CH275-15 Molecular Structure and Spectroscopy

24/25

Department
Chemistry
Level
Undergraduate Level 2
Module leader
Jozef Lewandowski
Credit value
15
Module duration
10 weeks
Assessment
20% coursework, 80% exam
Study location
University of Warwick main campus, Coventry

Description

Introductory description

This module will explore how molecules interact with electromagnetic radiation of different wavelengths – spanning from radio waves to UV/visible light – and the ultimate fate of photo-excited molecules.

Module web page

Module aims

This module will introduce the students to the physical origins of many of the analytical spectroscopic tools in use in a modern chemistry laboratory. The module will discuss several spectroscopic methods which utilize a range of electromagnetic wavelengths, from radio waves to UV/visible light, highlighting the different types of molecular processes probed. The module will introduce some of the quantum-mechanical models which underpin much of our understanding of spectroscopy (including harmonic oscillator and the rigid rotor), and their application to real-life spectroscopy. Student's knowledge of molecular symmetry and group theory will be developed by discussing its role in molecular structure and bonding, and the interpretation of electronic and vibrational spectra. The module will also provide students with a working knowledge of the various

relaxation pathways available to electronically-excited molecules. In addition, the module will link conceptually Nuclear Magnetic Resonance (NMR) to other discussed types of spectroscopy. The fundamentals of one-dimensional NMR spectroscopy will be introduced in the context of proton and carbon and then expanded to other nuclei in the periodic table. Finally, two-dimensional NMR will be qualitatively introduced.

Outline syllabus

This is an indicative module outline only to give an indication of the sort of topics that may be covered. Actual sessions held may differ.

- Quantum mechanics, light and energy quantisation
- Energy scales of electronic, vibrational and rotational motions in molecules, and nuclear spin energy levels
- The harmonic oscillator and its use in vibrational spectroscopy
- Vibrational spectroscopy of polyatomic molecules and using group theory to predict IR/Raman activity
- Quantum mechanics of rotating molecules and applications of rotational spectroscopy
- Electronic spectroscopy of diatomic molecules including vibronic structure and the Franck-Condon principle
- Electronic spectroscopy of polyatomic molecules – using group theory to explain electronic spectra
- Jablonski diagrams and the fate of electronically excited states; Excited-state kinetics and quantum yields for photochemical processes
- Fundamentals of one-dimensional NMR for spin ½ on the example of proton and carbon.
- Overview of NMR interactions including coupling to nuclei other than proton and carbon. Polarisation transfer and decoupling.
- Qualitative introduction to two-dimensional NMR.

Learning outcomes

By the end of the module, students should be able to:

- Appreciate how energy quantisation underpins important analytical methods that enable us to study the structure and dynamics of molecules
- Understand how and why molecules absorb light in different parts of the electromagnetic spectrum
- Explore how symmetry impacts on the bonding and vibrational/electronic properties of molecules
- Appreciate the range of possible fates of photo-excited molecules
- Explore the theory underpinning modern nuclear magnetic resonance (NMR) spectroscopy as a powerful analytical tool for chemists
- Develop skills in using python code to analyse spectroscopic properties

Indicative reading list

Physical Chemistry, P.W.Atkins and J. de Paula

Subject specific skills

Numeracy
Problem solving
Critical thinking
Organisation and time management
Digital skills and literacy

Transferable skills

Numeracy
Problem solving
Critical thinking
Organisation and time management
Digital skills and literacy

Study

Study time

Type	Required
Lectures	30 sessions of 1 hour (20%)
Tutorials	2 sessions of 1 hour (1%)
Practical classes	4 sessions of 1 hour (3%)
Private study	84 hours (56%)
Assessment	30 hours (20%)
Total	150 hours

Private study description

N/A

Costs

No further costs have been identified for this module.

Assessment

You do not need to pass all assessment components to pass the module.

Assessment group D

	Weighting	Study time
Assessed coding task	20%	30 hours

This assessment will build on the Python coding skills developed in year 1 of the course (CH168), and will focus on using Jupyter notebooks to analyse data from a variety of spectroscopic experiments. It will focus on using linear and non-linear regression methods to fit experimental data to extract e.g. disentangling overlapping spectral features before extracting spectral parameters

Examination	80%

- Answerbook Green (8 page)
- Students may use a calculator

Feedback on assessment

Individual assessment feedback provided via Moodle. Cohort level examination feedback will be provided after the June examination period.

Past exam papers for CH275

Availability

Pre-requisites

To take this module, you must have passed:

- All of
  - CH155-30 Practical and Professional Chemistry Skills I

Courses

This module is Core for:

- UCHA-4 Undergraduate Chemistry (with Intercalated Year) Variants
  - Year 2 of F101 Chemistry (with Intercalated Year)
  - Year 2 of F122 Chemistry with Medicinal Chemistry (with Intercalated Year)
- UCHA-3 Undergraduate Chemistry 3 Year Variants
  - Year 2 of F100 Chemistry
  - Year 2 of F100 Chemistry
  - Year 2 of F121 Chemistry with Medicinal Chemistry
- UCHA-F110 Undergraduate Master of Chemistry (with Industrial Placement)
  - Year 2 of F100 Chemistry
  - Year 2 of F110 MChem Chemistry (with Industrial Placement)
  - Year 2 of F112 MChem Chemistry with Medicinal Chemistry with Industrial Placement

- Year 2 of UCHA-F107 Undergraduate Master of Chemistry (with Intercalated Year)
- UCHA-F109 Undergraduate Master of Chemistry (with International Placement)
    - Year 2 of F109 MChem Chemistry (with International Placement)
    - Year 2 of F111 MChem Chemistry with Medicinal Chemistry (with International Placement)
- UCHA-4M Undergraduate Master of Chemistry Variants
    - Year 2 of F100 Chemistry
    - Year 2 of F105 Chemistry
    - Year 2 of F110 MChem Chemistry (with Industrial Placement)
    - Year 2 of F109 MChem Chemistry (with International Placement)
    - Year 2 of F125 MChem Chemistry with Medicinal Chemistry
- Year 2 of UCHA-F127 Undergraduate Master of Chemistry with Medicinal Chemistry(with Intercalated Year)