The University *of* Western Ontario
Department of Chemistry

Chemistry 3300B
COMPUTER METHODS IN CHEMISTRY
Winter 2024 (tentative)

Course Information

Instructor:	Viktor N. Staroverov E-mail: vstarove@uwo.ca Office: ChB 063

Lectures:	Monday, Wednesday, Friday, 10:30 am - 11:30 am, ChB 9
Tutorials:	Approximately every other week on Tuesdays, 1:30 pm - 3:30 pm, SSC 1000
Office hours:	By appointment (administrative matters)
Course web site:	`https://owl.uwo.ca/portal`

Prerequisites: Chemistry 1301A, Chemistry 1302B, and any 1.0 courses at the 1000 level or higher from Calculus, Applied Mathematics or Mathematics, with no mark less than 60% in any of the above. Integrated Science 1001X with a minimum mark of 60% may be used as a substitute for (Chemistry 1302A/B and Calculus 1301A/B).

Description: An introduction to computer methods and tools used in all branches of 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.

Course Topics

1. *Molecular visualization*. How to specify molecular structure on a computer. Z-matrices and internal coordinates. Introduction to WebMO.
2. *Mathematical techniques in chemistry*. Elements of linear algebra and their chemical applications. Curve fitting, basic statistical data analysis.
3. *General-purpose scientific software*. Introduction to MAPLE. Use of MAPLE as a calculator for evaluating derivatives and integrals, solving differential equations, and other mathematical tasks.
4. *Quantitative molecular orbital theory*. Calculation of atomic and molecular orbitals and orbital energies. Visualization of molecular orbitals. Frontier orbitals and chemical reactivity.
5. *Computational studies of reaction mechanisms*. Potential energy surfaces, reaction pathways, intermediates, and transition states. Calculation of thermodynamic state functions and reaction rates.
6. *Semi-classical molecular modelling methods*. Molecular mechanics and molecular dynamics. Molecular simulations.
7. *Model chemistries*. Computational methods beyond molecular orbital theory. Density-functional techniques.
8. *Calculation of molecular properties and spectra*. Dipole moments, electrostatic potential, atomic charges, bond orders. Simulation of IR, Raman, and UV-vis spectra.

Expected Learning Outcomes

- 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

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)
Assignments	16% (4% each)
Midterm test	14%
Final exam	40%