School of Physical and Chemical Sciences

UNIVERSITY OF CANTERBURY
Te Whare Wānanga o Waitaha
CHRISTCHURCH NEW ZEALAND

General Course Information

CHEM333
Chemical Physics and Spectroscopy

0.125 EFTS	15 Points
Second Semester	2022

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 (A/Prof. Sarah Masters; sarah.masters@canterbury.ac.nz)
2. Statistical mechanics & spectroscopy (A/Prof. Deb Crittenden; deborah.crittendon@canterbury.ac.nz)
3. Atmospheric chemistry (Prof. Alex Archibald; ata27@cam.ac.uk)

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.
- To discuss how computational methods can be combined with experimental methods to obtain the "best of both worlds".

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 so as 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
A/Prof. Sarah Masters, School of Physical and Chemical Sciences
Room 422 Beatrice Tinsley, 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:	40% (Masters 15%, Crittenden 15%, Archibald 10%)
Test:	20% (Masters 20%)
Exam:	40% (Crittenden 20%, Archibald 20%)

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? We 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: A/Prof. Sarah Masters, *sarah.masters@canterbury.ac.nz*

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

- Describe four 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*.
- Describe experimental methods that are complementary to computational methods.

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, *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: Prof. Alex Archibald, *ata27@cam.ac.uk*

At the end of the electronic states and photochemistry 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 the relevance to environmental issues such as urban air pollution and stratospheric ozone depletion.
- Calculate the steady state ozone distribution.
- Calculate photolysis rate constants.
- Describe different methods used to measure atmospheric composition.
- Understand the basic processes affecting trace gas and particle concentrations in the troposphere.

GENERAL INFORMATION 2022

Policy on 'Dishonest Practice'

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 ('Academic Integrity and Breach of Instruction Regulations').

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

- ***Plagiarism*** 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.
- ***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) (with, or without payment) to prepare all or part of an item of work submitted for assessment.

Additional Information

Special consideration of assessment**:** If you feel that illness, injury, bereavement or any other critical extenuating circumstance beyond your control has prevented you from completing an item of assessment or affected your performance in that assessment, you may apply for special consideration. Special consideration is not available for items worth less than 10% of the course. Applications for special consideration should be made **within five days** of the due date for the work or examination. In the case of illness or injury, medical consultation should normally have taken place shortly before, or within 24 hours after, the due date for the required work or the date of the test or examination. For details on special consideration, or to make an application, refer to the Examinations Office website http://www.canterbury.ac.nz/exams/. ***You have the right to appeal any decision.***

Extensions of deadlines: Where an extension may be granted for an assessment item, this will be decided by application to the course co-ordinator.

Late withdrawal from the 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**:** 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: these can be found on our website using the link below:
www.chem.canterbury.ac.nz/for/undergraduate.shtml

***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 will be at the discretion of the course coordinator. Please contact the coordinator if your assessment is likely to be late.

Marks and Grades: The following numbers should be considered as a guide to the expected grades under normal circumstances. The School reserves the right to adjust mark/grade conversions, if necessary.

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, and a C- at 300 level.

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**

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 (phone 3694228). 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.

Students with Disabilities: Students with disabilities should speak with someone at Equity and Disability Service, phone: 369 3334 (or ext. 93334), email: eds@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
2022