SNS COLLEGE OF PHARMACY AND HEALTH SCIENCES

Coimbatore -641035

COURSE NAME: INSTRUMENTAL METHODS OF ANALYSIS (BP 701 T)

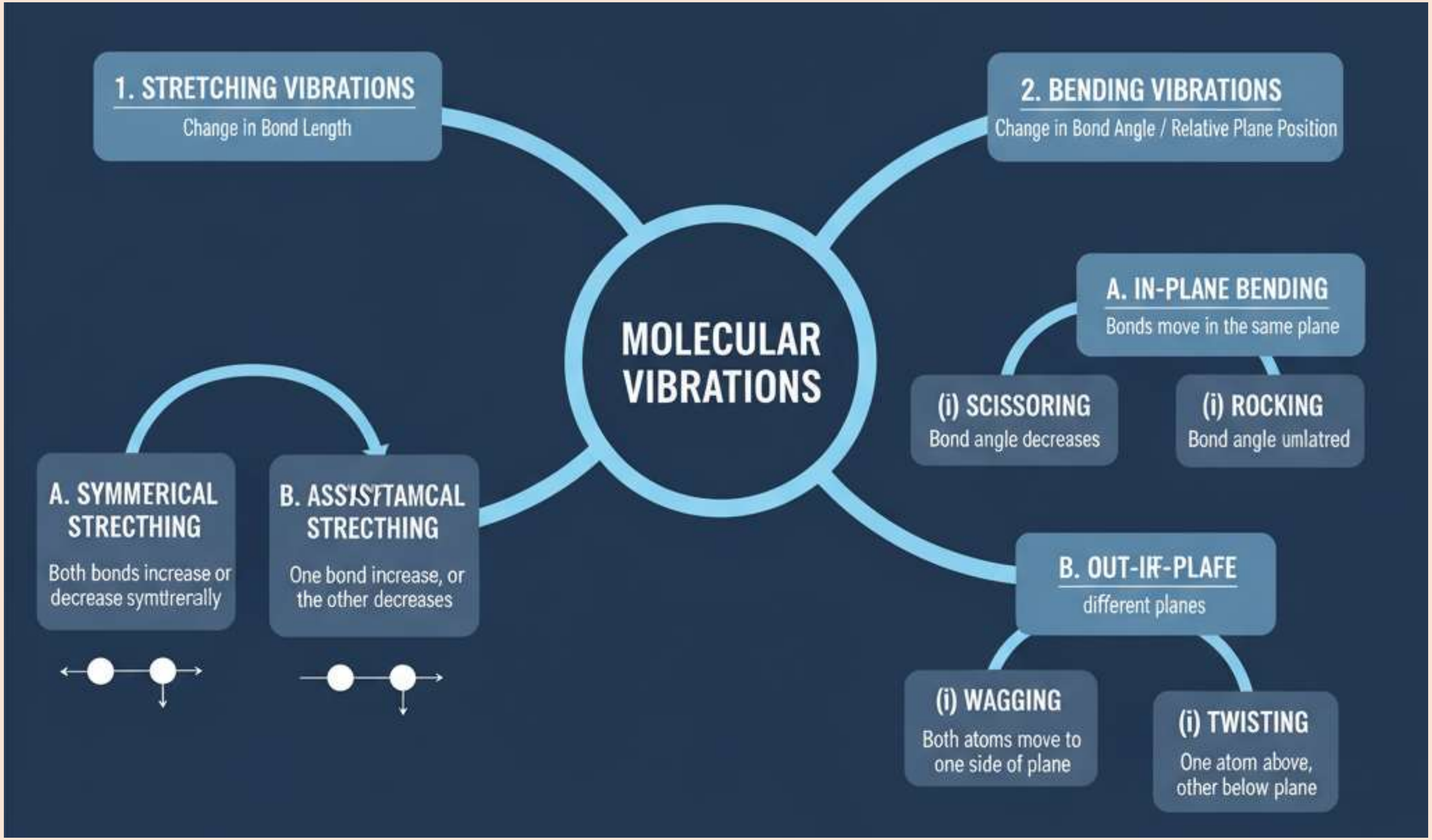
VII SEM/ IV YEAR

TOPIC 11: Principle & Modes of vibrations in IR Spectroscopy

Design Thinking for Understanding Principle & Modes of vibrations in IR Spectroscopy

1. **Empathize**: Understand the audience’s knowledge level to tailor explanations of stretching and bending vibrations.
2. **Define**: Create a clear PowerPoint to explain vibration types and subtypes using visuals
3. **Ideate**: Design slides with animated diagrams, color-coded visuals, and engagement tactics like quizzes.

MINDMAP

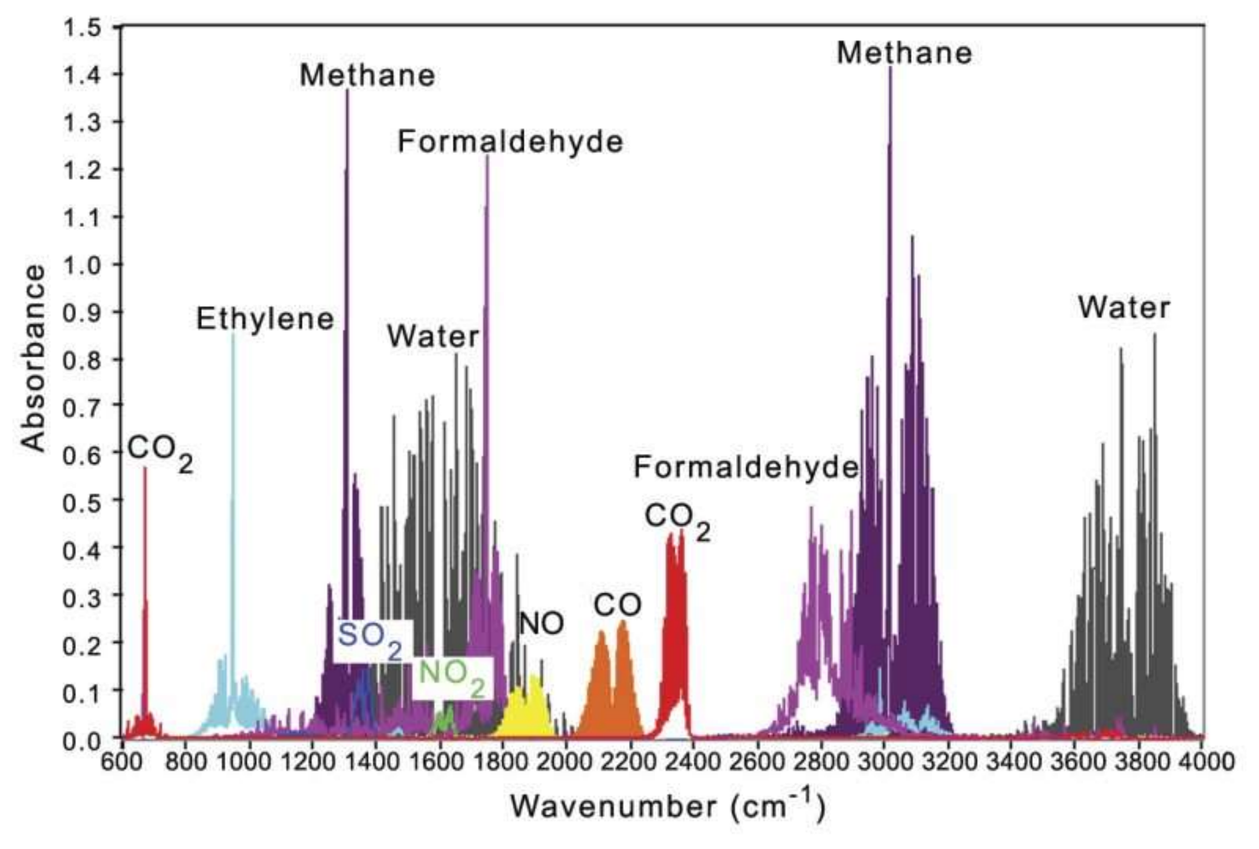

MOLECULAR VIBRATIONS
1. STRETCHING VIBRATIONS
Change in Bond Length
A. SYMMERICAL STRECTHING
Both bonds increase or decrease symtrerally
B. ASSISFTAMCAL STRECTHING
One bond increase, or the other decreases
2. BENDING VIBRATIONS
Change in Bond Angle / Relative Plane Position
A. IN-PLANE BENDING
Bonds move in the same plane
(i) SCISSORING
Bond angle decreases
(i) ROCKING
Bond angle umlatred
B. OUT-IF-PLAFE
different planes
(i) WAGGING
Both atoms move to one side of plane
(i) TWISTING
One atom above, other below plane

EMPHATHIZE

IR Spectroscopy

Who uses IR Spectroscopy?

- •Chemists, pharmacists, and researchers studying molecular structures.
- •Need to identify functional groups and molecular composition easily.



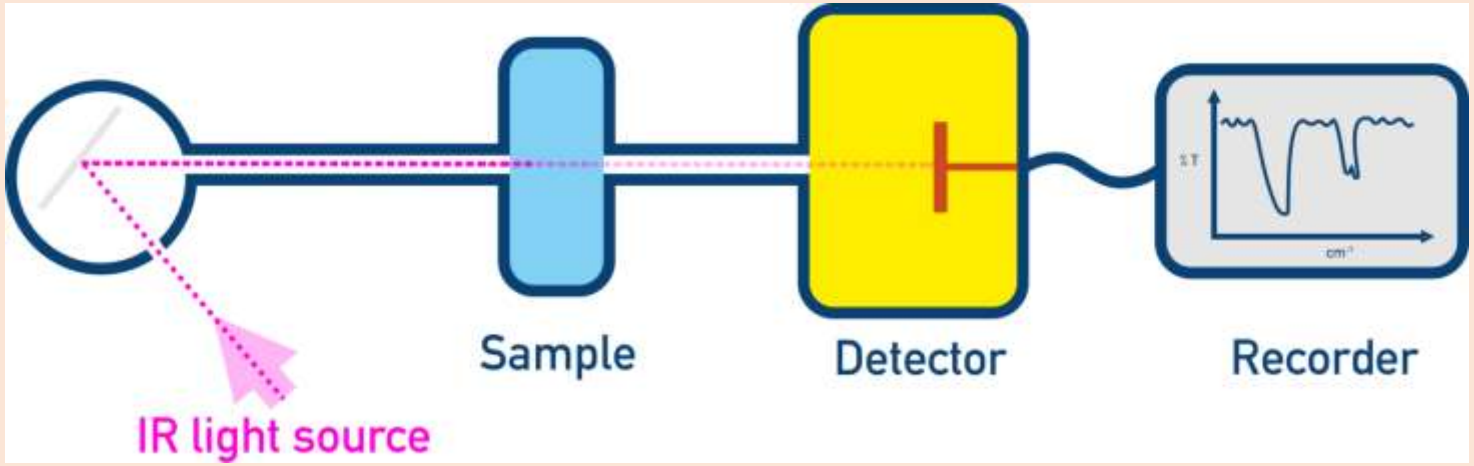
Why it matters?

- •IR spectroscopy helps in drug development, quality control, and material analysis.
- •Users want a reliable, non-destructive way to analyze compounds.

EMPHATHIZE

What is IR Spectroscopy?

- IR spectroscopy studies how molecules absorb infrared light to reveal their structure.
- IR light lies between visible and microwave regions in the electromagnetic spectrum.
- IR is a "fingerprint" tool to identify molecules based on their unique vibrational patterns.
- Widely used in pharmaceuticals to detect functional groups (e.g., -OH, C=O) and confirm compound identity.



DEFINE

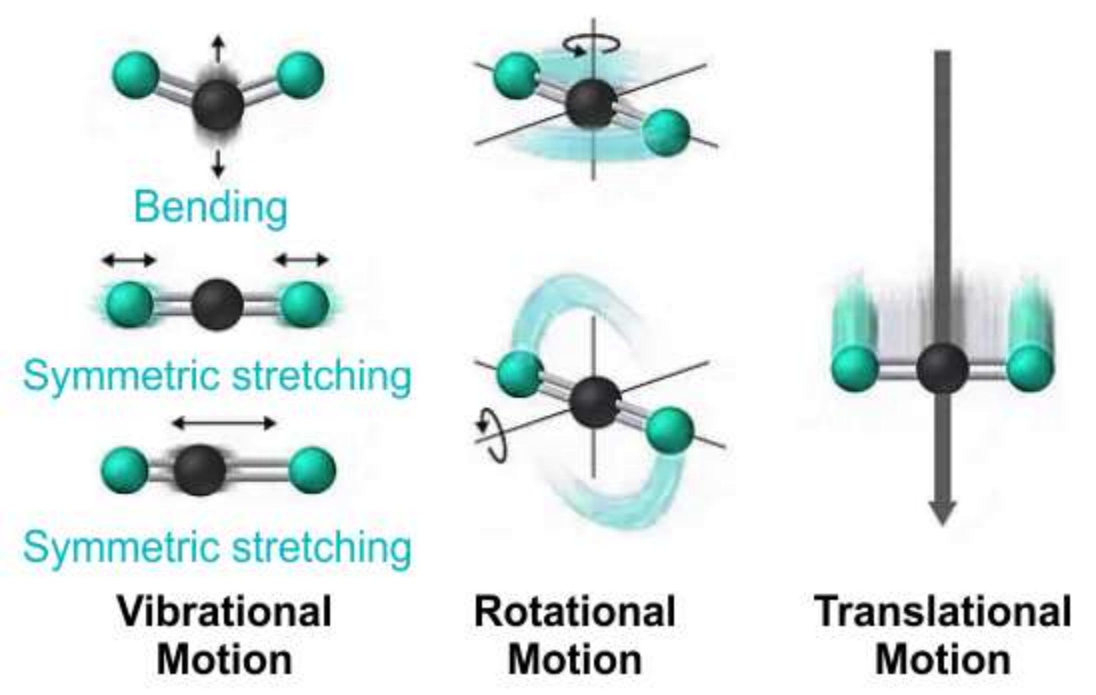
Principle of IR Spectroscopy

What’s Happening?

- ➢Molecules have energy (electronic + vibrational + rotational).
- ➢When IR light matches a molecule’s natural vibration frequency, it’s absorbed, creating peaks in the IR spectrum.

Key Requirement:

- ➢A molecule must change its dipole moment (polarity) to absorb IR light.
- ➢Example: CO_2’s asymmetric stretch creates a dipole, making it IR-active.



DEFINE

Conditions for IR Absorption

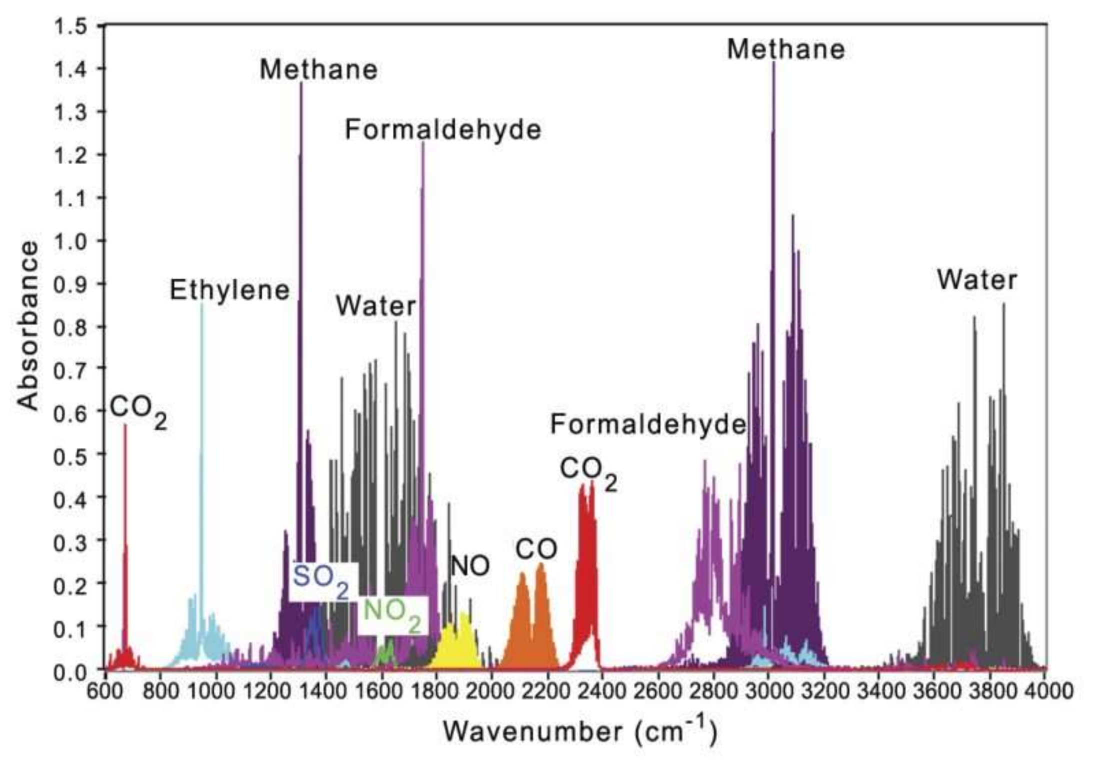
A compound can be analyzed by IR radiation only if:

➢There is a change in dipole moment during the vibration.

➢There is resonance between the applied and natural IR frequency.

➢For a vibration to be IR-active, the transition moment integral must be non-zero, and the photon's electric vector must align with the dipole change.

➢Symmetric molecules (e.g., O_2) do not absorb IR.



DEFINE

IR Spectral Regions

IR Regions:

Near IR (14000–4000 cm^{-1}): less common.

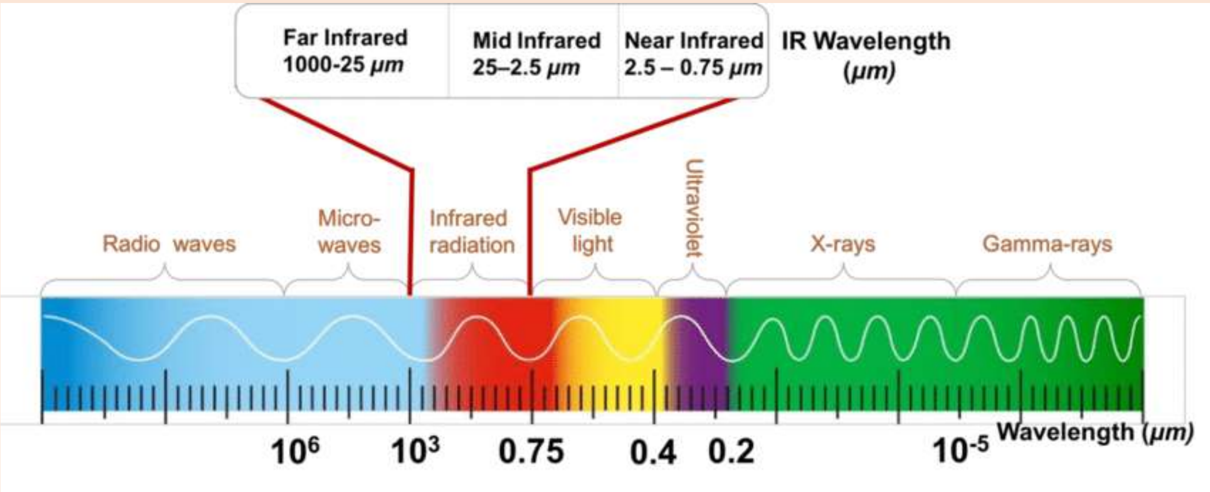
Mid IR (4000–400 cm^{-1}): Key for pharmaceuticals, shows functional group peaks.

Far IR (400–10 cm^{-1}): For inorganic compounds.

Two Key Zones in Mid IR:

Group Frequency Region (4000–1500 cm^{-1}): Shows peaks for specific functional groups (e.g., C=O at ~1,700 cm^{-1}).

Fingerprint Region (1500–400 cm^{-1}): Unique peaks for each molecule, like a molecular ID.

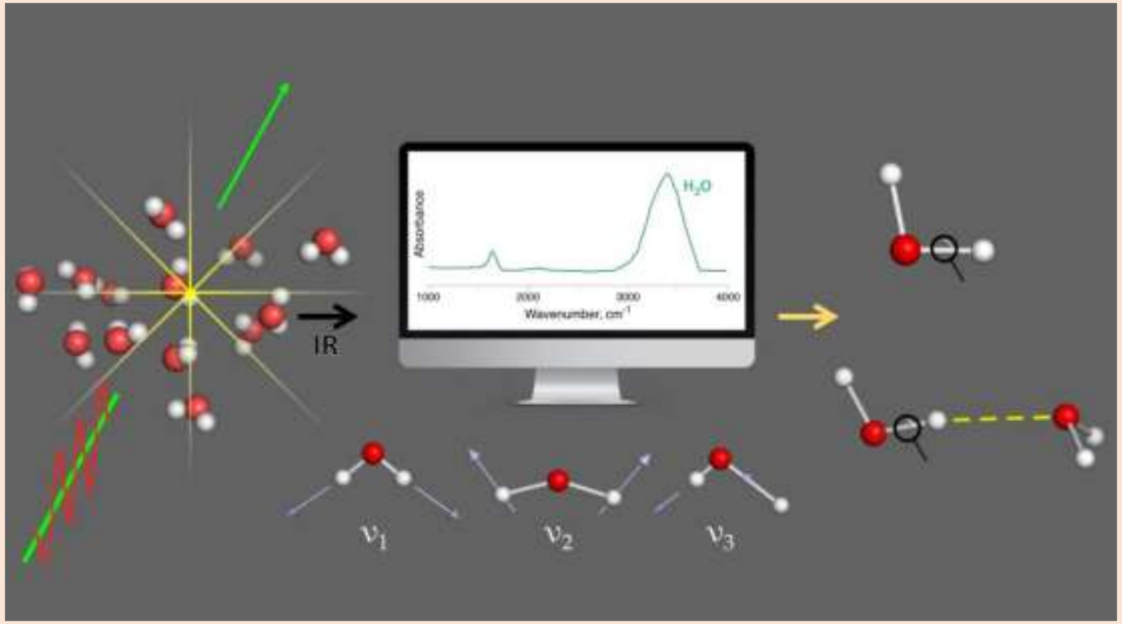


IDEATE

Types of Molecular Vibrations

Why Vibrations Matter?

Molecules vibrate because bonds act like springs, moving at specific frequencies.



IDEATE

Functional Groups and Their Frequency Regions

Functional Group	Bond	Range (cm^{-1})	Intensity
Alkanes	C-H stretch	2850-3000	Strong
Alkenes	=C-H stretch	3020-3100	Medium
Alkynes	≡C-H stretch	3300	Strong
Arenes	C-H stretch	3030	Variable
Alcohols & Phenols	O-H stretch (free)	3580-3650	Variable
Amines	N-H stretch (1°)	3400-3500	Weak
Aldehydes	C-H stretch (aldehyde)	2690-2840	Medium
Ketones	C=O stretch	1710-1720	Strong
Carboxylic Acids	O-H stretch	2500-3300	Strong, broad
Esters	C=O stretch	1735-1750	Strong
Amides	C=O stretch	1630-1695	Strong
Nitriles	C≡N stretch	2240-2260	Medium

IDEATE

Fundamental Modes of Vibrations in Polyatomic Molecules

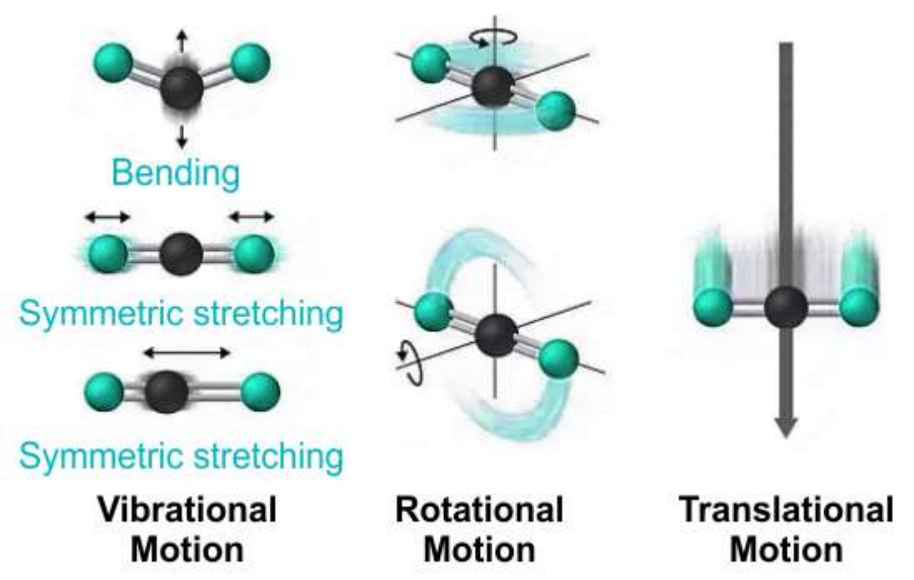
Number of Modes:

For a molecule with N atoms: Non-linear: 3N - 6 fundamental vibrational modes.

Linear: 3N - 5 fundamental vibrational modes.

Examples: H_2O (non-linear, N=3): 3 modes (symmetric stretch, asymmetric stretch, bend).

CO_2 (linear, N=3): 4 modes (symmetric stretch IR-inactive, asymmetric stretch active, two degenerate bends active).



IDEATE

Types of Molecular Vibrations

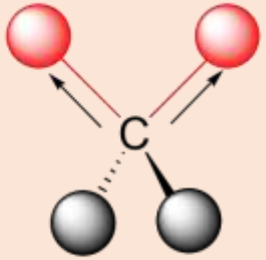
Two Main Types:

Stretching: Bonds get longer or shorter.

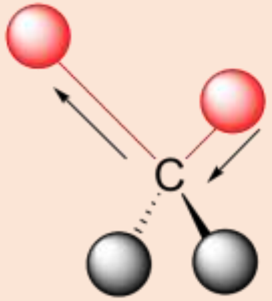
- Symmetric: Both bonds stretch together.
- Asymmetric: One bond stretches, the other shrinks.

Bending: Bond angles change.

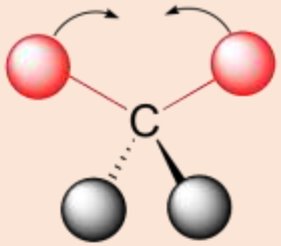
- In-plane: Scissoring (angle shrinks) or Rocking (bonds tilt together).
- Out-of-plane: Wagging (bonds move to one side) or Twisting (bonds move opposite ways).



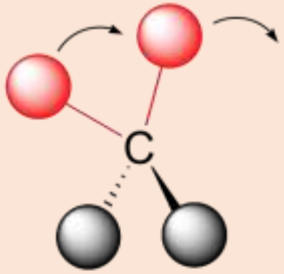
symmetric stretching



asymmetric stretching



scissoring



rocking

IDEATE

Stretching Vibrations

Stretching vibrations:

The bond length changes (increases or decreases).

Stretching requires higher energy than bending and appears at higher frequencies (e.g., 4000-1500 cm^{-1}).

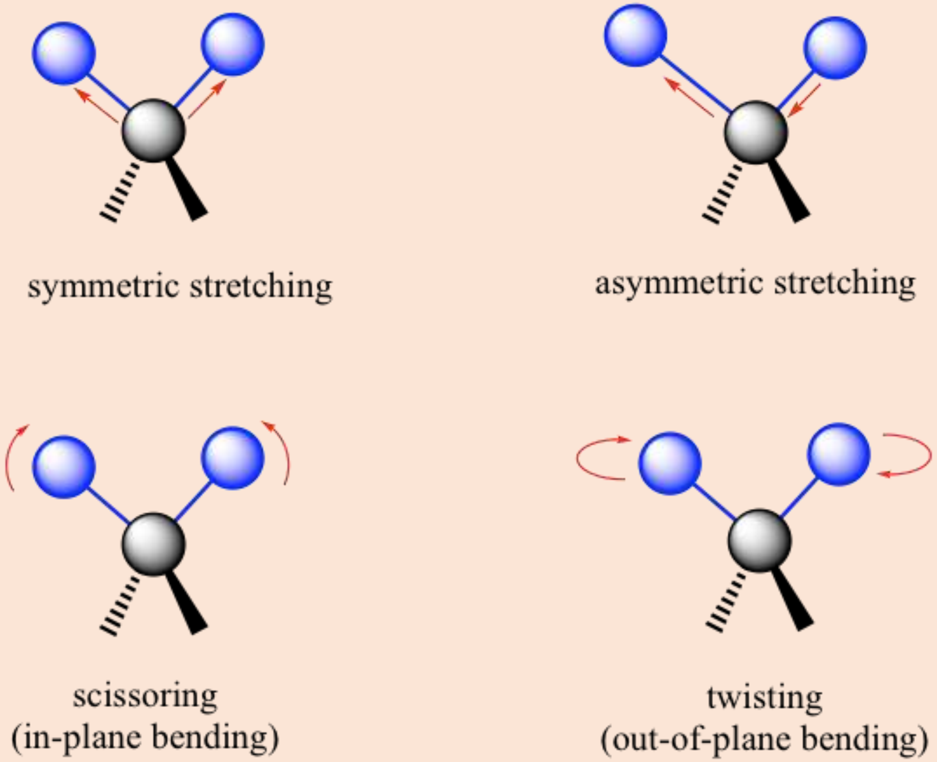
Types:

Symmetric stretching:

Both bonds increase or decrease in length symmetrically.

Asymmetric stretching:

One bond length increases while the other decreases.



Bending Vibrations

Bending vibrations:

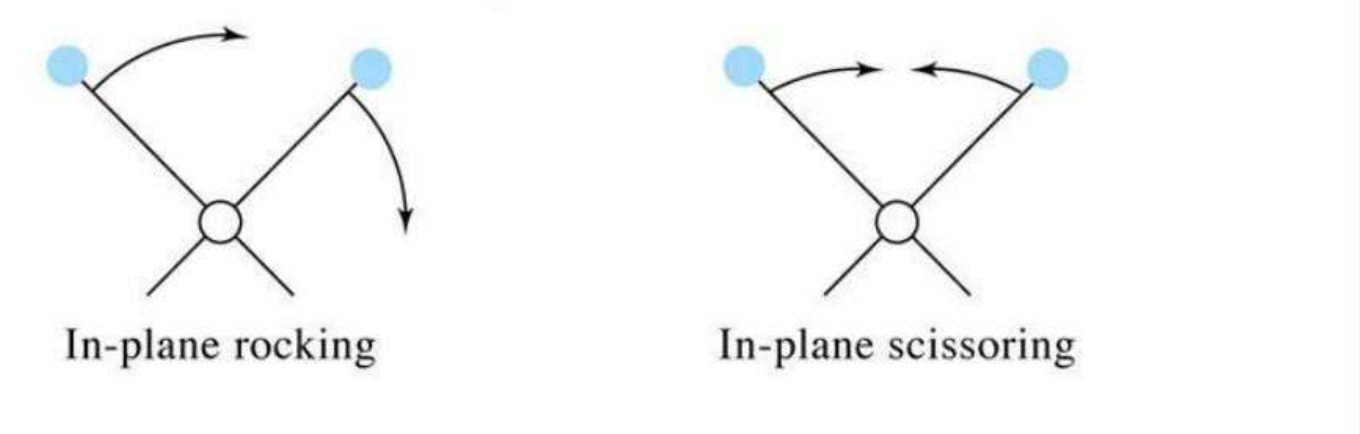
- Bending vibrations involve changes in bond angles.
- Bending appears at lower frequencies (e.g., 1500-400 cm^{-1}).

Types:

In-plane bending:

Bending occurs within the molecular plane.

- **Scissoring:** Bond angle decreases (like scissors closing).
- **Rocking:** Bond angle unchanged, but bonds move in the same direction within the plane.

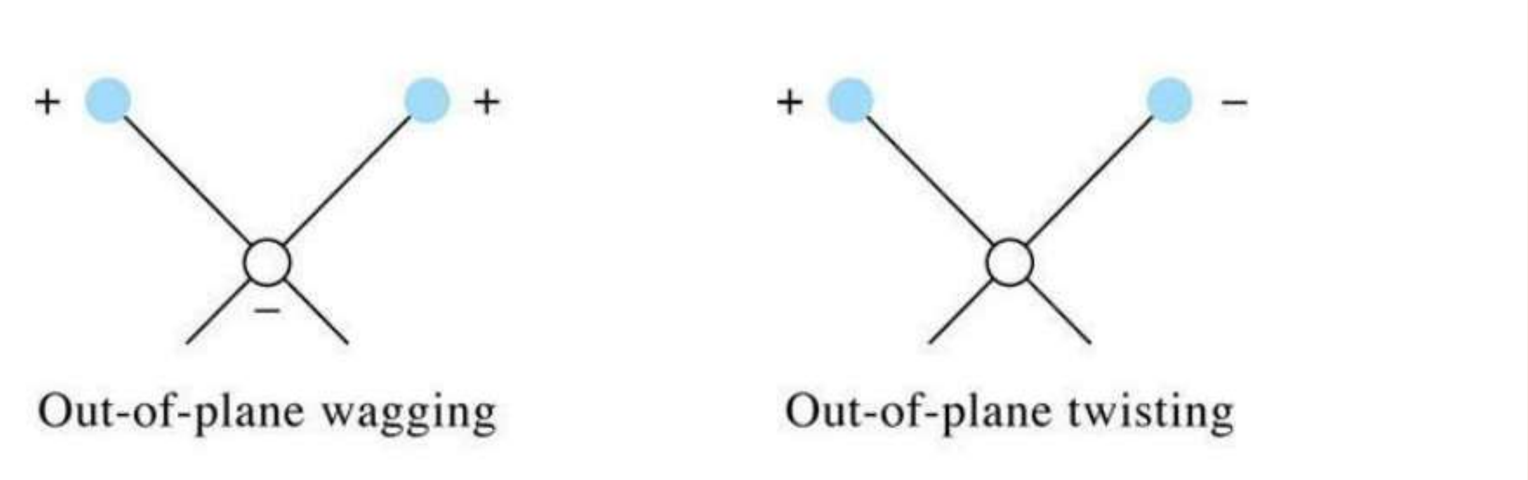


Bending Vibrations

Out-of-plane bending:

Bending occurs in different planes.

- **Wagging:** Both atoms move to one side of the plane.
- **Twisting:** One atom moves above the plane, the other below.



Summary

Vibration Type	**Sub-type**	**Description of Motion**	**Effect on Bond/Angle**	**Example (Functional Group)**
Stretching	A. Symmetrical	The two bonds connected to a central atom lengthen and shorten together in a symmetric pattern.	Change in Bond Length (Angle is maintained)	-CH2-, -NH2- symmetric stretch
	B. Asymmetrical	One bond lengthens while the other bond shortens (simultaneously, in an opposite pattern).	Change in Bond Length (Angle is maintained)	-CH2-, -NO2- asymmetric stretch

Summary

Vibration Type	**Sub-type**	**Description of Motion**	**Effect on Bond/Angle**	**Example (Functional Group)**
Bending	A. In-Plane: Scissoring	Two atoms move toward and away from each other within the same plane.	Change in Bond Angle (Angle decreases)	-CH2- scissoring
	A. In-Plane: Rocking	The entire group of atoms swings back and forth within the plane of the molecule.	Bond Angle is Unaltered	-CH2- rocking
	B. Out-of-Plane: Wagging	The group of atoms moves together above and below the plane of the molecule.	Change in Plane	-CH2- wagging
	B. Out-of-Plane: Twisting	One atom moves above the molecular plane while the other moves below the plane.	Change in Plane	-CH2- twisting

Assessment

Match the following:

Column A (Description of Motion)	Column B (Vibration Name)
1. Both bonds increase or decrease in length together.	A. Rocking
2. The bond angle decreases as two atoms move towards each other in a plane.	B. Asymmetrical Stretching
3. One bond lengthens while the other shortens.	C. Wagging
4. The entire group swings back and forth in the plane, with the bond angle staying constant.	D. Scissoring
5. Both atoms move to one side of the molecular plane.	E. Symmetrical Stretching
6. One atom moves above the plane, while the other moves below the plane.	F. Twisting

References

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Thank you!