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Teaching Assistant: Ivan Bosko

Lectures: Monday, Wednesday, Friday, 10:30 AM–11:30 AM, CHB 9 or Zoom

Labs: See the dates below, 6:00 PM, SSC 1000 or Zoom

Office hours: By appointment (administrative matters)

Course web site: https://owl.uwo.ca/portal

Prerequisites: Chemistry 2272F, 2281G, 2283G, 2384B

Description: An introduction to computer methods and tools available in chemistry. Topics include molecular structure visualization, calculation of molecular structure and properties, analysis of reaction mechanisms using potential energy surfaces, simulation of molecular spectra, numerical methods, data processing, and symbolic computation software.

Evaluation: The course grade will be determined as a weighted average of the following components:

- Computer labs 30% See the schedule below
- Assignments 15% See the schedule below
- Midterm test 15% Wednesday, March 2 (50 min, in class, written answers)
- Final exam 40% To be scheduled by the Registrar (3 hours, written answers)

Minimum requirements. The labs and assignments are essential components of this course. You must submit at least 4 out of 6 lab reports, at least 3 out of 4 assignments, and write the final exam. Students who fail to meet any of these requirements without accommodation will receive a course grade of no greater than 40%. If your accommodations reduce the number of completed labs and assignments below this minimum, you will be required to complete the missed items the next time the course is offered.

Course materials: There is no required textbook. All course materials (lecture notes, lab manuals, etc.) will be distributed via the course website.

Course Topics


3. *General-purpose scientific software.* Introduction to symbolic computation software. Using MAPLE to evaluate integrals, solve differential equations, plot functions, etc.


8. *Calculation of molecular properties and spectra.* Dipole moments, electrostatic potential, atomic charges, bond orders. Simulation of IR, Raman, and UV-vis spectra.

Learning Expectations

A student receiving credit for CHEM 3300G will be expected to:

- Recognize the utility of computer tools in chemistry research
- Understand the basic theoretical principles of molecular structure calculations
- Visualize, build, and manipulate molecular structures on a computer
- Understand the origin and meaning of molecular orbitals
- Know how to use the *Gaussian* program to predict the most stable structures of molecules, calculate reaction enthalpies and Gibbs energies, simulate vibrational spectra, correlate electronic structure with chemical properties
- Be able to perform basic operations of calculus and linear algebra using *Maple*
- Be able to perform least-squares fitting and regression analysis of data using *Excel*
- Be aware of the capabilities and limitations of computational chemistry techniques
All lab reports and assignments are due by 6:00:00 PM on the dates indicated above and must be submitted electronically via OWL. For lab reports, use the templates provided on OWL.

### Policies

**Fair evaluation.** All students will be evaluated using the same criteria described in this course outline. Private requests for any preferential treatment (e.g., bumping a grade, tweaking the evaluation method to achieve a higher course grade, offering additional assessments, etc.) will not be entertained under any circumstances. E-mails containing such requests are inappropriate and will not be responded to.

**Integrity.** Private requests to contravene or mitigate any regulation or provision set out in this course outline or in any university policy are unfair to the students abiding by the rules. E-mails containing such requests are inappropriate and will not be responded to.

**Inquiries about tests and exams.** All information about upcoming tests and exams that is meant to be known by the students will be provided in the form of general announcements. Further inquiries concerning any aspect of an upcoming test or exam will not be entertained.

**Academic offences.** All work submitted for a grade in this course must be your personal work. Use of answers obtained externally is prohibited. Plagiarism and cheating offences will be subject to disciplinary action as regulated by Western’s policy “Scholastic Discipline for Undergraduate Students”.

**Late submissions.** There is a penalty of 20% of the actual grade for all lab reports and assignments submitted within 24 hours after the deadline, increasing by 20% within each subsequent 24-hour period. In all cases, the OWL time stamp will be considered an official, indubitable record. Submissions flagged “late” by OWL (i.e., even if received 1 sec after 6:00:00 PM) will be treated as such.

**Missed labs.** There are no make-up labs. If you miss one or two labs and receive accommodation, the weight of the missed labs will be redistributed among the other labs. If you miss more than two labs and are excused, you will be required to complete the third and all subsequently missed labs the next time the course is offered.

**Missed assignments.** There are no make-up assignments. If you miss one assignment and receive accommodation, the weight of the missed assignment will be redistributed among the other assignments. If you miss more than one assignment and are excused, you will be required to complete the second and all subsequently missed assignments the next time the course is offered.

**Missed midterm test.** There is no make-up midterm test. If you are unable to write the midterm test, you must request academic consideration at [https://www.uwo.ca/sci/counselling/index.html](https://www.uwo.ca/sci/counselling/index.html) → PROCEDURES → Academic Consideration for Absences. If you miss the midterm test and receive academic accommodation, the weight of the missed midterm will be transferred to the final exam. Otherwise, the midterm test mark will be 0%.
Missed final exam. If you are unable to write the final exam, contact your faculty’s Academic Counselling Office as soon as possible. They will assess your eligibility to write the Special Exam (i.e., a makeup Final Exam). You may also be eligible to write the Special Exam if you are in a “Multiple Exam Situation”.

Class attendance. Class and lab attendance is mandatory. Information missed during absences cannot be considered as grounds for appeals.

Use of electronic devices. As a courtesy to your fellow classmates, please leave mobile devices at home or switch them to silent mode before lectures begin. If you use a laptop to take notes, please sit near the back of the classroom in order to minimize disruption to other students. During tests and exams, only basic electronic calculators are allowed; all other devices (cell phones, tablets, cameras, or iPod, etc.) are strictly prohibited. Those devices must be left either at home or with the student’s bag/jacket at the front of the room and must not be at the test/exam desk or in the individual’s pocket. Any student found with one of these prohibited devices will receive a grade of zero on the test or exam. The Department of Chemistry is not responsible for stolen/lost or broken devices.

Accessibility. Students with disabilities work with Accessible Education which provides recommendations for accommodation based on medical documentation or psychological and cognitive testing. For details, visit http://academicsupport.uwo.ca/accessible_education/index.html

Support Services. Counselors at the Student Development Centre (http://www.sdc.uwo.ca) can help you improve your learning skills. They offer presentations on strategies for improving time management, exam preparation/writing, textbook reading, and more. Individual support is offered in the drop-in Learning Help Centre and through individual counselling. Students who are in emotional/mental distress should refer to Mental Health at Western (http://www.health.uwo.ca/mental_health). Additional student-run support services are offered by the USC (http://westernusc.ca/services).

Use of Proctortrack. This course outline is subject to change with the evolving COVID-19 pandemic. Tests and examinations may be conducted using remote proctoring services such as Proctortrack. By taking this course, you are consenting to the use of such software and acknowledge that you will be required to provide personal information (including some biometric data) and that the session will be recorded. More information about this remote proctoring service is available in the Online Proctoring Guidelines at the following link: https://www.uwo.ca/univsec/pdf/onlineproctorguidelines.pdf Completion of this course will require you to have a reliable internet connection and a device that meets the technical requirements for this service. Information about the technical requirements are available at the following link: https://www.proctortrack.com/tech-requirements