Chemistry 6V91, 4V01 "Topics in Organic Chemistry: Computational Modeling"

Spring 2006 – MW 5:30-6:45 PM, BE3.102

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

Recommended Reference Text: "A Guide to Molecular Mechanics and Quantum Chemical Calculations," Warren G. Hehre, Wavefunction, Inc., 2003, ISBN 189066118X

Supplemental Reference texts: "Essentials of Computational Chemistry: Theories and Models", Christopher J. Cramer, Wiley 2002, ISBN 0471485527

"Molecular Modeling and Simulation: an interdisciplinary guide", Tamar Schlick, Springer 2002, ISBN 038795404X

Spartan '02 Windows: Tutorial and User's Guide, Wavefunction Inc., 2001, ISBN 1890661198

"A Brief Guide to Molecular Mechanics and Quantum Chemical Calculations", Warren J. Hehre, J. Yu, P.E. Klunzinger, and L. Lou, Wavefunction Inc. 1998, ISBN 1890661058

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, VMD/NAMD (www.ks.uiuc.edu)

Grading: There will be two homework assignments, comprising 30% of the grade. The two take-home exams will comprise 40%, and a project due on the last day of class will comprise 30%. There will be no scheduled final examination. Homework may be done collectively; individual effort is expected on all other work.

Outline

Week	Week of	Topic(s)
1	Jan 9	Introduction: force field and semiempirical calculations
2	Jan 19	Introduction: ab initio calculations (Jan 16 - holiday)
	Jan 21	Workshop - Spartan (tentative) - 10 AM - 3 PM
3	Jan 23	Force field calculations
4	Jan 30	Force field calculations; quantum mechanics refresher
5	Feb 6	QM refresher cont'd; Hückel MO calculations
6	Feb 13	Introduction to Molecular Dynamics; problem set 1 handed out
7	Feb 20	Feb 20 class to be rescheduled; semi-empirical calculations
8	Feb 27	Semi-empirical Calculations
	March 6	Spring break
9	March 13	ab-initio calculations; Exam 1 handed out
10	March 20	ab-initio calculations; problem set 2 handed out
11	March 27	Density functional calculations; selection of term paper topic
12	April 3	Biological applications
13	April 10	Databases
14	April 17	Oral reports
15	April 24	Oral reports: Exam 2 handed out (due May 1)