CH916-10 Magnetic Resonance

26/27

Department
Chemistry
Level
Taught Postgraduate Level
Module leader
Steven Brown
Credit value
10
Module duration
2 weeks
Assessment
50% coursework, 50% exam
Study location
University of Warwick main campus, Coventry

Description

Introductory description

Nuclear magnetic resonance (NMR) in both solution and the solid state as well as electron paramagnetic resonance (EPR) will be described. The course will cover the underlying theory of the experiments as well as practical aspects of recording spectra and their interpretation. The importance of magnetic resonance across science, in, e.g., organic chemistry, pharmaceuticals and proteins, will be demonstrated.

Module web page

Module aims

Nuclear magnetic resonance (NMR) in both solution and the solid state as well as electron paramagnetic resonance (EPR) will be described. The course will cover the underlying theory of the experiments as well as practical aspects of recording spectra and their interpretation. The importance of magnetic resonance across science, in e.g., organic chemistry, pharmaceuticals and proteins will be demonstrated.

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.

(1) Foundations of Nuclear Magnetic Resonance (NMR) (recap of material presented in CH921), e.g., spin angular momentum, Larmor frequency, instrumentation requirements, NMR interactions: chemical shifts, J and dipolar couplings, quadrupolar, Fourier transformation).

(2) Introduction to two-dimensional NMR (how the experiment works, phase- and amplitude modulation, schematic appearance of, e.g., NOESY spectra).

(3) Interpretation of solution-state NMR spectra of moderately sized organic molecules (e.g., diamagnetic and paramagnetic shieldings on 1H and 13C chemical shifts, effects of multiple bonds and rings, the -gauche effect, DEPT for interpreting 13C spectra, J coupling: 1J, 2J, 3J and 4JHH. 1JCH, Karplus relation, decoupling, both homo- and heteronuclear, 2D COSY for complex cases).

(4) Chemical exchange (effect on NMR spectra, extraction of dynamic information).

(5) NMR relaxation and saturation (experiments for measuring T1 and T2; solvent suppression).

(6) Basic overview of methods for calculating NMR chemical shifts.

(7) Using NMR for protein structure determination (2D experiments, the nuclear Overhauser effect).

(8) Basic concepts in solid-state NMR (magic-angle spinning, cross polarisation, 2D methods, applications to pharmaceuticals and biosolids).

(9) Introduction to electron paramagnetic resonance (basic concepts and hardware, dynamic nuclear polarisation).

Learning outcomes

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

- Understand the physical basis of magnetic resonance experiments and the role of the different elements of spectrometer hardware
- Assign NMR spectra, so as to identify the structure of small to moderately sized organic molecules
- Appreciate the wide applicability of magnetic resonances techniques

Indicative reading list

Reading lists can be found in Talis

Subject specific skills

Understand the physical basis of magnetic resonance experiments and the role of the different elements of spectrometer hardware
Assign NMR spectra, so as to identify the structure of small to moderately sized organic molecules
Use relevant databases and prediction programs
Appreciate the wide applicability of magnetic resonances techniques

Transferable skills

1 Critical thinking

- Recognise patterns, themes and key messages from sometimes confused and incomplete data.
- Make informed decisions on the value of a range of sources allowing an evidence based conclusion based on this analysis.
  2 Problem solving
- Use rational and logical reasoning to deduce appropriate and well-reasoned conclusions.
- Retain an open mind, optimistic of finding solutions, thinking laterally and creatively to look beyond the obvious.
- Knows how to learn from failure.
  3 Self-awareness
- Actively seek opportunities for personal development in the context of employment and life.
- Aware of personal strengths and emotional intelligence
- Reflect on learning, seeking feedback on and evaluating personal practices, strengths and opportunities for personal growth.
  4 Communication
- Communicate orally in a clear and sensitive manner which is appropriately varied according to different audiences.
- Written: Present arguments, knowledge and ideas, in a range of formats. Active listening: questioning, reflecting, summarising.
  5 Teamwork and working effectively with others
- Operate within, and contribute to, a respectful, supportive and cooperative group climate.
- Sensitive to the impact of actions on others.
  6 Information literacy (research skills)
- Critical awareness of how information is gathered, used, managed and synthesised.
- Understanding of the relative value of different sources and the importance of provenance.
- The systematic collection, analysis and evaluation of information in the investigation of a topic.
  7 Digital literacy
- Has the capabilities that enable living, learning and working in a digital society.
- Comfortable with using digital media to communicate, solve problems, manage information, collaborate, create and share content.
  11 Professionalism
- Prepared to operate autonomously.
- Aware of how to be efficient and resilient.
- Manages priorities and time.
- Self-motivated, setting and achieving goals, prioritising tasks.
  12 Organisational awareness
- Understanding of business, government and third sector issues and priorities.
- Awareness of the responsibilities of organisations in society.
- Understanding organisational norms of behaviour

Study

Teaching split

Provider	Weighting
Physics	80%
Chemistry	20%

Study time

Type	Required
Lectures	10 sessions of 2 hours (20%)
Demonstrations	1 session of 2 hours (2%)
Practical classes	4 sessions of 3 hours (12%)
Private study	66 hours (66%)
Total	100 hours

Private study description

66 hours self study (reading, preparation, data analysis, write-ups)

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 C6

Assessment component	Weighting	Study time	Eligible for self-certification
Mixed assessment	50%		No
Assessment based on practicals, demonstrations and presentations			
Reassessment component is the same			

Assessment component	Weighting	Study time	Eligible for self-certification
Written Examination (Locally Held) Standard written exam	50%		No

Reassessment component is the same

Feedback on assessment

Written work will be annotated and returned to students. Feedback on workshop presentation will be provided verbally.

Past exam papers for CH916

Availability

Courses

This module is Optional for:

- Year 1 of TCHA-F1PY Postgraduate Taught Analytical Science and Instrumentation
- Year 1 of TCHA-F1PX Postgraduate Taught Analytical and Polymer Science
- Year 1 of TCHS-F1PK Postgraduate Taught Polymer Chemistry
- Year 1 of TCHA-F1PW Postgraduate Taught Polymer Science