CH162-30 Introduction to Physical Chemistry

21/22

Department
Chemistry
Level
Undergraduate Level 1
Module leader
Vasilios Stavros
Credit value
30
Module duration
20 weeks
Assessment
20% coursework, 80% exam
Study location
University of Warwick main campus, Coventry

Description

Introductory description

To provide the student with a quantitative appreciation of four branches of physical chemistry:

1. Quantum mechanics
2. Kinetics
3. Thermodynamics
4. Spectroscopy

The 6 CATS of skills-based assessed work is part of 18 CATS of skills-based content across the three year 1 theory modules. An example of this overall content would be maths, coding, general IT, specific chemistry software and career development skills.

Provide skills development for a range of transferrable and chemistry-specific skills to support their studies and careers e.g. being able to use a range of generic software, chemical software, plus access relevant databases.

For the Maths skills component, this provides the mathematical learning support for the Year 1 modules and more advanced modules in Years 2/3/4, enabling students to solve problems in the main branches of chemistry. The mathematical skills taught allow students to understand the

concepts behind much of chemistry and allow the processing of their own data.

The majority of the module content is drawn from components of A-level syllabuses. As such, most students will already be familiar with some aspects of the module syllabus, but the pattern of familiarity will be heterogeneous across the class. The primary aim of the module is to equip all students with the necessary mathematical skills to succeed in their chemistry degree at Warwick. The module is structured to allow individual students to concentrate their time on those bits of the module with which they are unfamiliar.

Module web page

Module aims

To provide the student with a quantitative appreciation of four branches of physical chemistry:

1. Quantum mechanics
2. Kinetics
3. Thermodynamics
4. Spectroscopy

The 6 CATS of skills-based assessed work is part of 18 CATS of skills-based content across the three year 1 theory modules. An example of this overall content would be maths, coding, general IT, specific chemistry software and career development skills.

Provide skills development for a range of transferrable and chemistry-specific skills to support their studies and careers e.g. being able to use a range of generic software, chemical software, plus access relevant databases.

For the Maths skills component, this provides the mathematical learning support for the Year 1 modules and more advanced modules in Years 2/3/4, enabling students to solve problems in the main branches of chemistry. The mathematical skills taught allow students to understand the concepts behind much of chemistry and allow the processing of their own data.

The majority of the module content is drawn from components of A-level syllabuses. As such, most students will already be familiar with some aspects of the module syllabus, but the pattern of familiarity will be heterogeneous across the class. The primary aim of the module is to equip all students with the necessary mathematical skills to succeed in their chemistry degree at Warwick. The module is structured to allow individual students to concentrate their time on those bits of the module with which they are unfamiliar.

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.

The module will be taught in distinct sections. Here follows an illustrative syllabus for each section of the module.

Quantum Mechanics

- TOPIC 1: General concepts: What is quantum mechanics, and why do we need it?
- TOPIC 2: Fundamental principles of quantum mechanics: Postulates, Hamiltonians and operators.
- TOPIC 3: Solvable systems
  o Solvable system I: Particle in a box
  o Solvable system II: Free-particle motion
  o Solvable system III: Harmonic oscillator
  o Solvable system IV: Rigid rotor
  o Solvable system V: One-electron systems
- TOPIC 4: Spin
- TOPIC 5: Many electron systems

Kinetics

- TOPIC 1: Reaction potential energy surfaces and kinetics at the molecular level
- TOPIC 2: Rates of reaction and rate laws
- TOPIC 3: Determining the rate law from experimental data
- TOPIC 4: Multistep reactions including unimolecular, bimolecular, enzyme and chain reactions
- TOPIC 5: Temperature dependence of reaction rates

Thermodynamics

- TOPIC 1 : Foundations: ideal gas, enthalpy and entropy
- TOPIC 2 : Chemical equilibrium, liquids and gases in equilibrium, vapour pressure
- TOPIC 3 : Phase diagrams of pure substances
- TOPIC 4 : The thermodynamic description of mixtures
- TOPIC 5 : The First, Second and Third Laws of thermodynamics

Spectroscopy

- TOPIC 1. Properties of electromagnetic radiation
- TOPIC 2. The H-atom spectrum and the Rydberg equation
- TOPIC 3. Factors influencing transition intensities
- TOPIC 4. Rotational spectroscopy
- TOPIC 5. Vibrational spectroscopy

An example collective skills syllabus may include elements from the following:

1. Maths
   Perform routine algebraic manipulations.
   Manipulation of units and dimensions.
   Solve simple equations.
   Understand the basis of differential calculus, be able to differentiate and, find maxima and minima.
   Integrate functions and solve simple differential equations.
   Determine the limits of simple functions.
   Manipulate logarithmic and exponential functions.

Introduction to error propagation.
Perform routine trigonometric manipulations.
Expand simple series.
Manipulate complex numbers, vectors, and matrices.

2. Probability and statistics
3. Coding
4. General IT skills
5. Specific chemistry software training
6. Career development skills

Learning outcomes

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

- Understand core concepts in physical chemistry, spanning thermodynamics, kinetics, quantum mechanics, and spectroscopy.
- Apply core concepts from physical chemistry in a range of exercises, often mathematically based.
- Use physical chemistry concepts to understand and explain practical science problems and applications.
- Tackle physical chemistry concepts of similar complexity and depth on the periphery of, or even outside, the syllabus.
- Perform routine algebraic manipulations. Solve simple equations, including both quadratic and simultaneous. Manipulate logarithmic functions and powers. Determine the limiting values of functions.
- Differentiate functions and find maxima and minima. Integrate functions and solve simple differential equations.
- Perform routine trigonometric manipulations. Expand simple series. Manipulate complex numbers and matrices. Solve simple eigenvalue problems
- Become familiar with the use of a range of general IT software packages and coding.
- Be able to use a range of chemical software, plus access relevant databases to support their practical chemistry.

Indicative reading list

Core textbook:
Physical Chemistry, P.W. Atkins and J. de Paula (Oxford University Press)

Further (non-compulsory) reading:

THERMODYNAMICS:
Physical Chemistry: A Molecular Approach, D. A. McQuarrie and J. D. Simon (University Science Books)

KINETICS:
Reaction Kinetics, M. J. Pilling and P. W. Seakins (Oxford University Press)

QUANTUM MECHANICS:

Molecular Quantum Mechanics, P. W. Atkins (Oxford University Press)
Physical Chemistry: A Molecular Approach, D. A. McQuarrie and J. D. Simon (University Science Books)

SPECTROSCOPY:
Modern Spectroscopy, J. M. Hollas (Wiley)
Symmetry and Spectroscopy, D. C. Harris & M. D. Bertolucci (Oxford University Press)

Maths skills component:
Maths for Chemists, 2nd Ed., M. Cockett and G. Doggett, RSC Publishing.
Foundation Maths, 4th Ed., A. Croft and R. Davison, Pearson Prentice Hall.
Calculus with Analytical Geometry, 2nd Ed., G. F. Simmons, McGraw Hill.

Subject specific skills

Numeracy
Problem solving
Organisation and time management

Transferable skills

Numeracy
Problem solving
Organisation and time management

Study

Study time

Type	Required
Lectures	40 sessions of 1 hour (13%)
Tutorials	6 sessions of 1 hour (2%)
Other activity	20 hours (7%)
Private study	234 hours (78%)
Total	300 hours

Private study description

N/A

Other activity description

Skills component
6 Lectures

2 workshops

Costs

No further costs have been identified for this module.

Assessment

You must pass all assessment components to pass the module.

Assessment group D1

	Weighting	Study time	Eligible for self-certification
Assessment component			
Assessed	20%		No
Reassessment component is the same			
Assessment component			
Online Examination ~Platforms - AEP	80%		No

- Answerbook Green (8 page)
- Periodic Tables
- Graph paper
- Students may use a calculator

Reassessment component is the same

Feedback on assessment

Homework sets, with worked answers, will be made available online throughout the module.

Workshops will go through a number of problem-solving exercises; again, worked answers will be provided online.

Informal oral (optionally, written) feedback will be provided on work handed-in prior to small-group

tutorials.
Cohort level examination feedback provided via Moodle following the Exam Board.

Written feedback for assessed work components.

Past exam papers for CH162

Availability

Post-requisite modules

If you pass this module, you can take:

- CH273-15 Properties of Solutions and Foundations of Electrochemistry and Statistical Mechanics
- CH3F1-15 Advanced Physical Chemistry and Laboratory

Courses

This module is Core for:

- UCHA-4 Undergraduate Chemistry (with Intercalated Year) Variants
  - Year 1 of F101 Chemistry (with Intercalated Year)
  - Year 1 of F122 Chemistry with Medicinal Chemistry (with Intercalated Year)
- UCHA-3 Undergraduate Chemistry 3 Year Variants
  - Year 1 of F100 Chemistry
  - Year 1 of F121 Chemistry with Medicinal Chemistry
- UCHA-F110 Undergraduate Master of Chemistry (with Industrial Placement)
  - Year 1 of F100 Chemistry
  - Year 1 of F110 MChem Chemistry (with Industrial Placement)
  - Year 1 of F112 MChem Chemistry with Medicinal Chemistry with Industrial Placement
- Year 1 of UCHA-F107 Undergraduate Master of Chemistry (with Intercalated Year)
- UCHA-F109 Undergraduate Master of Chemistry (with International Placement)
  - Year 1 of F109 MChem Chemistry (with International Placement)
  - Year 1 of F111 MChem Chemistry with Medicinal Chemistry (with International Placement)
- UCHA-4M Undergraduate Master of Chemistry Variants
  - Year 1 of F100 Chemistry
  - Year 1 of F105 Chemistry
  - Year 1 of F110 MChem Chemistry (with Industrial Placement)
  - Year 1 of F109 MChem Chemistry (with International Placement)
  - Year 1 of F125 MChem Chemistry with Medicinal Chemistry
- Year 1 of UCHA-F127 Undergraduate Master of Chemistry with Medicinal Chemistry(with Intercalated Year)