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Structure Identification by Combined Spectral Evidence

Practical 13 - Spectral interpretation practical

Aim

To identify a candidate structure by integrating UV, IR, NMR and mass evidence.

Principle

Each technique constrains different structural features. A defensible assignment must satisfy formula, unsaturation, functional-group, proton and fragment evidence together.

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. Derive candidate formulae and unsaturation from mass and composition evidence.
4. Create a joint assignment table for UV chromophore, IR groups, proton/carbon NMR environments and mass fragments; reject candidates that fail essential observations.
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

- Double-bond equivalents for an ordinary closed-shell CHNX formula = (2C + 2 + N - H - X)/2; oxygen and sulfur do not enter this simple expression.

Worked Example

Illustrative C8H9NO2 has DBE = (16 + 2 + 1 - 9)/2 = 5.

An aromatic ring plus one carbonyl accounts for five, but further evidence is needed to identify the substitution pattern.

Carbon NMR evidence

• Record the carbon NMR solvent, reference, acquisition and decoupling conditions. Compare carbonyl, aromatic/alkene and aliphatic carbon environments with the proposed structure.

• A broadband proton-decoupled carbon spectrum generally does not show ordinary proton n+1 splitting, and peak areas are not automatically quantitative carbon counts.

• Use symmetry and overlap when comparing the number of observed environments with the molecular formula; DEPT or two-dimensional correlations can add constraints when available.

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 combine techniques?

They constrain different aspects of a structure.

What is DBE?

A formula-based count of rings and pi-bond equivalents under stated valence assumptions.

What if evidence conflicts?

Recheck data and candidates rather than ignoring the conflict.

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