SYLLABUS
CHEMISTRY 332, Physical Chemistry Laboratory
Spring 2008

Instructor:

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Office Hours

Monday, Tuesday and Thursday 3:00-5:00 pm
Look for Dr. King in rooms 330, 331, 335

Teaching Assistants:

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Text Book

There is no required textbook. Extensive notes for experiments, lab lectures, and optional project will be distributed. Students should maintain these notes in a three-ring binder.

Course Content

Students are required to perform four experiments, submit a written Lab Report for each, and attend related lectures. In addition, students can perform an optional computer project for extra credit.

Exams

There are no quizzes nor examinations.

Course Grade

Each of the four experiments and related Lab Report are weighted equally in determining the course grade. A student who conscientiously attends all assigned lab and lecture sessions, and responsibly participates in preparation of the four Lab Reports will earn a grade not lower than a $C+$, and possibly as high as $A-$. Completing the optional Computer Project can not lower, and usually will raise, a student's grade. The Computer Project is required for a course grade of A. 15% of the course grade is based on the joint-instructor-TA general evaluation of a student's performance in lab and lectures during the semester,

Lab Reports

Preparation of the Lab Report is a major component of che 332, at least as important as performance of the experiment itself. Note that technical writing will most likely be an essential part of a student's future professional experience in either industry, academia, or government laboratory. Assigned Lab Reports should be viewed as preparation for this. Students work in pairs (or triples) when performing an experiment. A student may have different lab partners for different experiments. In any case, preparation of the Lab Report is the joint responsibility of the pair (or triple) of students who performed the experiment, and both (or all three) student names should

appear in the cover sheet of the Report. Both (or all three) students receive the same grade for that work.

Lab Reports are due three weeks from the day the experiment was performed, with the exception of the FTIR Report and the optional Computer Project Reports which are due by some date late in the semester, to be announced.

Lectures

Lectures are given on aspects of Fourier transform infrared spectroscopy and various other subjects related to che 332. The lecture on any given subject is repeated at least once for students unable, for any reason, to attend the first presentation. Students are required to attend one lecture on each subject.

Error Analysis

When reporting the measured value of a physical quantity the Report should include the numerical value (with physical units) of the measured quantity, and a quantitative estimate of the reliability of that numerical value.

Required Lab Experiments

1. **Carbon dioxide critical point** The goal of this experiment is to determine the critical temperature and density of carbon dioxide, and the liquid-vapor coexistence curve (temperature vs density) in the region just below the critical point, and relate the results to Wilson's theory of critical exponents.
2. **Virial coefficients of real gases** The goal of this experiment is to measure the second and third virial coefficients of carbon dioxide and helium at a temperature near room temperature.
3. **Bomb calorimetry** The goal of this experiment is to measure heat of combustion using a Parr adiabatic calorimeter, and determine related enthalpy changes.
4. **FTIR** The goal of this experiment is to understand the principles of the Fourier transform spectrometer, to measure the infrared absorption spectrum of a mixture of four isotopes of hydrogen chloride gas, assign the spectrum, interpret the spectrum in terms of quantum mechanical energy levels, and extract from the spectrum values of the following spectroscopic constants: harmonic vibration frequency, force constant, moment of inertia, vibration-rotation coupling constant, and anharmonic constant.

Optional Computer Project

The optional project can be carried out by just one students working on his/her own, or jointly by a pair of students (no triples). Students make those decisions for themselves. Student pairs for the Computational Project are not necessarily the same as pairs that performed lab experiments together.

The optional computer project is concerned with molecular aspects of the virial coefficient experiment and the critical point experiment. The goal of the Computer Project is to see how well one can reproduce the carbon dioxide liquid-vapor coexistence curve by statistical mechanical theory (Monte Carlo sampling) using a simple expression for the intermolecular interaction potential. The project does not require the student to

write any computer code. Using an existing computer program, developed by Professor Kofke and collaborators, the student evaluates the parameters in the approximate potential energy function by fitting to supplied data for the temperature-dependent second virial coefficient using the theoretical relationship between intermolecular interaction energy and $B(T)$. The resulting potential function is used for Monte Carlo (MC) simulation of the liquid-vapor equilibrium to predict the liquid and vapor densities at a given temperature. The MC computation is repeated for several different temperatures, and the theoretical results are then fitted in much the same way as were the experimental densities measured in the laboratory. The project requires a bit of background reading, and attendance at an additional lecture. The computations, which can be performed on essentially any computer, are a bit time consuming if one is to achieve reliable statistical samples. Thus, students choosing to carry out this project should begin to plan reasonably early in the semester, and inform the instructor, or TA, of that intention. The following schedule allows ample time.

Deadlines:

February 29. Inform us of your intent to do the Computational Project.
March 31. Submit a brief, written current Progress Report.
April 30. Submit the Final Report.