CHEMISTRY 3398
Physical Chemistry Laboratory – II
Spring 2020

Lectures:  Wednesday  12:00 pm to 12:50 pm Beury 415

Labs:

<table>
<thead>
<tr>
<th>Section</th>
<th>Time</th>
<th>Location</th>
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<tbody>
<tr>
<td>Section 001, Thursday</td>
<td>12:00 pm to 2:50 pm</td>
<td>Beury 207, 404, or 220</td>
</tr>
<tr>
<td>Section 002, Friday</td>
<td>1:00 pm to 3:50 pm</td>
<td>(check your Master Schedule)</td>
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Instructors:

Dr. Jun Han  Beury 203  215-204-2836  junhan@temple.edu
Office Hours:  Monday and Tuesday, 1–2:30 pm; Wednesday, 10-11 am; or by appointment

Dr. Elizabeth Cerkez  Beury 448  215-204-7821  cerkeze1@temple.edu
Office Hours:  Wednesday 1-3pm; Thursday 9-11am; or by appointment

Text:  Experimental and analysis background can be found in:
(2) “Experimental Physical Chemistry - A Laboratory Textbook,” by Arthur M. Halpern and George McBane (referred to as H, out of print but relevant sections are posted on Canvas), and supplemental materials.

Prerequisites:  C- or higher in Chemistry 3103 (0215), C- or higher in 3105 (0217), and C- or higher in 3302 (0232).

INTRODUCTION

Welcome to the Physical Chemistry Laboratory II course! We will apply quantum mechanics and spectroscopic techniques to study the properties of chemical substances.

Physical chemistry is the application of physical methods to the study of molecular processes and properties. It has a long and illustrious history founded primarily on experiment, although the advent of quantum mechanics has allowed for the calculation of molecular properties without the input of experimental information. While much of modern physical chemistry is technically quite sophisticated, there are many wonderful experiments that can be performed to demonstrate and study basic physical and chemical properties of matter.

In this writing-intensive course, you will learn to write formal laboratory reports using both brief and full paper formats as detailed below. Thus, getting the right answer is not enough! A significant part of your grade will be based on writing style and clarity. Please set aside enough time to achieve this goal.
Major writing-related learning goals:

- Acquire and develop fundamental skills for Scientific Technical Writing through oral and written communication based on quantitative experimental measurements. This will be achieved through the preparation and revision of formal laboratory reports, including argument-driven research-style papers in a format consistent with the American Chemical Society guidelines [http://portal.acs.org/corg/content, search: “writing skills”].

- Incorporate accurate description and detailed argument-driven interpretation of quantitative physical chemistry measurements with topic-specific calculations and thorough data analyses.

- Adequately apply the scientific method: define a problem clearly, develop testable hypotheses, execute experiment(s), analyze data, and draw appropriate conclusion(s).

- Demonstrate the ability to retrieve specific information from the chemical literature and to make effective use of peer-reviewed publications through integration and use of this information in the reports.

STRUCTURE OF THE COURSE

You will each complete four experiments, spanning thermodynamics, kinetics to quantum mechanics and molecular spectroscopy, and then write individual lab reports. You will see each experimental setup twice. First, guided by an instructor, you will visit the laboratory during the lab time in the second week. In the first three weeks, known as "Round Robins", lectures will be given to cover the theoretical background necessary to understand the “what” and “how” of each experiment.

In your second encounter with the setup, you and your partner will actually perform the experiment. In the lecture prior to each lab, you will be given a pre-lab quiz that will test your understanding of the experiment you are going to do. You are expected to be capable to collect and analyze the data with little input from your instructors. Following each experiment, there will be a mandatory data analysis period (CL-Computer Lab) held in the Chemistry Department Computer Lab (BE220). The purpose of these sessions is to work up your raw data to the point where we are sure you are on the right track and to reassure us that you have sufficient knowledge and strategy to write the required sections and assemble them competently into a high-quality report. A Writing Workshop (WW) is scheduled prior to submission of each full format report. In WW, you should bring your printed first draft of the full format report to be peer-reviewed for revision.

All of these elements are summarized in the Master Schedule for each section respectively.

EXPERIMENTS:

After the Round Robin sessions are completed, experiments will be performed according to the master schedule for your section. You are welcome to make a written request for a laboratory partner before the start of the first set of labs. If no request is made, you will be assigned a group.

Come prepared to take data! The instructors will examine your notebooks and your grade will be adversely affected if you do not take your preparation seriously. Your preparation should include an introduction and purpose for the experiment, any relevant calculations or constants you need (molecular weight, density, etc.), answers to any assigned pre-lab questions, and prepared tables into which you can write the data as you take it. A USB flash-drive is also needed to save the data from your experiment.


<table>
<thead>
<tr>
<th>EXPERIMENTS TO BE PERFORMED (4 in all)</th>
<th>Abbreviation</th>
<th>duration</th>
<th>reports</th>
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</thead>
<tbody>
<tr>
<td>Molecular Constants of Diatomic Molecules (Computational, Handout)</td>
<td>Comp</td>
<td>1 lab period</td>
<td>1</td>
</tr>
<tr>
<td>Vibrational-Rotational Spectra of HCl and DCl (GNS #37, H#36)</td>
<td>IR</td>
<td>1 lab period</td>
<td>1</td>
</tr>
<tr>
<td>Absorption Spectra of Conjugated Dyes and Nanoparticles</td>
<td>Abs</td>
<td>1 lab period</td>
<td>1</td>
</tr>
<tr>
<td>(GNS #34 + handout, also look at H #39)</td>
<td>2-Naphthol: Excited State Acidity Constant (H #33)</td>
<td>pKa*</td>
<td>1 lab period</td>
</tr>
<tr>
<td>Deprotonation and Protonation Rate Constants (H #34)</td>
<td>S-V</td>
<td>1 lab period</td>
<td>1</td>
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Each experiment will take one lab period. You are expected to work independently. However, things sometimes may go unexpectedly, so do not hesitate to point out a problem or ask a question that requires an instructor's attention.

**While you will work in groups performing the experiments and collecting data, each of you will be required to take your own notes.** Your lab report will be graded alongside that of your partner's to confirm that each of you took independent notes during the experiment and worked independently on the report.

**QUIZZES and FINAL EXAM:**

Quizzes, based on each experiment topic (see Master Schedule), will be given during the Wednesday lecture prior to each experiment. Each quiz will include questions about concepts, experimental details, and calculations with sample data. The purpose of the quiz is to ensure you have properly prepared for the laboratory experimentation, thus a passing score (minimum 60%) on the quiz is a prerequisite to proceed with each corresponding experiment in the laboratory. A failing quiz grade for any experiment will prevent the student from completing that experiment and to receive any related credit. Students have an opportunity for one make-up quiz before the corresponding lab time.

A closed notes/closed book Final Exam will be held as scheduled (see Master Schedule) based on all lectures and experiments studied, including data analysis and fundamental concepts. The Final Exam will be completed independently. Calculator will be needed.

**PRESENTATIONS:**

Two groups will collaborate to make one oral presentation during the Wednesday lecture in the 8th or 10th week. The presentation should be made in PowerPoint and include five sections: 1) Title page; 2) Background and the scientific questions investigated, 3) Experimental approach, 4) Key results: Tables and Figures, 5) Conclusions.

**ERROR ANALYSIS AND USE OF COMPUTER SOFTWARE:**

The importance of error analysis in this course cannot be overstated, but often students find the amount of error analysis required to be daunting. You should remember much of this from Analytical Chemistry. To help remind you of this material, please read Chapters 2 and 3 of GNS. Chapter 2 is concerned with the mathematical processing of data (calculations and presentation issues) to obtain desired quantitative results and correct evaluation of uncertainties. The use of computer software (spreadsheets such as Excel, Quattro Pro) for data analysis is discussed in Chapter 3. A lecture on these topics will be given in class and selected problems will be discussed. The methods reviewed are expected be applied in your lab reports. It is very important to work on the end-of-chapter problems and assure adequate background prior to writing your lab reports.
GRADING:

a. Pre-lab Quizzes: Passed

b. Lab reports: [scientific content and writing/presentation style]
   1) Brief Report I: 15% (7.5% First version, 7.5% Revised version)
   2) Full Paper Report I: 25% (12.5% First version, 12.5% Revised version)
   3) Brief Report II: 15% (No Revision)
   4) Full Paper Report II: 25% (No Revision)

c. Final Exam: 20%

"Scientific content" means the precision, accuracy, and competent interpretation of your results, and further the quality of your error analysis, graphs, and tables. "Writing/presentation style" means how well you tell the story, how carefully you match verb to subject, your use of tense, and other aspects of style. All graded work will contribute to the final grade as shown above.

Attendance Policy: Attendance of all scheduled classes is required. Missing an experiment without a medical excuse will result in an “F” grade for the corresponding report(s). An unexcused absence from any scheduled computer lab (CL) or writing workshop (WW) will result in a penalty of 25% from the final grade of corresponding report. Up to a 25% penalty can also be applied if a student is physically present in any of the classes, but not adequately prepared (homework assignments, etc.).

Late report penalty: Your lab report score will be reduced by one full grade for each day that a lab report is late (without a medical excuse).

LABORATORY NOTEBOOKS:

You must have a lab notebook, which may be any brand, but should be ~8.5"x11", solidly bound (not wire-bound), with at least 100 numbered pages. All data taken in the lab must be recorded in this notebook neatly and clearly identified so that it is traceable to your report. At the end of each lab period you and the instructor must sign your notebook. This laboratory notebook should be brought to all classes, including computer lab (CL) and writing workshop (WW) lab periods, with detailed sample calculations written prior to the corresponding CL class. These sample calculations should be completed by the end of the computational lab class, then signed and dated by both the student and lab instructor. A Xeroxed copy or a carbon copy of the signed data and sample calculations must be submitted with your laboratory report as an appendix.

Your notebook should contain a detailed account of all work you performed in the lab. Since your reports can be written only if you have a good record of your work and data, you must keep your notebook readable and up to date. For example, numbers must be accompanied by appropriate units and be labeled as to what quantity was measured. Unavoidable deviations from the established procedure, problems encountered, mishaps suffered, and other pertinent events/observations should also be recorded. Be a pro and record your work as you go along, not at the end of the day when you’ve forgotten much of what happened.

LABORATORY REPORTS:

Reading Assignment: Chapters 1-3 from GSN and at least 2 papers (from an ACS journal http://pubs.acs.org, free access on campus) for each full format report.

For each experiment you will prepare a laboratory report using the format described below. The knowledge gained from an experiment is of little value unless it can be communicated. You should write your report in a lucid,
easy-to-follow manner, readily comprehensible by anyone with a basic background in physical chemistry. Since this course has been designated a writing-intensive course, a great deal of importance will be attached to the quality of your technical writing.

Two of the major channels for scientific communication are poster presentations at professional meetings and papers published in peer-reviewed scientific journals. A poster is presented in-person by the author(s) and includes a brief summary of experimental method(s), data, and conclusions illustrated by figures and tables. You can find many posters on the walls of our Chemistry Department from a variety of scientific meetings.

When a scientific paper is published in a journal, the author is not immediately available to answer questions, so the experiment itself, all data obtained, and all conclusions drawn are clearly explained and well argued in writing. The authors place their work in context with the most recent achievements in the scientific field.

During this course you will use both styles to present your experimental data. Please note that prior to writing your full paper reports, it is very helpful to analyze your data carefully and develop a brief report as a skeleton of your work, then add the detailed descriptive part as outlined below.

Please take note of the following points:

1. **Your report is to be entirely your own work.** Although you may gather data with your group, you must do the calculations and write-up yourself. Evidence of unacknowledged collaboration in the preparation of your report will result in a penalty. (As stated above, your report will be graded alongside your partner's.)

2. You are expected to keep all original files (complete spreadsheets with graphs, original spectra, word document files etc.) related to any reports you submit for the duration of this course and be ready to present them upon request.

3. **Reports are due two weeks after the day the experiment was completed.** Revised papers are due one week from the day graded originals are returned. Revised papers should be submitted together with graded originals. All changes must be indicated (highlighted) and all questions arising from the original papers must be answered in the revised versions.

4. All reports must be typed with a word-processor and double-spaced. Use a word processor with an equation editor, to generate calculations and special characters. If you do not know how to install this feature, please ask. NEATNESS COUNTS TOWARD YOUR GRADE! **Do not** hand in reports that are too lightly printed, with excessive amounts of text, figures, or tables, or that are otherwise hard to read.

5. **Plagiarism** – As stated, you will complete each experiment with your partner but each partner is responsible for his/her own report. **Duplication of text, graphs, calculations, tables, or formatting used by other students is not acceptable. Copying of any fragments from websites, textbooks, and other sources is not permissible and your lab report will be given an "F" grade and may be reported to the Chair, Dean, and/or Provost.**

6. **The files for all four lab reports must be submitted electronically via Canvas to receive a grade.** This must be done by the time you submit your hardcopy report and the file submitted electronically must be identical to the printed paper copy submitted in class. An “F” grade will be assigned if your printed copy is found to differ from the corresponding electronic file. To submit a file, go to the Chem 3398 Canvas site and click on the assignment you wish to upload. **Do not re-submit!**

7. **Calculations:** Calculations should be consistent with the measured data, i.e., do not arbitrarily discard significant figures and, conversely, do not include long strings of meaningless digits. If you have trouble with any calculation, you are encouraged to see one of the instructors. Always bring your notebook with you to help the instructor locate the source of your difficulties.
“FULL PAPER FORMAT” LAB REPORT (REQUIRED CONTENT AND FORMATTING):

1. **Cover page:** The first page template should be used exactly as downloaded from Canvas and updated with your information:
   a. your name and student ID number, section #, group #, type (format) of the report, and report #
   b. title of the experiment
   c. the name(s) of partners, if any
   d. the dates on which you started and finished the experiment
   e. the date on which you are submitting the report. The cover page template is provided in Canvas.

   Do not change text font(s) or the arrangement of the cover page!

   **Caution:** An incorrectly labeled cover page may result in your report being misplaced or lost! An “F” grade will be assigned to any missing lab reports.

2. **Abstract:** A concise summary (250 words or less) of the purpose of the experiment, what was measured, by what technique, and the relevant results and associated errors. A comparison of the results with theoretical models or known literature values is also appropriate.

3. **Introduction:** A 1-3 page introduction can include background information and the purpose of the experiment, relevant mathematical expressions, theoretical information, etc. This should be in the form of a narrative (tell a story!), that prepares another chemist to understand your work.

4. **Experimental:** This should include
   a. **Materials** section: list chemicals (and manufacturers) used in a paragraph format.
   b. **Methods and/or Techniques** section: names of equipment (with manufacturers) and/or discussion of methods used. Discussion of procedures (e.g. how the values were measured with reference to any corresponding sample calculations in appendix) used for the experiment. It is not necessary to include pictures of instruments, unless the experimental apparatus is unique.

5. **Results:**
   a. A clear description of your results must be given, together with the established errors and all appropriate units. It is important to write clearly and in complete sentences indicating where the results are presented (e.g. Table 1, Figure 2, Graph 1, Appendix 1 etc.). A reminder: you are telling a story! Use a narrative style. Important intermediate results should also be given (for example, averages of several experimental runs, data from chart recordings, etc.).
   b. **Make use of figures and tables** whenever possible to show clearly the effect of an independent variable (e.g. temperature, concentration, etc.) on the observable (dependent variable). For graphs make sure you label all axes clearly using the appropriate units. When graphing a model calculation (e.g. a linear fit) it is best to plot the data as points and the fit as a solid line on the same graph.

   **Make sure you apply a legend to the plot to identify what each line or symbol stands for.** Briefly (within 2-3 text lines) describe the corresponding content using figure and table caption(s).
   c. **Errors:** Results with error analyses should be included with adequate interpretation. The error estimates on the final results may require that you use the propagation of errors technique. Whenever appropriate, perform a suitable statistical analysis of your results. Add error bars to your plots as needed. If you question the validity of one or more experimental data points and wish to discard them, you will have to provide a reasonable (quantitative, if possible) justification. The extent of the error analysis required will vary greatly depending on the experiment. Sample calculations of error analysis must be included in an appendix.
   d. **Sample calculations:** Describe briefly the operations you performed to reduce your raw data to the final results. For example, if data of the same kind were obtained at three different temperatures, only one sample calculation should be given. On the other hand, if the same set of data was used to obtain two different derived quantities, two sample calculations are expected, one for each different type of quantity. These samples calculations should appear in an appendix. Start with a symbolic mathematical expression, then show one numerical example with corresponding dimensional analysis of each type of calculation using your own data. You must write a complete sentence directing the reader to the appendix.
e. Model calculations: This will be appropriate only for some experiments and should be skipped entirely for others. State briefly the basic premises and results of the model. Then use the model to obtain a theoretical estimate of only those quantities derived from your experimental data. Show a sample of each different type of theoretical calculation in an appendix.

6. Discussion: This section should include comments on the significance of your results and your confidence in them. It should include, where appropriate, comparisons of your results with those in the literature and with the predictions of a theoretical model. Are the results in reasonable agreement with your expectations? Are they consistent with each other? Why or why not? Keep this section to the point, i.e., directly related to the actual results you obtained. Questions which you are asked in the notes, Halpern and/or in GNS should be answered here. A clear, concise, and specific discussion of errors, together with a numerical estimate of their effect on your data and on the derived quantities you calculated, should be included. In some cases only a very minimal discussion of errors is needed, while others may require considerable effort.

7. Conclusions: This section includes a brief explanation of why you did what you did, the reason for the observed behavior of the atoms and molecules of the materials involved, how your results compare with what is already known, and why any discrepancies exist in your data. Further, you should present suggestions for further interesting experiments that would resolve some of the problems you encountered and make some comments about the broader implications of your results.

8. References: List all cited literature references in consecutive series by order of appearance in the text, with the citations presented as superscript Arabic numbers. The ACS Style Guide should be followed for the appropriate style in citations of journal articles, books, and other publications.

9. Appendices: The appendices will include Xeroxed or carbon copies of your laboratory notebook pages for the experiment in question, sample calculations, error analyses, and copies of any cited papers.

BRIEF LABORATORY REPORT (REQUIRED CONTENT AND FORMATTING):
(numbering based on “Full Format Report” above):

1. Cover page
2. Abstract
4a-b. Experimental
5b-d. Results (include 5e if necessary; note that 5a is not included.)
7. Conclusions (~1/2 page)
8. References
9. Appendices

Assemble your report with the different sections in the order given above.

STYLISTIC CONSIDERATIONS:

1. Figures
   a. Figures must be computer generated with the axes clearly labeled, including units if applicable. Try to scale data or curves to occupy a significant fraction of the graph area, i.e., do not bunch all of the information in one corner of the space.
   b. Plot each set of data clearly, using different symbols or colors for different sets of data.
   c. Each graph must have a figure caption that describes what kind of information is shown. The figure caption is always located below the figure. When a caption is included, a title should not be located above or on the graph.
   d. Whenever appropriate, properly computed error bars should be shown for your experimental data points and errors of calculated slopes and intercepts reported (with specified confidence limits and corresponding degrees of freedom).

2. Tables must include titles and numbering. All rows and columns should have clear labels which include units in parenthesis when necessary. The table caption is always above the table.
3. References: In most reports you will refer to theoretical and/or literature information. Each time you do this you must give a complete reference and include a copy of the relevant page of a cited paper in your appendix with the corresponding text highlighted.

4. Write in third person with passive voice; do not use “I” or “we”.

5. Do not wait until the last minute to prepare your report. You may run into unexpected trouble – and help may not be available then.

LABORATORY CLEAN-UP:

Before you leave at the end of each lab period your group must:

1. Empty and clean all glassware, except for containers (properly labelled with name of chemical and date) storing those materials which are to be used by other students later.
2. Clean the bench (and balance area, if you have used it) and surrounding areas.
3. Store all glassware and equipment the same way you found it.
4. Turn off power to all equipment.

Your instructor will not sign your lab notebook until you have cleaned up.

SAFETY:

***Violation of safety rules outlined below may result in expulsion from the laboratory.***

Serious accidents in Physical Chemistry Laboratories, although rare, are not unheard of. Understand how the apparatus works and what you are asked to do with it before you begin. Do not exert force on the equipment or try to do anything to which you encounter resistance – a sure symptom that you are doing something wrong or that there is equipment malfunction. Equipment malfunctions can have serious safety consequences, especially for experiments using gases at very high pressures, or experiments where potentially lethal voltages may exist. If you are not sure that you understand a particular operation, or if you think that the apparatus may not be functioning properly, ask your instructor.

You must observe the following safety rules for the protection of yourself and those working near you:

1. Eye protection – wear approved safety goggles at all times, as required by state law.
2. Fire hazards – determine the location of the fire extinguisher(s), shower, and eye wash, which will be shown to you by your instructor. Any use of flammable organic solvents constitutes an obvious fire hazard. Organics must not be disposed of in the sink drains; organic waste containers are provided.
3. Electrical hazards – In addition to the usual hazards found in chemistry labs, some experiments require the use of electrical circuits carrying potentially lethal voltages. Voltage is not in itself a reliable indication of danger because, since the body's resistance varies so widely, it is not possible to predict in general how much current will exist in response to a given voltage. Prevention is the best medicine for electric shock. That means having a healthy respect for all voltages, and always following safety procedures when working with electrical equipment.
4. High pressure – In some experiments you will use gases stored at very high pressure. Gas cylinders must remain securely tied to the benches at all times; you must never attempt to move a cylinder, or change regulator settings. If you run out of gas, tell your instructor.
5. Broken glass – You should already be aware, from your previous lab work, of the hazards of broken glass. Observe the appropriate precautions; clean up broken glass immediately (Dustpan and brush, not fingers!) and report any broken or sharp edges to your instructor at once. Never use glass apparatus with cracks or chips.
6. Mercury – Handle with care any apparatus containing mercury. Be sure to report any spills, since mercury constitutes a potential health hazard and must be taken care of promptly. Be careful also to keep gold or silver jewelry, watches, etc., out of contact with mercury, which can amalgamate with them.
7. Pipetting – Never pipet any liquid by mouth; rubber bulbs are provided for this purpose.
8. Report every accident, no matter how minor, to your instructor.
9. If chemicals are to be used for more than 1 period, they must be labeled with the name of chemical (not abbreviated), and the date.
10. **Dispose** of chemicals (glass) in chemical waste (disposable glass) containers provided.

11. **Food and beverages are not allowed** inside the lab.

**INCOMPLETES / DROPS / WITHDRAWALS:**

This course will adhere to the Department and the University Policies regarding the last date to drop or withdraw from the course. For the university policy please see [http://policies.temple.edu/getdoc.asp?policy_no=02.10.14](http://policies.temple.edu/getdoc.asp?policy_no=02.10.14). The last date to **drop** is **Monday, January 27**. The last date to **withdraw** is **Wednesday, March 18**. To obtain an “incomplete”, an incomplete contract must be signed upon sufficient completion of 60% of the work. The student's accumulated total to that point should be more than 75% of the possible points. Non-attendance to the lab does not constitute "dropping" the course. Official withdraws can only be done through the Registrar's office.

**HELP!**

Make certain you take full advantage of all the academic support services available at Temple - on the Main Campus. These include instructor office hours and the STEM Learning Lab ([http://www.temple.edu/class/](http://www.temple.edu/class/)) in Tuttleman 100. The services provided through the Student Success Center include one-on-one tutoring, computer lab, weekly group tutorials/supplementary instruction, final exam review sessions, and a resource library. For additional information check [http://www.temple.edu/class](http://www.temple.edu/class). Assistance with editing the text of your written draft(s) can be obtained at the **Temple Writing Center** ([https://www.temple.edu/class/programs/writing/index.html](https://www.temple.edu/class/programs/writing/index.html) for more information). You can also ask for assistance at the library reference desks concerning literature search.

**DISABILITY RESOURCES AND SERVICES:**

Any student who has a need for accommodations based on the impact of a documented disability or medical condition should contact Disability Resources and Services (DRS) in 100 Ritter Annex (drs@temple.edu; 215-204-1280) to request accommodations and learn more about the resources available to you. If you have a DRS accommodation letter to share with your instructors, or you would like to discuss your accommodations, please contact Dr. Han or Dr. Cerkez as soon as practical. We will work with you and with DRS to coordinate reasonable accommodations for all students with documented disabilities. All discussions related to accommodations will be confidential.