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UV Absorption and Woodward-Fieser Calculations

Practical 1 - Spectral interpretation practical

Aim

To calculate a model UV absorption maximum using the applicable Woodward-Fieser rules.

Principle

Empirical base values and increments estimate absorption maxima for specified conjugated systems. Correct chromophore classification is essential; these rules do not apply to every aromatic or medicinal molecule.

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. Draw the conjugated chromophore and identify whether the adopted table covers a diene or an alpha,beta-unsaturated carbonyl system.
4. Record the selected base, substituent, ring-residue and exocyclic increments from the same rule set.
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

- Predicted wavelength = applicable base value + justified increments

Worked Example

Illustrative acyclic diene model: base 217 nm plus two alkyl/ring-residue increments of 5 nm gives 227 nm, assuming no additional increments.

Report the chosen rule convention and compare with an actual spectrum; the estimate is not a measured wavelength.

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 classify the chromophore?

Different conjugated systems use different empirical rules.

What is a bathochromic shift?

A shift to longer wavelength.

Why can observation differ?

Solvent, conformation and rule limitations can affect the spectrum.

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