

Chemistry 3374A – Quantum Chemistry and Spectroscopy: Course Outline

1 Course Information

- **CHEM 3374A:** Quantum Chemistry and Spectroscopy, Fall 2024
- **Lecture times and location:** [REDACTED]
- **Tutorials:** [REDACTED]
- **First lecture:** [REDACTED]

1.1 Prerequisites

The prerequisites for this course are: Chemistry 1301A/B, Chemistry 1302A/B, 0.5 course from Calculus 1000 A/B, Calculus 1500A/B, Numerical and Mathematical Methods 1412A/B, and any other 0.5 course at the 1000-level from Calculus, Applied Mathematics, Mathematics, or Numerical and Mathematical Methods. Integrated Science 1001X may be used as a substitute for the combination of Chemistry 1302A/B and Calculus 1301A/B.

Unless you have either the requisites for this course or written special permission from your Dean's Designate (Department/Program Counsellors and Science Academic Advisors) to enroll in it, you may be removed from this course and it will be deleted from your record. This decision may not be appealed. You will receive no adjustment to your fees in the event that you are dropped from a course for failing to have the necessary prerequisites.

1.2 Antirequisites

Anti-requisite: Physics 3200A/B.

2 Instructor Information

- Instructor: Dr. Mikko Karttunen. Email: mkarttu at uwo dot ca.
 - Students must use their Western (@uwo.ca) email addresses when contacting by email.
 - **IMPORTANT:**
If/when you email me, the subject line *MUST ABSOLUTELY* have the following text exactly as given below:
CHEM3374A-2024
Failure to do so will lead to your email not being answered.
 - Office: CHB072

- Office hours: By appointment: Office hours will be in-person meetings that will be scheduled by appointment only.

3 Course Syllabus, Schedule, Delivery Mode

Brief Course Description: The course builds a background in quantum chemistry/mechanics needed to understand the physical and chemical behaviour of matter on the atomic scale. Quantum-mechanical concepts are developed and applied to model systems such as a particle in a box, the harmonic oscillator, the rigid rotor, and the hydrogen atom. The results are used to explain the principles of electronic, vibrational and rotational spectroscopy, atomic electronic structure, and chemical bonding.

3.1 Learning outcomes

Course-Specific Expectations:

- Recognize the importance of quantum chemistry and its applications.
- Think critically about, explain, integrate, and apply physical models to describe material and energy levels associated with atoms.
- Learn a variety of physical principles and to solve models.
- Solve a variety of novel problems, both qualitatively and quantitatively.
- Draw scientific conclusions from experimental results or data.

Soft-Skill Expectations:

- Analyze and critically assess problems and take a systematic approach to solve them.
- Execute mathematical calculations accurately.
- Communicate thoughts, ideas, and observations verbally and in writing.

3.2 Schedule and delivery mode

- Lectures: [REDACTED]
- Tutorials: [REDACTED]

3.3 Key Dates:

- First class: Friday September 6, 2024
- Fall Reading Week: October 12–20, 2024
- Classes end: December 6, 2024
- Exam period: December 9–22, 2024

4 Course Materials

The primary material of the course consists of your lecture notes – you must take notes during the classes and tutorials – material that is worked-out on the board, material distributed in the class, tutorials, and/or posted at the OWL website of the course, and your work on the assignments.

The following textbook is optional: “Physical Chemistry: Quanta, Matter and Change” by P. Atkins, J. de Paula, R. Friedman. (2nd Edition, W. H. Freeman & Co, New York 2014). The course covers Chapters 1-5.

Students are responsible for checking the course OWL site (<https://westernu.brightspace.com/>) regularly for news and updates. This is the primary method by which information will be disseminated to all students in the class.

If students need assistance with the course OWL site, they can seek support on the [OWL Brightspace Help](#) page. Alternatively, they can contact the Western Technology Services Helpdesk. They can be contacted by phone at 519-661-3800 or ext. 83800.

4.1 Technical Requirements

You will need pen & paper, or a tablet, for taking notes.

5 Methods of Evaluation

5.1 Grading Scheme and Assessment Dates

The overall course grade will be calculated as listed below:

Component	Date	Value
Midterm 1	Friday Oct 11, in-class.	20 %
Midterm 2	Friday Nov 15, in-class.	20 %
Final exam	Scheduled by the Registrar	60 %

Assignments: Every week, an assignment will be posted on the course website. The assignments will be neither collected nor marked, and no solution key will be provided. However, all the midterm questions, and at least 80% of the questions from the final exam will come from the assignment problems.

Midterms & if you miss them: Two 50 min midterms are scheduled (above) during regular class hours on Friday Oct 11 and Friday Nov 15. The format will be problems and short answers (can be calculations or/and verbal answers). Closed book, calculator needed. No cheat sheet will be provided. There will be no make-up midterms. If you miss the first midterm, the value (percentage) will be moved toward the second midterm, and if you miss the second midterm, the value will be moved to the final exam. If you miss both midterms, the final exam will carry the value of 100% of the assessment. No documentation of any kind is required to activate these re-weightings, and students do not even need to contact the instructor.

Final exam: Three-hour exam. The date is decided by the Registrar’s Office. The final exam will cover the whole course material. The format of the exam will be problems and answers (calculations and verbal). Closed book, calculator needed. No cheat sheet will be provided.

5.2 General information about missed coursework

Students must familiarize themselves with the *University Policy on Academic Consideration – Undergraduate Students in First Entry Programs* posted on the Academic Calendar:

https://www.uwo.ca/univsec/pdf/academic_policies/appeals/academic_consideration_Sep24.pdf.

This policy does not apply to requests for Academic Consideration submitted for **attempted or completed work**, whether online or in person.

The policy also does not apply to students experiencing longer-term impacts on their academic responsibilities. These students should consult [Accessible Education](#).

For procedures on how to submit Academic Consideration requests, please see the information posted on the Office of the Registrar’s webpage: https://registrar.uwo.ca/academics/academic_considerations/

All requests for Academic Consideration must be made within 48 hours after the assessment date or submission deadline.

All Academic Consideration requests must include supporting documentation; however, recognizing that formal documentation may not be available in some extenuating circumstances, the policy allows students to make one Academic Consideration request **without supporting documentation** in this course. However, the following assessments are excluded from this, and therefore always require formal supporting documentation:

- Examinations scheduled during official examination periods (Defined by policy)

When a student *mistakenly* submits their one allowed Academic Consideration request **without supporting documentation** for the assessments listed above or those in the **Coursework with Assessment Flexibility** section below, the request cannot be recalled and reapplied. This privilege is forfeited.

5.3 Evaluation Scheme for Missed Assessments

See Section [5.1](#).

When a student misses the Final Exam and their Academic Consideration has been granted, they will be allowed to write the Special Examination (the name given by the University to a makeup Final Exam). See the Academic Calendar for details (under [Special Examinations](#)), especially for those who miss multiple final exams within one examination period.

6 Additional Statements

6.1 Religious Accommodation

When conflicts with a religious holiday that requires an absence from the University or prohibits certain activities, students should request an accommodation for their absence in writing to the course instructor and/or the Academic Advising office of their Faculty of Registration. This notice should be made as early as possible but not later than two weeks prior to the writing or the examination (or one week prior to the writing of the test).

Please visit the Diversity Calendars posted on our university's EDID website for the recognized religious holidays:

<https://www.edi.uwo.ca>.

6.2 Accommodation Policies

Students with disabilities are encouraged to contact Accessible Education, which provides recommendations for accommodation based on medical documentation or psychological and cognitive testing. The policy on Academic Accommodation for Students with Disabilities can be found at:

https://www.uwo.ca/univsec/pdf/academic_policies/appeals/Academic_Accommodation_disabilities.pdf.

6.3 Academic Policies

The website for Registrar Services is <https://www.registrar.uwo.ca/>.

In accordance with policy,

https://www.uwo.ca/univsec/pdf/policies_procedures/section1/mapp113.pdf,

the centrally administered e-mail account provided to students will be considered the individual's official university e-mail address. It is the responsibility of the account holder to ensure that e-mail received from the University at their official university address is attended to in a timely manner.

Electronic devices in tests and exams: Only calculators without internet access are allowed. No computers or tablets

6.4 Scholastic Offences

Scholastic offences are taken seriously and students are directed to read the appropriate policy, specifically, the definition of what constitutes a Scholastic Offence, at the following Web site:

https://www.uwo.ca/univsec/pdf/academic_policies/appeals/scholastic_discipline_undergrad.pdf.

6.5 Support Services

Please visit the Science & Basic Medical Sciences Academic Advising webpage for information on adding/dropping courses, academic considerations for absences, appeals, exam conflicts, and many other academic-related matters:

<https://www.uwo.ca/sci/counselling/>.

Students who are in emotional/mental distress should refer to Mental Health@Western (<https://uwo.ca/health/>) for a complete list of options about how to obtain help.

Western is committed to reducing incidents of gender-based and sexual violence and providing compassionate support to anyone who has gone through these traumatic events. If you have experienced sexual or gender-based violence (either recently or in the past), you will find information about support services for survivors, including emergency contacts at

https://www.uwo.ca/health/student_support/survivor_support/get-help.html.

To connect with a case manager or set up an appointment, please contact support@uwo.ca.

You may also wish to contact Accessible Education at http://academicsupport.uwo.ca/accessible_education/index.html if you have any questions regarding accommodations.

Learning-skills counsellors at Learning Development and Success (<https://learning.uwo.ca>) are ready to help you improve your learning skills. They offer presentations on strategies for improving time management, multiple-choice exam preparation/writing, textbook reading, and more. Individual support is offered throughout the Fall/Winter terms in the drop-in Learning Help Centre, and year-round through individual counselling.

Additional student-run support services are offered by the USC, <https://westernusc.ca/services/>.