UNIVERSITY of BRADFORD

Module Descriptor

Module Details	
Module Title	Spectroscopy
Module Code	CFS7030-B
Academic Year	2023/4
Credits	20
School	School of Chemistry and Biosciences
FHEQ Level	FHEQ Level 7

Contact Hours	
Type	Hours
Interactive Learning Objects	18
Practical Classes or Workshops	10
Directed Study	164
Laboratories	8

Availability	
Occurrence	Location / Period
BDA	University of Bradford / Semester 1

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 with theoretical overview of 1D and 2D NMR experiments.
1D experimentation including nuclei other than 1H and 13C (31P, 19F, 15N 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
Solid-state NMR including cross polarisation, magic angle, molecular and symmetry considerations, nuclei
Quantitative NMR including T1 relaxation, internal and external referencing, ERETIC

Practical considerations for NMR experimentation:
Lock signal in modern spectrometers (2D lock)
Shimming
Calibration of 90 degree pulse
Sensitivity and S:N
Pulse programmes
Working in protonated solvents
Advanced Spectral processing
FID manipulation, FFT, Phasing, Baseline corrections, integration

Vibrational Spectroscopy
Recap of fundamentals of vibrational spectroscopy, including energy units and molecular spectra, vibrations of diatomic and polyatomic molecules, factors determining vibrational frequencies, Raman versus Infrared spectroscopy, depolarization ratios, point symmetry elements, classification of normal vibrations by symmetry, symmetry selection rules.
Critical review of vibrational spectroscopy applied to structural chemistry, biochemistry and materials chemistry. Solid-state and industrial applications will be examined.
Development of vibrational spectroscopic techniques for the solution of structural chemical problems in interdisciplinary case studies; remote sensing probes; handling of difficult samples.
Develop a systematic understanding of knowledge, and a critical awareness of current problems and/or new insights, much of which is at, or informed by, the forefront of the academic field.

Learning Outcomes

Outcome Number	Description
01	Evaluate and apply knowledge and understanding of the theories of instrumental analysis, including sample preparation and analysis.
02	Describe recent advances in the subject area.
03	Manipulate samples for selection, preparation and analysis.
04	Analyse, interpret and critically review experimental data generated with the selected techniques.
05	Identify poor quality analytical results and suggest/apply remedial action.
06	Apply skills in problem solving and written communication.

Learning, Teaching and Assessment Strategy

The module uses a blended approach to support learning and achievement. Students will engage with a series of online learning packages. These will include short videos that address key concepts, a set of structured activities (reading, online discissions etc.) that 'scaffold' the learning, and a range of formative tasks that generate feedback on progress.

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 assessments 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	Weighting
Summative	Examination - Open Book	Student will submit a report detailing analysis of sample(s) and interpretation of experimental data (2 Hrs)	50%
Summative	Examination - Closed Book	A formal closed book exam covering the taught syllabus. Short questions followed by longer essay type questions (2 Hrs)	50%

Reading List

To access the reading list for this module, please visit https://bradford.rl.talis.com/index.html

Please note:
This module descriptor has been published in advance of the academic year to which it applies. Every effort has been made to ensure that the information is accurate at the time of publication, but minor changes may occur given the interval between publishing and commencement of teaching. Upon commencement of the module, students will receive a handbook with further detail about the module and any changes will be discussed and/or communicated at this point.
