

Chemistry 251 — Physical Organic Chemistry

Instructor:	Severin T Schneebeli
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Office Hours:	10:00–11:30 am Tuesdays and Thursdays
Class Meetings:	8:30–9:45 am Tuesdays and Thursdays, Aiken Center 112
Meeting Dates:	19 Jan – 04 May 2016
UVM Holidays:	Classes will not be held on: March 7–11, 2016

Learning Objectives:

In this course, you will develop a quantitative understanding of chemical transformations and the properties of molecules. Everyone who has taken this course should also be able to judge and apply molecular mechanics (MM) modeling and density functional theory (DFT) calculations as a basic research tool for organic chemistry.

Computational Chemistry Software:

We will use software programs from Schrödinger, Inc. to perform some basic MM and DFT calculations during the course. Please follow the instructions posted on blackboard to install the Schrödinger software package on your personal computers.

Required Textbook / On reserve at the UVM Bailey/Howe Library:

- (1) Anslyn, E. V., and Dougherty, D. A. *Modern Physical Organic Chemistry*, 3rd ed., ISBN: 978-1-891389-31-3.

450-Point Grading Scale:

Problem Sets	100 points	Four Sets, Handed out two weeks before due dates
In-Class Examination	100 points	In class, March 15
Short Student Presentations	100 points	In class, April 28 and May 3, Groups of two
Final Examination	150 points	May 12, 10:30–1:15 pm, Aiken Center 112

Please note: The final examination will be cumulative!

In-Class Examinations and Problem Sets:

One 75 minute-long examination will be given in class on March 15. You will also be assigned five problem sets (each counting 20 points towards your final grade) throughout the semester to aid in your learning of the course material. The problem sets will be due at the BEGINNING of class on February 16, March 1, March 29, April 12, and April 26.

Short Student Presentations:

In groups of two or three, students will give short (ca. 15 min + ca. 5 min of questions) presentations to critically discuss a recent research paper. A list of papers to choose from will be provided during the course.

Course Grading

Course grading will be structured according to the 450-point scale (*vide supra*). Failure to complete an assignment in a timely fashion will result in a numerical score of zero. Proposals for “extra credit” will not be considered.

Academic Conduct:

Cheating or plagiarism will be considered grounds for failing the course (a numerical score of zero). All graded assignments must be your own work. Cases of cheating or plagiarism will lead to further disciplinary action, which may include dismissal from the University according to the rules set forth in the University of Vermont’s Code of Academic Integrity:

<http://www.uvm.edu/~uvmppg/ppg/student/acadintegrity.pdf>

Course Topics:

1. Brief Review of Quantum Mechanics and Molecular Orbital Theory
2. Conformational Analysis with the Molecular Mechanics (MM) Calculations
3. Thermochemistry and the Basics of Hartree-Fock Theory
4. Solvation and Noncovalent Binding Forces
5. The Basics of DFT Applied to Acid-Base Chemistry
6. Molecular Recognition and Supramolecular Chemistry
7. Reaction Kinetics and Transition State Calculations
8. Supramolecular Recognition Applied to Catalysis
8. Introduction to Organic Polymer and Materials Chemistry

Religious Holidays:

Students have the right to practice the religion of their choice. If you need to miss class to observe a religious holiday, please submit the dates of your absence to me in writing by the end of the second full week of classes. You will be permitted to make up work within a mutually agreed-upon time.

Student Learning Accommodations:

In keeping with University policy, any student with a documented disability interested in utilizing accommodations should contact ACCESS, the office of Disability Services on campus. More information (including contact information) can be found online at www.uvm.edu/access. ACCESS works with students and faculty in an interactive process to explore reasonable and appropriate accommodations via an accommodation letter to faculty with recommended accommodations as early as possible each semester.

Promoting Health & Safety:

The University of Vermont's number one priority is to support a healthy and safe community. If you have any concerns whatsoever regarding anybody’s health and/or safety, please contact UVM’s center for Health and Wellbeing. More information can be found online at <http://www.uvm.edu/~chwb/>. If you would like to remain anonymous, you can report your concerns online at <http://www.uvm.edu/~dos/>.