UNIT 6: SPECTROSCOPIC TECHNIQUES AND APPLICATIONS

1. Introduction to Spectroscopy

Spectroscopy is the study of how matter interacts with electromagnetic radiation. It helps determine the structure, composition, and properties of substances. Different types of spectroscopy include:

- **Electronic Spectroscopy (UV-Visible)**
- **Vibrational Spectroscopy (Infrared, IR)**
- **Rotational Spectroscopy (Microwave, MW)**

2. Principle of Spectroscopy

- Atoms and molecules absorb or emit radiation at specific wavelengths.
- This interaction causes transitions between **energy levels**:
  - **Electronic transitions** (UV-Vis spectroscopy)
  - **Vibrational transitions** (Infrared spectroscopy)
  - **Rotational transitions** (Microwave spectroscopy)
- The spectrum obtained gives valuable information about the molecular structure.

3. Instrumentation of Spectroscopy

Basic Components of a Spectrometer:

1. **Radiation Source** – Provides electromagnetic radiation (UV, IR, MW).
2. **Monochromator** – Selects a specific wavelength of light.
3. **Sample Holder** – Holds the substance under study.
4. **Detector** – Measures absorbed or emitted radiation.
5. **Recorder & Display Unit** – Shows the obtained spectrum.

Types of Spectroscopy & Their Instrumentation

(A) Electronic Spectroscopy (UV-Visible Spectroscopy)

- Studies **electronic transitions** in molecules.
- **Wavelength Range:** 200-800 nm (UV-Vis region).

Instrumentation:

- **Light Source**: Deuterium (UV), Tungsten (Visible).
- **Monochromator**: Diffraction grating to select wavelengths.
- **Sample Cell**: Quartz cuvette for UV, Glass cuvette for Visible.
- **Detector**: Photomultiplier tube, Photodiode.

Applications:

- Identification of organic compounds.
- Determination of **conjugation** in molecules (chromophores).
- Used in **DNA/protein analysis**.

(B) Vibrational Spectroscopy (Infrared Spectroscopy - IR Spectroscopy)

- Studies **molecular vibrations** (bond stretching and bending).
- **Wavelength Range:** 2.5-25 μm (Mid-IR).

Instrumentation:

- **Light Source**: Globar (heated SiC rod).
- **Monochromator**: Grating or prisms.
- **Sample Holder**: Salt plates, KBr pellet for solid samples.
- **Detector**: Thermocouple, Pyroelectric detectors.

Applications:

- Identifies **functional groups** in organic molecules.
- Used in **pharmaceutical analysis**.
- Detects **impurities** in samples.

(C) Rotational Spectroscopy (Microwave Spectroscopy - MW Spectroscopy)

- Studies **molecular rotation** in gases.
- **Wavelength Range:** 1 mm - 1 m (Microwave region).

Instrumentation:

- **Microwave Source**: Klystron oscillator.
- **Sample Holder**: Gas cell under low pressure.
- **Detector**: Crystal detector.

Applications:

- Determines **bond length and bond strength**.
- Used in **remote sensing and space research**.
- Helps in **structural elucidation of small molecules**.

4. Spectroscopy of Diatomic Molecules

(A) Electronic Spectroscopy of Diatomic Molecules

- Involves **electronic transitions** between different energy states.
- Governed by **Franck-Condon Principle**, which states that electronic transitions occur faster than nuclear motion.
- Spectral bands depend on **vibrational & rotational energy levels**.

Applications:

- Used in **astronomy** to study interstellar molecules.
- Determines **electronic structures of diatomic gases**.

(B) Vibrational Spectroscopy of Diatomic Molecules

- Describes how atoms vibrate within a molecule.
- Governed by **Hooke's Law**: where **k** = bond force constant, **μ** = reduced mass.

Applications:

- Used in **molecular fingerprinting**.
- Helps in **gas analysis**.

(C) Rotational Spectroscopy of Diatomic Molecules

- Involves **pure rotational transitions**.
- Energy levels given by: where **J** = rotational quantum number, **B** = rotational constant.

Applications:

- Determines **bond lengths of gases**.
- Used in **atmospheric studies**.

5. Summary & Outcomes

- Spectroscopy helps in **structural analysis of molecules**.
- **Electronic spectroscopy** deals with **UV-Vis transitions**.
- **Vibrational spectroscopy** (IR) identifies **functional groups**.
- **Rotational spectroscopy** (MW) gives information about **molecular geometry**.
- Understanding spectroscopic techniques is crucial for **chemical, biological, and industrial applications**.