



CHEM2401

Physical Chemistry I

Session 1, In person-scheduled-weekday, North Ryde 2023

School of Natural Sciences

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General Information

Unit convenor and teaching staff

Convenor

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Contact via 9850 8293

4WW 236

Drop in

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://www.mq.edu.au/study/calendar-of-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.

General Assessment Information

To pass this unit you must:

- Achieve a total mark equal to or greater than 50%, and
- Participate to an acceptable level in the hurdle activities, as described below.

Attendance at practical classes:

- You must attend and participate in the practical classes to pass CHEM2401. This is a hurdle requirement.
- You must obtain an average mark of 50% for your practicals (prelab, prac report, lab book). Resubmission of the practical report will be allowed for practicals that are assessed at between 40% and 50%. The maximum mark upon resubmission is 50%
- Note: If you miss a practical class class you are NOT automatically entitled to a make-up class. Such an opportunity may be offered, if possible, provided sufficient warning is provided.

In-Session Tests (20%):

- The In-Session Tests will be held as iLearn Quizzes. You will be given a window of approximately 3 1/2 days within which you must start and complete the test. Once started the test must be completed in the indicated time (between 45 minutes and an hour, depending on the test).

Final Exam (50%):

- The final examination will be three (3) hours in length (unless otherwise notified), The final examination will cover all sections of the unit (lectures, lab practicals, workshops and assignments) and is designed to address specific understanding of all the concepts

presented within the course.

Information on Supplementary exams:

- If you receive a special consideration for the final exam, a supplementary exam will be scheduled in the interval between the regular exam period and the start of the next session. By requesting a special consideration for the final exam you are declaring yourself available for a resit during the supplementary examination period and will not be eligible for a second special consideration approval based on pre-existing commitments. Please ensure that you are familiar with the policy prior to submitting an application.

Your marks will be displayed on iLearn. It is your responsibility to regularly verify that the records displayed at iLearn (Tools->Grades) are correct.

If you have difficulty attending and participating in a hurdle assessment task, please contact the Unit Convenor, in ADVANCE if possible, and immediately after if not, as there may be alternatives available to make-up a missed task. If there are circumstances that mean you miss a hurdle assessment task, you may apply for a special consideration. To support your extension, you must submit a "Special Consideration Request" request via www.ask.mq.edu.au. See the [SPECIAL CONSIDERATIONS](#) web page for instructions on how to do this. Please note that evidence must be given to support your request for an extension. You have a limited time after the event to submit a special consideration request (see [SPECIAL CONSIDERATIONS](#) web page).

Submission Deadlines:

Online quizzes, in-class activities, or scheduled tests and exam must be undertaken at the time indicated in the unit guide. Should these activities be missed due to illness or misadventure, students may apply for Special Consideration.

Unless a Special Consideration request has been submitted and approved, a 5% penalty (of the total possible mark of the task) will be applied for each day a written report or presentation assessment is not submitted, up until the 7th day (including weekends). After the 7th day, a grade of '0' will be awarded even if the assessment is submitted. Submission deadlines are given on the iLearn page.

For any late submission of time-sensitive tasks, such as scheduled tests/exams, performance assessments/presentations, and/or scheduled practical assessments/labs, please apply for Special Consideration.

Assessment Tasks

Name	Weighting	Hurdle	Due
In-Semester Tests	10%	No	Week 7, Week 12
Final Examination	50%	No	Final Exam Period

Name	Weighting	Hurdle	Due
<u>Assignments</u>	20%	No	Week 7, Week 12
<u>Practicals</u>	20%	Yes	Approx. Fortnightly

In-Semester Tests

Assessment Type ¹: Quiz/Test

Indicative Time on Task ²: 16 hours

Due: **Week 7, 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 Exam 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.

Assignments

Assessment Type ¹: Problem set

Indicative Time on Task ²: 16 hours

Due: **Week 7, Week 12**

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: **Approx. 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.

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 [Writing Centre](#) 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

Communication

During the semester, the CHEM2401 iLearn site will be used to communicate important information to you. In addition, emails will be sent to your student email account. Please check your messages frequently.

We cannot overstate the importance of **regularly checking your emails and the CHEM2401 iLearn site**.

Please feel free to communicate directly with your unit convenor using the contact details provided on the iLearn. Questions about the unit content and administration that may be of general interest will be best posted the Student Q&A on the iLearn site so that everybody can see the answer.

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 during the tutorial classes.

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

Covid-19

For the latest information on the University's response to COVID-19, please refer to the Coronavirus infection page on the Macquarie website: <https://www.mq.edu.au/about/coronavirus-faqs>. Remember to check this page regularly in case the information and requirements change during semester. If there are any changes to this unit in relation to COVID, these will be communicated via iLearn.

Unit Schedule

The following schedule is tentative and may change.

CHEM2401 Lecture and Tutorial Schedule					
Week	Lecture 1	Lecture 2	Tutorial	Pracs	Assessments
1	Introductions; Empirical Kinetics	Empirical Kinetics	-	-	
2	Molecular Basis of Kinetics	Molecular Basis of Kinetics	Kinetics	Data Analysis W/S	
3	Reaction Mechanisms	Reaction Mechanisms	Kinetics	Kin 1 (Thu A)	
4	Collision Theory	Collision Theory	Kinetics	Kin 1 (Thu B)	

5	Principles of Spectroscopy	Principles of Spectroscopy	Spectroscopy	Kin 2 (Thu A)		
6	Rotational Spectroscopy	Rotational Spectroscopy	Spectroscopy	Kin 2 (Thu B)		
7	Vibrational Spectroscopy - Diatomics	Rotational Fine Structure & Polyatomics	Spectroscopy	Infrared (Thu A)	Assignment 1	In-Session Test 1
	Recess	Recess	Recess	Recess		
	Recess	Recess	Recess	Recess		
8	Rotational Fine Structure & Polyatomics	UV-Visible Spectroscopy	Spectroscopy	Infrared (Thu B)		
9	UV-Visible Spectroscopy	NMR Spectroscopy	Spectroscopy	UV-Vis (Thu A)		
10	Thermodynamics	Thermodynamics	Thermodynamics	UV-Vis (Thu B)		
11	Thermodynamics	Thermodynamics	Thermodynamics	Thermo W/ S (Thu A)		
12	Transport and Fate	Transport and Fate	Transport and Fate	Thermo W/ S (Thu B)	Assignment 2	In-Session Test 2
13	Transport and Fate	Revision	Transport and Fate	-		

Policies and Procedures

Macquarie University policies and procedures are accessible from [Policy Central \(https://policies.mq.edu.au\)](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](#)
- [Assessment Procedure](#)
- [Complaints Resolution Procedure for Students and Members of the Public](#)
- [Special Consideration Policy](#)

Students seeking more policy resources can visit [Student Policies \(https://students.mq.edu.au/support/study/policies\)](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 \(https://policies.mq.edu.au\)](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

Academic Integrity

At Macquarie, we believe [academic integrity](#) – honesty, respect, trust, responsibility, fairness and courage – is at the core of learning, teaching and research. We recognise that meeting the expectations required to complete your assessments can be challenging. So, we offer you a range of resources and services to help you reach your potential, including free [online writing and maths support](#), [academic skills development](#) and [wellbeing consultations](#).

Student Support

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

The Writing Centre

[The Writing Centre](#) provides resources to develop your English language proficiency, academic writing, and communication skills.

- [Workshops](#)
- [Chat with a WriteWISE peer writing leader](#)
- [Access StudyWISE](#)
- [Upload an assignment to Studiosity](#)
- [Complete the 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 Services and Support

Macquarie University offers a range of [Student Support Services](#) including:

- [IT Support](#)
- [Accessibility and disability support](#) with study

- Mental health [support](#)
- [Safety support](#) to respond to bullying, harassment, sexual harassment and sexual assault
- [Social support including information about finances, tenancy and legal issues](#)
- [Student Advocacy](#) provides independent advice on MQ policies, procedures, and processes

Student Enquiries

Got a question? Ask us via [AskMQ](#), or contact [Service Connect](#).

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.

Changes since First Published

Date	Description
06/02/2023	Unit Schedule section updated