WESTERN UNIVERSITY
DEPARTMENT OF CHEMISTRY

CHEM 3374a-Quantum Chemistry and Spectroscopy
September-December 2013

COURSE OUTLINE

Welcome to CHEM 3374A!

Instructor Dr. Styliani Constas, Room 071-Chemistry Building, ext. 86338

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Location and Class hours CHB-9, Chemistry Building
Lectures Monday, Wednesday, Thursday 11:30 am-12:30 pm
Tutorial Friday 11:30 am-12:30 pm

Office hours Monday, Wednesday, Friday 12:30-2:30 pm or by appointment

Course website https://owl.uwo.ca/portal

Notice from the Registrar Unless you have either the prerequisites for this course or written special permission from your Dean to enroll in it, you will 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, which are Chemistry 2384B or the former Chemistry 2284B**. Antirequisite is Physics 3200A/B.

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); or
- "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.

Course Evaluation

Course Grade The course grade, out of 100, will be calculated as listed below:
five quizzes with the highest marks-25%
the midterm test 35%
the final exam 40%

Midterm Exam Two-hour exam on Saturday, October 20, 2012, 1:00 pm-3:00 pm. The format of the exam will be problems and short answers.

Final Exam Three-hour exam. The date is to be decided by the Registrar's Office. The final exam will be cumulative, with emphasis on the material 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 web site (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.

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.

Table 1: Assignment/Quiz Schedule

#	*Assignment posted*	*Due date*	*Quiz*
1	September 12	September 19	September 20
2	September 26	October 3	October 4
3	October 10	October 17	October 18
4	October 24	November 7	November 8
5	November 14	November 21	November 22
6	November 28	December 5	December 6

Accessibility

Please contact the course instructor if you require material in an alternate format or if you require any other arrangements to make this course more accessible to you. You may also wish to contact Services for Students with Disabilities (SSD) at 661-2111 x 82147 for any specific question regarding an accommodation.

Absences, Missed Exams/Quizzes, Code of Conduct

- 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.

- **Missed exam:** If you miss the final exam, contact your Dean's office to obtain an SPC form. Students who are ill, for all exams and tests yet choose to write the final exam, must accept the mark that they receive.

- **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 course will communicate that decision to the Dean of the Faculty of registration.

- **Scholastic Offense Policy:** You should be familiar with the Scholastic Offense Policy in the Academic Calendar. Scholastic offenses are taken seriously and students are

directed to read the appropriate policy, specifically, the definition of what constitutes a Scholastic Offense, at the following Web site:
http://www.uwo.ca/univsec/handbook/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.

- **Exam Distress Policy:** It is the policy of the Department of Chemistry that when a student takes a test or an examination, one should have deemed oneself fit to do so. Claims of distress or medical issues after the fact will not be considered as a basis of a grade appeal.

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

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 Schrödinger equation.* Differential equations. The differential equation for classical waves. The Schroedinger 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 Schroedinger 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 Schroedinger 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. *The structure of many-electron atoms.* The orbital approximation for many-electron wave functions. Fermions and bosons. The Pauli exclusion principle. Slater determinants. The Aufbau principle and the periodic table. HartreeFock self-consistent field method. Spin multiplicity (singlet, doublet, triplet, etc. states).

Important Dates (2013)
September 9, Classes start
October 14, Thanksgiving Holiday
October 31 and November 1st, Fall Study Break
November 5, Last day to drop a first-term half course without academic penalty
Midterm date Saturday, October 19, 2013, 1:00 pm-3:00 pm
December 6, Fall/Winter Term classes end
December 7, Study day
Final Exam date, Registrar's office decision