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Interpretation of FTIR Spectra

Practical 2 - Spectral interpretation practical

Aim

To identify functional-group evidence and compare fingerprint regions in FTIR spectra.

Principle

IR absorption arises from vibrations associated with a change in dipole moment. Band position, shape and the complete pattern matter; hydrogen bonding and sample preparation can change appearances.

Materials and Requirements

- Recorded qualified spectra with acquisition settings
- Candidate formulae and structures
- Peak-assignment worksheet
- Approved method or teaching-data pack and a dated record sheet

Procedure

1. Define the preparation or dataset, study question and method version. Record identities, units and the criteria to be used before examining the outcome.
2. Check axis, units, calibration, solvent or reference and acquisition quality.
3. Inspect background, accessory and spectral quality before interpreting the spectrum.
4. Evaluate broad O-H/N-H regions, carbonyl features and the full fingerprint pattern against a suitable reference.
5. Assign features with multiplicity, intensity or fragmentation context and list alternative explanations.
6. Compare all available evidence with the candidate structures, distinguishing a provisional assignment from a confirmed identity.
7. Retain the original observations and calculations. State deviations, missing information and the limits of the conclusion; do not replace measured values with expected results.

Observations and Record

Enter actual measurements or the supplied teaching data. Record the method, material identity, conditions and units.

Feature / region	Observed value	Proposed assignment	Supporting / conflicting evidence
Major feature	Enter	Assign	Assess
Diagnostic feature	Enter	Assign	Assess
Missing feature	State	Explain	Assess

Calculations

- Wavenumber (cm^-1) = 1 / wavelength (cm)

Worked Example

Illustrative a strong band near 1715 cm^-1 supports some carbonyl environments, but cannot alone identify a specific compound.

A broad acid O-H region and other evidence are needed before assigning a carboxylic acid.

Result and Interpretation

• Provide an annotated spectrum and a reasoned structural conclusion with limitations.

Precautions

• Do not read isolated peaks without context.
• Retain unprocessed data and processing choices.
• Use orthogonal evidence when an assignment is ambiguous.

Viva Questions and Answers

Why is the fingerprint useful?

The combined pattern can distinguish many compounds.

Does every vibration absorb IR?

The vibration must produce a dipole-moment change.

Can one carbonyl band establish identity?

Several structures may have overlapping carbonyl regions.

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