CHEM 3101: Quantum Chemistry - Fall 2026

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 Rowley (christopherrowley@cunet.carleton.ca)

Department: Chemistry

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

Preclusions: None

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 midterms, online computational assignments, a contribution to the course wikibook, in class assessments (participation), and a written final exam.

Class Schedule

Days: Mondays and Wednesdays, 1:05 PM - 2:25 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)
Students are not required to purchase textbooks or other learning materials for this course.

Communication

You may call the instructor by his first name (Chris). Please advise Chris of how you would like to be called (name/pronouns) if you would like to. You may communicate with Chris through Carleton email (christopherrowley@cunet.carleton.ca).

Student Hours:
Chris's office is in HS 6304, on the 6th floor of the Health Sciences Building. Because this floor is restricted access, you will need to make an appointment to meet with Chris in his office.
Each exercise and the term project will be discussed in class.

Evaluation

Component	Weight
midterm 1	17.5
midterm 2	17.5
final exam	40
assignments	10
participation	10
wiki project	5

Midterm Dates

The midterms are tentatively scheduled for:

Midterm	Date
1	October 7
2	November 9

You will be notified on Brightspace if these need to be rescheduled.

Academic Accommodations and Regulations

Carleton is committed to providing academic accessibility for all individuals. You may need special arrangements to meet your academic obligations during the term. The accommodation request processes, including information about the Academic Consideration Policy for Students in Medical and Other Extenuating Circumstances, are outlined on the Academic Accommodations website: https://students.carleton.ca/course-outline/ https://students.carleton.ca/course-outline/ .

Practice Quizzes

There are optional online quizzes intended for you to make a self-assessment of your understanding. These do not contribute to your final grade.

Problem Sets

There are sample long-form written problem sets intended to provide practice with the course material examples of midterm and exam questions. You may ask the instructor about the solutions, but they are not submitted, graded, and do not contribute to your final grade.

Participation

There will be some form of in-class assessment at every lecture, excluding midterms and reviews. Your three lowest assessments will be waived automatically. There is no alternative form of assessment, so a grade of zero will be assigned if you are absent.

Midterm Tests

There will be 2 midterm tests, worth 17.5% 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 in the regular lecture

location. 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.

These dates 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 for arriving at a solution with your classmates, but 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. Please consult the university policy on plagiarism.

There is no explicit prohibition on the use of generative AI, although the quality of the results for the material in this course is generally extremely poor and usually does not align with the expectations. Accordingly, many submissions generated by generative AI have been given a grades of zero. Even if cited, the use of generative AI is not a justification for providing an incorrect answer or one that does not reflect the expectations.

As our understanding of the uses of generative AI and its relationship to student work and academic integrity continue to evolve, students are required to discuss their use of generative AI in any circumstance not described here with the course instructor to ensure it supports the learning goals for the course.

Course Schedule

Lecture	Topic
1	Introduction and Hamiltonian Mechanics
2	Operators and the Schrödinger Equation
3	Particle in a One-Dimensional Box
4	Particle in a One-Dimensional Box, Uncertainty Principle, and Particles in Two and Three Dimensions
5	Particle in a Square and Cube
6	Quantum Mechanical Model for a Rotating Molecule
7	Rotational Spectroscopy
8	Midterm 1 Review
9	**Midterm Test 1**
10	The Quantum Harmonic Oscillator
11	Vibrational Spectroscopy of Diatomic Molecules

12	Rovibrational Spectroscopy and Vibrational Spectroscopy of Polyatomic Molecules
13	Blackbody Radiation
14	Vibrational Spectroscopy of Polyatomic Molecules, Combination Bands, and Population of States
15	Quantum Mechanics of Rotating Molecules
16	Operators of the Rigid Rotor
17	Rotational-Vibrational Spectroscopy
18	Midterm 2 Review
19	**Midterm Test 2**
20	Hydrogen Atom
21	Atomic Orbitals
22	More Orbitals and Atomic Emission Spectroscopy
23	The Helium Atom
24	Electron Spin
25	Final Examination Review

Note: The course schedule is approximate and may be adjusted as needed. Any changes will be communicated through Brightspace.

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.

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.

Late and Missed Work Policy

All assignments must be submitted electronically through Brightspace by the posted deadline. Late submissions will not be accepted and will receive a grade of zero.

Students who are unable to meet a deadline due to illness or other extenuating circumstances must follow Carleton University's Academic Consideration Policy. Requests for extensions, deferred deadlines, or other accommodations must be submitted in accordance with the University's procedures and may require submission of the Academic Consideration Form.

Academic consideration is not granted automatically. Students are responsible for submitting requests in a timely manner and for providing any documentation or information required under University policy.

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

Academic Accommodations and Regulations

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Student Rights & Responsibilities

Students are expected to act responsibly and engage respectfully with other students and members of the Carleton and the broader community. See the 7 Rights and Responsibilities Policy for details regarding the expectations of non-academic behaviour of students. Those who participate with another student in the commission of an infraction of this Policy will also be held liable for their actions.