NMR Spectrum Interpretation

Experiment 22 - Practical Notes

Name: _____ Roll no.: _____ Date: _____

Aim

To interpret the supplied nmr spectrum interpretation.

Principle

Chemical shift, integral and splitting describe nuclei in a molecular environment. Reliable interpretation uses the nucleus, solvent and the assigned spectrum conditions.

Requirements

- Instructor-provided labelled diagrams, traces or data for this activity.
- Calculator, graph paper or spreadsheet, and the activity record.

Procedure

1. Read the spectrum

Record nucleus, chemical-shift scale, solvent and supplied frequency.

2. Assign signals

Mark chemically distinct signals and compare integral ratios for appropriate non-exchangeable signals.

3. Analyse splitting

Use the assigned simple coupling model where suitable; complex spectra are not resolved by a universal n+1 rule.

4. Compare structure

Check whether the proposed structure accounts for the full pattern, integration and known exchange/overlap limitations.

Observations and Record

Record item	Entry
Activity / material identifier	_____
Measurement or visible feature	_____
Comparison / calculated outcome	_____
Interpretation and limitation	_____

Worked Example

The numbers below are illustrative; enter your own observations in the record.

- Integral ratios support relative proton numbers in the applicable 1H spectrum.
- Example: clean integral values 2:3 support a 2:3 relative proton ratio, subject to the stated integration conditions.

Result

The recorded finding is ____; the supporting observation or calculation is ____. The main limitation is ____.

Precautions

- Use the supplied teaching material; distinguish a measured observation from an assumed value.
- Keep units, axes, labels and measurement conditions consistent.
- Record limitations and seek instructor review before applying a conclusion to a live case.

Viva Questions and Answers

1. What is the main endpoint?

Interpret the supplied nmr spectrum interpretation.

2. Does one observed result prove a general conclusion?

No. Controls, repeatability and the limitations of the method must be considered.

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