Unit - 6

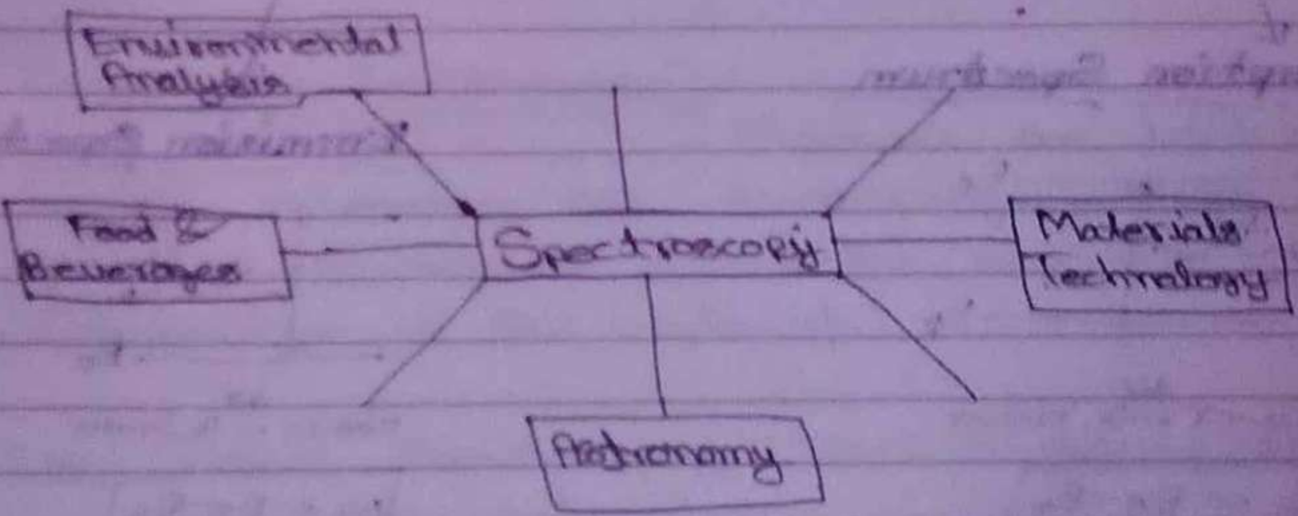
Spectroscopic techniques and applications

Spectroscopy

→ It is a branch of science which deals the study of intraction of EMR with matter.

→ It deals with the transition that a molecule undergoes b/w its energy levels.

→ Spectroscopic refers to the study of the interaction between matter and electromagnetic radiation. This field encompasses a variety of techniques used to analyze and understand the composition, structure, and properties of substances by observing how they absorb emit, or scatter light.



Unit - 6

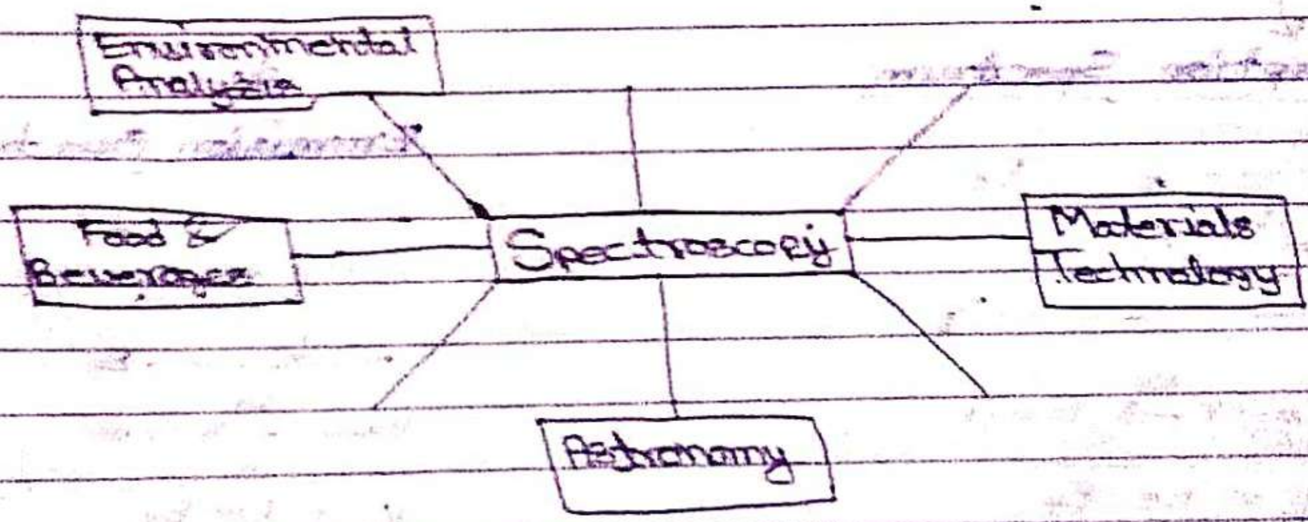
Spectroscopic techniques and application

Spectroscopy

→ It is a branch of science which deals the study of intraction of EMR with matter.

→ It deals with the transition that a molecule undergoes b/w its energy levels.

→ Spectroscopic refers to the study of the interaction between matter and electromagnetic radiation. This field encompasses a variety of techniques used to analyze and understand the composition, structure, and properties of substances by observing how they absorb, emit, or scatter light.



Teacher's Signature ....

Key Concepts

Page No.
Date

- **Electromagnetic Radiation:**

This includes various types of light, such as visible light, ultraviolet light, infrared light, x-rays, and more.

- **Interaction with matter:**

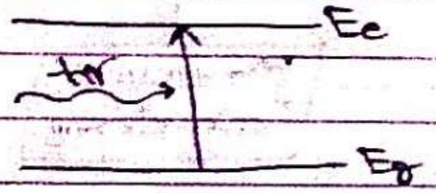
When light interacts with matter, it can be absorbed, emitted, or scattered. These interactions provide valuable information about the material's properties.

Spectrum:

Consider two energy levels of an atom/molecule.

1) Ground state energy level (E_g)
2) Exited state energy level (E_e)

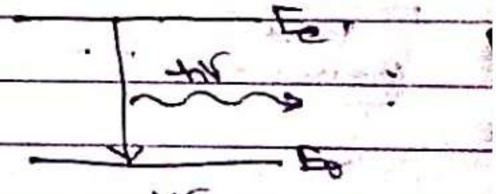
Absorption Spectrum



Lower $\xrightarrow{h\nu}$ higher

$\boxed{\Delta E = E_e - E_g}$

Emmision Spectrum



Higher $\xrightarrow{h\nu}$ lower

$\boxed{\Delta E = E_e - E_g}$

Teacher's Signature ....

Types of Spectroscopy

Page No.
Date

- **Absorption Spectroscopy:-** Measures the amount of light absorbed by a sample at different wavelengths. Each substance absorbs light in a unique pattern, Creating a spectrum that acts like a fingerprint

Exg: UV-visible spectroscopy used to determine the Concentration of Solutions.

- **Emission Spectroscopy:-** Measures the light emitted by a substance. When atoms or molecules are excited (by heat or light), they emit light as they return to their ground state.

Exg: Flame tests in chemistry, where different elements emit different Colours.

- **Scattering Spectroscopy:-** Measures the light scattered by a substance. The scattering pattern can provide information about the structure and Composition of the material.

Exg: Raman Spectroscopy used to study vibrational modes in molecules.

Importance & Applications of Spectroscopy

Page no.
Date

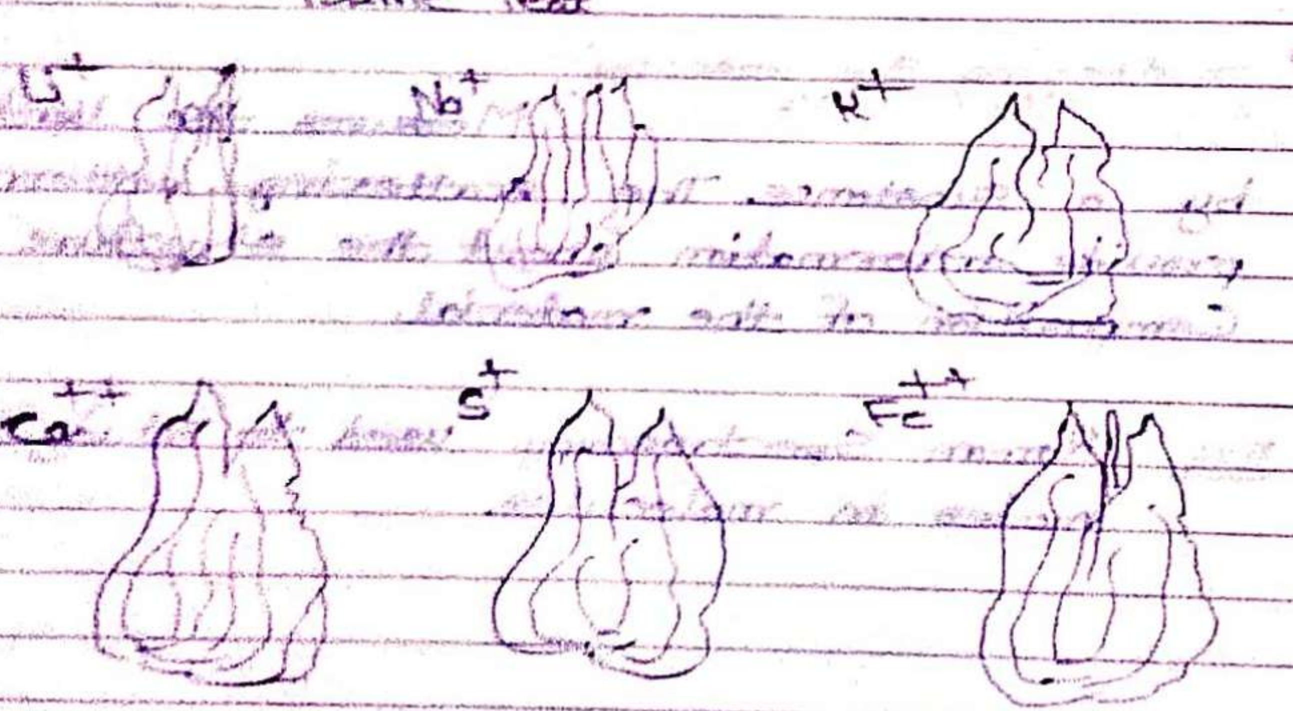
① Identification of Substances:

* Real-Life Example: Flame Tests in chemistry

* Description:
When different elements are heated in a flame, they emit light of specific colors. For instance sodium emits a yellow colour, while Copper emits blue

* Importance:
This helps in identifying elements based on the colors of the flame they produce. It is a simple yet powerful way to detect the presence of certain elements.

Flame Test



Teacher's Signature ....

Page No.
Date / /

② Medical Diagnostics:-

- Example: MRI (Magnetic Resonance Imaging)

- Description:-
MRI uses principles from NMR (Nuclear magnetic Resonance) Spectroscopy to create detailed images of the inside of the body.

- Importance:-
It helps doctors diagnose conditions like tumors, brain disorders and spinal injuries without invasive surgery.

③ Environmental Monitoring:-

- Example: Mass spectrometry for pollution Detection

- Description:-
Mass spectrometry can detect and measure pollutants in air, water, and soil.

- Importance:-
This ensures environmental safety and helps in the detection of harmful substances enabling timely actions to protect ecosystems and human health.

Teacher's Signature ....

Page No.
Date

(4) Astronomical Discoveries:-

- Example: Spectroscopy in Space Exploration

- Description:-
Spectroscopy analyzes the light emitted by stars and planets to determine their Composition.

- Importance:-
It helps scientists understand the makeup of celestial bodies and the universe's overall structure and origins.

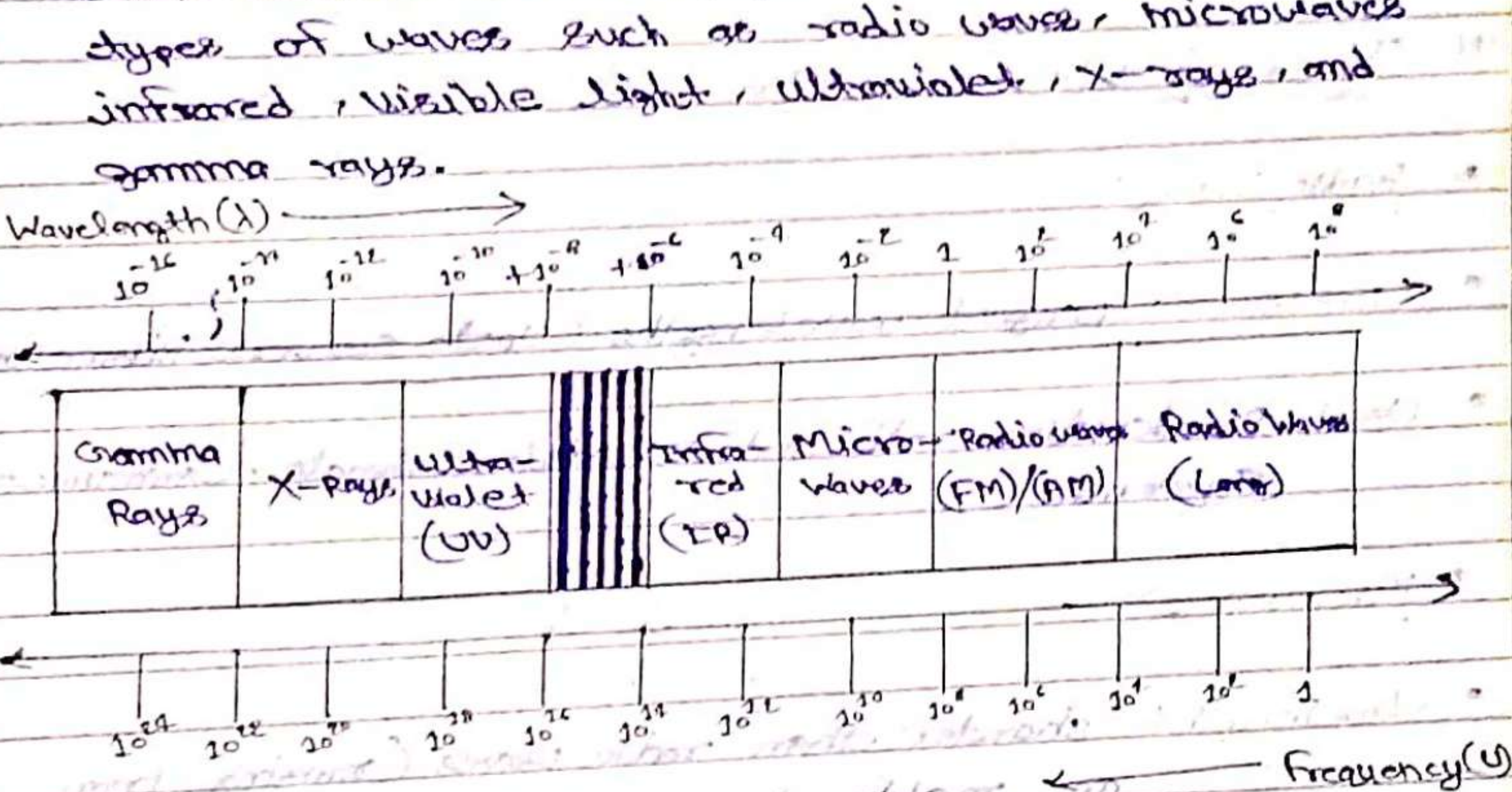
Teacher's Signature ....

EMR (Electromagnetic Radiation)

→ Electromagnetic Radiation (EMR) is a form of energy that travels through space at the speed of light.

→ It is composed of oscillating electric and magnetic fields that move perpendicular to each other and to the direction of the wave travel.

→ EMR covers a broad spectrum, including various types of waves such as radio waves, microwaves, infrared, visible light, ultraviolet, X-rays, and gamma rays.



Key characteristics:

- Wavelength and Frequency:
- Wavelength: The distance between successive peaks of the wave.
- Frequency: The number of wave cycles that pass a given point per second. It is measured in hertz (Hz).

Page No. | Date

- Relationship: Wavelength and Frequency are inversely related. Higher frequency waves have shorter wavelengths and vice versa.

- Speed of Light:-

EMR travels at the speed of light (approximately 300,000 kilometers per second or 186,000 miles per second in a vacuum).

Types of Electromagnetic Radiation (EMR):-

- Radio Waves:-

- Wavelength: Longest wavelengths (Up to serveral kilometres).

- Use: Broadcasting radio and television signals, Communication Systems.

- Microwaves:-

- Wavelength: shorter than radio waves (ranging from one metter to one millimeter)

- Use: Cooking (microwave ovens), radar, and wireless Communications.

- Infrared (IR):-

- Wavelength: Longer than visible light but shorter than microwaves.

Teacher's Signature ....

Page No.
Date

- Use: Remote Controls, thermal imaging, and heating.

- Visible Light:
  - Wavelength: The range that the human eye can see (approximately 400–700 nanometers).
  - Use: Enables vision, used in lighting and photography.

- Ultraviolet (UV):
  - Wavelength: Shorter than visible but longer than X-rays.
  - Use: Sterilization, fluorescent lighting, and suntanning.

- X-Rays:
  - Wavelength: Shorter than UV rays but longer than gamma rays.
  - Use: Medical imaging, security scanning.

- Gamma-Rays:
  - Wavelength: Shortest wavelengths, highest energy.
  - Use: Cancer treatment, sterilizing medical equipment.

Teacher's Signature ________

Page No. | Date

Spectroscopic Techniques:-

→ It is a technique for chemical analysis of molecules or Compounds.

→ Spectroscopy techniques are methods scientists use to study how substance interact with light and other form of electromagnetic radiation.

→ These techniques provides valuable information about the Composition, structure, and properties of substances.

- Earlier:- Molecular formula and chemical reaction.
- Nowdays:- chemical analysis through Spectroscopy.

Some Common Spectroscopy techniques:-

→ UV-Visible Spectroscopy (UV-Visible)
→ Vibrational and Rotational/IR Spectroscopy.
→ Nuclear magnetic Resonance (NMR) Spectroscopy.
→ Mass Spectroscopy (MS).
→ X-ray diffraction (XRD).

Teacher's Signature ....

Page No.
Date

UV-Visible Spectroscopy (UV-Visible):-

- How it works: Measures how much ultraviolet (UV) or Visible light a substance absorbs

- Example:- Think about a glass of colored juice. If you shine a light through it, the juice absorbs some colours more than other. This technique helps determine the concentration of the juice.

- Real-life Use:- Used in hospitals to measure the concentration of substances in blood samples.

Vibrational and Rotational/IR Spectroscopy:-

- How it works: Measures how a substance ~~absorbs~~ absorbs infrared light. Causing its molecules to vibrate.

- Example:- Imagine a tuning fork that vibrate when you hit it. Similarly, molecules vibrate in specific ways when they absorb infrared light.

- Real-life Use: Used in forensics to identify unknown substances found at crime scenes.

Teacher's Signature ....

Nuclear Magnetic Resonance (NMR) Spectroscopy:-

- How it works: Uses magnets and radio waves to study the magnetic properties of certain atoms in a substance.

- Example:- Like how MRI scans use magnetic to take pictures inside your body. NMR helps scientists see the structure of molecules.

- Real-life Use: Scientists use NMR to determine the structure of new molecules.

Mass Spectroscopy (MS):-

- How it works:- Measures the mass of defference particles in a substance.

- Example:- Imagine sorting a bag of mixed candies by their weights. Mass spectroscopy similarly helps identify substance by their "weight."

- Real-life Uses: Used in airports to detect explosive materials in luggage.

Page No.
Date

X-Ray Diffraction (XRD):-

- How it works: Measures how X-rays bounce off the atoms in a crystal to determine its substance.
- Example: Think of shining a flashlight through a prism to see a rainbow. XRD helps see the "rainbow" pattern of atom in a crystal.
- Real-life Use: Used to determine the structure of minerals and metals.

Raman Spectroscopy:-

- How it works: Measures the scattering of light as it passes through a substances, changing its energy slightly.
- Example: Think of a ball bouncing off a wall and losing a bit of energy each time. Raman Spectroscopy measures these small energy changes.
- Real-Life Use: Used in art Conservation to analyze pigments without damaging the artwork.

Teacher's Signature ....

Principle of UV-Visible spectroscopy:-

- **Analysis:-**
  It is the quantitative and qualitative determination of any sample.

- **Spectroscopy:-**
  It is the branch of science which is used for quantitative analysis of matter / sample by using light (electromagnetic radiations)

  eg- amount of substance in sample etc.

Spectrum + Scopy

EMR ← Light To determine

- Gamma Rays :-→ < 0.001 NM
- X - Rays → < 0.01 — 10 NM
- UV → 200 → 400 NM
- Visible → 400 → 800 NM
- Infrared → 0.8 → 200 NM
- Microwaves → 0.01 → 1 M
- Radio waves → 1 → 10^7 M

ENERGY

Page No. ____ Date ____

- **UV Visible Spectroscopy:**

→ Used for quantitative analysis of matter/sample by using UV (ultraviolet) and Visible light.

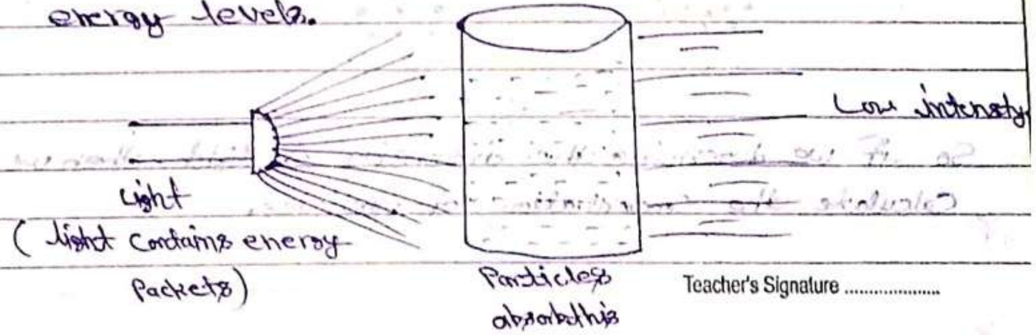
→ The overall range of wavelength of UV Visible is 200 – 800 NM.

200 – 400 → UV
400 – 800 → Visible
200 – 800 NM

→ EMR Light Contains packets of energy (photos). Now when this light passes through the sample, A particle/Molecules of sample absorb the light.

→ In other words, on passing EMR (UV-Visible range 200 – 800 NM) to Compound. A part of the radiation is absorbed by the Compound. After the absorption of energy the electrons in the orbital of lower energy are excited to the orbital of higher energy levels.

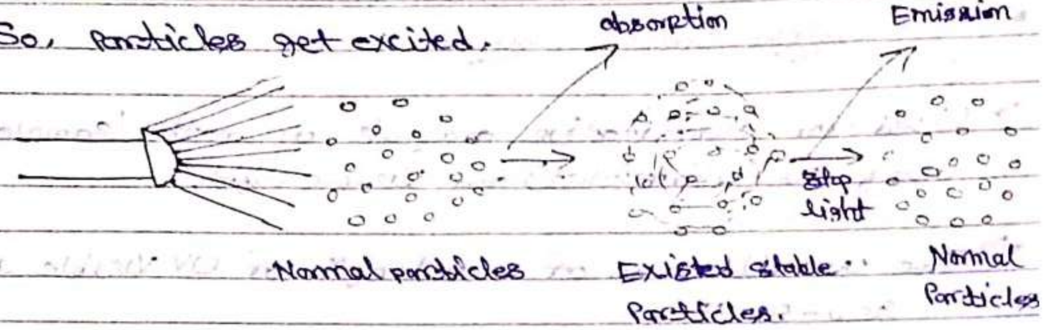
The energy absorbed by the electrons will equal to the energy difference between two energy levels.



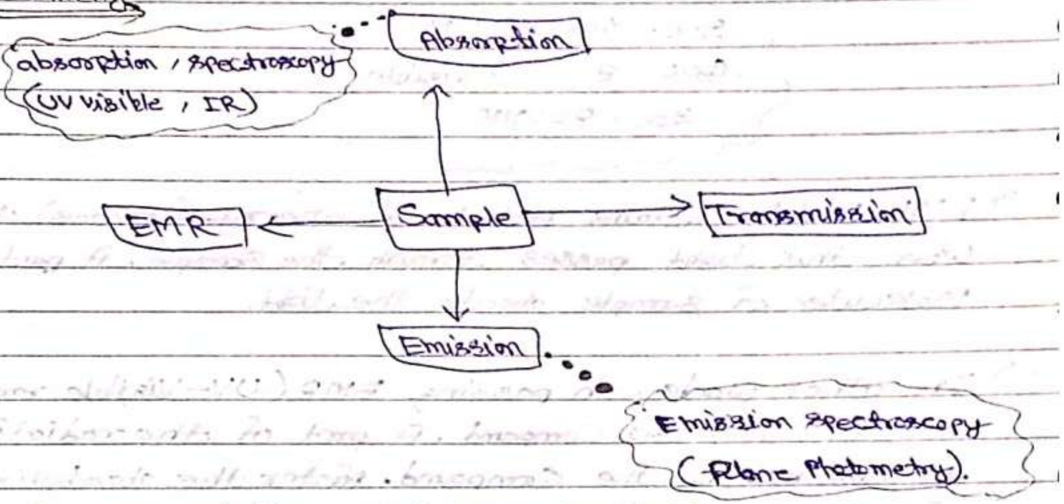
Teacher's Signature ....

Page No.
Date

So, particles get excited.

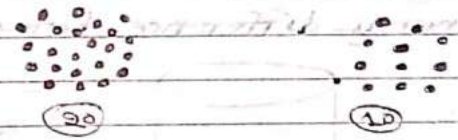


• Summary:-



Now, UV-Visible spectroscopy principle depends upon the absorption of light.

Question → Who absorb more light?



So, if we determine the intensity of light, then we calculate the concentration of particles.

Teacher's Signature ....

Page No.
Date

Absorption $\propto$ Concentration of particle

Absorption $\uparrow$ = Concentration $\uparrow$

Absorption $\downarrow$ = Concentration $\downarrow$

So, Now we have to calculate the absorption.

Teacher's Signature ....

Page No.
Date

Q.1 Write notes on applications of I.R. ?

or State the application of I.R. spectroscopy?

Ans. The important applications of I.R. spectroscopy are as follows.

① **Qualitative Analysis:-**

I.R. Spectroscopy is particularly useful in the qualitative determination of compound or component in a mixture. I.R. spectroscopy was successful used in identification of various organic compounds such as alkynes, aromatic, inorganic ions.

② **Quantitative Analysis:-**

The quantitative determination of given compound is based on the determination of concentration of one of functional group of compound being estimated. Suppose there is a mixture of hexane and hexanol and then concentration of hexanol can be calculating the concentration.

$$A = \log I/I_0 = abC$$

Where. A absorbance

$I \longrightarrow$ Intensity of radiation after leaving the sampl

$I_0 \longrightarrow$ Intensity of radiation befor entering the sampl

Page No.
Date

$a \rightarrow$ Absorptivity of cell.
$b \rightarrow$ Initial path length of same cell and
$c \rightarrow$ Concentration of solution.

If a and b are Constant then.

$A \propto C$

Hence. C Can be measured by knowing A.

(3). In Identifying Compounds:-
The I.R. Spectroscopy of the Compound is compared with that of known Compound and from the resemblance of two spectra The nature of the Compound Can be established due to the particular group of atoms give to characteristics absorption band in the I.R. Spectrum A particular group absorb light of certain wavelength in I.R. spectrum no matter to which Compound it belongs.

(4) In detecting Impurities in a Sample:-
I.R. Spectroscopy is useful to detect impurities of the sample I.R. spectroscopy of impure sample will show extra absorption bands by comparison with I.R. Spectroscopy of pure Compound. Hence these bands if impure sample indicates the impurity of given sample.

Teacher's Signature ______

Page No.
Date

(5) To Distinguish between intra and inter molecular Hydrogen bonding :-

We know that generally, it is not possible to distinguish between intra and inter molecular hydrogen bonding. This can be done, by taking a series of I.R. spectroscopy of the Compound of different Concentration as the concentration increased, the absorption of bond, due to hydrogen bonding increases, while that due to H. bonding remains unchanged.

(6) Elucidation of Structure :- Elucidation of structure is possible by I.R. Spectroscopy because it gives valuable information regarding molecular Symmetry, dipole moments, bond Lengths, bond strength etc.

(7) In the study of Reaction kinetics :- We know that any reaction, there is always bond breaking and making in the reactants. I.R. Spectroscopy arises from the different modes of vibrations in bonds. So if we withdraw the sample from reaction mixture in a regular interval of time and study its I.R. Spectroscopy. We can draw some inference regarding the kinetics of reaction.

Page No.
Date

(8) In study of Polymers:-

$\Rightarrow$ Infrared techniques have been used in the detection of end groups and chain branching found in polymers. Use of polarise infrared radiation has been made in the study of certain properties of polymers.

Example: Strength of rubber.

Teacher's Signature ....