

IR Spectroscopy (Infrared Spectroscopy)

Introduction to IR Spectroscopy

Principle:

- Infrared (IR) spectroscopy involves the interaction of IR light with molecules, leading to vibrations within molecular bonds.

How it Works:

1. Absorption:

- Molecules absorb specific IR frequencies, causing vibrational transitions in bonds (e.g., stretching or bending).

2. Spectrum Generation:

- Remaining radiation passes to a detector, generating a spectrum of intensity vs. frequency, revealing absorbed regions indicative of chemical bonds.

3. Fingerprinting:

- Each molecule has a unique IR absorption pattern, with bonds like C-H, N-H, and O-H showing distinct absorptions.

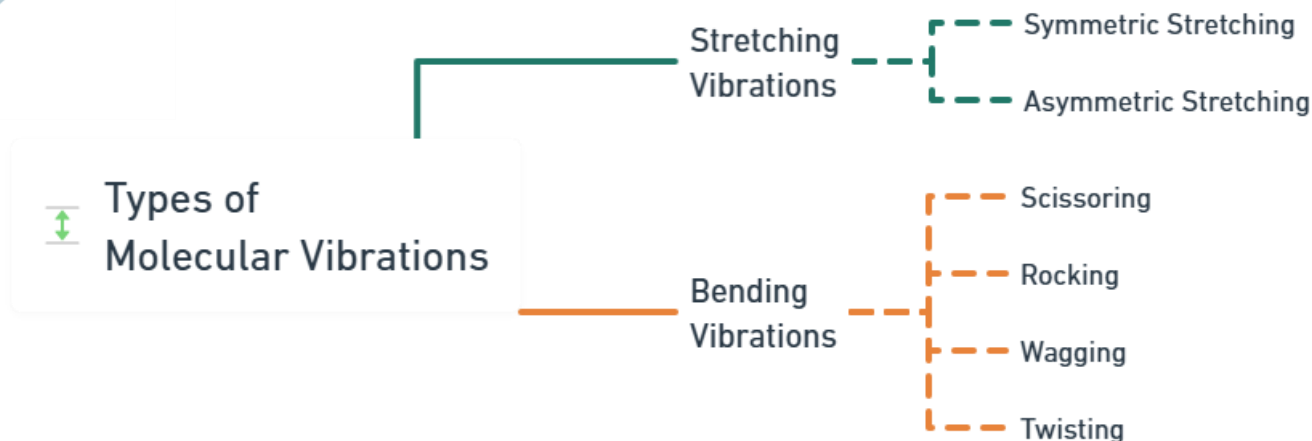
Pharmaceutical Applications:

1. **Identification:** Verifies the chemical composition, ensuring purity and consistency.
2. **Quantitative Analysis:** Measures the amount of a specific compound in a sample.
3. **Formulation Analysis:** Ensures correct ingredients and detects impurities in drug formulations.
4. **Physical State:** Identifies whether a drug is crystalline or amorphous.

Fundamental Modes of Vibrations in Polyatomic Molecules

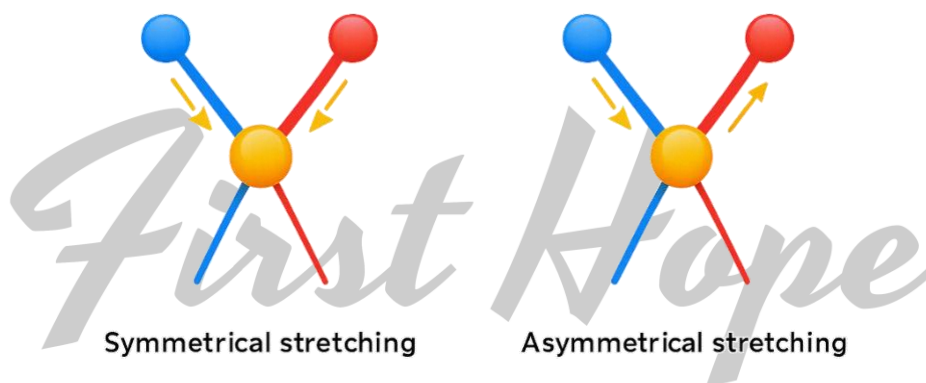
Molecular Vibrations

- In polyatomic molecules, atoms are not stationary but vibrate around their equilibrium positions.
- These vibrations can be described as periodic motions and are quantized, meaning they occur at specific energy levels.
- The two main types of molecular vibrations are:



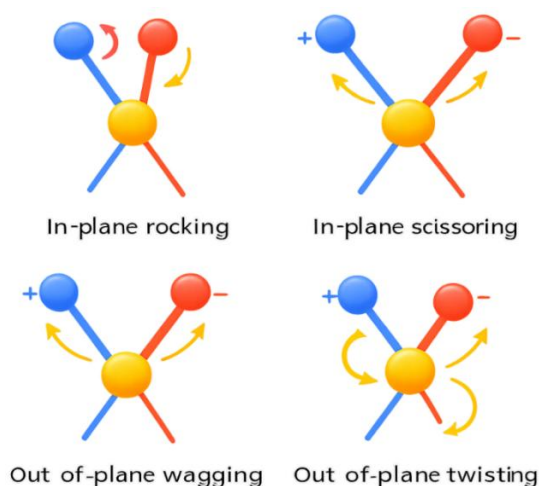
1. Stretching Vibrations:

- Involve changes in the bond length between atoms.
 - Symmetric Stretching:** Bonds expand and contract simultaneously in the same direction.
 - Asymmetric Stretching:** One bond shortens while another lengthens.



2. Bending Vibrations:

- Involve changes in the bond angle between atoms.
 - Scissoring:** Two atoms move toward and away from each other.
 - Rocking:** Atoms move in the same direction, rocking back and forth.
 - Wagging:** Atoms move up and down out of the plane.
 - Twisting:** One atom moves up while another moves down, causing a twist.



Degrees of Freedom

- **Translational Degrees:** Movement of the entire molecule in space (three degrees).
- **Rotational Degrees:** Rotation of the molecule around its axes (three degrees for nonlinear, two for linear molecules).
- **Vibrational Degrees:** Calculated using the formula:
 - **Nonlinear Molecules:** $3N - 6$
 - **Linear Molecules:** $3N - 5$
 - Where N is the number of atoms in the molecule.

Sample Handling Techniques in Infrared (IR) Spectroscopy

- Proper sample preparation is essential for obtaining accurate IR spectra.
- Techniques vary based on the sample's physical state: solid, liquid, gas, or solution.



A. Solid Sampling:

KBr Pellet Technique:

- Solid is ground with potassium bromide (transparent to IR) and pressed into a pellet.

Mull Technique:

- Solid is mixed with mineral oil to form a mull, then spread between NaCl salt plates.

Diffuse Reflectance (DRIFT):

- Used for solids unsuitable for other methods. The sample is mixed with a reflective medium, and the reflected IR radiation is analyzed.

B. Liquid Sampling:

Thin Film:

- A thin liquid film is placed between NaCl plates for analysis, suitable for non-corrosive liquids.

Solution Technique:

- Sample dissolved in an IR-transparent solvent and analyzed in a liquid cell or between salt plates.



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