Concepts of Physical Chemistry II-Laboratory

Chemistry 352, Fall 2006

Lab: W 3:30-6 in Sci 278
Office hours: M 3:30-5:00 or by appointment
www.csub.edu/chemistry/352/

Dr. Carl Kemnitz
Sci 252, ☎ 664-2013
ckemnitz@csub.edu

Required:

Atkins, Peter and De Paula, Julio *Physical Chemistry* 8th Ed, W.H. Freeman and Company: New York, NY, 2006.

Reference:

- Foresman, J. B. and Frisch, A. *Exploring Chemistry with Electronic Structure Methods*, 2nd ed., 1996 Gaussian Inc. Pittsburgh.

Schedule of Topics/Course Objectives

I. Introduction
- Theoretical basis of computational chemistry
- Potential energy surface (hypersurface)
- Familiarization with the use of Gaussian and GaussView Programs
- Geometry optimizations and single point calculations
- Local and global minima
- Frequency calculations

II. Symmetry
- Understanding symmetry elements
- Determination of point groups
- Use of Gaussian to classify point groups
- Understanding ramifications of symmetry to conformational changes

III. Calculating reaction enthalpies
- Use of isodesmic reactions
- Single point energy calculations at higher level of theory
- Utilizing frequency calculations for corrections to electronic energies

IV. Visualizations

- Animating vibrational modes
- Characterizing transition states
- Visualizing molecular orbitals
- Visualizing charge distributions

V. Different types of electronic structure calculations

- Molecular mechanics, semi-empirical, ab initio methods
- Understanding basis set notation
- Transition state searches

VI. Additional electron correlation

- Variational theory
- Configuration Interaction (CI) methods
- Complete Active Set (CASSCF) methods
- Density Functional Theory (DFT) methods

***Grading*:**

Four laboratory experiments are required. One will be written up as formal laboratory report (100 pts), two will be written up informally (50 pts each), and one will be done as a class exercise (-10 pts if absent).

Laboratory Reports

Deadlines for the formal laboratory reports will be given near the conclusion of each experiment. Formal lab reports will be typewritten, chemical structures will be drawn using a professional chemical drawing program (e.g., ChemDraw), three-dimensional geometries will be shown within the lab report for each geometry, and your electronic notebook will be appended to the report. The formal report will contain:

- an ***introduction***, describing the theoretical basis for your calculations and the relevance to chemistry. This is the place where the student demonstrates an understanding of the theoretical background of quantum calculations.
- a ***methods*** section which *concisely* describes the computational methodology, such that the results could be reproduced by a peer.
- a ***results*** section that includes data gathered into one or more organized and readable table(s). Include:
    - images of each molecular geometry
    - completed data tables (as supplied within each experiment)
- an in-depth ***discussion*** section in which all of the results are discussed. Any questions from the laboratory report should be addressed. You should make any

conclusions that can be drawn from your results. The information should be analyzed and explained in terms of its chemical and theoretical significance. Comparison to experiment should be made whenever possible.

- a ***conclusion*** section (set-apart or as the final paragraph of the discussion section) is nice and should always be included for lengthy reports.

Informal lab notes will consist of all completed data tables (submitted electronically), answers to all discussion questions (may be neatly hand-written), and your electronic notebook.

Policy on Academic Dishonesty

The principles of truth and honesty are recognized as fundamental to a community of teachers and scholars. The University expects that students will honor these principles and in so doing will protect the integrity of all academic work and grades. Students are expected to do all work assigned to them without unauthorized assistance and not to give unauthorized assistance.

There are certain forms of conduct that violate this community's principles. *Academic dishonesty* is a broad category of actions that use fraud and deception to improve a grade or obtain course credit. Academic dishonesty arises whenever students attempt to gain an unearned academic advantage. *Plagiarism* is a specific form of academic dishonesty which consists of the misuse of any works of another by claiming them as ones own. It may consist of using ideas, paragraphs, sentences, or phrases written by another, or using data or statistics compiled by another without giving citation. Other examples of academic dishonesty include falsification of data and the *submission of essentially the same assignment* for credit in two courses without prior approval.

When a faculty member discovers a violation of the community's principles, the faculty member is required to notify the department chair, the school dean, and the Coordinator for Student Discipline & Judicial Affairs.