**Study Material: Spectroscopic Techniques**

**I. Core Principle of Spectroscopy**

**Definition:** Spectroscopy is the study of the interaction between **matter** and **electromagnetic radiation (light)** as a function of wavelength or frequency.

**The Fundamental Concept:**
When light (energy) hits a molecule, the molecule can **absorb** a specific amount of that energy, promoting it to a higher energy state. The amount of energy absorbed depends on the type of transition occurring within the molecule (e.g., electronic, vibrational, nuclear spin). Each transition requires a specific, quantized amount of energy.

The key equation is: **E = hν = hc / λ**

* **E** is the energy difference between two states.
* **h** is Planck's constant.
* **ν** (nu) is the frequency of the radiation.
* **c** is the speed of light.
* **λ** (lambda) is the wavelength of the radiation.

**The Output: A Spectrum**
A plot of the intensity of light absorbed or emitted by a sample versus the wavelength or frequency. This spectrum acts as a **"fingerprint"** for a molecule, providing information about its structure, composition, and environment.

**II. The Electromagnetic Spectrum & Corresponding Techniques**

The type of information obtained depends on the energy of the radiation used, which correlates to different regions of the EM spectrum.

| **Region of Spectrum** | **Wavelength Range** | **Energy Transition** | **Techniques** |
| --- | --- | --- | --- |
| **Radiofrequency** | 1 m - 1 km | Nuclear Spin (in a magnetic field) | **Nuclear Magnetic Resonance (NMR)** |
| **Microwave** | 1 mm - 1 m | Molecular Rotation | Rotational Spectroscopy |
| **Infrared (IR)** | 0.7 µm - 1 mm | Molecular Vibration | **Infrared (IR) Spectroscopy** |
| **Visible/Ultraviolet (UV-Vis)** | 200 nm - 800 nm | Electron Energy (outer electrons) | **UV-Visible Spectroscopy** |
| **X-ray** | 0.01 nm - 10 nm | Electron Energy (inner core electrons) | X-ray Crystallography |

**III. Major Spectroscopic Techniques (Deep Dive)**

**1. Infrared (IR) Spectroscopy**

* **Principle:** Measures the absorption of IR light, which causes **vibrational transitions** in molecules (bending and stretching of bonds).
* **Information Obtained:** Identifies **functional groups** present in a molecule (e.g., C=O, O-H, N-H, C≡N).
* **Key Output:** A spectrum plotted as % Transmittance vs. Wavenumber (cm⁻¹).
* **How to Analyze:** Look for characteristic absorption peaks (e.g., strong peak at ~1700 cm⁻¹ for a carbonyl group, C=O). The fingerprint region (1500-500 cm⁻¹) is unique to each molecule.
* **Applications:** Quick functional group identification, monitoring chemical reactions (disappearance/appearance of peaks), quality control.

**2. Ultraviolet-Visible (UV-Vis) Spectroscopy**

* **Principle:** Measures the absorption of UV or visible light, which causes **electronic transitions** (promotion of electrons from π or n orbitals to π\* anti-bonding orbitals).
* **Information Obtained:** Reveals the presence of **chromophores** (light-absorbing groups), especially conjugated systems (e.g., benzene rings, carotenoids).
* **Key Output:** A spectrum plotted as Absorbance (A) vs. Wavelength (λ, in nm). The λ\_max is the wavelength of maximum absorption.
* **Applications:** Quantitative analysis (using Beer-Lambert Law: **A = εlc**), determining concentration of solutions, studying conjugated systems, reaction kinetics.

**3. Nuclear Magnetic Resonance (NMR) Spectroscopy**

* **Principle:** In a strong magnetic field, the nuclei of certain atoms (e.g., ¹H, ¹³C) absorb radiofrequency radiation, which causes a flip of their **nuclear spin**.
* **Information Obtained:** Provides detailed information about the **carbon-hydrogen framework** of a molecule. It is the most powerful tool for determining molecular structure.
* **Key Parameters:**
	+ **Chemical Shift (δ, ppm):** Indicates the electronic environment of a nucleus (e.g., what groups are nearby).
	+ **Integration:** Reveals the number of equivalent protons giving rise to a signal.
	+ **Spin-Spin Coupling (Splitting):** Shows the number of adjacent, non-equivalent protons.
* **Types:** ¹H-NMR (proton NMR), ¹³C-NMR (carbon NMR).
* **Applications:** Elucidating the complete structure of unknown organic molecules, determining purity, studying molecular dynamics.

**4. Mass Spectrometry (MS) - Not strictly spectroscopy, but paired with it**

* **Principle:** **Not based on light absorption.** It involves ionizing chemical compounds to generate charged molecules or fragments and measuring their **mass-to-charge ratio (m/z)**.
* **Information Obtained:** Determines the **molecular weight** of a compound and provides information about its structure based on fragmentation patterns.
* **Key Output:** A mass spectrum plotted as Abundance vs. m/z.
* **Key Features:**
	+ **Molecular Ion Peak (M⁺⁺):** The peak with the highest m/z, corresponding to the intact molecular ion (gives the molecular weight).
	+ **Base Peak:** The tallest peak in the spectrum (most abundant fragment).
	+ **Fragmentation Pattern:** The way the molecule breaks apart, which is characteristic of its structure.
* **Applications:** Determining molecular weight, elucidating structures of unknown compounds, identifying compounds in complex mixtures (when coupled with GC or LC).

**IV. Putting It All Together: Structure Elucidation**

The true power of spectroscopy is using these techniques **together** to solve a molecular puzzle.

**Example Workflow for an Unknown Compound:**

1. **Mass Spectrometry (MS):** Provides the molecular weight.
2. **Infrared (IR) Spectroscopy:** Identifies the main functional groups (e.g., OH, C=O, C-O).
3. **Nuclear Magnetic Resonance (NMR):** ¹H-NMR and ¹³C-NMR maps out the carbon-hydrogen framework, showing how the atoms are connected.