Infrared Spectroscopy

Molecular Vibrations

Stretch, bend, rock, wag, twist modes. Each unique to molecular structure.

IR Regions

4000-2500: O-H, N-H | 2000-1500: C=O, C=C | 1500-400: Fingerprint

ATR-FTIR

Attenuated Total Reflectance. No sample prep required.

Water Interference

Strong O-H absorption. Use D_2O or dry samples.

Detailed Examples & Illustrations

1. Molecular Vibrations

Stretching Vibrations: Bond length changes periodically

• Symmetric stretch: Both bonds extend/contract together

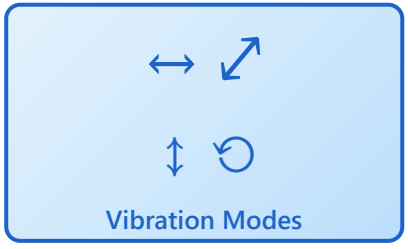
• Asymmetric stretch: One extends while other contracts

Bending Vibrations: Bond angle changes

• In-plane bending: Scissoring, rocking

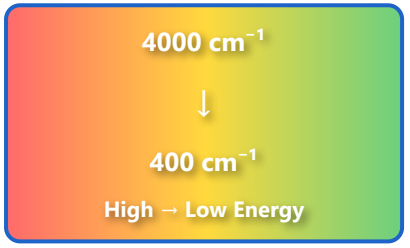
• Out-of-plane bending: Wagging, twisting

Typical Frequencies:



- C-H stretch: ~3000 cm^{-1}
- C=O stretch: ~1700 cm^{-1}
- C-C stretch: ~1000 cm^{-1}

2. IR Spectral Regions



Functional Group Region (4000-1500 cm^{-1}):

- 3600-3200: O-H stretch (alcohols, phenols)
- 3500-3300: N-H stretch (amines, amides)
- 3000-2850: C-H stretch (alkanes, alkenes)
- 1750-1650: C=O stretch (carbonyls)
- 1680-1600: C=C stretch (alkenes)

Fingerprint Region (1500-400 cm^{-1}):

- Complex pattern unique to each molecule
- Used for definitive compound identification
- C-O, C-N, C-C stretches and various bending modes

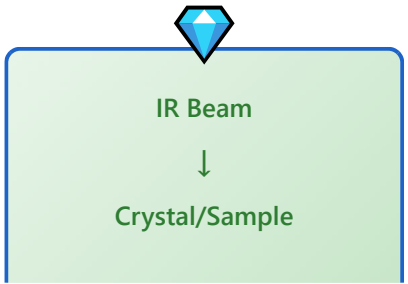
3. ATR-FTIR Technique

Working Principle:

- IR beam undergoes total internal reflection at crystal-sample interface
- Evanescent wave penetrates sample (~0.5-5 µm depth)
- Sample absorbs specific wavelengths
- Reflected beam carries absorption information

Key Advantages:

- No sample preparation needed
- Works with solids, liquids, powders, films
- Quick analysis (1-2 minutes)



• Non-destructive

Common Crystals:

• Diamond: Hardest, most durable, wide range

• ZnSe: Good for most organic samples

• Ge: Best for strongly absorbing samples

4. Water Interference Problem

The Problem:

• Water shows very strong O-H stretching (~3400 cm^{-1})

• H-O-H bending band at ~1640 cm^{-1}

• Overlaps with important functional groups (O-H, N-H)

• Moisture in air can interfere with measurements

Solutions:

• **Use D_2O:** Deuterium shifts O-D stretch to ~2500 cm^{-1}

• **Dry samples:** Store in desiccator before measurement

• **Background subtraction:** Measure pure water spectrum first

• **Purge instrument:** Continuously flow dry N_2 or air

• **Use ATR-FTIR:** Less sensitive to atmospheric water

Best Practice:

Always record background in same conditions as sample measurement

💡 Key Tips for IR Analysis

• Always run a blank/background spectrum first

• Clean ATR crystal thoroughly between samples

- Apply consistent pressure on ATR crystal
- Use correlation tables to identify unknown peaks
- Compare fingerprint region with reference spectra
- Consider both presence and absence of peaks
- Multiple complementary techniques (NMR, MS) confirm structure