

CHEM 3101: Quantum Chemistry - Fall 2023

Calendar Entry

Quantum Chemistry

Classical equations of motion, harmonic oscillator, diatomic molecules, quantum mechanics, Schrödinger equation and wave functions, vibrational spectra, hydrogen atom, quantum numbers, electronic spectra.

Lectures and problems three hours a week.

Instructor: Christopher N. Rowley (christopherrowley@cunet.carleton.ca)

Prerequisites: CHEM 2103, MATH 2007, and MATH 2008.

Required Text: None

Course Format

Wherever possible, the course instruction and evaluation will be completed **in person** in the designated class hours. You will be assessed through written assignments, online quizzes, a writing project, and a written final exam.

Class Schedule

Date: September 7, 2023 to December 7, 2023

Days: Tue Thu **Time:** 11:35 - 12:55

Days: Tuesday and Thursdays, 11:35 AM - 12:55 PM

Location: In-person, Richcraft Hall Room: 1200

Course Materials

An online text with the relevant material will be available on Brightspace

<https://brightspace.carleton.ca/d2l/home>

CHEM3101A Quantum Chemistry (LEC)

Communication

You may communicate with Chris through Carleton email (christopherrowley@cunet.carleton.ca). You will also be able to communicate with Chris and other members of the class through the online messaging system, Slack. To join the Slack group for this course, use the following link:

<https://join.slack.com/t/chem3101/signup>

The URL to access the slack channel is <https://chem3101.slack.com/>

A demonstration on how to use Slack is available here:

<https://youtu.be/m2JuAa6-ors>

Each exercise and the term project will be discussed in class.

Evaluation

Component	Weight
midterm 1	15
midterm 2	15
final exam	35
written assignments	20
online quizzes	10
wiki project	5

Online Quizzes

There will be at least one online quiz each week. They can be completed at any point during the week but will generally be due Friday at 10 PM. My recommendation is for you to read the course material and attend the lectures before attempting the quiz. You will have two attempts to complete each quiz. To preserve the academic integrity of the quizzes, the solutions will not be released. You are encouraged to speak to the instructor if there are questions you got wrong but do not understand why.

Academic Integrity on Quizzes: You may not share the answers to quizzes, post the content or solutions to quizzes in any public forum, or submit answers that have been determined by other people.

Tests

There will be 2 midterm tests, worth 15% each. They will be held in person during the scheduled class time. They will generally be held on the scheduled dates during the class time (11:30 AM to 1 PM ET) in the regular lecture locations. You should study for these tests and prepare for them based on the course material covered to date in the class. You will be informed of the specific expectations of these tests the week prior to them.

You do not have to provide documentation if you do not complete a midterm; if you do not complete them, the grades for these assessments will be transferred to the final exam. There will be no makeup tests. You are strongly encouraged to complete them because they will be much easier than the final exam. If you receive a lower grade on a midterm than on the final exam, the midterm grade will be dropped and the weight will be added to the final exam, so you can only improve your grade by writing the midterms. Historically, the grades on the midterms have been significantly higher than on the final exam.

Academic Integrity on Tests: The tests will only be administered in person under exam conditions. You will only be allowed the use of a non-programmable calculator (i.e., you will not be allowed to use a smartphone, tablet, laptop, or any other device that connects to the internet/SMS). You will be provided with an equation sheet and scrap paper, but will not be allowed any other materials.

The tentative schedule for these tests is:

Midterm	Date
1	October 3
2	November 2

Assignments

There will be four written assignments.. The assignments must be submitted as a PDF through Brightspace. Assignments that are not submitted by the deadline will be given a grade of zero. To allow for assignments to be graded and returned in a timely manner, no late assignments will be accepted.

The tentative due dates will be:

Assignment	Date
1	September 26
2	October 17
3	November 7
4	November 28

These date may be adjusted as necessary. You should consult with the Brightspace entry for the assignment for the due date

Academic Integrity on Assignments. You are free to ask the instructor questions about the assignments. You are encouraged to discuss the strategy. Please consult the [university policy on plagiarism](#). You may not share the answers to quizzes, post the content or solutions to quizzes in any public forum, or submit answers that have been written by other people.

General Academic Integrity Policy

In addition to the specific academic integrity requirements for each component, the general Carleton University academic integrity policy also applies. Except where indicated, all course materials, quiz questions, tests, etc. are under copyright. Uploading or distributing these materials without permission is a violation of this copyright and of the academic integrity policy.

Wikibook

There is a term-long independent writing assignment where you will write an an example problem and its solution. These solutions will become part of a text for this course and will be available to students in later years. Your assignment and its specific solution are available on the BrightSpace page.

The wikiproject assignment will contribute 5% of your final grade.

It is due November 17, 2022

Academic Integrity on the Wikibook Project. The specific requirements are provided in the the text of the wikibook assignment PDF. Your entry must be written entirely by you. Please consult the [university policy on plagiarism](#). You may only make use of images provided to you, those that are already on wikimedia, or have been created by you.

Additional Material

If you wish to make use of additional resources, there are several books in the library that include the material covered in this course:

- Quantum Chemistry, McQuarrie, Donald A., 2008
 - https://ocul-crl.primo.exlibrisgroup.com/permalink/01OCUL_CRL/1gorbd6/alma991013018219705153

- Quantum Chemistry, Levine, I, 2009
 - https://ocul-crl.primo.exlibrisgroup.com/permalink/01OCUL_CRL/1gorbd6/alma991013483489705153

Excepted materials from appropriate texts are available for viewing on the Course Materials page of BrightSpace.

Intended Student Learning Outcomes

At the end of CHEM 3101, students will be able to:

- Understand the postulates and general principles of quantum mechanics as they pertain to chemistry
- Solve and understand the solution to the Schrödinger equation for the particle in a box model
- Solve and understand the solution to the rigid rotor model for molecular rotation and understand how this relates to microwave spectroscopy
- Solve and understand the solution to the harmonic oscillator model for molecular vibration and understand how this relates to infrared spectroscopy
- Solve and understand the solution to the hydrogen atom and explain and interpret orbitals and periodic trends in atoms based on it
- Understand and apply the concept electron spin based on quantum mechanics
- Develop models for the helium atom using the variational principle and perturbation theory. Be able to explain interelectron repulsion and screening based on these models

This contributes to the learning outcomes for the B.Sc. Chemistry program:

- 3: Demonstrates competency in theoretical and practical aspects of organic, inorganic, physical and analytical chemistry.
- 4: Integrates theoretical and practical knowledge of subdisciplines of chemistry to solve complex chemistry problems.
- 14: Practices meta-cognition and applies learned knowledge to new situations.

Standard University Outline Items

Survivors of Sexual Violence

As a community, Carleton University is committed to maintaining a positive learning, working and living environment where sexual violence will not be tolerated and is survivors are supported through academic accommodations as per Carleton's Sexual Violence Policy. For more information about the services available at the university and to obtain information about sexual violence and/or support, visit: carleton.ca/sexual-violence-support

Requests for Academic Accommodation

You may need special arrangements to meet your academic obligations during the term. Please contact your instructor with any requests for academic accommodation (pregnancy, religion, disability, etc.) during the first two weeks of class, or as soon as possible after the need for accommodation is known to exist.

For an accommodation request, the processes can be found here:

carleton.ca/equity/wp-content/uploads/Student-Guide-to-Academic-Accommodation.pdf

Academic Accommodations for Students with Disabilities

If you have a documented disability requiring academic accommodations in this course, please contact the Paul Menton Centre for Students with Disabilities (PMC) at 613-520-6608 or pmc@carleton.ca for a formal evaluation or contact your PMC coordinator to send your instructor your Letter of Accommodation at the beginning of the term. You must also contact the PMC no later than two weeks before the first in-class scheduled test or exam requiring accommodation (if applicable). After requesting an accommodation from PMC, meet with your instructor as soon as possible to ensure accommodation arrangements are made.

carleton.ca/pmc

Accommodation for Student Activities

Carleton University recognizes the substantial benefits, both to the individual student and for the university, that result from a student participating in activities beyond the classroom experience. Reasonable accommodation must be provided to students who compete or perform at the national or international level. Please contact your instructor with any requests for academic accommodation during the first two weeks of class, or as soon as possible after the need for accommodation is known to exist. <https://carleton.ca/senate/wp-content/uploads/Accommodation-for-Student-Activities-1.pdf>

For more information on academic accommodation, please contact the departmental administrator or visit: students.carleton.ca/course-outline

COVID

It is important to remember that COVID is still present in Ottawa. The situation can change at any time and the risks of new variants and outbreaks are very real. There are a number of actions you can take to lower your risk and the risk you pose to those around you including being vaccinated, wearing a mask, staying home when you're sick, washing your hands and maintaining proper respiratory and cough etiquette.

Feeling sick? Remaining vigilant and not attending work or school when sick or with symptoms is critically important. If you feel ill or exhibit COVID-19 symptoms do not come to class or campus. If you feel ill or exhibit symptoms while on campus or in class, please leave campus immediately. In all situations, you must follow Carleton's symptom reporting protocols.