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Interpretation of Mass Spectra

Practical 11 - Spectral interpretation practical

Aim

To interpret molecular-ion or adduct and fragmentation evidence in mass spectra.

Principle

Mass spectrometry records mass-to-charge ratios of ions. Ionisation method determines whether a molecular radical cation, protonated/deprotonated molecule or another adduct is expected.

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 ionisation mode, polarity and mass accuracy; identify plausible charge and adduct states.
4. Compare isotope patterns and exact or nominal mass with candidate formulae, then rationalise diagnostic fragments and neutral losses.
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

- Mass error (ppm) = (observed - calculated m/z) / calculated m/z x 10^6

Worked Example

Illustrative calculated m/z 200.1000 and observed 200.1004 give +2.0 ppm.

Whether this supports an assignment depends on instrument performance, isotope evidence and candidate ambiguity.

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

Is the base peak always the molecular ion?

No; it is the most intense recorded peak.

Why specify ionisation?

It determines likely ion types and fragmentation.

What does m/z mean?

Ion mass divided by its charge number.

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