

Organic Spectroscopy

Second Year, Michaelmas term, 8 lectures: Dr TDW Claridge & Prof BG Davis

Lectures 1-4 highlight the importance of spectroscopic methods in the structural elucidation of organic molecules starting with an introduction to the NMR phenomenon; these four lectures will enable you to interpret ^1H and ^{13}C spectra of simple organic molecules and to identify simple organic structures from their NMR spectra.

Content: (1) Organic absorption spectroscopy, nuclear spin and resonance, chemical shifts; (2) factors that influence ^1H chemical shifts, spin-spin coupling, coupling patterns and resonance multiplicities, coupling to chemically equivalent spins, weak and strong coupling; (3) chemical and magnetic equivalence, ^1H spin couplings and chemical structure—geminal, vicinal and long-range couplings, chirality and NMR, chiral solvating agents; (4) ^{13}C NMR spectroscopy, NMR instrumentation, Fourier transform NMR, interpretation.

Lectures 5-7 will introduce those aspects of UV (0.5 lect.), IR (1.5 lect.) and MS techniques (1 lect.) that you will need in order to suggest candidate structures given raw experimental data in each case. Coverage of the underlying theory and instrumentation associated with each method will be kept to a bare minimum since these aspects are covered elsewhere. In modern research laboratories, NMR spectroscopy and MS are usually the first choice method for gaining structural information, with IR information routinely acting in a supporting capacity and UV spectra only being required in specialised circumstances (e.g. polymers, porphyrins). Lecture 8 will show how IR and MS data can be used in combination with NMR spectra to assign structures in a selection of real examples.

Previous examination questions for practice

Part IA: 2004 (Q7), 2005 (Q2), 2006 (Q1), 2007 (Q8), 2008 (Q9), 2009 (Q1)

Bibliography

- Introduction to Organic Spectroscopy: LM Harwood & TDW Claridge

Basic text for this course

- Spectrometric Identification of Organic Compounds (7th ed): RM Silverstein, FX. Webster & DJ. Kiemle

Comprehensive description of IR, MS and NMR with many problems: highly recommended

- Spectroscopic Methods in Organic Chemistry (5th Edn): DH Williams & I Fleming

Broad coverage of UV, IR, NMR and MS

- Organic Structures from Spectra: LD Field, S Sternhell & JR Kalman

Workbook of ^1H and ^{13}C NMR spectra of increasing complexity

- Structure Elucidation by NMR in Organic Chemistry: E Breitmaier

Workbook of example NMR spectra

- Experimental Organic Chemistry (2nd Edition): L M Harwood, C J Moody & J M Percy

Chapter 5 and Appendix 3 provide useful background and reference tables