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Interpretation of Proton NMR Spectra

Practical 3 - Spectral interpretation practical

Aim

To assign a proton NMR spectrum using shift, integration and coupling evidence.

Principle

Chemical shift reflects electronic environment, integration approximates relative proton populations under suitable acquisition conditions, and coupling provides connectivity clues. Exchange and second-order effects can complicate simple patterns.

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. Record solvent, spectrometer frequency and reference; identify solvent, water and exchangeable signals.
4. Normalise integrals and examine multiplicities and coupling constants without forcing the n+1 rule on complex signals.
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

- Chemical shift delta (ppm) = frequency difference (Hz) / spectrometer frequency (MHz)

Worked Example

Illustrative shift difference 800 Hz at 400 MHz gives delta = 2.00 ppm.

An ethyl pattern can show a 3H triplet and 2H quartet with matching coupling, but the surrounding structure determines their shifts.

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

What does integration measure?

Relative signal area, related to proton count under suitable conditions.

Why quote solvent?

It affects shifts and introduces its own signals.

When can n+1 fail?

Strong coupling, nonequivalent neighbours and exchange can complicate patterns.

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