

Infrared (IR) Spectroscopy

Principle:

Infrared spectroscopy is a technique used to study the vibrational transitions of molecules. Molecules absorb infrared radiation when the frequency of the radiation matches the vibrational frequency of a particular bond or functional group. The principle is based on the fact that different bonds vibrate at characteristic frequencies, and the absorption of infrared light causes these vibrations.

Instrumentation:

Infrared (IR) spectroscopy instrumentation typically consists of several key components that work together to analyze the interaction of infrared radiation with a sample. Here is an overview of the main components in an IR spectroscopy setup:

IR Light Source:

- The IR light source emits infrared radiation. Common sources include Nernst glowers, Globar sources, and more modern sources like quantum cascade lasers.

Beam Splitter:

- The beam splitter divides the incident infrared beam into two paths: one that interacts with the sample and another that serves as a reference.

Sample Compartment:

- The sample compartment holds the sample being analyzed. It allows the infrared light to pass through the sample.

Chopper:

- The chopper is a mechanical device that modulates the IR light beam. It periodically interrupts or modulates the light beam, creating a pulsed beam. This modulation is essential for the subsequent detection process.

Monochromator: Separates the dispersed infrared radiation based on its wavelength. It selects specific wavelengths to reach the detector.

Detector:

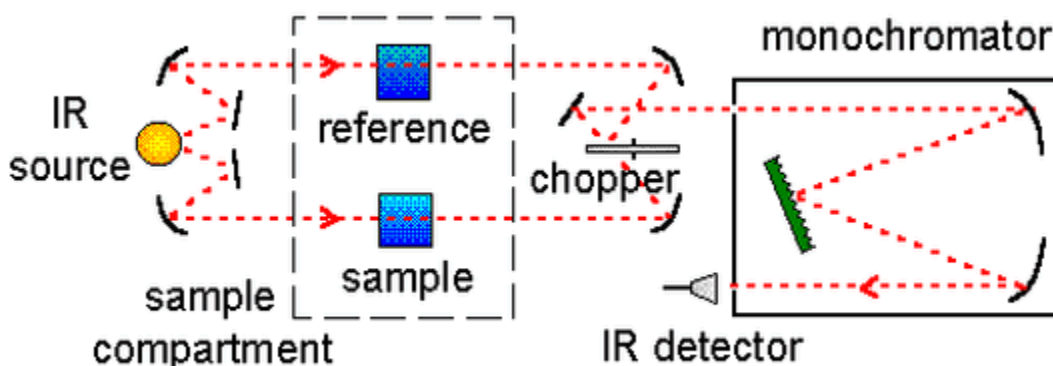
- The detector measures the intensity of the infrared light that has interacted with the sample. Common types of detectors include thermal detectors (such as pyroelectric detectors) and photoconductors.

Data System/Processor:

- The data system processes the signals from the detector and converts them into a spectrum.

Display/Output Device:

- The processed spectrum is displayed on a computer monitor or other output device. The spectrum shows peaks at specific wavenumbers, providing information about the vibrational modes in the sample.



IR spectroscopy range

Infrared (IR) spectroscopy covers a range of wavelengths or wavenumbers that correspond to the vibrational transitions of molecules. The IR spectrum is typically divided into three main regions based on the energy of the absorbed radiation:

Near-Infrared (NIR): Wavenumber Range: $12,800\text{ cm}^{-1}$ to $4,000\text{ cm}^{-1}$

Mid-Infrared (MIR): Wavenumber Range: $4,000\text{ cm}^{-1}$ to 400 cm^{-1}

Far-Infrared (FIR): Wavenumber Range: 400 cm^{-1} to 10 cm^{-1}

The mid-infrared region is of primary interest in routine IR spectroscopy, as it corresponds to the fundamental vibrations of chemical bonds.

Vibrational modes

Infrared (IR) spectroscopy is a powerful analytical technique used to study the vibrational transitions of molecules. It involves the interaction of infrared radiation with matter, where

molecules absorb specific frequencies of infrared light corresponding to vibrational modes. The resulting spectrum provides information about the functional groups and molecular structure of a sample.

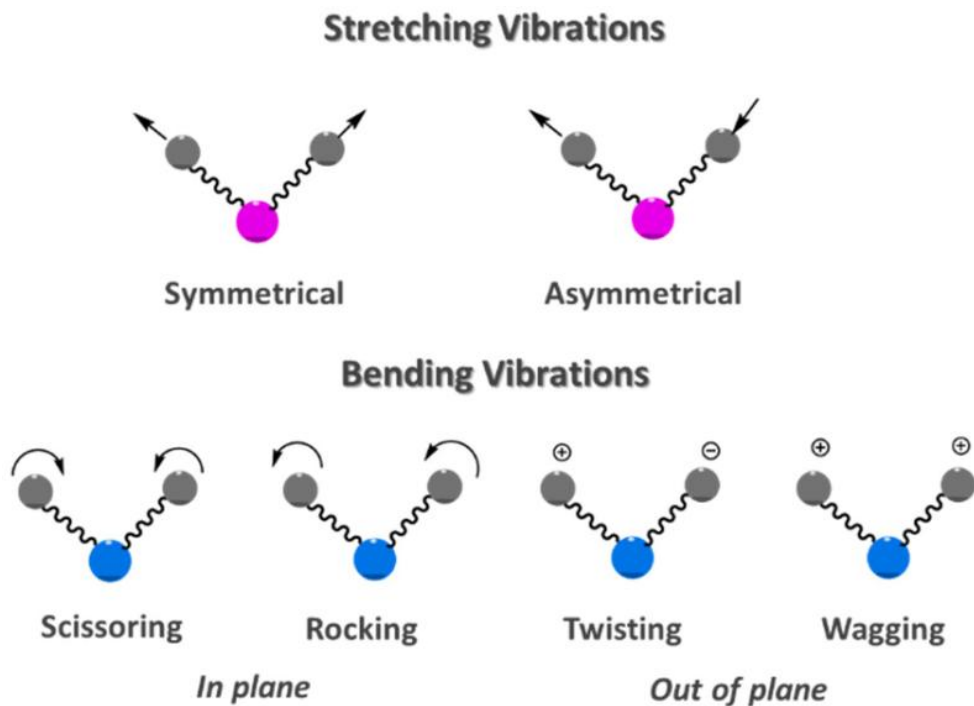
Molecules consist of atoms connected by chemical bonds, and these bonds can vibrate in different ways. The vibrational modes in IR spectroscopy are broadly categorized into three main types:

1. Stretching Vibrations:

- **Symmetrical Stretch (ν_1):** Both atoms move toward or away from the central atom simultaneously.
- **Asymmetrical Stretch (ν_2):** Atoms on either side of the central atom move in opposite directions.

2. Bending Vibrations:

- **In-Plane Bending (ν_3):** Atoms within the same plane move toward or away from each other.
- **Out-of-Plane Bending (ν_4):** Atoms move above and below the plane of the molecule.



Selection rules

The selection rules for infrared (IR) spectroscopy describe which vibrational modes are allowed (IR active) or forbidden (IR inactive) in a given molecule. These rules are based on changes in the dipole moment of a molecule during vibrational transitions. Here are the general selection rules:

IR Active Vibrations:

1. Change in Dipole Moment (μ):

- An IR-active vibrational mode must involve a change in the dipole moment of the molecule during the vibration.

Eg. Hydrogen Fluoride (HF), Hydrogen Chloride (HCl), Water (H₂O)

- A molecule is IR active if it has a permanent dipole moment, and a vibrational mode results in a change in the dipole moment.

2. Vibrational Modes that Are IR Active:

- Vibrations that involve changes in bond length (stretching) or bond angle (bending) often result in a change in the dipole moment and are, therefore, IR active.
- Asymmetrical stretches and bends are typically IR active.

IR Inactive Vibrations:

1. No Change in Dipole Moment:

- Vibrations that do not result in a change in the dipole moment are IR inactive.

E.g. Diatomic Molecules with Identical Atoms (e.g., N₂, O₂, H₂)

- For example, symmetrical stretches, which involve equal and opposite changes in bond length, do not result in a net change in dipole moment and are typically IR inactive.

2. Centrosymmetric Molecules:

- In centrosymmetric molecules (molecules with a center of inversion), only vibrational modes with an odd change in symmetry are IR active.

- Symmetrical stretches and certain symmetrical bends are often IR inactive in centrosymmetric molecules.

3. **Conjugated Systems:**

- In some cases, vibrational modes involving changes in conjugated systems may be IR inactive.