

Infrared Spectroscopy

Introduction to IR Spectroscopy

- Infrared (IR) Spectroscopy is a powerful analytical technique based on the interaction of infrared radiation with matter, primarily used to determine the functional groups, molecular structure, and purity of pharmaceutical substances.
- It relies on the fact that molecules absorb specific frequencies of infrared light that cause vibrational transitions in the bonds between atoms.
- This technique is particularly useful for:
 - Identifying functional groups
 - Confirming molecular structure
 - Detecting polymorphs
 - Quality control of raw materials and finished products

Applications of IR Spectroscopy

- **Identification of functional groups:** Based on characteristic absorption bands.
- **Purity testing:** Extra bands indicate impurities.
- **Monitoring chemical reactions:** Disappearance or appearance of specific bands.
- **Structure elucidation:** Combined with other techniques (NMR, MS).

Vibrational Transitions

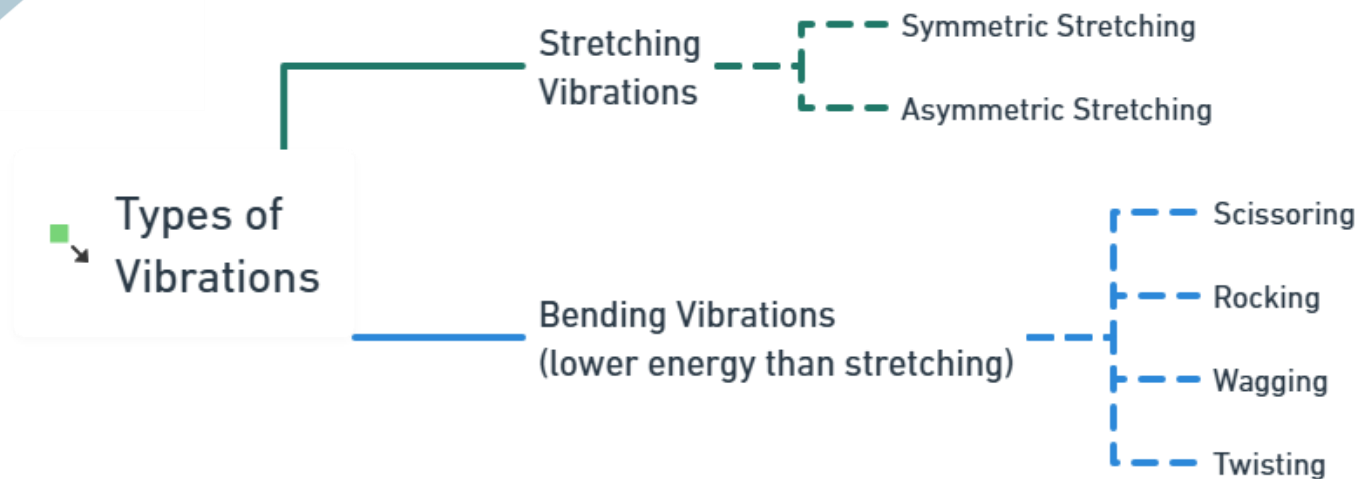
Basic Concept

- Molecules are not rigid bodies; their atoms are constantly in motion – stretching, bending, twisting, etc.
- These motions are known as **vibrations**.
- When a molecule absorbs infrared radiation, the energy is transferred to the molecule, causing a transition from one **vibrational energy level** to another.
- This is called a **vibrational transition**.

Quantized Vibrational Energy

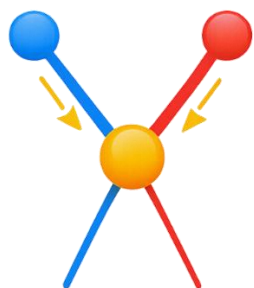
- Vibrational energy levels are **quantized**, meaning that only specific discrete energy values are allowed.
- The energy difference between these levels corresponds to the energy (or frequency) of the absorbed IR radiation.

Types of Vibrations

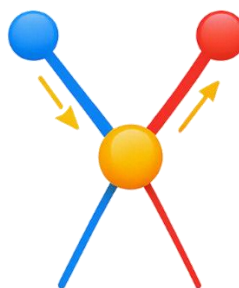


A. Stretching Vibrations:

- **Symmetric stretching:** atoms move in and out together.
- **Asymmetric stretching:** one atom moves in while the other moves out.



Symmetrical stretching



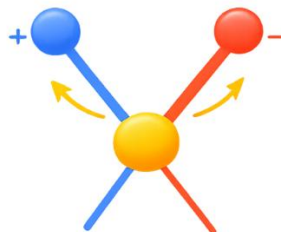
Asymmetrical stretching

B. Bending Vibrations (lower energy than stretching):

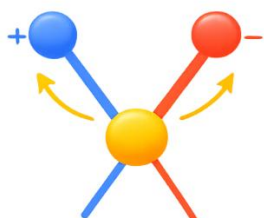
- **Scissoring:** atoms move toward and away from each other.
- **Rocking:** atoms move side to side.
- **Wagging:** atoms move up and down together.
- **Twisting:** atoms move in opposite directions out of plane.



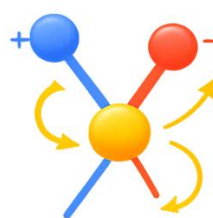
In-plane rocking



In-plane scissoring



Out of-plane wagging



Out of-plane twisting

- A molecule must experience a change dipole moment in during vibration for it to absorb IR radiation.

Selection Rules

- For a vibration to be IR-active (i.e., capable of absorbing IR radiation), the **dipole moment** of the molecule must change during the vibration.
- This is a quantum mechanical requirement derived from electromagnetic theory.

IR Frequency (Wavenumber)

- The frequency of IR radiation is usually expressed in **wavenumbers (cm⁻¹)**.
- Wavenumber is directly proportional to energy: higher wavenumber = higher energy.

Dependence on Bond Strength and Mass

- The vibrational frequency of a bond depends on:
 - The **strength of the bond** (stronger bonds vibrate at higher frequencies)
 - The **masses of the atoms** involved (lighter atoms vibrate at higher frequencies)
- This relationship can be modeled by Hooke's Law (approximate model of bond vibration):

$$\tilde{\nu} = \frac{1}{2\pi c} \sqrt{\frac{k}{\mu}}$$

- **Where:**
 - $\tilde{\nu}$ = wavenumber (cm⁻¹)
 - c = speed of light
 - k = bond force constant (proportional to bond strength)
 - μ = reduced mass of the two atoms in the bond

Characteristic Absorption Frequencies

- Different types of bonds absorb IR radiation at characteristic frequencies:

Bond Type	Typical IR Absorption Range (cm ⁻¹)
O-H (alcohol)	3200–3600 (broad)
N-H (amine/amide)	3300–3500
C-H (alkane)	2800–3000
C≡C, C≡N	2100–2300
C=O (carbonyl)	1650–1750

C=C (alkene)	1600–1680
C–O (ether/ester)	1000–1300

- Thus, analyzing these absorption bands allows chemists to infer structural features of the molecule.

Infrared Absorption Bands

Definition

- When a molecule absorbs IR radiation, it produces a peak (or band) in the IR spectrum.
- Each peak corresponds to a specific vibrational transition of a bond or group in the molecule.
- The position, intensity, and shape of the absorption band give information about the bond type and molecular environment.

Types of Bands

- **Sharp Bands:** Indicate isolated bond stretching (e.g., C≡C).
- **Broad Bands:** Usually due to hydrogen bonding (e.g., O–H in alcohols, N–H in amines).
- **Weak or Missing Bands:** If the bond does not involve a change in dipole moment, it may not appear even though the vibration exists (e.g., symmetrical C≡C in alkynes).

Band Intensity

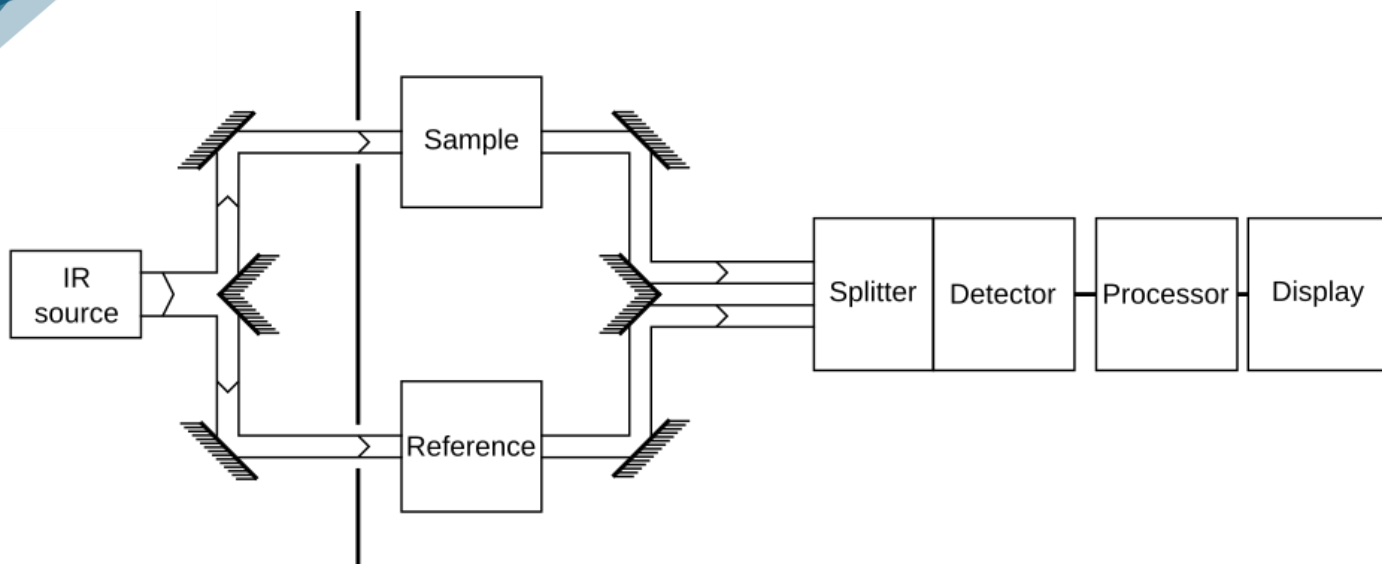
- Depends on the magnitude of the change in dipole moment during vibration.
- Polar bonds generally show strong absorption.
- Nonpolar or symmetric bonds show weak or no absorption.

Band Shape

- **Influenced by:**
 - Hydrogen bonding
 - Coupling between vibrations
 - Overtones (multiples of fundamental frequencies)
 - Fermi resonance (interaction of vibrational modes)

Instrumentation – IR Spectrometer

- An **Infrared (IR) spectrometer** is an analytical instrument used to measure the absorption of infrared radiation by a sample.
- The basic function is to record how much of the IR radiation is absorbed at each frequency (wavenumber), producing an IR spectrum.



Basic Components of an IR Spectrometer:

1. **IR Source:** produces IR radiation.
2. **Collimating System:** focuses the radiation into a beam.
3. **Monochromator:** separates IR radiation into individual frequencies.
4. **Sample Cell or Holder:** holds the sample to be analyzed.
5. **Detector:** measures the intensity of transmitted or absorbed IR radiation.
6. **Signal Processor and Recorder:** amplifies the signal and displays the spectrum.

There are two main types of IR spectrometers:

- **Dispersive IR Spectrometers:** use monochromators (prisms or gratings).
- **FTIR (Fourier-Transform Infrared) Spectrometers:** use interferometers (usually a Michelson interferometer).

How It Works

- The IR source emits radiation that passes through the sample.
- The sample absorbs specific frequencies corresponding to vibrational transitions.
- The transmitted (or reflected) light reaches the detector.
- The resulting spectrum displays % **transmittance** or **absorbance** vs **wavenumber** (cm^{-1}).

Sources of IR Radiation

- The **IR source** in a spectrometer must emit **stable**, **continuous**, and **broad-spectrum** infrared radiation over the required wavenumber range (typically $4000\text{--}400\text{ cm}^{-1}$).

Common IR Sources

Source Type	Temperature	Wavenumber Range	Notes
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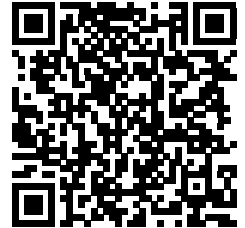


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