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.

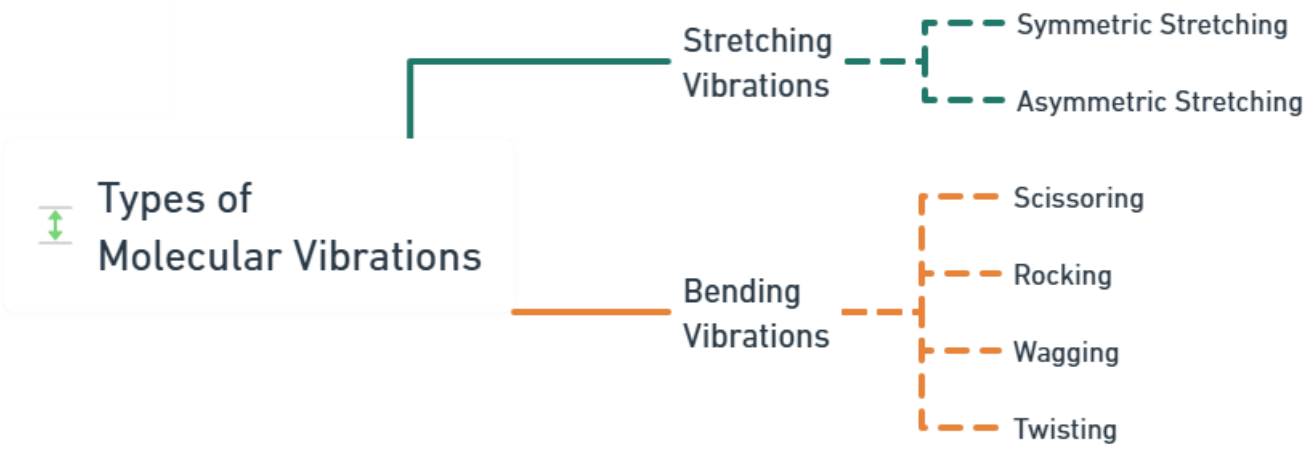
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Fundamental Modes of Vibrations in Polyatomic Molecules

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:

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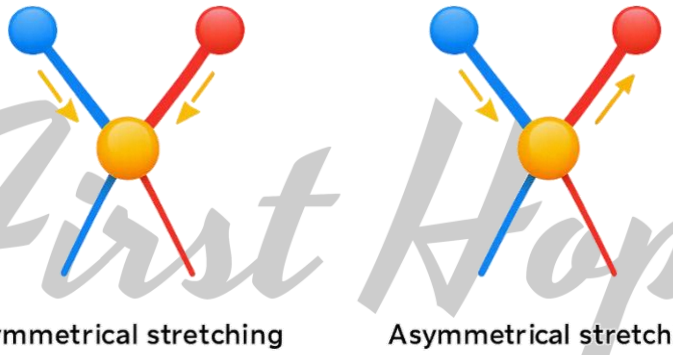


1. Stretching Vibrations:

- Involve changes in the bond length between atoms.

a) **Symmetric Stretching**: Bonds expand and contract simultaneously in the same direction.

b) **Asymmetric Stretching**: One bond shortens while another lengthens.



2. Bending Vibrations:

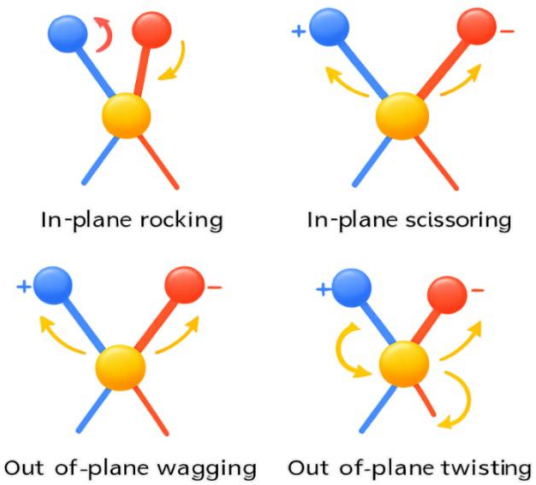
- Involve changes in the bond angle between atoms.

a) **Scissoring**: Two atoms move toward and away from each other.

b) **Rocking**: Atoms move in the same direction, rocking back and forth.

c) **Wagging**: Atoms move up and down out of the plane.

d) **Twisting**: One atom moves up while another moves down, causing a twist.



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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−63N - 63N−6
  - **Linear Molecules**: 3N−53N - 53N−5
  - Where NNN 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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