

CHEMISTRY 330 B SYLLABUS Spring 2008  
Physical Chemistry Laboratory  
Molecular Modeling

**Location** Room 335 in the Natural Sciences Complex (NSC).

**Instructor:** Prof. Harry King, Office room 330 NSC

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**Office hours:** Monday, Tuesday, Thursday 3:00-5:00 pm

Look for Dr. King in rooms NCS 330, 331, 335

**Teaching Assistants**

(Monday) Matthew Kundrat, mkundrat@buffako.edu, room 345

(Tuesday) Shaohui Zheng, szheng3@buffalo.edu, room 345

## 1 Overview

This course provides an introduction to modern computational methods for the study of molecular structure, chemical reactivity, and molecular spectroscopy. Students will use computers to construct molecular models, study chemical bonding, compute thermodynamic and kinetic information, and predict IR, NMR and UV/VIS spectra (emphasis on chemical bonding and IR spectra). Methods studied include: molecular mechanics (using the Merck and SYBYL force fields), semi-empirical models (MNDO, AM1 and PM3), Hartree Fock, Møller Plesset and other correlated *ab initio* methods, and density functional theory using BP, BLYP, EDF1 and B3LYP functionals. Students will perform calculations using the Spartan program, acquire a good understanding of the underlying theory, gain some appreciation for the reliability of various theoretical models, and incidentally, learn some chemistry.

No previous knowledge of the subject is assumed other than a general background in organic and inorganic chemistry, familiarity with the elementary physical concepts of force and potential energy, and the thermodynamic concept of energy.

The course consists of 14 scheduled, four-hour, laboratory sessions, plus, on average, two hours per week of unscheduled time (for outside reading, computer practice, and preparation of project reports). There is no final examination. A typical scheduled laboratory session consists of “hands-on” computer use interspersed with lectures, quizzes and class discussion.

## 2 Textbooks

**textbook** *Spartan for windows Tutorial and User's Guide*, published by Wavefunction Inc. ISBN 1-890661-23-6

An adequate number (hopefully) of shared copies are available in the laboratory, so students need not purchase their own personal copies, but if you want one to take home then you must purchase a new copy from the company, or a used copy on the web. Versions '02, '04 and '06 do not differ from one another significantly, so any version is adequate for the purposes of che 330.

**reference textbook** W. J. Hehre, *A Guide to Molecular Mechanics and Quantum Chemical Calculations*, published by Wavefunction Inc. ISBN 1-890661-18X, List price is \$50 paperback, but students are not expected to purchase a copy.

A few department-owned, paperback copies are available in the lab. Students can take them out of the lab on loan. Please record your name and the check-out and return dates on the sign-out sheet in room 335.

**class notes** Each registered student must obtain a three-ring, loose-leaf binder in which to preserve copies of extensive class notes distributed, from time to time during the semester. Each student is responsible for keeping and maintaining his/her notebook.

## 3 Schedule

### 3.1 Part I (first three weeks)

During the first three weeks of the semester students are expected to master the main features of the Spartan program, and begin to understand the underlying theory. Students will complete a total of six tutorials. These are to be performed during scheduled lab time. After completing a tutorial the student will be given a short quiz to refresh his/her memory and understanding of that material. Students may use the computer and consult the User's Guide while taking the quiz. Tutorial quizzes are graded, but not recorded, *i.e.* they do not contribute to the final course grade. Students are encouraged to consult with other students and/or the TA while performing these tutorials, but not when taking a quiz.

In addition, there will be class discussion, lectures and additional quizzes covering more fundamental and theoretical aspects of the subject. These quizzes are graded and recorded.

**January 15** Introductory remarks, Chapters 4 and 5 tutorials: Organic molecules and Groups of Organic Molecules. Lecture 1, The Concept of Molecular Energy and the Potential Energy Surface (PES).

**January 22** Chapters 6 and 7 tutorials: Organic Reactions and Medicinal Chemistry. Quiz on Lecture 1. Lecture 2, Methods for computing the PES.

**January 29** Chapters 8 and 9 tutorials: Polypeptides to Proteins, Inorganic and Organometallic Molecules. Quiz on Lecture 2. Lecture 3. Further Discussion of Methods for Computing the PES.

### **3.2 Part II (weeks 4, 5, 6, and 7)**

Lectures and quizzes continue during Part II. In addition, there is a class project. Unlike Part I, in which all students perform the same computer exercises, Not all students are performing exactly the same computations in Part II. The entire class will collaborate on one, rather large, original research project consisting of several long computations. The class is partitioned into pairs of students, each pair performing its own computations. Results from all pairs are then combined. The last lab session before Spring Break consists entirely of brief class presentations by pairs of students, and related class discussion.

### **3.3 Part III (after Spring Break)**

Lectures and quizzes continue. In addition, each student selects and performs his/her own individual computer project. Several topics will be suggested. A student may pick one of the suggested topics, may modify one of the suggested topics, or may propose a project related to something discussed in another course, or in an undergraduate research project in the Chemistry Department, or any other appropriate project. A short, written, Preliminary Project Report is due by March 31. This Preliminary Report defines the goal of the student project, outlines the proposed procedure, and reports current progress.

### **3.4 Oral Presentation and Written Report**

A written Final Project Report is due by April 30 by all students. In addition, students have the option of presenting a brief oral presentation of his/her work in class on the last day of the semester, Tuesday, 22.

## **4 Course Grade**

Students who master the Part I material and actively participate in Parts II and III activities will get a grade of *C+* or better. Students who achieve a total of at least 50 points on quizzes (tutorial quiz grades are not counted toward this total), and submit a well conceived and executed Project Report will get a grade of *B+* or better. To earn an *A*, a student must demonstrate a command of the Spartan program and the underlying theory, and complete and submit a particularly well executed and well reported Student Project.

## 5 Specific concepts, methods, and computer techniques to be covered

1. Use of the SPARTAN program. Becoming familiar with program functions and how to execute them using the graphical user interface: keystrokes, mouse pointer, menus, tools, and dialog boxes.
2. Graphics methods. Building and viewing molecular models and graphical representation of electron density and related molecular properties.
3. The concept of the potential energy surface (PES), the potential energy of a molecular system expressed as a function of geometrical parameters such as bond lengths and angles.
4. Search techniques for finding local minima on the PES. Local minima correspond to stable molecular conformations.
5. Search techniques for finding saddle points on the PES. Saddle points correspond to transition states connecting pairs of local minima.
6. Standard approximate methods of computing the PES (items 7 to 12 below).
7. Molecular mechanics (MM) using the SYBYL and MMFF94 force fields. MM methodology is not expressed in terms of molecular orbitals, but is based instead on empirical information about equilibrium bond lengths and angles and force constants.
8. Quantum mechanical (QM) methods (items 9 to 12 below)
9. Semi-empirical methods, MNDO, AM1, and PM3.
10. Hartree Fock theory (HF)
11. Density Functional theory (DFT)
12. Quantum mechanical theories involving electron correlation including Møller Plesset (MP2 and MP3) and configuration interaction (CI).
13. Standard molecular orbital basis sets.
14. Performance of various methods, *i.e.* their computational cost and reliability.
15. Molecular properties related to potential energy including: rotational energy barriers, reaction barriers,  $\Delta E$ ,  $\Delta H$ , and  $\Delta G$  of reaction, force constants and normal modes of vibration.
16. Molecular properties related to electron density including: dipole and quadrupole moments and electrostatic potential.

17. Molecular spectroscopy including: infrared, electronic transitions, and NMR.
18. Applications to organic, inorganic, organometallic, and biochemistry.

## **6 Course Structure and Philosophy**

All of the various subjects listed above are encountered in the course, but not with equal emphasis. These topics are not taken up one-at-a-time, but rather, they reoccur in one context or another throughout the semester. For example, students will apply MM and QM methods very early in the semester, before being taught the underlying theory. In this way students become familiar with the terminology and the utility of the underlying ideas. We aspire to gradually improve the student's understanding of the fundamental physical principles and motivate future study of them.