

Chemistry 6V39, "Topics in Organic Chemistry: Computational Modeling"
Spring 2005 – TR 11AM – 12:15 PM, BE3.102

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Prerequisites: One year of physical chemistry and one semester of advanced organic chemistry, or consent of instructor.

Text: "A Guide to Molecular Mechanics and Quantum Chemical Calculations," Warren G. Hehre, Wavefunction, Inc., 2003. Recommended supply: USB pocket drive, 64Mbyte.

Goals: The student will become familiar with the physical basis for molecular modeling and will learn to apply some of the currently available modeling packages to problems of interest in organic chemistry and structural biology. The emphasis will be on utility: How well do particular techniques reproduce reality and how much insight do they provide about chemistry?

Software: Spartan, Gaussian 03, the Insight suite.

Outline:

Week	Week of	
1	Jan 10	Introduction to modeling
2	Jan 17	Force field calculations.
3-4	Jan 24, 31	Review of quantum mechanics
5	Feb 7	Hückel calculations as intro. to LCAO-MO calculations.
6	Feb 14	Semiempirical calculations.
7-8	Feb 21, 28	RHF calculations.
9-10	Mar 14, 21	Density Functional calculations.
11	Mar 28	Molecular Dynamics calculations.
12	Apr 4	Accessing structural databases (esp. the Protein Data Bank).
13-14	Apr 11, 18	Project oral reports.

Grading: There will be several homework assignments, comprising 20% of the grade. The two take-home exams will comprise 50%, and a project due on the last day of class will comprise 30%. There will be no final examination. Homework may be done collectively; individual effort is expected on all other work.