UNIVERSITY OF MASSACHUSETTS BOSTON
CHEMISTRY DEPARTMENT

Physical Chemistry Structure Laboratory

General Information

Purpose of the course:

- Laboratory experiments in CHEM 379 are meant to introduce the students to the fundamental concepts of different spectroscopic techniques. These concepts are based on the application of quantum mechanics to molecular systems and to their interaction with the electromagnetic radiation over a wide wavelength range.

- We will review the quantization of energy for the electronic states of molecules, their vibrational and rotational states, and the interaction of electronic and nuclear spins with radiation in the presence of an external magnetic field.

- We will relate the symmetry properties of the molecules with the quantified energy levels and with the selection rules.

- We will apply various spectroscopic techniques, such as Infrared, Raman, UV-visible, NMR, etc. For each technique, we will analyze the type of information it can provide concerning the chemical composition, the structure, the energy levels or the dynamics of the system.

In many cases, the experimental procedures themselves are easily carried out, but transforming the data into meaningful quantitative results is often not trivial. Consequently, the major emphasis in this laboratory course is placed on the theory and calculations relating to the experimental measurements, rather than the instrumentation used to obtain the data. This emphasis is not unlike the focus of research work in physical chemistry today (although instrumental design and operational technique are often major obstacles to success).

Instructor & Schedule:
Dr. Timothy Dransfield, Chemistry Department, S-1-085 (617-287-6143).
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Course web page: http://alpha.chem.umb.edu/chemistry/ch379

Lecture: Th 12:30-1:45 (Room S-1-089).
Lab: Th 2:00-5:00 (Room S-2-041)
Office Hours: Tu 10:00-11:30, or by appointment.

Required Text and Course Materials:

The main text for this course is Experiments in Physical Chemistry, *Carl W. Garland, David P. Shoemaker, and Joseph W. Nibler, 8th ed., McGraw-Hill, New York 2003*. Earlier editions of the text are available through various online vendors, and the 7th and 6th editions are both perfectly serviceable for this course. Most of the experiments are described in this text and in addition, it contains helpful information about theory, equipment, techniques and numerical analysis. It may be a valuable reference material later on in your career. Instructions for the experiments not found in this textbook will be distributed at appropriate times during lectures. Many other textbooks can be useful for specific subjects:

1) Physical Chemistry, P.W. Atkins, J. de Paula, 8th ed. W.H. Freeman and Co, 2006. *Basic reading.*

2) Physical Chemistry. Principles and Applications in Biological Sciences, I. Tinoco Jr., K. Sauer, J.C. Wang, J.D. Puglisi, 4th ed. Prentice Hall, 2002. *Recommended reading with examples on biological molecules.*

3) Introduction to Spectroscopy**,** 2nd edition. D.L. Pavia, G.M. Lampman G.S. Kriz. Saunders, 1996. *Complementary reading for IR, uv-visible and NMR.*

4) Molecular Physics and Elements of Quantum Chemistry, H. Haken and H.C. Wolf, Springer, 1995. *Complementary reading with many examples.*

5) Molecular Quantum Mechanics. P.W. Atkins and R.S. Friedman, 3rd ed. Oxford University Press,1997. *Complementary reading.*

Grades:

Grades will be based on:

- Laboratory reports are worth a total of **225 points** (see values on schedule).
- Quizzes given before each experiment are worth **80 points** (see values on schedule).
- Based on historical class performances, the approximate cutoff points for letter grades are:

A ≥ 92%; 85% ≤ **A-** < 92%; **B-** → **B+** = 70% → 85%; **C-** → **C+** = 55% → 70%; Grades lower than C- represent dramatically incomplete work, and there are no real numerical guidelines. I reserve the right to award grades *more generously* than this, but I promise not to grade more harshly.

Attendance:

It is very difficult and sometimes impossible to schedule "make-up labs." Therefore, you must attend your assigned laboratory session. If you must miss a lab session for any reason, contact the Instructor as soon as possible to discuss the possibility of an alternative.

Experimental Work:

Experiments will generally be performed in groups of two or more students. In certain cases, the laboratory section as a whole will carry out the measurements and all students will share data obtained. Although data will be collected by groups of students, each student must write and submit his/her own report. Collaboration in collecting and analyzing the data is perfectly acceptable, but if it is evident that two or more students have jointly written a lab report, the grade for that experiment will be divided equally among the participants in this joint effort. Preparation for each experiment, collection of data, and writing of reports should follow the guidelines and suggestions on Chapter I of the Text (pp. 1 - 26). The following points are especially important:

1. Each student should have a lab notebook in which the details of an experimental procedure and data obtained are recorded as the experiment is carried out.
2. Each student should keep a back-up copy of his/her report. This can be a computer file or a print-out copy. Keeping a back-up copy is your insurance in case your report gets misplaced somehow.
3. Reports must be prepared with a word processor**,** using graphic software suitable for statistical analyses particularly linear least-squares regression, and printed on a good-quality printer (e.g., laser or ink-jet printer)**.** Read Chapter III in Shoemaker et al. for suggestions on using computer software for report preparation. For details on least squares analysis, see appropriate sections of Chapters II, III, and XXII of the Text. Many current spreadsheet programs (e.g., Quattro Pro, Lotus, Excel) and graphing programs (e.g., SigmaPlot, Axum, Origin) are suitable for these purposes and are available on the Department's student-accessible computers. In addition to Departmental resources, Computing Services has personal computers and software available for student use.
4. Reports should be concise and free of redundant presentation of readily available information**.** Specifically, do not paraphrase the theory and procedures in the book or handout. However, do note significant departures from the standard procedure or events in the conduct of the experiment that may affect the data and results. Furthermore, the discussion section should provide evidence of command of the theory relevant to the experiment.
5. Data and calculated results should be neatly and completely presented with appropriate units. Large data sets should be presented in tabular form with clearly labeled column heads. Show sample calculations to demonstrate how you obtained your numerical results.
6. Numerical results must be presented with the appropriate number of significant figures. Where appropriate, calculate standard deviations for the data. For an overview of matters pertaining to error and the treatment of experimental data in general, see Chapter II of the Text.
7. Except for generally recognized constants (e.g., anything listed on the inside front cover of Shoemaker et al.), cite the source of any value or information you obtain from the literature**.** Occasionally students find data that are unknown to the instructor; a citation can help validate the data and your appropriate use of it.

Specifications for laboratory reports

All laboratory reports are due at 5:00, two weeks after completion of the experiment unless otherwise announced or noted in the laboratory schedule. Late reports will be penalized 1 point plus 1 additional point for each 24 hours that passes before they are turned in. Reports WILL NOT BE ACCEPTED more than one week late. In keeping with the analogy to research work, the laboratory reports in this course follow the format of published research papers in the field, as might appear in one of the standard journals (e.g., *Journal of Physical Chemistry*, *Journal of the American Chemical Society*). Reports should emulate the overall style of published work in physical chemistry, and you are encouraged to peruse the journals in the library for examples of standard scientific presentation. In addition, you should consult *The ACS Style Guide* for guidelines on style, reference format, illustrations, and all other matters pertaining to preparation of chemical reports. Some specific guidelines are presented in a separate handout posted on the course web page.