CHEM2401

Physical Chemistry I

Session 1, Weekday attendance, North Ryde 2021

Department of Molecular Sciences

Contents

Notice

As part of Phase 3 of our return to campus plan, most units will now run tutorials, seminars and other small group activities on campus, and most will keep an online version available to those students unable to return or those who choose to continue their studies online.

To check the availability of face-to-face activities for your unit, please go to timetable viewer. To check detailed information on unit assessments visit your unit's iLearn space or consult your unit convenor.

General Information

Unit convenor and teaching staff
Unit Convenor
Ian Jamie
ian.jamie@mq.edu.au
Contact via 02 9850 8293
4WW 236
Open Hours

Credit points
10

Prerequisites
CHEM1002

Corequisites

Co-badged status

Unit description
Physical chemistry permeates all of modern chemistry and many adjoining disciplines and fields. In this unit the fundamental chemical principles of quantum chemistry, chemical thermodynamics and chemical kinetics will be explored through their application to the environmental issues that are of foremost concern in the world today. The environment depends on complex interactions of chemical and physical processes. Using environmental chemistry examples and contexts, we explore the what, why and how fast of chemistry: structure, energy and rate. These topics are examined in terms of the origin, transport and fate of chemicals in the biosphere, atmosphere, hydrosphere and lithosphere.

Important Academic Dates

Information about important academic dates including deadlines for withdrawing from units are available at https://students.mq.edu.au/important-dates

Learning Outcomes

On successful completion of this unit, you will be able to:

ULO1: Explain the underlying molecular and quantum processes relating to kinetics, quantum mechanics (spectroscopy) and thermodynamics.
ULO2: Solve problems in kinetics, quantum mechanics (spectroscopy), thermodynamics and chemical transport, by identifying the essential parts of, and formulating a strategy

for solving, them. You will be able to rationally estimate the solution to a problem, apply appropriate techniques to arrive at a solution, test the correctness of the solution, and interpret the results.

ULO3: Discuss the use of models in theory and be able to critical analyse the strengths and weaknesses of the models used in the context of this unit.

ULO4: Communicate conclusions based on experiments in the form of written reports.

ULO5: Demonstrate intermediate chemistry-laboratory skills and an understanding of general laboratory safety procedures.

ULO6: Collect, record and analyse experimental data, describing the numerical significance of experimental results and the source and significance of uncertainty in scientific investigations.

Assessment Tasks

Name	Weighting	Hurdle	Due
Assigments	20%	No	Week 6 and Week 11
Practicals	20%	Yes	Fortnightly
In-Semester Tests	10%	No	Week 7 and Week 12
Final Examination	50%	No	Final Examination Period

Assigments

Assessment Type [1]: Problem set
Indicative Time on Task [2]: 16 hours
Due: **Week 6 and Week 11**
Weighting: **20%**

Assignment are issued so that students will have the opportunity to use the information provided in the lectures and textbook to explore their extent of understanding of those topics. The two assignments will each consist of approximately ten short-answer quantitative and qualitative questions.

On successful completion you will be able to:

- Explain the underlying molecular and quantum processes relating to kinetics, quantum mechanics (spectroscopy) and thermodynamics.
- Solve problems in kinetics, quantum mechanics (spectroscopy), thermodynamics and

chemical transport, by identifying the essential parts of, and formulating a strategy for solving, them. You will be able to rationally estimate the solution to a problem, apply appropriate techniques to arrive at a solution, test the correctness of the solution, and interpret the results.
- Discuss the use of models in theory and be able to critical analyse the strengths and weaknesses of the models used in the context of this unit.
- Collect, record and analyse experimental data, describing the numerical significance of experimental results and the source and significance of uncertainty in scientific investigations.

Practicals

Assessment Type [1]: Lab report
Indicative Time on Task [2]: 35 hours
Due: **Fortnightly**
Weighting: **20%**
This is a hurdle assessment task (see assessment policy for more information on hurdle assessment tasks)

Laboratory exercises are designed to provide a concrete example of the abstract topics covered in the course work, and to give you the opportunity to discover the principles and applications for yourself. Laboratory exercises also offer the opportunity to explore the uncertainty inherent in scientific investigations and the limitations of models and theories by allowing comparison with real systems. Practicals are composed of a laboratory session, in which an experiment is conducted and data acquired (or a workshop in which data are given) and a practical report in which the acquired data is presented, along with manipulations of that data to provide information on a chemical process.

On successful completion you will be able to:

- Solve problems in kinetics, quantum mechanics (spectroscopy), thermodynamics and chemical transport, by identifying the essential parts of, and formulating a strategy for solving, them. You will be able to rationally estimate the solution to a problem, apply appropriate techniques to arrive at a solution, test the correctness of the solution, and interpret the results.
- Discuss the use of models in theory and be able to critical analyse the strengths and weaknesses of the models used in the context of this unit.
- Communicate conclusions based on experiments in the form of written reports.
- Demonstrate intermediate chemistry-laboratory skills and an understanding of general

laboratory safety procedures.
- Collect, record and analyse experimental data, describing the numerical significance of experimental results and the source and significance of uncertainty in scientific investigations.

In-Semester Tests

Assessment Type [1]: Quiz/Test
Indicative Time on Task [2]: 16 hours
Due: **Week 7 and Week 12**
Weighting: **10%**

Two in-semester tests will be held after the first two major sections. The intention of these tests is to allow students to consolidate their learning of those sections of the unit. The tests provide students with a measure of their understanding of those sections and will direct them to areas on which they need to spend more study. They will be administered through iLearn.

On successful completion you will be able to:

- Solve problems in kinetics, quantum mechanics (spectroscopy), thermodynamics and chemical transport, by identifying the essential parts of, and formulating a strategy for solving, them. You will be able to rationally estimate the solution to a problem, apply appropriate techniques to arrive at a solution, test the correctness of the solution, and interpret the results.
- Discuss the use of models in theory and be able to critical analyse the strengths and weaknesses of the models used in the context of this unit.
- Collect, record and analyse experimental data, describing the numerical significance of experimental results and the source and significance of uncertainty in scientific investigations.

Final Examination

Assessment Type [1]: Examination
Indicative Time on Task [2]: 20 hours
Due: **Final Examination Period**
Weighting: **50%**

The final examination will be 3 hours in length and will cover all sections of the unit (lectures, tutorials, assignments and laboratory exercises). Students will be allowed to take with them a single double-sided A4, handwritten study sheet.

On successful completion you will be able to:

- Solve problems in kinetics, quantum mechanics (spectroscopy), thermodynamics and chemical transport, by identifying the essential parts of, and formulating a strategy for solving, them. You will be able to rationally estimate the solution to a problem, apply appropriate techniques to arrive at a solution, test the correctness of the solution, and interpret the results.
- Discuss the use of models in theory and be able to critical analyse the strengths and weaknesses of the models used in the context of this unit.
- Communicate conclusions based on experiments in the form of written reports.
- Demonstrate intermediate chemistry-laboratory skills and an understanding of general laboratory safety procedures.
- Collect, record and analyse experimental data, describing the numerical significance of experimental results and the source and significance of uncertainty in scientific investigations.

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[1] If you need help with your assignment, please contact:

- the academic teaching staff in your unit for guidance in understanding or completing this type of assessment
- the Learning Skills Unit for academic skills support.

[2] Indicative time-on-task is an estimate of the time required for completion of the assessment task and is subject to individual variation

Delivery and Resources

Classes

Timetable: Please check www.timetables.mq.edu.au for the official timetable of the unit.

Lectures: The material presented in the lectures is important and you should not assume that all examinable material is available in the textbook or in the printed notes. On the other hand, do not assume that all examinable material is to be found in the lecture notes.

Tutorial: Tutorial problems, which may form part of the material submitted for assessment, will be distributed by the lecturer.

Laboratory Work: You will undertake practicals both at the bench (wet-labs) and in the "write-up room" dry-lab workshops.

A laboratory roster will be issued to indicate which experiments you will be undertaking in which week.

Before commencing an experiment, you are required to complete a laboratory preparation exercise (“prelab”). You will not be allowed to commence the experimental work until the preparation exercise is completed in a satisfactory manner. A delay in starting the experimental work due to poor preparation will have a detrimental effect on your ability to perform the laboratory work. You should attempt the prelab exercises well in advance of each practical class. You are advised to carefully read the notes for each experiment.

Students unable to attend laboratory classes due to illness or misadventure (as defined in the Handbook of Undergraduate Studies) must provide formal documentary evidence to the University as soon as possible after the absence, via the Special Consideration mechanism. For any unjustified absences, a mark of zero will be given.

Some practical work may be undertaken before the corresponding material has been covered in lectures. The notes have been written with this in mind and some allowance will be made in the marking of reports.

Reports must be submitted no later than 6 pm on the day of the next practical session, except for the last practical report which will be submitted at the end of the lab session. Penalties for late submission will accumulate at 10% per day overdue. Reports are to be **word-processed and submitted via iLearn**. All supplementary files (spreadsheets, spectra, etc) are to be uploaded along with the report.

Required and Recommended Texts and/or Materials

Recommended Textbook: Atkins & de Paula "Elements of Physical Chemistry" 7th Ed, Oxford University Press is recommended. The larger "Atkins' Physical Chemistry" 11th ed, Oxford University Press is better but more expensive. The 10th edition is also acceptable.

Recommended Supplementary Text: Monk "Maths for Chemistry: a Chemist's Toolkit of Calculations" or some equivalent book might be useful.

Alternative Text Books: Raymond Chang "Physical Chemistry for the Chemical and Biological Sciences", 3rd ed, University Science Books (2000) is reasonable, and somewhat more readable than "Elements of Physical Chemistry", but is a bit light in the spectroscopy section. Some students find "Physical Chemistry" by R.A. Alberty and R.J. Silbey provides readable introductions to some topics but is less helpful when it comes to problem-solving. Two older books that can provide an alternative introduction to aspects of molecular spectroscopy are "Fundamentals of Molecular Spectroscopy" by C.N. Banwell and "Introduction to Molecular Spectroscopy" by G. M. Barrow. You can find several textbooks with "Physical Chemistry" in the title in the University library. All cover similar material but often use different notation. You may find that some of these other books explain certain topics more clearly.

Texts entitled *Environmental Chemistry* or similar tend to be too broad with respect to the chemistry, and there is limited depth of discussions on Physical Chemistry aspects. However, good background information on the broader aspects of Chemistry in the environmental context can be obtained from these texts. Examples of good Environmental Chemistry texts are S.E. Manahan "Environmental Chemistry" (TD193.M36), G.W. VanLoon and S.J. Duffy "Environmental Chemistry: A Global Perspective" (TD193 .V36) and C. Baird and M. Cann "Environmental Chemistry" (TO192 .B35)

There are also many web resources, but material placed on the web is not necessarily checked for accuracy, so be careful when using it.

Technology Used and Required

Your reports will be submitted electronically (through iLearn), so it is important that you have access to a word processor, and the ability to manipulate PDF files.

Use will be made of Excel and other data processing and display software. Computers carrying this software are available in the teaching laboratories. Items of interest and links to other on-line material will be placed on the unit iLearn website. While spreadsheets are recommended for most calculations during session, it is important that you have a scientific calculator as this will be used in the final examination. Note that text-retrieval calculators are not allowed in the final examination.

General use computers are provided by the University, but it would be advantageous to have your own computer and internet access.

Microsoft Office is available free-of-charge to Macquarie University students. See https://wiki.mq.edu.au/display/microsoftstu/About

Unit Web Page: The URL of the CHEM2401 web site is: ilearn.mq.edu.au. You will be asked for a username and password. Your username is your student MQID. Your MQID and password have been mailed to you by the University. If you have lost them go to the student portal: my.mq.edu.au

Unit Schedule

CHEM2401 Physical Chemistry Schedule 2021

The schedule below is indicative and may be altered as required.

			Lecture 1	Lecture 2	Tutorial		Practicals
			Tuesday	Tuesday	Friday		Thursday
MQ Week	Week starting		Zoom 11am – 12n	Zoom 12n – 1pm	11WW230 11am-12n or 11WW230 12n-1pm		E7B 349 2:00 - 6:00 pm
1	22-Feb-21		Introductions; Empirical Kinetics	Empirical Kinetics			-
2	1-Mar-21		Molecular Basis of Kinetics	Molecular Basis of Kinetics	Kinetics		Data Analysis W/S
3	8-Mar-21		Reaction Mechanisms	Reaction Mechanisms	Kinetics		Kin 1 (Thu A)
4	15-Mar-21		Collision Theory	Collision Theory	Kinetics		Kin 1 (Thu B)
5	22-Mar-21		Principles of Spectroscopy	Principles of Spectroscopy	Spectroscopy		Kin 2 (Thu A)
6	29-Mar-21		Rotational Spectroscopy	Rotational Spectroscopy	Good Friday		Kin 2 (Thu B)

	5-Apr-21		Recess	Recess	Recess	Recess
	12-Apr-21		Recess	Recess	Recess	Recess
7	5-Apr-21		Vibrational Spectroscopy - Diatomics	Rotational Fine Structure & Polyatomics	Spectroscopy	Infrared (Thu A)
8	19-Apr-21		Rotational Fine Structure & Polyatomics	UV-Visible Spectroscopy	Spectroscopy	Infrared (Thu B)
9	26-Apr-21		UV-Visible Spectroscopy	NMR Spectroscopy	Spectroscopy	UV-Vis (Thu A)
10	3-May-21		Thermodynamics	Thermodynamics	Thermodynamics	UV-Vis (Thu B)
11	10-May-21		Thermodynamics	Thermodynamics	Thermodynamics	Thermo W/S (Thu A)
12	17-May-21		Transport and Fate	Transport and Fate	Transport and Fate	Thermo W/S (Thu A&B)
13	24-May-21		Transport and Fate	Revision	Transport and Fate	

Policies and Procedures

Macquarie University policies and procedures are accessible from Policy Central (https://policies.mq.edu.au). Students should be aware of the following policies in particular with regard to Learning and Teaching:

- Academic Appeals Policy
- Academic Integrity Policy
- Academic Progression Policy
- Assessment Policy
- Fitness to Practice Procedure
- Grade Appeal Policy
- Complaint Management Procedure for Students and Members of the Public
- Special Consideration Policy

Students seeking more policy resources can visit Student Policies (https://students.mq.edu.au/support/study/policies). It is your one-stop-shop for the key policies you need to know about throughout your undergraduate student journey.

To find other policies relating to Teaching and Learning, visit Policy Central (https://policies.mq.edu.au) and use the search tool.

Student Code of Conduct

Macquarie University students have a responsibility to be familiar with the Student Code of Conduct: https://students.mq.edu.au/admin/other-resources/student-conduct

Results

Results published on platform other than eStudent, (eg. iLearn, Coursera etc.) or released directly by your Unit Convenor, are not confirmed as they are subject to final approval by the University. Once approved, final results will be sent to your student email address and will be made available in eStudent. For more information visit ask.mq.edu.au or if you are a Global MBA student contact globalmba.support@mq.edu.au

Student Support

Macquarie University provides a range of support services for students. For details, visit http://students.mq.edu.au/support/

Learning Skills

Learning Skills (mq.edu.au/learningskills) provides academic writing resources and study strategies to help you improve your marks and take control of your study.

- Getting help with your assignment
- Workshops
- StudyWise
- Academic Integrity Module

The Library provides online and face to face support to help you find and use relevant information resources.

- Subject and Research Guides
- Ask a Librarian

Student Enquiry Service

For all student enquiries, visit Student Connect at ask.mq.edu.au

If you are a Global MBA student contact globalmba.support@mq.edu.au

Equity Support

Students with a disability are encouraged to contact the Disability Service who can provide appropriate help with any issues that arise during their studies.

IT Help

For help with University computer systems and technology, visit http://www.mq.edu.au/about_us/offices_and_units/information_technology/help/.

When using the University's IT, you must adhere to the Acceptable Use of IT Resources Policy. The policy applies to all who connect to the MQ network including students.