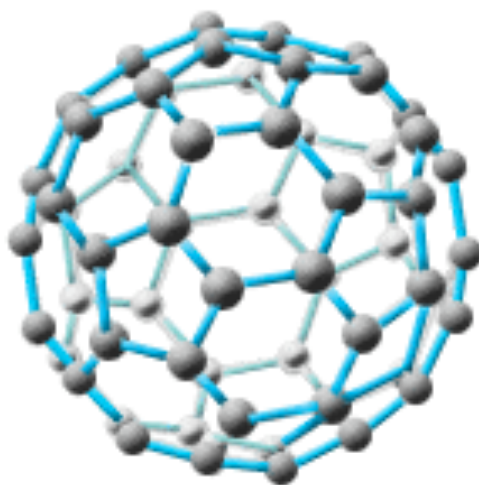


Laboratory Manual for Computational and Experimental Physical Chemistry I (CHEM 3710L)

Tom Rybolt and Douglas Kutz

Department of Chemistry
University of Tennessee at Chattanooga
2010



Organization of Laboratory Manual web pages

Introduction

- Cover page
- Table of Contents
- List of Experiments
- Literature Values
- Course Information
- Directions for Lab Work
- Lab Notebook
- Lab Reports – Important Style Issues

Experiments

AS	Adsorption from Solution
EX	Exothermic Reaction
FP	Freezing Point Depression
HV	Heat of Vaporization
IS	Reaction Rate of the Inversion of Sucrose
LV	Liquid–Vapor Equilibrium
ME	Molecular Energy of Isomers
MM	Molecular Modeling and Equilibrium
RO	Determination of Reaction Order
SM	Spectra of Conjugated Molecules

Appendices

- A. Safety**
- B. Significant Figures and Errors**
- C. Computer, Balances, And Equipment Use**
- D. Molecular Modeling Tutorial**

INTRODUCTION

LIST OF EXPERIMENTS

General PChem Topic

AS	Adsorption from Solution	equilibrium, surfaces
EX	Exothermic Reaction	thermodynamics, heat
FP	Freezing Point Depression	thermodynamics, solutions
HV	Heat of Vaporization	thermodynamics, phases, heat
IS	Reaction Rate of Sucrose Inversion	kinetics
LV	Liquid Vapor Equilibrium	thermo, phase diagrams
ME	Molecular Energy of Isomers	modeling, structures
MM	Molecular Modeling	equilibrium, modeling
RO	Determination of Reaction Order	kinetics
SM	Spectra of Conjugated Molecules	quantum, spectroscopy

In this laboratory course you will have an opportunity to study some of the physical properties of matter that are associated with various chemical substances. The Physical Chemistry Laboratory is designed to demonstrate the application of principles covered in the lecture portion of the course. **You should strive to integrate your knowledge of theory and experiment and understand how these two aspects of Physical Chemistry are interrelated. Each week, you should read the textbook pages that deal with the specific experiment you are doing that week. Lecture can help you understand lab, but lab can also help you understand lecture.**

The laboratory experiments and computational chemistry experiments to be conducted during this semester are listed above. This information packet contains information and gives background theory as well as specialized instructions for your experimental activities, computational work, data analysis, and lab reports. If corrections or updates are needed during the semester, they may be placed on a page placed in the experiment lab drawer. Be sure to note any of these corrections or additions prior to starting your experiment.

LITERATURE VALUES

Sources for each experiment

Reference material is available on the bookshelf in the physical chemistry lab and in the in the main library reference section. Do not remove books from the room where they are located. Be gentle with books as many people use them. The list below are suggested sources of information to obtain accepted literature values or if no such value is needed. The word “literature” as used for scientific literature or information means published and accepted as correct.

AS	Adsorption from Solution	no specific value to compare depends on equilibration time but for your powder probably between 10 to 50 m ² /g
EX	Exothermic Reaction	CRC Handbook or Lange's Handbook
FP	Freezing Point Depression	Periodic Table and molecular formula or CRC or Lange's Handbook
HV	Heat of Vaporization	Lange's Handbook use value at boiling point of methanol
IS	Inversion of Sucrose	Atkin's Textbook Appendix on Kinetics Arrhenius parameters
LV	Liquid Vapor Equilibrium	Lange's Handbook
ME	Molecular Energies	none, just compare molecules in each pair
MM	Molecular Modeling	lab packet gives experimental results for ratio no other literature values needed
RO	Determination of Reaction Order	Atkin's Textbook Appendix on Kinetics Arrhenius parameters shows order with sucrose and order with acid Table 22.1 8 th edition
SM	Spectra of Conjugated Molecules	Compare your theoretical, calculated, and experimental results – no literature value needed

Use of Books (lit values)

This semester you will be asked to find literature values of various quantities. You are directed to specific sources that you should use and find literature values **before you leave lab. Do not remove reference books from the room in which you use them.**

In other scientific activities in the future, you may need to find published or accepted (literature) values. Below are some valuable sources to consult.

Printed Information (lit values)

1. General and Physical Chemistry *textbooks* normally have a number of important tables in the appendices.
2. *CRC Handbook of Chemistry and Physics*
3. *Lange's Handbook of Chemistry*
4. *The Merck Index*
5. Chemical company catalogs such as *Sigma-Aldrich*

The kind of information that appears in handbooks slowly changes. Hence, if you do not find something in a newer edition of a handbook, check in an older version as well.

If after checking many sources, you do not find what you are looking for, it may be that it is just not readily available.

Web based Sources – Internet (lit values)

For a useful collection of links to the chemical literature use UTC Chemistry Dept homepage www.utc.edu/Academic/Chemistry/ then select Finding Chemical Information. You will observe a variety of chemistry information sites on the web listed. Occasionally links may be out of date and new sites frequently appear. The NIST (Chemistry) WebBook (collection of data of the National Institute of Standards and Technology) has a great deal of structural, spectroscopic, and thermodynamic information. This is often place to look. Catalogs are also online such as <http://www.sigma-aldrich.com> for the Sigma-Aldrich Catalog.

COURSE INFORMATION for 371 Lab

Attendance

You are expected to attend all sessions of the laboratory. You must make up any missed work. One time will be available at end of the semester for a make-up lab. If you miss lab, discuss with instructor as soon as possible. If you miss the day that labs are due, then you should see instructor when you return to school with labs ready to be turned in to your lab instructor.

Breakage

Equipment breakage is usually the result of carelessness or not considering consequences of your actions. Students who break an item may have their lab grade for that experiment reduced. The damage of a major piece of equipment or an instrument may result in a 0 for that experiment.

Grades

The lab grade comprises 25% of your course grade. Your grade is based on the average of lab reports and the successful completion of computational and molecular modeling assignments at the beginning of the semester. Although your laboratory grade will be based on your written lab reports, improper conduct in lab or lack of preparation for lab could affect your grade. You need to keep up during the semester and strive to understand what you are doing. You need to prepare before lab.

Honesty

One of the distinguishing features of Science as a human endeavor is its emphasis on absolute honesty and truthfulness. You should cultivate this habit in all your undergraduate work and life in general. In this lab as in all others whether your data is "good" or "bad" it is real and thus what you have to work with, analyze, and try to understand. You are expected to do your own data analysis and write your own report. Although you may discuss the experiment with other students and your lab partner, you may not copy, paraphrase, or rewrite portions of another person's report. You are not allowed to permit other persons to use your reports for unethical purposes. Discussions for the purpose of understanding are fine; whereas, copying for the purpose of generating a lab report without understanding is not an acceptable practice and will result in a 0 on that lab and possibly an F in the course.

Notebook

A bound laboratory notebook is required. All recorded information is to be written directly in this notebook. You must use ink. You are not allowed to record information temporarily on scraps of paper or tear pages out of the notebook. You should include enough information so that it is clear what type of data and units are being recorded. You should date each data page. Some data is collected directly by computer, but it never hurts to write key numbers in a lab notebook. You should have work that needs to be done prior to lab recorded in your lab notebooks before you enter lab to begin.

Textbook

Refer to your lecture textbook for needed background information and read sections that go along with your lab work each week. You are assumed to have read and prepared prior to lab and your lab instructors are in lab to assist as needed, but not to tell you what to do.

DIRECTIONS FOR LAB WORK

Prior To Lab You Should:

Read the experiment carefully.

Read the supplemental information provided in this lab packet for the experiment.

Locate and study information in your textbook that pertains to the experiment.

Plan your activities for the lab period.

Estimate the amount of materials to be used for the experiment.

During Lab You Should:

Be prepared with goggles, lab notebook, pen, calculator, structures of molecules you are using drawn, preliminary work done if any needed, and a general plan of what you are doing

Record data and other information related to the experiment directly in your bound lab notebook.

Think about what you are doing and try to relate your experimental observations to theoretical explanations.

Learn as much as possible regarding the operation of any equipment or instruments you are using. The lab textbook has supplemental information on these topics that you should read.

Take only the amount of chemicals that you will use.

Follow the safety rules and dispose of chemical wastes according to the directions given in the safety instructions.

Find and record literature values that might be needed.

Safety:

You must sign a copy of the UTC Chemistry Department safety rules before working in the laboratory. This packet has information related to safety rules and the proper disposal of chemical waste. **Safety Goggles must be worn at all times in the lab room.**

LAB NOTEBOOK

You are required to record all information in a bound laboratory notebook.

Begin each experiment on a new page. Record the title of the experiment and date each page. List your name and identify any partners.

Record information in chronological order. The notebook should read like a diary of events. Do not leave blank spaces to be filled in at a latter time. The first few pages of the notebook should left blank to be used for a table of contents.

When making a measurement always include units.

If you are preparing a solution, describe the procedure you are following listing what glassware you are using and what volumes are involved.

If you are using an instrument, record its model number and the settings you selected.

Record all information in ink, and not in pencil. You must record directly in the notebook, not on scraps of paper.

You should record measurements in original units.

If a large number of similar measurements are being performed, prepare a table of data. Label the numbers with headings indicating the units.

It should be clear to the reader that numbers are measurements that you performed and which numbers are quantities that you have calculated.

You should record literature values in the notebook. You may perform the calculations in the notebook, but this is not required. However, it is beneficial to have all information in one place.

You should know or learn the molecular structure of any organic chemicals you use in an experiment. Draw the structures of any organic molecules in your lab notebook.

LAB REPORTS - IMPORTANT STYLE ISSUES

Different experiments may involve varied styles or requirements so you must refer to specific information your instructor gives you about what is required for the specific report you are writing.

In general when Writing Your Lab Reports Make Sure You:

Follow the format given by professor in charge of your lab section for that specific experiment.

Write or type your lab report on standard 8.5 x 11 inch paper stapled together in the upper left hand corner. Do not use paper ripped out of a spiral binder. Xeroxes are not allowed.

Your report must be legible and neat, or it will not be accepted.

Strive for conciseness, clarity, and logic.

Use proper English (this includes grammar, spelling, punctuation, syntax, etc.) Your report grade will be lowered if there are errors in language usage. You must use conventional scientific style and write reporting what was done not as if giving directions to do.

Unacceptable: "I dissolved 4.0g of NaCl in 100mL of water."

Unacceptable: "Dissolve 4.0g of NaCl in 100mL of water." You are not giving directions.

Acceptable: "4.0g of NaCl were dissolved in 100mL of water."

Label each main section in the report.

Identify all **symbols** used by name and indicate **units**.

Number in order any **equations** used. Place the number of the equation in parentheses to the right of the equation. Just use numbers such as (1), (2), (3), etc. Do not write (Eq. 1). Each such numbered equation should be on a line by itself with a space above and below it and all the symbols defined and units indicated.

Present numerical data in **tables** with columns labeled and units indicated.

Include on your **figures** a title, labeled axes with units indicated, and even incremental spacing along each axis with the increments clearly shown. Have symbols such as a circle that represent each data point and can be clearly seen. If more than one type of data is on the figure distinguish the points by using a different symbol for each type. Figures should be referred to by number and should be included in your report.

References should be numbered in order of appearance in the body of your lab report and referred to in the report by number. List the author, journal, pages, and year for articles. List the author, title, publisher, location, year and pages for a book.