The University of Western Ontario  
Department of Chemistry  

Chemistry 3300G  
COMPUTER METHODS IN CHEMISTRY  
Winter 2019  

Course Information  

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Teaching Assistant: Amer El-Samman  
E-mail: aelsamm@uwo.ca  

Lectures: Monday, Wednesday, Friday, 10:30–11:20 am, ChB 9  

Labs: Monday, 6:00–9:00 pm, SH 1310  

Office hours: By appointment  

Course web site: owl.uwo.ca  

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

Description: The course provides a theoretical background and practical experience in using computer-based tools for solving chemistry problems. Students learn basic computational chemistry methods and then apply those methods to calculate molecular structure and properties, study reaction mechanisms, and simulate molecular spectra. Numerical methods and symbolic computation software are also introduced.  

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

<table>
<thead>
<tr>
<th>Component</th>
<th>Weight</th>
<th>Description</th>
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<tbody>
<tr>
<td>Labs</td>
<td>32%</td>
<td>8 computer labs</td>
</tr>
<tr>
<td>Quizzes</td>
<td>8%</td>
<td>8 in-class quizzes (based on the problem assignments)</td>
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<tr>
<td>Midterm exam</td>
<td>20%</td>
<td>Wednesday, February 27, in class</td>
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<tr>
<td>Final exam</td>
<td>40%</td>
<td>cumulative, to be scheduled by the Registrar</td>
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To obtain a passing grade, a student must write all exams and submit all lab reports. A mark of zero will be assigned for each quiz missed without a valid reason.  

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

Lecture Topics


6. *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.

Lab, Assignment, and Quiz Schedule

All labs are on Mondays at 6:00 pm in SH 1310

All assignments will posted on the lab dates and due on the lab report due dates

All quizzes will be on the due date of the corresponding assignment

<table>
<thead>
<tr>
<th>Lab #</th>
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<tbody>
<tr>
<td>1</td>
<td>January 21</td>
<td>5</td>
<td>March 11</td>
</tr>
<tr>
<td>2</td>
<td>January 28</td>
<td>6</td>
<td>March 18</td>
</tr>
<tr>
<td>3</td>
<td>February 4</td>
<td>7</td>
<td>March 25</td>
</tr>
<tr>
<td>4</td>
<td>February 11</td>
<td>8</td>
<td>April 1</td>
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1. Lab reports are due at 6:00 pm on Monday one week after the lab (exception: Lab 4 report is due after the Reading Week, on February 25).

2. Lab attendance is mandatory.

3. Lab manuals will be posted on OWL. Read the manual before coming to the lab.

4. All lab reports and other required files must be submitted electronically via OWL. Use Lab Report templates provided on OWL.

5. Late submission penalty: 30% if submitted within 24 hours after the deadline. Reports will not be accepted 24 hours after the deadline.
Learning Expectations

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

• Recognize the utility of computer tools in chemistry research
• Explain 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

Policies

Course website. Students should check OWL (https://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.

Assignments. 8 problem assignments will be posted on the lab dates and due on the lab report dues dates (see the schedule above). Assignments themselves will not be marked.

Quizzes. Each quiz will ask you to solve a short problem similar to one of the problems from the current take-home assignment. Each quiz will be marked out of 10.

Attendance. Any student who, in the opinion of the instructor, is absent too frequently from class without valid reasons will be given a warning. Failure to take this warning seriously may result in being barred from sitting the final exam.

Missed exams. If you are unable to write the midterm exam or the final exam 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. The Academic Counselling Office of the Faculty of Science website is: https://www.uwo.ca/sci/counselling. A student requiring academic accommodation due to illness must use the Student Medical Certificate when visiting an off-campus medical facility. For further information, please consult the university’s medical illness policy at https://www.uwo.ca/univsec. Missed midterm: A makeup will be offered. Missed 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”.

Missed labs. There are no make-up labs. If you miss a lab and do not wish to receive a zero mark for it, you must request in writing (by e-mail) accommodation from the instructor. If the accommodation is granted, you must submit a complete lab report as if you had attended the lab. Medical documentation in such cases is not required.
**Missed quizzes.** There are no make-up quizzes. If you miss a quiz and do not wish to receive a zero mark for it, you must request in writing (by e-mail) accommodation from the instructor. If the accommodation is granted, you will be excused and your quiz mark will be re-weighted. Medical documentation in such cases is not required.

**Academic accommodation.** Students seeking academic accommodations based on medical (physical or mental) illness should begin by contacting the Academic Councillors of their home faculty.

**Scholastic offences.** 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 website: [https://www.uwo.ca/univsec](https://www.uwo.ca/univsec)

**Use of electronic devices.** With the exception of calculators, no electronic devices may be in your possession during exams.

**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.

**Support Services:** Learning counsellors at the Student Development Centre ([http://www.sdc.uwo.ca](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 ([https://www.uwo.ca/health](https://www.uwo.ca/health)) for a complete list of options about how to obtain help.