Typically a Globar (SiC rod) or Nernst Glower.

Sample Holder – Solid (KBr pellet), liquid (salt plates), or gas cell.

Monochromator – Disperses IR radiation into component frequencies.

Detector – Detects transmitted/absorbed IR radiation (e.g., DTGS, MCT).

Recorder/Computer – Plots intensity vs. wavenumber.

Output: IR Spectrum — peaks correspond to functional groups and bond types.
Q.26: Explain the applications of IR Spectroscopy.

Applications of IR Spectroscopy:

Identification of Functional Groups:
Each functional group (–OH, –NH , –COOH) has characteristic absorption bands.

Structure Elucidation:
Helps in determining molecular structure and bonding.

Monitoring Reactions:
Used to track the progress of chemical reactions.

Purity Analysis:
Impurities show additional peaks in the IR spectrum.
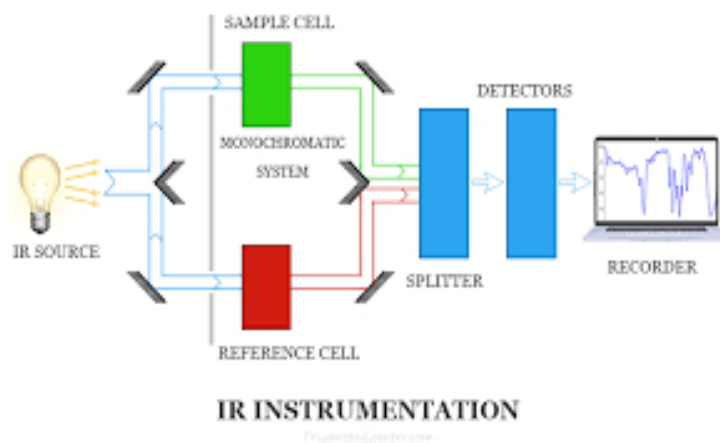
Polymer and Material Science:
Characterizing polymers and their interactions.

Pharmaceuticals:
Quality control and drug verification.

Environmental Testing:
Detection of pollutants and contaminants.

IR INSTRUMENTATION

Q.27: Discuss in detail the Intermolecular Forces.

Intermolecular Forces (IMFs):
These are forces of attraction between molecules and are weaker than intramolecular (covalent or ionic) bonds.
Types of IMFs:

London Dispersion Forces (Van der Waals Forces):

Present in all molecules (especially non-polar).

Caused by momentary dipoles due to electron movement.

Weakest but significant in large atoms/molecules.

Dipole-Dipole Interactions:

Occur between polar molecules.

Partial positive of one molecule attracts partial negative of another.

Hydrogen Bonding:

Strong dipole-dipole interaction.

Involves H bonded to highly electronegative atoms (F, O, N).

Example: Water, DNA base pairing.

Ion-Dipole Forces:

Occur between an ion and a polar molecule.

Important in ionic compounds dissolved in polar solvents like water.

Importance:

Determines boiling/melting points, solubility, viscosity.

Influences biological structure (protein folding, DNA structure).