CHEM 3374A: Quantum Chemistry and Spectroscopy  
2016–17 Course Outline

Prerequisite Requirements

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 or the former 2284B. Anti-requisite is Physics 3200A/B.

Course Website

Students should check OWL (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. Students are responsible for checking OWL on a regular basis. Always check your UWO email rather than your other email adress.

Accessibility

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 Services for Students with Disabilities (SSD) at 661-2111 ext. 82147 if you have questions regarding accommodation.

Support Services

Learning-skills counsellors at the Student Development Centre (http://www.sdc.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.
Students who are in emotional/mental distress should refer to Mental Health@Western (http://www.health.uwo.ca/mental_health) for a complete list of options about how to obtain help.
Additional student-run support services are offered by the USC, http://westernusc.ca/services.
The website for Registrarial Services is http://www.registrar.uwo.ca.

**Course Website**

Students should check OWL (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. The missing of critical information due to your failure to check OWL cannot be used as a basis for appeal.

**Course Materials**

**Textbooks**
Any of the following textbooks is optional:
“Physical Chemistry” by P. Atkins and J. de Paula, 9th ed. (Freeman, 2010); or “Physical Chemistry” by R. J. Silbey, R. A. Alberty, M. G. Bawendi, 4th ed. (Wiley 2005)
“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 webct site 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.

**Lecture and Instructor Information**

<table>
<thead>
<tr>
<th>Section</th>
<th>Time</th>
<th>Room</th>
<th>Instructor</th>
<th>Office</th>
<th>Email</th>
</tr>
</thead>
<tbody>
<tr>
<td>Course</td>
<td>M-W-Th 11:30−12:30pm</td>
<td>SEB-2100</td>
<td>Prof. François Lagugné-Labarthet</td>
<td>MSA0202</td>
<td><a href="mailto:flagugne@uwo.ca">flagugne@uwo.ca</a></td>
</tr>
<tr>
<td>Tutorial</td>
<td>Friday 11:30−12:30pm</td>
<td>KB-K106</td>
<td>Prof. François Lagugné-Labarthet</td>
<td>MSA0202</td>
<td><a href="mailto:flagugne@uwo.ca">flagugne@uwo.ca</a></td>
</tr>
<tr>
<td>Office</td>
<td>Mondays and Wednesdays 5:00-6:30pm or by appointment</td>
<td>MSA0202</td>
<td>Prof. François Lagugné-Labarthet</td>
<td>MSA0202</td>
<td><a href="mailto:flagugne@uwo.ca">flagugne@uwo.ca</a></td>
</tr>
</tbody>
</table>
If you are contacting your instructor, please use your Western email address.

**Evaluation Components**

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.

<table>
<thead>
<tr>
<th>Component</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Five Quizzes with the highest mark</td>
<td>25%</td>
</tr>
<tr>
<td>Midterm Test</td>
<td>35%</td>
</tr>
<tr>
<td>Final Exam Scheduled by the Registrar</td>
<td>40%</td>
</tr>
</tbody>
</table>

**Midterm exam:** two hours exam on **Oct 26th 2015- 6-8 pm** Room to be announced. The format of the exam will be problems and short answers.

**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 problems and short answers.

**Assignments and quizzes:** Every two weeks, an assignment will be posted on the course website (see the schedule below). Hints and short answers will be made available on the due date. The assignments will not be collected. 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 written solutions prepared at home, but not any other materials. 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 5 out of the total of 6 quizzes. If and only if you take all the 6 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, during the tutorial time and will last for 20 minutes.

<table>
<thead>
<tr>
<th>#</th>
<th>Assignment posted</th>
<th>Due date</th>
<th>Quiz</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Sept 15th</td>
<td>Sept 22nd</td>
<td>Sept 23th</td>
</tr>
<tr>
<td>2</td>
<td>Sept 29th</td>
<td>Oct 6th</td>
<td>Oct 7th</td>
</tr>
<tr>
<td>3</td>
<td>Oct 13th</td>
<td>Oct 20th</td>
<td>Oct 21st</td>
</tr>
<tr>
<td>4</td>
<td>Oct 27th</td>
<td>Nov 3rd</td>
<td>Nov 4th</td>
</tr>
<tr>
<td>5</td>
<td>Nov 10th</td>
<td>Nov 17th</td>
<td>Nov 18th</td>
</tr>
<tr>
<td>6</td>
<td>Nov24th</td>
<td>Dec 1st</td>
<td>Dec 2nd</td>
</tr>
</tbody>
</table>

**To pass the course,** you must obtain a minimum of 50% in the average of quizzes, midterm and final. One should write the midterm and final exam to pass the course. Obtaining a good average grade in the quizzes and midterm is not sufficient to pass the course.
Absences, Missed Course Components, Code of conduct

If you are unable to meet a course requirement due to illness or other serious circumstances, you must provide valid medical or supporting documentation to the Academic Counselling Office of your home faculty as soon as possible.

If you are a science student, the Academic Counselling Office of the Faculty of Science is located in WSC 191, and can be contacted at 519-661-3040 or scibmsac@uwo.ca. Their website is http://www.uwo.ca/sci/undergrad/academic_counselling/index.html.

Accommodation for illness. Students seeking academic accommodations based on medical (physical or mental) illness should begin by contacting the Academic Counsellors of their home faculty. Please visit the following link for policy on Accommodation for Illness: http://www.uwo.ca/univsec/pdf/academic_policies/appeals/accommodation_illness.pdf

Exam Distress Policy. It is Faculty of Science policy that a student who chooses to write a test or exam deems themselves fit enough to do so, and the student must accept the mark obtained. Claims of medical, physical, or emotional distress after the fact will not be considered.

Scholastic offences are taken seriously and students are directed to read the appropriate policy, specifically, the definition of what constitutes a Scholastic Offence, at this website: http://www.uwo.ca/univsec/pdf/academic_policies/appeals/scholastic_discipline_undergrad.pdf.

Plagiarism is a serious Scholastic Offense. Students should write their essays and assignments individually. Copying of assignments will involve penalties in the grades. In essays, whenever a student takes an idea or a passage from another source, appropriate reference should be given.

Failure to complete or write the midterm, or the final, or quiz will result in a mark of zero for the missed item, and potential failure in the course, unless a valid medical or compassionate reason has been approved and an exemption has been granted. The Policy of Accommodation for Medical Illness is found in the web site: https://studentservices.uwo.ca/secure/index.cfm and for further policy information please visit http://www.uwo.ca/univsec/handbook/appeals/accommodation medical.pdf

Missed quizzes: One quiz may be skipped without any penalty. Students who have to miss more than one quiz must: (a) ask the instructor for prior permission not to write the quiz; (b) submit a complete assignment by the appropriate due date (see above). No formal documentation for this accommodation is required. However, if the student cannot complete the assignment by the due date or write the quiz then formal documentation is required otherwise the quiz will receive zero mark. If formal documentation that justifies the missing quiz and the completion of the assignment is received then the mark for the quizzes will be based on the average of the written quizzes.
If you miss the Midterm Exam, the weight of the midterm (35%) will be reported on the final exam. The weight of the final will therefore be 75%.

If you miss the Final Exam, contact your faculty’s Academic Counselling Office as soon as possible. They will assess your eligibility to write the Special Exam (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” (see http://www.registrar.uwo.ca/examinations/exam_schedule.html).

Code of Conduct: Students are reminded of the University’s Code of Conduct found on the university website. To maintain a high standard of learning environment in our classrooms, those who are disruptive, rude, or show unacceptable behavior, either to the instructor, or the other students, will be asked to leave.

Attendance: Any student who, in the opinion of the instructor, is absent too frequently from class or laboratory periods in any course will be reported to the Dean of the Faculty offering the course (after due warning has been given). On the recommendation of the Department concerned, and with the permission of the Dean of that Faculty, the student will be debarred from taking the regular examination in the course. The Dean of the Faculty offering the offering the course will communicate that decision to the Dean of the Faculty of registration.

**CHEM 3374 Learning Expectations**

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.
Anticipated Lecture Topics

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.

Lecture Topics:


7. The structure and spectra of hydrogenic atoms. The Schrödinger equation for hydrogenic atoms. Energy levels, eigenfunctions (atomic orbitals) and probability densities for hydrogenic


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 relation between electron, energy and spectroscopy.

Social Media

Twitter - Follow us @westernuchem (to know what s going on in your favorite field!)
Follow me @lagugne (I am a crazy tweeter!)
Facebook - www.facebook.com/ChemistryatWestern

Important dates 2016

September 8th, Class starts
October 10th, Thanksgiving Monday
October Wednesday 26th, 6-8 pm, mid-term
October 27-28, Fall study break
Dec. 7th- Last day of class
Dec 10-21, Exam period

No courses on: Wednesday September 21st, Thursday November 10th