

## Chemistry 3374A Course Outline

### 1. Course Information

#### Course Information

Quantum Chemistry and Spectroscopy, Fall 2022

Courses: Monday, Wednesday, Friday, 10h30-11h30, Location VAC-100

Tutorial: Thursday, 11h30-12h30, Location AHB-1B06

**First Course: Friday September 9<sup>th</sup>, 10h30, VAC-100**

#### List of Prerequisites

Unless you have either the prerequisites for this course or written special permission from your Dean 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. The prerequisite for this class is CHEM 2384B. Anti-requisite is Physics 3200A/B.

### 2. Instructor Information

Instructors	Email	Office	Phone	Office Hours
Dr. Francois Lagugne-Labarthet	flagugne@uwo.ca	CH16	5196612111 ext 81006	By appointment

Students must use their Western (@uwo.ca) email addresses when contacting their instructors.

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 four model systems: 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.

#### Learning outcomes.

#### Course-Specific Expectations :

- Recognize the importance of quantum chemistry and of its application.
- 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 qualitative and quantitative.
- 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.

**Courses:** Monday, Wednesday, Friday, 10h30-11h30, Location VAC-100, in person courses.

**Tutorials:** Thursday, 11h30-12h30, Location AHB-1B06, in person tutorial.

**Midterm 1:** Wednesday October 12<sup>th</sup>, in class midterm, 50 min

**Midterm 2:** Wednesday Nov 16<sup>th</sup>, in class midterm, 50 min.

Fall Reading Week: October 31 – November 6, 2022

Classes end: December 8, 2022

Exam period: December 10 – 22, 2022

**Contingency plan for an in-person class pivoting to 100% online learning:** In the event of a COVID-19 resurgence during the course that necessitates the course delivery moving away from face-to-face interaction, affected course content will be delivered entirely online, either synchronously (i.e., at the times indicated in the timetable) or asynchronously (e.g., posted on OWL for students to view at their convenience). The grading scheme will **not** change. Any remaining assessments will also be conducted online as determined by the course instructor.

### 4. Course Materials

#### Textbooks

Any of the following textbooks is optional:

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

“Quantum Chemistry and Spectroscopy” by T. Engel, 2nd ed. (Prentice Hall, 2010).

All books are on reserve at the Taylor library for a two-hour loan. The primary material of the course consists of your lecture notes, material that is worked-out on the board, material distributed in the class and posted on the OWL website of the course and your work on the assignments and quizzes. References to parallel material in various books available in the library may also be made.

Students are responsible for checking the course OWL site (<http://owl.uwo.ca>) on a regular basis for news and updates. This is the primary method by which information will be disseminated to all students in the class.

All course material will be posted to OWL: <http://owl.uwo.ca>.

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

## 5. Methods of Evaluation

The overall course grade, out of 100, will be calculated as listed below. Listed next to the respective components are their maximum contributions toward the course grade.

Component	dates	Value
Quizzes	See table below	20%
Midterm Test 1	Wednesday Oct 12 <sup>th</sup> - 50 min	15%
Midterm Test 2	Wednesday Nov 16 <sup>th</sup> - 50 min	15 %
Final	Scheduled by the Registrar	50%

**Midterm exams:** Two 50 min mid terms are scheduled during regular class hours on Wednesday Oct 12<sup>th</sup> and Wednesday Nov. 16<sup>th</sup>. The format of the exam will be problems and short answers. Closed book, calculator needed.

**Final exam:** Three-hour exam. The date is decided by the registrar’s Office. The final exam will be cumulative, with emphasis on the materials that was not examined in the midterm exam. The format of the exam will be multiple choice questions. Closed book, calculator needed.

**Home Assignments and Quizzes:** Every two weeks, an assignment will be posted on the course website (see the schedule below). Correction of the assignments and questions will be done during the tutorial hour on the due date of the assignments. The assignments will not be collected nor marked. However, on the day following the due date there will be a quiz asking you to solve a problem that is similar to one of the problems of the assignment. During the quiz, you will be allowed to use your hand written solutions of the prepared home assignments. No other material is authorized (no tablet or computers allowed, calculator are ok) . The quizzes will be collected and marked by the instructor. Detailed solutions to the problems will be released after the quiz. You are required to take at least 4 out of the total of 5 quizzes. **If and only if** you take all the 5 quizzes, you will earn a **bonus**: the quiz for which you received the lowest score will not be counted toward your final course grade. A table with the

dates of quizzes and assignments is included below. The quizzes will take place on a Friday and will last for 10-15 min and will be followed by the class.

#	Assignment posted on Thursdays	Due dates on Thursdays	Quiz on Fridays
1	Sept 15 <sup>th</sup>	Sept 22 <sup>th</sup>	Sept 23rd
2	Sept 29th	Oct 6th	Oct 7 <sup>th</sup>
3	Oct 20 <sup>th</sup>	Oct 27 <sup>th</sup>	Oct 28 <sup>th</sup>
4	Nov 3rd	Nov 10th	Nov 11th
5	Nov 24 <sup>th</sup>	Dec 1st	Dec 2nd

### Topics covered.

1. The wave character of particles. Inability of classical mechanics to describe microscopic phenomena. Quanta of light and energy. Wave-particle duality of matter. Diffraction by a double slit. De Broglie waves and their experimental observation.

2. The Schrodinger equation. Differential equations. The differential equation for classical waves. The Schrödinger equation for a particle. Probability and probability density. Complex numbers and functions. Wave functions and their physical interpretation. Operators, eigenfunctions and eigenvalues. The Hamiltonian operator.

3. Simple quantum-mechanical problems. A free particle. A particle in a box in one, two, and three dimensions. Chemical applications of the particle-in-a-box model. Rectangular-box model of the chemical bond. Quantum tunneling through a barrier. The scanning tunneling microscope. Tunneling in chemical reactions. Quantum wells and quantum dots.

4. General quantum mechanical principles. Construction of operators for physical observables. Superposition of wave functions. Individual measurements and expectation values. Relation between commutability and precision of measurement. The uncertainty principle. The postulates of quantum mechanics.

5. Principles of vibrational spectroscopy. The classical and quantum-mechanical harmonic oscillators. Vibrations of diatomic molecules. Allowed and forbidden transitions. The origin of selection rules. Infrared and Raman transitions.

6. Principles of rotational spectroscopy. The Schrödinger equation for rotation in two and three dimensions. Angular momentum and its quantization. Spherical harmonics. The rigid rotor and rotational spectroscopy of diatomic molecules.

7. The structure and spectra of hydrogenic atoms. The Schrödinger equation for hydrogenic atoms. Energy levels, eigenfunctions (atomic orbitals) and probability densities for hydrogenic atoms. Complex and real orbitals. Radial distribution functions. Orbital angular momentum and electron spin.

8. Many electron atoms and molecules. Exact and approximate solutions to the Schrodinger equation. Variation method. Basis-set expansion. Orbitals and electron configurations Pauli exclusion principle. Hartree-Fock method. How quantum chemistry predicts molecular geometry.

**Upon successful completion of this course, the student will be able to:**

- Solve basic differential equations used to model electron energy and wavefunction
- Understand energies associated with electron transitions between energy levels.
- Calculate wavefunctions associated with orbitals
- Understand the concepts of electron density probabilities and represent them.
- Perform quantum mechanics common problems such as particles in 1D and 3D box.
- Understand the intimate relationship between electron, energy and spectroscopy.

**To pass the course**, you must write at least one midterm, write the final exam, and obtain an overall grade of at least 50% according to the marking scheme on page 3. Students who fail to write at least one midterm, whether excused or not, will receive a final grade of not greater than 40%, even if the calculated grade is higher.

## 6. Student Absences

If you are unable to meet a course requirement due to illness or other serious circumstances, please follow the procedures below.

**Assessments worth less than 10% of the overall course grade:**

If one Quiz is missed: no consequence on the total Quiz mark and the 4 written quizzes will be used for the total mark of the Quiz Portion.

If two or more quizzes are missed:

-if no valid medical or supporting documentation is provided, the mark associated with the missed quizzes will be 0/5 for each of the missed quizzes.

-if valid medical or supporting information is provided\* for each of the missed quizzes, the weight of the excused quizzes will be transferred to the final exam.

\*Note that in all cases where documentation (medical or otherwise) is required, it can *only* be collected by the student's Dean's Office Academic Counselling unit.

**Assessments worth 10% or more of the overall course grade:**

For work totalling 10% or more of the final course grade, you must provide valid medical or supporting documentation to the Academic Counselling Office of your Faculty of Registration as soon as possible. For further information, please consult the University's medical illness policy at

[https://www.uwo.ca/univsec/pdf/academic\\_policies/appeals/accommodation\\_medical.pdf](https://www.uwo.ca/univsec/pdf/academic_policies/appeals/accommodation_medical.pdf).

The Student Medical Certificate is available at

[https://www.uwo.ca/univsec/pdf/academic\\_policies/appeals/medicalform.pdf](https://www.uwo.ca/univsec/pdf/academic_policies/appeals/medicalform.pdf).

Only one make-up exam will be given and will be cumulative on the material covered during Midterms 1 and 2.

## Absences from Final Examinations

If you miss the Final Exam, please contact the Academic Counselling office of your Faculty of Registration as soon as you are able to do so. They will assess your eligibility to write the Special Examination (the name given by the University to a makeup Final Exam).

You may also be eligible to write the Special Exam if you are in a “Multiple Exam Situation” (e.g., more than 2 exams in 23-hour period, more than 3 exams in a 47-hour period).

If a student fails to write a scheduled Special Examination (SPC), the date of the next Special Examination (if granted) normally will be the scheduled date for the final exam the next time this course is offered. Students who fail to write an approved SPC examination on that date forfeit that privilege and must apply again. The maximum course load for the term in which the SPC was granted will be reduced by the appropriately. See the Academic Calendar for details (under [Special Examinations](#)).

**Note:** missed work can *only* be excused through one of the mechanisms above. Being asked not to attend an in-person course requirement due to potential COVID-19 symptoms is **not** sufficient on its own.

## 6. Accommodation and Accessibility

### Religious Accommodation

When a course requirement conflicts with a religious holiday that requires an absence from the University or prohibits certain activities, students should request accommodation for their absence in writing at least two weeks prior to the holiday to the course instructor and/or the Academic Counselling office of their Faculty of Registration. Please consult University's list of recognized religious holidays (updated annually) at

<https://multiculturalcalendar.com/ecal/index.php?s=c-univwo>.

### 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](https://www.uwo.ca/univsec/pdf/academic_policies/appeals/Academic_Accommodation_disabilities.pdf).

## 7. Academic Policies

The website for Registrarial Services is <http://www.registrar.uwo.ca>.

In accordance with policy,

[https://www.uwo.ca/univsec/pdf/policies\\_procedures/section1/mapp113.pdf](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.

No electronic devices other than calculators are permitted on tests (quizzes) and exams.

**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:

[http://www.uwo.ca/univsec/pdf/academic\\_policies/appeals/scholastic\\_discipline\\_undergrad.pdf](http://www.uwo.ca/univsec/pdf/academic_policies/appeals/scholastic_discipline_undergrad.pdf).

In the event of a lock down due to pandemic issues, tests and examinations in this course will be conducted using a remote proctoring service. By taking this course, you are consenting to the use of this software and acknowledge that you will be required to provide **personal information** (including some biometric data) and the session will be **recorded**. Completion of this course will require you to have a reliable internet connection and a device that meets the technical requirements for this service. More information about this remote proctoring service, including technical requirements, is available on Western's Remote Proctoring website at:

<https://remoteproctoring.uwo.ca>.

**Note:** use of online proctoring for in-person courses requires approval from the Dean's Office.

## 8. Support Services

Please visit the Science & Basic Medical Sciences Academic Counselling 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](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](mailto:support@uwo.ca).

Please contact the course instructor if you require lecture or printed material in an alternate format or if any other arrangements can make this course more accessible to you. You may also wish to contact Accessible Education at

[http://academicsupport.uwo.ca/accessible\\_education/index.html](http://academicsupport.uwo.ca/accessible_education/index.html)

if you have any questions regarding accommodations.

Learning-skills counsellors at the Student Development Centre (<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.