Chemistry 3300B

COMPUTER METHODS IN CHEMISTRY

Winter 2024

Course Information

[redacted]

[redacted]

Lectures: [redacted]

Tutorials: [redacted]

Office hours:

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

Prerequisites: Chemistry 1301A/B, Chemistry 1302A/B and ... 1.0 courses at the 1000 level or higher ...

1301A/B).

... using potential energy surfaces, simulation of molecular spectra, numerical meth... reaction mechanisms

Expected Learning Outcomes

- Recognize the utility of computer tools in chemistry research
- Understand the basic theoretical principles of molecular structure calculations
- Visualize, build, and manage 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

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

Recommended textbook: E. G. Lewars, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, 2nd ed., Springer, Dordrecht, 2011, ISBN 978-90-481-3862-3. Online access is available through the Western Library Catalogue.

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

Tutorials	30% (5% each)
Quizzes	16% (4% each)
Midterm test	14% (in class on Wednesday, February 28)
Final exam	40%

4287(ei)1781314)av course grade-243.363(o)-1.87468(5e)2.35254(n)o18.1873(u)t3.3525406egre-3.04891(a)2.3505

Policies