

Module Details	
Module Title	Spectroscopy
Module Code	CFS7030-B
Academic Year	2020/1
Credits	20
School	School of Chemistry and Biosciences
Subject Area	Chemistry
FHEQ Level	FHEQ Level 7
Pre-requisites	N/A
Co-requisites	N/A

Contact Hours	
Type	Hours
Learning Objects Interaction	18
Practical Classes or Workshops	18 (online workshop)
Directed Study	156
Laboratories	8

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

Module Aims
<p>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.</p> <p>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.</p>

## 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  $^1\text{H}$  and  $^{13}\text{C}$  ( $^{31}\text{P}$ ,  $^{19}\text{F}$ ,  $^{15}\text{N}$  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.

## 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 weekly online learning packages. These will include short videos that address key concepts, a set of structured activities (reading, online discussions etc.) that 'scaffold' the learning, and a range of formative tasks that generate feedback on progress. Online workshops and tutorials will also be used to support learning and monitor progress as students move through the curriculum.

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
Summative	Laboratory Report	Student will submit a laboratory report detailing analysis of sample(s) and interpretation of experimental data	N/A	50%
Summative	Examination - Open Book	A formal open book exam covering the taught syllabus. Short questions followed by longer essay type questions.	2 hour	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.*