The University of Western Ontario
Department of Chemistry

Advanced Quantum Chemistry and Spectroscopy, Chem 4474b
January-April 2012

COURSE OUTLINE

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 is 3374A/B.

Course website: http://webct.uwo.ca

Lectures

- Tuesday and Thursday at 11:30 am – 12:30 pm, CHB115 (Chemistry Building, Room 115) and Wednesday at 9:30 am – 10:30 am, CHB115
- Instructor: Dr. Styliani Constas, Chemistry Building, Room 071.

  Phone: 519-661-2111 x 86338

  e-mail : sconstas@uwo.ca, styliani.constas@gmail.com

Office hours : Wednesdays 12:30pm-14:00pm and Friday 12:30-2:30 pm in Chemistry Building, Room 071 or another day by appointment.

Materials

- Lecture notes and assignments posted in the course website in webct.uwo.ca.
- Problems worked-out in the class.
- *Recommended textbooks:*

  Quantum Chemistry and Spectroscopy by T. Engel (Pearson, 2nd Ed.);

  Spectra of Atoms and Molecules by P. F. Bernath, 1st or 2nd ed., Oxford University Press, 1995 or 2005 .

  These books are on reserve in the library (2 hour loan).

- Alternative texts may be:

  R. J. Silbey, R. A. Alberty, and M. G. Bawendi, *Physical Chemistry*, 4th ed., Wiley &Sons, 2005 ;

  D. A. McQuarrie, *Quantum Chemistry*, 1st or 2nd ed., University Science Books, Sausalito, CA, 1983 or 2008 ;

  I. N. Levine, *Quantum Chemistry*, 4th, 5th, or 6th ed. Prentice Hall, Englewood Cliffs, NJ, 1991–2009

Course evaluation

- The course grade, out of 100, will be calculated as listed below:
  - 5 problem sets (25 marks).
  - Two-hour midterm exam (35 marks) on Wed. February 29, 5:30 pm-7:30 pm (the date will be discussed in the class on January 10, 2012 for the availability of the students. If the students are not available because of a conflict with another course the date might change.)
  - Three-hour final exam (40 marks), date set by the Registrar. This exam is cumulative, but it will emphasize the material not covered in the midterm exam.

- To pass the course, you must obtain a minimum of 50% or greater in the average by all the tests (Mid-term and Final exam) and assignements estimated with the described weight.
- **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.
- **Plagarism** 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.

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, Code of Conduct

- Failure to complete or write the midterm, or the final, 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

  (notice the underscore in accomodation_medical.pdf in the above web address).

- **Missed exam:** If you miss the midterm exam or 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 midterm or 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 and laboratories those who are disruptive, rude, or show unacceptable behavior, either to the instructor, the TA, 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.

Brief Course Description

The course discusses applications of quantum mechanics to atomic and molecular spectroscopy (including electronic, vibrational and rotational spectroscopy) and introduces the basics of advanced quantum chemistry methods (variation method, perturbation theory, Hartree-Fock method) that are used to study the chemical bondin g.

Lecture Topics

1. *Foundation of Spectroscopy.* Review of the postulates and theorems of quantum mechanics. Dirac notation. Atomic units. Schroedinger equation for nuclear motion. Interaction of radiation with matter. Einstein coefficients and introduction to the selection rules.

2. *Symmetry and group theory.* Molecular symmetry. Elements of point group theory. Matrices and determinants. Matrix representations of symmetry operations. Reducible and irreducible representations. Great orthogonality theorem. Character tables.

3. *Group theory in quantum chemistry.* Symmetry operations on functions. Symmetry of the molecular Hamiltonian. Symmetry-adapted functions. Selection rules.

4. *Rotational spectroscopy.* Rotation of rigid bodies. Diatomic and linear molecules. Symmetric and asymmetric tops. Centrifugal distortion. Selection rules. Structure determination.

5. *Vibrational spectroscopy.* Wave functions and energy levels for harmonic and anharmonic oscillators. Vibrational and vibration-rotational spectra of diatomic molecules. Vibrational spectra of polyatomic molecules. Normal modes of vibration. Symmetry of normal modes. Raman spectra. IR and Raman active modes.

6. *Approximate methods in quantum chemistry.* Review of the exactly solvable quantum-mechanical models. Variation method. Trial functions that depend linearly on the variational parameters. Secular determinant. Perturbation method. Time-independent perturbation theory: nondegenerate and degenerate cases.

7. *Angular momentum in atomic and molecular spectroscopy.* Orbital and spin angular momentum. Spin eigenfunctions. Addition of angular momenta. Clebsch–Gordan coefficients. Atomic and molecular term symbols. Spin-orbit coupling. Fine structure of atomic spectra.

8. *Electronic spectroscopy of molecules.* Electronic energy levels. Electronic absorption spectra of diatomic molecules. Franck–Condon principle. Oscillator strength. Electronic spectra of polyatomic molecules. Beer–Lambert law. Huckel molecular orbital theory. Canonical and localized molecular orbitals. Koopmans' theorem. Photoelectron spectroscopy. Lasers. Fluorescence and phosphorescence. Optical activity and optical rotation. Jahn–Teller effect.

9. *Magnetic resonance spectroscopy.* ***(if time allows)*** Nuclear magnetism and nuclear magnetic resonance. Energy levels in nuclear magnetic resonance (NMR). Fourier transforms. Nuclear magnetic spectrometry. Chemical shift. Internuclear spin-spin coupling. Electron spin resonance.

Important Dates (2012)

January 9	Classes resume
January 17	Last day to add a second-term half course, or a second-term full course
Feb. 15	Last day to drop a second-term half course, or a second-term full course without academic penalty
see Course Evaluation	*Midterm date*
Feb. 20-24	Reading week
April 11	Fall/Winter Session classes end
Registrar's Office decision	*Final Exam date*