School of Physical and Chemical Sciences

General Course Information

CHEM333
Chemical Physics and Spectroscopy

0.125 EFTS 15 Points
Second Semester 2024

Description (and Lecturers)
This course develops concepts and models needed to realistically describe and characterize useful properties of molecules and materials. The following topics are covered (in the given order):
1. Applied quantum chemistry (Prof. Sarah Masters; sarah.masters@canterbury.ac.nz)
2. Statistical mechanics & spectroscopy (A/Prof. Deb Crittenden; deborah.crittenden@canterbury.ac.nz)
3. Atmospheric chemistry (Dr Catherine Hardacre; catherine.hardacre@canterbury.ac.nz)

Goals of the Course
As well as being an important component of a broad degree in chemistry, this course will prepare students for higher-level study in physical chemistry and will provide a satisfying culmination to previous physical chemistry studies. Students will learn how to apply theory to real-world problems, providing both qualitative and quantitative explanations of observed properties of matter on both the nano- and macro-scales. There will be development of scientific problem-solving skills through lecture examples and assignment problems. Appreciation of the fundamentals of physical chemistry and chemical physics will be honed to a high level via in-depth thinking about molecules and processes.

More specifically, the goals of each component of the course are:

Applied Computational Chemistry
- To develop an understanding of the various methods that comprise computational chemistry.
- To understand the fundamental concepts that underpin each method.
- To appreciate the practical applications of computational methods in the field of structural chemistry.
- To understand the differences in accuracy and precision afforded by different computational methods.
- To illustrate how theoretical methods can be used to interpret molecular properties.

Statistical Mechanics and Spectroscopy
- To learn how microscopic and macroscopic properties of molecules and materials are related through statistical distribution of thermal energy
- To apply mathematical models to predict and explain the properties of collections of molecules
- To explain the molecular behaviour that underpins spectroscopic transitions and their intensities.

Atmospheric Chemistry
- To understand the chemical and physical structure of the troposphere and stratosphere
- To explore the different spatial and chemical scales of atmospheric gases
- To develop an understanding of stratospheric photochemistry and how to calculate the steady-state ozone distribution
- To calculate photolysis rate constants
- To appreciate different methods used to measure atmospheric composition
- To illustrate the basic processes affecting trace gas and particle concentrations in the troposphere

Timetable and Course Structure
Four contact hours per week, typically comprising three lectures and one tutorial. There are three blocks of lecture material.

Assignments: You will be required to complete assignment work for all blocks of lectures. You will be informed about the timing and nature of your assignment/s by the relevant lecturer. These may take a non-traditional form, e.g. an essay, a data-analysis exercise, a quiz during a tutorial, or use of a computational package, but will be set and structured to impinge minimally on the following block of lectures.

NOTE: If you do not submit an assignment for assessment, you will be allotted zero marks which will affect your final result. You should ensure that you pick up marked assignments and keep them until the end of the course as evidence that the work was completed and marked in case either is disputed. To guard against accidental loss, it would be prudent to keep photocopies or electronic copies of anything submitted. If you submit work electronically, please cc a copy to yourself in lieu of keeping a physical copy.

Students should note that in the Faculty of Science they are responsible for *about three hours of additional study or work on assignments for each hour of lectures or tutorials* at the 300-level.

Course Coordinator
Professor Sarah Masters, School of Physical and Chemical Sciences
Room 633 Julius von Haast, tel. 369 4229, email *sarah.masters@canterbury.ac.nz*
*Email me **at any time** if you have **any** questions about the course.*

Examination and Formal Tests
Test: As advertised in My Timetable and UC's Course Information System;
1 hour in length; on **lecture topic 1**.
Exam: Time and date to be advised, including through My Timetable and the examinations timetable;
2 hours in length; on **lecture topics 2 and 3** only.

Assessment
Component contributions to the overall course mark will be as follows (with individual lecturer components in brackets):

Assignments:	30% (Masters 10%, Crittenden 10%, Hardacre 10%)
Test:	20% (Masters 20%)
Exam:	50% (Crittenden 25%, Hardacre 25%)

Please note that for **all assignments** a formal application (i.e., through the University) for **special consideration** *will not be considered*. Rather, if a student is unable to complete an assignment by the given deadline, then *an **extension** should be sought by direct application to the **lecturer concerned*** or, if necessary, the course coordinator.

Prerequisites/Restrictions
P: CHEM251 or CHEM243

Web-Based Resources
Learning resources (lecture material, reference links, quizzes, discussion forums etc.) for this course will be available via http://learn.canterbury.ac.nz/.

COURSE CONTENT / LEARNING OUTCOMES

APPLIED COMPUTATIONAL CHEMISTRY (12 lectures & 4 tutorials)

The field of computational chemistry has grown to find uses in almost all areas of chemistry. Most properties of a molecule can be predicted by computational chemistry methods. But how reliable are these methods? Can a non-expert using a "black box" hope to be able to run such calculations? This topic will build on your existing knowledge of quantum chemistry to show the calculation of approximate solutions to the Schrödinger equation can be used to study structural chemistry. There are several different methods that are covered by computational chemistry; we will study molecular mechanics, semi-empirical methods, density functional theory and *ab initio* approaches to gain an appreciation of when such methods can be used to aid experimental structure determination.

Lecturer: Prof. Sarah Masters, Room 633 Julius von Haast, *sarah.masters@canterbury.ac.nz*

At the end of the applied computational chemistry topic, students should be able to:

- Describe different computational methods that can be applied to determine molecular structure.
- Understand which methods are most applicable to certain problems.
- Discuss the relative accuracies of the different methods compared to the length of time taken to calculate various properties.
- Summarize why computational methods are used to augment experimental structural information.
- Describe at least five molecular properties that can be calculated *ab initio*.
- Understand the basis of common functional forms used in molecular mechanics, and the origin and role of specific parameters within this;
- Recognise the strengths and weaknesses of this approach and identify suitable cases for its use;
- Extract relevant parameters from potential energy surface and reconstruct potential energy surfaces from given parameters.

STATISTICAL MECHANICS AND SPECTROSCOPY (12 lectures & 4 tutorials)

These lectures will cover the following topics: molecular modes of motion (electronic, vibrational, rotational, translational), the microcanonical ensemble, partition functions, the Boltzmann distribution; statistical mechanical definition of thermodynamic quantities (entropy, enthalpy, internal energy, heat capacity); using the Boltzmann distribution to explain intensities of spectroscopic transitions.

Lecturer: A/Prof. Deb Crittenden, Room 520 Julius von Haast*, deborah.crittenden@canterbury.ac.nz*

At the end of the statistical mechanics and spectroscopy topic, students should be able to:

- Describe the different modes of motion that molecules, atoms and subatomic particles undergo.
- Define (in a statistical mechanics context) the following terms: macrostate, microstate, configuration.
- Construct all possible configurations obeying a given microcanonical rule, and determine their weights.
- Use the Boltzmann distribution to determine the distribution of particles among energy levels for systems with large numbers of particles in their most probable configuration.
- Calculate partition functions for diatomic molecules.
- Calculate heat capacities of gases and explain how and why the heat capacity of a gas varies with temperature.
- Interpret and explain the intensities of transitions in electronic emission, IR, UV-Vis and microwave spectra.
- Explain the relationship between statistical mechanics, the ideal gas equation and the kinetic theory of gases.

ATMOSPHERIC CHEMISTRY (12 lectures & 4 tutorials)

Earth's atmosphere is thin, and vital for sustaining life. In this section of the course we will explore atmospheric chemistry and its consequences for habitability. We will first explore the basic chemical and physical structure of the atmosphere. We will review the kinetics of gas-phase reactions, learn how photolysis rate constants are calculated, and explore the consequences of photolysis of common atmospheric gases. We will then go on to explore stratospheric chemistry and ozone depletion. Methods used to determine atmospheric composition will be discussed. The last part will focus on the chemistry of the troposphere, including air pollution, acid deposition, trace gas oxidation and tropospheric ozone.

Lecturer: Dr Catherine Hardacre, *catherine.hardacre@canterbury.ac.nz*

At the end of the atmospheric chemistry topic, students should be able to:

- Describe the chemical and physical structure of the troposphere and stratosphere
- Understand the different spatial and chemical scales of atmospheric gases and aerosols and the relevance to environmental issues such as urban air pollution and stratospheric ozone depletion.
- Calculate the steady state ozone distribution.
- Calculate photolysis rate constants.
- Calculate concentrations and rates of production/destruction of atmospheric gases using the ideal gas law and chemical kinetics.
- Describe different methods used to measure atmospheric composition.
- Understand the basic processes affecting trace gas and particle concentrations in the troposphere.

GENERAL INFORMATION | TE KIMI MŌHIOHIO 2024

Policy on 'Dishonest Practice'| Ngā Takahitanga me ngā Tinihanga

The University has strict guidelines regarding 'dishonest practice' and 'breach of instructions' in relation to the completion and submission of examinable material. In cases where dishonest practice is involved in tests or other work submitted for credit, a department may choose to not mark such work – see the online guidelines in relation to 'Academic Integrity'.

The School of Physical and Chemical Sciences upholds this policy. It considers plagiarism, collusion, copying and ghost writing – all detailed below – to be unacceptable and dishonest practices:

- ***Plagiarism | Tārua Whānako*** is the presentation of any material (text, data or figures, on any medium including computer files) from any other source without clear and adequate acknowledgement of the source. Note that the use of **AI generative tools such as ChatGPT** for assessment work is *strictly forbidden*, except where the lecturer concerned has specifically granted approval.
- ***Collusion*** is the presentation of work performed in whole, or in part, in conjunction with another person or persons, but submitted as if it has been completed by the named author alone. This interpretation is not intended to discourage students from having discussions about how to approach an assigned task and incorporating general ideas that come from those discussions into their own individual submissions, but acknowledgement is necessary.
- ***Copying*** is the use of material (in any medium, including computer files) produced by another person or persons with or without their knowledge and approval. **This includes copying of the lab reports (raw data may be shared within the group if permitted or required by the experiment) – data analysis and interpretation of obtained results MUST be performed individually.**
- ***Ghost writing*** is the use of other person(s) (whether with or without payment) to prepare all or part of an item of work submitted for assessment.

Special consideration of assessment | Ngā Pairuri Motuhake

'Special Consideration' for an item of assessment is for students who have covered the work involved but have been prevented from demonstrating their knowledge or skills at the time of the assessment due to unforeseen circumstances, whether illness, injury, bereavement, car crash or any other extenuating circumstance *beyond one's control*. Special Consideration for a test/exam may be because a student has not sat it or has done so with impaired performance. Applications can be submitted via the above link and must be made **no later than five working days after the assessment due date**. Note that special consideration is **not available for items worth less than 10% of the overall course mark**. In the case of illness or injury, medical consultation should normally have taken place either shortly before or within 24 hours after the due date for the required work or test/examination.

Note that you may be required to sit a special exam or your grade may not be changed if there is insufficient evidence of your performance from other invigilated assessment items in the course. ***You have the right to appeal any decision.***

It is important to understand that Special Consideration is only available *where course work has been covered*, and the inability to demonstrate this fully is both *no longer possible* AND is due to *unexpected circumstances beyond one's control*. Thus Special Consideration **is NOT available for:**

- essays, assignments or quizzes where an extension of time is available to complete the assessment item (see below for the process to involved);
- missed lectures during the semester;
- experiencing examination anxiety;
- having several examinations or assessments close together;
- known impairment, such as chronic illness (medical or psychological), injury or disability unless medical evidence confirms that the circumstances were exacerbated, despite appropriate management, at the time of assessment;
- mistaking the date or time of an examination (this is a circumstance one can control!);
- failing to turn up to an examination or test because of sleeping in (a circumstance as above!);
- where applications are repeatedly made for the same or similar reason, then the application may be declined on the grounds that the reason is not unexpected;
- where the application is made at the time of the assessment but the supporting documentation is received significantly after this date or after the date results are released; or
- the application is made following the release of results (unless under exceptional circumstances).

Extensions of deadlines | Tononga Wā Āpiti
Where an extension may be granted for an assessment item, this will be decided by application to the course co-ordinator and/or the lecturer concerned.

Late withdrawal from a course
If you are prevented by extenuating circumstances from completing the course after the final date for withdrawing from the course, you may apply for special consideration for late discontinuation. For details on special consideration, or to make an application, refer to the Examinations Office website http://www.canterbury.ac.nz/exams/. Applications must be submitted ***within five days*** of the end of the main examination period for the semester.

Missing of tests | Te Matangaro i ngā Whakamātautau
In rare cases a student will not be able to sit a test. In such cases, the student should consult with the course co-ordinator to arrange alternative procedures. **This must be done well in advance of the set date for the test.**

Past tests and exams
Past tests can be found on our Chemistry Undergraduate website. Past exams can be found on the Library website.

Submission of reports and assignments
Reports (including lab reports) and assignments should be handed in on time. Extensions will be granted only in exceptional circumstances (such as illness or bereavement). If an extension is required, as early as possible you should request it from the lecturer concerned.
Note: If you do not submit an assignment for assessment, you will be allotted zero marks, which will affect your final result. You should ensure that you pick up marked assignments and keep them until the end of the course as evidence that the work was completed and marked in the case that either is disputed. To guard against accidental loss, it would be prudent to keep photocopies or electronic copies of anything submitted.

Late Work
Acceptance of late work for assessment will be at the discretion of the course coordinator and/or the lecturer concerned. If your assessment is likely to be late, please contact the relevant of these people ***before the assessment is due***. Never assume that an extension will be automatically granted – some courses have the policy of no late work being accepted. A commonly exercised policy is to deduct 10% of the total marks for each day that the work is late, where weekends and public holidays also count as such days.

Marks and Grades | Taumata Ako
The following numbers should be considered as a guide to the expected grades under normal circumstances.

Please note that for all invigilated assessments (tests and exams) worth 33% and above, failure to obtain a mark of at least 40% will result in a final grade no higher than an R at 100 and 200 level; in

general this requirement will not be applied at 300 level, but if it is then the course coordinator will inform the class and it will result in a final grade no higher than a C–.

Grade:	**A+**	**A**	**A−**	**B+**	**B**	**B−**	**C+**	**C**	**C-**	**D**	**E**
Minimum mark %:	**90**	**85**	**80**	**75**	**70**	**65**	**60**	**55**	**50**	**40**	**0**

The School reserves the right to adjust this mark/grade conversion, up or down, to achieve consistency of assessments standards.

Reconsideration of Grades
Students should, in the first instance, speak to the course co-ordinator about their marks. If they cannot reach an agreeable solution, or have questions about their grade in a course, students should then speak to the Director of Undergraduate Studies, Assoc Prof Greg Russell. Students can appeal any decision made on their final grade. You can apply at the Registry for reconsideration of the final grade within four weeks of the date of publication of final results. Be aware that there are time limits for each step of the appeals process.

Student Accessibility Services | Te Whaikaha
Students can speak with someone at Student Accessibility Service, phone: 369 3334 (or ext. 93334), email: sas@canterbury.ac.nz).

Academic Advice
Assoc Prof Greg Russell is the coordinator of undergraduate chemistry courses. His interest is in the academic performance and well-being of all such students. Anyone experiencing problems with their chemistry courses or requiring guidance about their B.Sc. in Chemistry should get in contact with Greg.

Staff-Class Rep Liaison
Assoc Prof Greg Russell is in charge of liaison with students in chemistry courses. Your class will appoint a student representative to the liaison committee at the start of the semester. Please feel free to talk to the Academic Liaison or the student rep about any problems or concerns that you might have.

Greg Russell (greg.russell@canterbury.ac.nz, tel. 369 5129)
Director of Undergraduate Studies
School of Physical and Chemical Sciences
2024