**CHEM 3101: Quantum Chemistry - Fall 2021**

## Course Format

The course instruction, assigned work, evaluation, and communication will be completed exclusively through remote learning facilities (BrightSpace and Zoom). There will be a set of online evaluations conducted over BrightSpace. Your primary source of the course content will be reading online texts on quantum chemistry. There will be weekly lectures summarizing this material. You will be assessed through written assignments, online quizzes, online tests, and a writing project.

**CHEM 3101 [0.5 credit]**

**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.

# Class Schedule

**Date:** Sep 08, 2021 to Dec 10, 2021 **Days:** Tue Thu **Time:** 08:35 - 09:55

| Tuesday  8:30 - 10 AM | Summary Lectures | https://carleton-ca.zoom.us/j/94068416178 |
| --- | --- | --- |
| Thursday  8:30 - 10 AM | Optional Q/A and tests | https://carleton-ca.zoom.us/j/95392541119 |

**Tuesday’s 8:30–10 AM**. I will give short (20–30 minutes) lectures summarizing the week’s materials on Zoom. You are strongly advised to attend and there is no guarantee that the content we discuss will be available later, although I will attempt to post the notes and lecture recordings, when possible.

**Thursday’s 8:30–10 AM** are reserved for completing the real-time online tests during the weeks they are scheduled. You must be available during these times to complete this course requirement. If there is no test scheduled that week, these times will be reserved for Q/A sessions with Chris. Attendance at the Q/A sessions is recommended but optional.

## 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/shared_invite/zt-tcsls3bn-YiAfIh3bDrROtE7PyQOkwA>

The URL to access the slack channel is [https://chem3101.slack.com/](https://chem3102-2020.slack.com/)

A demonstration on how to use Slack is available here:

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

I will schedule online meetings to discuss each exercise and the term project stages. The dates and times of these sessions and the connection information will be posted on Brightspace.

## Evaluation

| **Component** | **Weight** |
| --- | --- |
| online quizzes | 26 |
| online tests | 24 |
| written assignments | 35 |
| wiki project | 15 |

## Online Quizzes

There will be approximately one online quiz per week. The can be completed at any point during the week, but will generally be due Friday at 10 PM. My recommendation is that you will read the course material and attend the online lecture before attempting the quiz. You will have two attempts to complete each quiz. If you do not complete a quiz by the deadline, you will be able to complete the quiz at any later date until the end of the course, but you will be given a 30% penalty for that quiz.

## Online Tests

There will be 4 online tests, worth 6% each. They will generally be held on Thursdays during the class time (8:30 AM to 10 AM ET). You should study for these tests and prepare for them based on the quizzes you have already completed and the course material covered to date in the class. The questions on the test will be similar to those you’ve already seen on the quizzes. You must complete them online during the 90 minute scheduled class period. You do not have to provide documentation if you do not complete a test; If you do not complete them, the grades for these assessments will be redistributed evenly to the other requirements. There will be no makeup tests. You are strongly encouraged to complete them because they will probably be much easier than the other course requirements. If you receive a lower grade on these assessments than the other components of the course, they will be dropped and the weight will be added equally to the other forms of assessment.

You may not communicate with other people, including your classmates, during these tests. I can’t stop you from using your notes or google during the tests, but I will design the tests so that this won’t help and it will be difficult for you to complete the test in time if you try to search for the answers or learn the material on the fly..

The tentative schedule for these tests is:

| **Quiz** | **Date** |
| --- | --- |
| 1 | September 30 |
| 2 | October 21 |
| 3 | November 11 |
| 4 | December 2 |

## 

## Wikibook

Part of your assessment will be to write an example problem and its solution, which will become part of an online textbook for students in later years of this class. Your assignment and its specific solution are available on the BrightSpace page.

**The wikiproject assignment will be worth 15% of your final grade.**

**It is due November 19, 2021**

## 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

## 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