



PHYSICAL CHEMISTRY LABORATORY

CHEMISTRY 3550L W (SPRING, 2008)

Course Outline

This laboratory course is designed to familiarize the student with the physical basis and applications of chemical measurements. Activities will be based on electronics, optical spectroscopy, thermodynamics, kinetics and computational chemistry. This course has been designated as a writing intensive course for the *Writing Across the Curriculum Program* (WAC) and will include writing informal and formal laboratory reports and a term paper.

Learning Objectives

After successful completion of the course, the student should be able to:

- Design and perform simple experiments (spectroscopy, thermodynamics, kinetics and electronics) to study chemical systems;
- Operate independently and interpret results using common chemical instrumentation and modeling;
- Use quantum mechanical based theory and software to explore and explain experimental data;
- Develop a positive attitude towards research and laboratory experimentation, which often involves unexpected difficulties in reaching research goals; and
- Communicate scientific ideas effectively in oral and written presentations.

General Information

Instructors

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Farooq A. Khan

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Office Hours

T 11:00 – 1:00 pm; 2:00 -4:00 pm

R 1:00 -4:00 pm

M, W 12:45 - 1:45 pm

T 10 am – 12:00 pm; 1:00 – 4:00 pm

Additional office hours can be arranged by appointment.

General Information (Continued)

Textbook Handouts will be provided.

Attendance **Required.** A student may be awarded a failing grade in the course if more than 30% of activities are missed.

Grades

Your grade will be calculated based on the following components:

Formal Reports (4 @ 40 points each)	160 points
Informal Reports (4 @ 20 points each)	80 points
In-class Reports (4 @ 10 points each)	40 points
Term paper	60 points
Presentation	60 points
Oral Examinations (2 @ 50 points each)	100 points
TOTAL	500 points

Letter grades

Score	Grade
85% - 100%	A
75% - 84%	B
65% - 74%	C
50% - 64%	D
0% - 50%	F

Writing Lab Reports

One of the purposes of an advanced laboratory course is to provide experience in writing scientific reports. In accordance with the WAC requirement, we will edit and grade each report. Resubmission of your report may occur if we deem it necessary. Please pay close attention to avoiding calculation errors, since these can ruin the most carefully gathered data. Please visit the library and look at articles from a current issue of the journal, *Physical Chemistry*, to get an idea of the writing style used. To the end of your report, staple photocopies of your lab notebook pages

(including calculations) which contain your data and instructor initials. **Please see the sections below on laboratory notebooks and laboratory reports.**

Policy on Late Laboratory Reports

The schedule of experiments will be provided after the add-drop period. All laboratory reports are due one week after the experiment is completed. A 10% per day penalty will be assessed for each day the report is late. If the report is not turned in by the fifth late day, the laboratory report will not be accepted. It is our policy to administratively withdraw a student from this course with a WF if they fail to turn in more than two laboratory reports within the stipulated time.

Laboratory Notebook

A laboratory notebook should provide a permanent record of details in procedure, raw data, observations, calculations and results. The criterion for sound record keeping is that someone else should be able to readily locate and understand the pertinent results for an experiment. Although reasonable legibility and neatness are required to meet this criterion, the utility of a record is determined largely by whether it is original, systematic, and complete, not by whether it is a work of art. The following are guidelines for keeping a proper experimental record:

1. A bound notebook is required for this lab. Numbered pages are required.
2. Enter all data in **ink** as soon as it is taken. Never recopy numbers or use loose sheets of paper. Cancel errors or rejected data by drawing a single line through them. Do not erase or remove pages. Set aside the first two pages of the notebook for a table of contents, which you will organize at the end of the course.
3. Enter data only on the right page of the two facing pages (optional). Use the left side as a scratch sheet for calculations.
4. Clearly label all entries, including the units (e.g. grams). To facilitate direct recording of experimental work, it is helpful to set up a data page for each experiment before coming to the lab.
5. Even if the calculation of final results from the data taken in lab is done at a later time, record these calculations in your notebook for future reference. To avoid errors in the calculations, write out each step of the calculation.

Report Format

All reports will be on 8.5 x 11-inch sheets and should be written on a word processor. Students are encouraged to make use of spreadsheet and plotting software in their reports. They are encouraged to plot data as soon as it is obtained, if possible, so that problems may be detected early and not the night before the write-up is due. Sloppy reports will not be graded and will be returned to be rewritten. Correct use of English is expected in all reports. If in doubt about spelling, look the word(s) up in a dictionary or run a spell checker. Be specific and concise in reports, especially in the introduction and discussion. Do not put reports in fancy binders or folders. Use a single staple in the upper left-hand corner of the report.

Formal Reports

The student will be graded using the following format:

1. **Title:** Title of experiment, together with your name, department, and college should appear on a separate title page which is not counted in the 10-page limit.
2. **Abstract:** A one-paragraph (five to 10 sentences) abstract must be included on the lower half of the title page. The purpose of the experiment should be stated and the results summarized.
3. **Introduction:** Outline the theory of the experiment; use schematics when possible. The line of reasoning upon which the experiment is based must be presented in a careful and logical manner.
4. **Experimental:** A brief but descriptive outline or statement of the procedure should be included. Emphasize any changes of the procedure prescribed in the experiment handout. A neat sketch of the apparatus is useful. Label all parts of the drawing.
5. **Data:** Organize the data carefully into tables and/or graphs where appropriate. Include with every numerical entry an estimate of its uncertainty and the units. When several determinations are made of the same quantity, the standard deviation of the average should be used to indicate uncertainty. A spreadsheet and plotting program **must be used** for the graphs.
6. **Calculations and Results:** One example of each calculation should be given. Each result should be accompanied by an estimate of its uncertainty (standard deviation). For replicate determinations, the final value of each sample can be calculated, the results averaged and the standard deviation can be calculated. Alternatively, an uncertainty may be estimated by propagating the uncertainties with the raw data. Learning to estimate errors and see how they propagate through the calculations into the final result is one of the most important aspects of this laboratory experience. For linear data, use

least-squares analysis when appropriate.

7. **Discussion with error analysis:** Discuss how the results correlate to the theory presented in the introduction. From the statistical analysis data, discuss the significance of the results obtained. Consider whether the precision of the results is reasonable for the particular method of analysis. Describe any potential sources of determinate or systematic error.

Informal Reports

Informal reports must not exceed 5 total pages.

1. **Title:** Title of experiment, together with your name, department, and college should appear on a separate title page which is not counted in the 5-page limit.
2. **Abstract:** A one-paragraph abstract must be included on the lower half of the title page. In the abstract, you must briefly state the purpose of the experiment and summarize your findings. This paragraph should be limited to no more than five sentences.
3. **Data:** Organize the data carefully into tables and/or graphs where appropriate. Include with every numerical entry an estimate of its uncertainty and the units.). For replicate determinations, the final value of each sample can be calculated, the results averaged and the standard deviation can be calculated. You must use a spreadsheet and plotting program for the graphs. **No hand-drawn graphs will be accepted.**
4. **Calculations and Results:** One example of each calculation should be given. Deviation of experimental results from theoretical data should be presented. A detailed error analysis is **not** required for these reports.
5. **Discussion:** Discuss how the results correlate to the theory presented in the introduction.

In-class Reports

In-class reports must not exceed 2 total pages.

1. **Title:** Title of experiment, together with your name, department, and college should appear on a separate title page which is not counted in the 2-page limit.
2. **Abstract:** A one-paragraph abstract must be included on the lower half of the title page. In the abstract, you must briefly state the purpose of the experiment and summarize your findings. This paragraph should be limited to no more than five sentences.
3. **Data:** Organize the data carefully into tables and/or graphs where appropriate. Include with every numerical entry an estimate of its uncertainty and the units. For replicate determinations, the final value of each sample can be calculated, the results averaged and the standard deviation can be calculated. You must use a spreadsheet and plotting program for the graphs. **No hand-drawn graphs will be accepted.**
4. **Calculations and Results:** One example of each calculation should be given.

Term Paper on Spectroscopic Techniques

Each student will choose an analytical/physical technique that is not explicitly covered in this course and write a 10-page, double spaced, font size 12, 1 inch margins term paper. The paper should discuss the scope, theory and impact/application of the technique in the form of examples published in the chemical literature. In addition, each student will give a 20 minute presentation in class on the selected technique, preferably using Powerpoint.

The assignment on the term paper will be broken into four parts:

- I. **Topic Selection** – submit an abstract of your topic with five references. The references must be recent (last 3 years) and cannot be textbooks, internet sites. Please attach the abstracts from the five references. **Due on February 6, 2008.**
- II. **Initial Draft** – submit a 10-page (excluding figures) draft of your paper for editing. **Due on March 5, 2008.**
- III. **Final Paper** – submit the 10-page final draft of your paper along with a copy of your initial draft. **Due on April 9, 2008.**
- IV. **Oral Presentations will be held on April 28 and April 30, 2008.**

Policy on cheating

Occurrences of cheating are rare. However, cheating by one individual raises questions about fairness for the rest of the class, and indeed, endangers the honor code that governs our examination system. It is after considerable thought and agonizing that we have arrived at the following formula.

If an individual cheats on a report for the first time, he/she will obtain a score of zero for that particular report. If an individual is caught cheating a second time during the semester, he/she will receive a grade of F for the entire course.

Tentative Time Table for Experiments

Week of	Subject
7-Jan	Introduction
14-Jan	Error Analysis (Khan), Heat of Vaporization
21-Jan	MLK (Monday) Conjugated Dyes (Wednesday)
28-Jan	IR Spectroscopy of HCL/ DCL
4-Feb	Raman Spectroscopy of Functional Groups
11-Feb	Intro to Mass Spectrometry
18-Feb	Nanoparticle Adsorption Isotherm
25-Feb	Oral Exams
3-Mar	Rotation
10-Mar	Rotation
17-Mar	<i>Spring Break - No Lab</i>
24-Mar	Rotation
31-Mar	Computation (Dr. Dutt)
7-Apr	Projects
14-Apr	Projects
21-Apr	Oral Exams
28-Apr	Oral Presentations