

Spectroscopy

Module Code:	CFS7030-B
Academic Year:	2018-19
Credit Rating:	20
School:	School of Chemistry and Biosciences
Subject Area:	Chemistry and Forensic Science (ceases 2016)
FHEQ Level:	FHEQ Level 7 (Masters)

Pre-requisites:

Co-requisites:

Contact Hours

Type	Hours
Lectures	18
Practical classes and	18
Directed Study	164

Availability Periods

Occurrence	Location/Period
BDA	University of Bradford / Semester 1 (Sep - Jan)

Module Aims

This module will provide you with specialist knowledge in the principles and application of IR, Raman and NMR. This covers; sample preparation, instrumental fundamentals and design, including case studies related to applications in specialist areas and recent advances.

The specialist knowledge is reinforced by the 'hands on' practical component and will include use of the analytical centre instruments, collecting and analysing data, troubleshooting and method development/enhancement. The practical sessions will also

involve following written experimental protocols, working in a small group, and working to deadlines.

Outline Syllabus

Advanced Nuclear Magnetic Resonance

An introduction to NMR spectroscopy: Theoretical overview of 1D and 2D NMR experiments.

1D experimentation including nuclei other than ^1H and ^{13}C (^{31}P , ^{19}F , ^{15}N etc.)

2D experiments including COSY, HSQC, HMBC, H2BC etc.

NOE experiments including NOEDIFF, NOESY and ROESY

Hands on training in the Structure Elucidation of organic molecules using 1D and 2D NMR spectral data in association with other sources of data.

Practical considerations for NMR experimentation:

- Lock signal in modern spectrometers (2D lock)
- Shimming
- Calibration of 90° pulse
- Sensitivity and S:N
- Pulse programmes
- Working in protonated solvents

Advanced Spectral processing

- FID manipulation
- FFT, Phasing, Baseline corrections, integration

Solid state NMR – an introduction (cross polarisation, magic angle, molecular and symmetry considerations, nuclei). Quantitative NMR – an introduction (T_1 relaxation, internal and external referencing, ERETIC)

Vibration Spectroscopy

Module introduction. Vibrational spectroscopy: advanced applications of IR and Raman spectroscopy and microscopy in the derivation of molecular structural information. Energy units and molecular spectra, vibration of a diatomic molecule. Factors determining vibrational frequencies. Vibrations of polyatomic molecules. Selection rules for Infrared and Raman spectra. Raman versus Infrared spectroscopy. Depolarization ratios. The concept of symmetry: point symmetry elements. The character tables. Classification of normal vibrations by symmetry, symmetry selection rules. Applications: to structural chemistry, to biochemistry, biology, and medicine. Solid state application. Industrial applications; development of vibrational spectroscopic techniques for the solution of structural chemical problems in interdisciplinary case studies; remote sensing probes; handling of difficult samples.

Module Learning Outcomes

On successful completion of this module, students will be able to...

- 1 Evaluate and apply knowledge and understanding of the theories of instrumental analysis, including sample preparation and analysis.
- 2 Describe recent advances in the subject area.
- 3 Manipulate samples for selection, preparation and analysis.
- 4 Analyse, interpret and critically review experimental data generated with the selected techniques.

- 5 Identify poor quality analytical results and suggest/apply remedial action.
- 6 Apply skills in problem solving and written communication.

Learning, Teaching and Assessment Strategy

This module will be presented as a series of lectures and workshops/laboratory sessions. The lectures will describe sample preparation and instrumental techniques covering the fundamentals to recent developments. The lectures will include case studies enabling you to think across your own discipline and explore other fields. The lectures will be supported by practical workshops and 'hands-on' sessions with relevant samples. Formative progress tests will be used to revise previous content with feedback and questions from students. The assessment will be used to assess your learning and to enable you to demonstrate your problem solving and interpretation skills.

Mode of Assessment

Type	Method	Description	Length	Weighting	Final Assess'
Summative	Laboratory Report	Student will submit a laboratory report detailing analysis of sample(s) and interpretation of experimental data.	-2000 words	50%	No
Summative	Examination - closed book	A formal exam covering the taught syllabus. Short questions followed by longer essay type questions.	2 hours	50%	Yes

Legacy Code (if applicable)

Reading List

To view Reading List, please go to [rebus:list](#).