CHEM 3420: Physical Chemistry II - Spring 2016

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Office Hours Tuesday 2–3:30
Wednesday 3–4:30
By appointment: call or email and we can find a time to meet

Lecture MWF 8:30–9:45 AM

Labs Tuesday, 8:30-11:10 AM, USC 354

Textbook *Physical Chemistry for the Chemical Sciences*, Chang & Thoman (*University Science Books*)

Experiments in Physical Chemistry, Garland, Nibler, and Shoemaker, 8th edition (*available on reserve in the library*)

Lab Manual *Physical Chemistry Lab Manual*, Spring 2016 Edition, Available for download on Blackboard.

Website Course materials are available on the course website at `http://blogs.stockton.edu/pchem`

The website will be the place to find announcements, lecture summaries & slides, homework, exams, and solutions. In addition, a series of podcasts will be available aimed at helping you review the important mathematics skills necessary for success in physical chemistry. Please check the site frequently for new materials and announcements.

Copyright or other restricted material will be posted on the course Blackboard site. The lab manual will be posted on Blackboard.

Course Goals

1. **Learning fundamental principles, generalizations, or theories (Program Competence, Quantitative Reasoning)**
   You will develop an understanding of quantum mechanics and its application to atomic and molecular structure. These concepts will be applied to spectroscopic techniques used to probe structure.
2. **Learning to apply course material to improve thinking, problem solving, and decisions (Program Competence, Critical Thinking, Quantitative Reasoning)**
   You will apply concepts from quantum mechanics to develop problem-solving expertise enabling the solving of both quantitative and qualitative problems. In addition, concepts from across physical chemistry will be utilized to complete experimental work in the laboratory.
3. **Developing skill in expressing oneself orally or in writing (Communication Skills)**
   You will prepare scientific manuscripts using a variety of formats to report on experimental work from the laboratory. In addition, a written proposal, oral presentation, and final written report will be submitted detailing the student's independent project work. Writing assignments will be evaluated using rubrics posted on the course website.

Procedures and Policies

Lecture Regular attendance is important and expected. **Please arrive on time.** Late arrivals are disturbing for the entire class. The lecture will cover new material and sample/group problem solving. Since we will be doing problem solving during class, please bring your calculator with you. Mobile phones, pagers, and other sound-producing devices must be turned off or silenced during class meetings.

Laboratory

Attendance is mandatory. You must complete all laboratory assignments & reports in order to pass the course. No unexcused absences are permitted. If it is necessary to be absent from a regular lab period for important reasons, you must contact me in advance. Your ride leaving early on Tuesday during the week before Spring Break does not qualify as an important reason. You must wear goggles and shoes with closed toes (no sandals) at all times in the lab. No exceptions.

Homework

Homework will be posted on the course website on a regular basis. Homework will not be collected but a suggested completion date will be included on all assignments. Solutions will be posted after the suggested completion date.

Completing problems on your own or in groups is essential for learning physical chemistry. Watching someone else solve problems or reading the solutions will not prove to be an effective way to master the material in this course. Do not put off working on problems to just before exams. You must keep up with the problems in order to be successful in this course. Please come to class with questions on the current assignment or bring your questions to office hours.

Additional assignments may be handed out periodically during the semester. These assignments will be due on the indicated date.

Lab Reports

Read the general lab guidelines and advice on lab reports, data analysis, preparation of graphs, note keeping, etc. in the lab manual before your first lab and refresh your memory after a few weeks. There are examples for all of the above in the lab manual as well as help files online. Full lab reports are due in lab **two weeks** after completing an experiment. Summary (short) lab reports are due in lab **one week** after completing a lab. You will write full reports for Experiments 1 & 5. The remaining reports will be summary reports. Reports will be evaluated using the rubric posted on the course website.

Late Policy

I realize that your semester will create some busy periods so you are given 10 days of extensions for **lab reports only**, which must be used in one-day units. **These extension days include weekends.** To use an extension, please write "# days extension used" on the title page. However, I do not want to encourage procrastination, so beyond that I will have to reduce your lab report or other late assignment grade by 25% for each day that it is late.

Extension days for lab reports can only be used until Monday, April 18. Beyond that date, all reports will be considered late and penalized accordingly.

Exams

There will be at most a total of three exams tentatively scheduled for **February 26, March 25, and April 25**. Our final class session as determined by the exam schedule is on **Friday, May 6, 8:30–10:30 am**.

Exams will cover lecture material and homework. Exams will emphasize concepts and understanding, so no need to memorize lots of equations. The format of the exams will be discussed in class.

I will grant permission to make up an exam if the absence is due to any of the following: (1) serious illness; (2) an order from the US Military; (3) officially representing the College; (4) death in the immediate family. All such instances will require documentation before a make-up exam will be given.

Academic Honesty

Collaboration is important part of learning, especially in the sciences. Working in groups to discuss homework and class material is encouraged. When turning in written work sources must be cited in the appropriate format. Remember, you cannot copy someone else's words even if you have a proper citation. Direct quotes are not appropriate in scientific writing.

Your written work must be your own. Handing in someone elses work as your own is cheating. Plagiarism will result in a grade of zero for the assignment. Please review the college's academic honesty policy available on the Academic Affairs website. **All incidents of academic dishonesty will be reported to the Office of the Provost as required by college policy.**

Other Issues

Students with disabilities who may need disability related classroom accommodations (or other considerations) for this course are encouraged to speak with the Learning Access Program, located in J-204 or by calling 652-4988.

Grading

Your written work for this course will receive numerical grades. Each component of the course will be weighted as follows:

Laboratory	35%
Exams	35%
Project	25%
Participation (Class/Lab)	5%

There are no set ranges for particular letter grades. The grading scale will depend in part on my assessment of the difficulty of exams and the final. The grading scale for students completing all course requirements will not be raised above the 90–100% = A-range, 80–90% = B-range, 70–80% = C-range, 60–70% = D-range scale. This means if you receive an overall percentage of 90% and complete all course requirements, you will get a grade in the A-range. If you have an overall percentage of 89% and you have completed all course requirements you will be guaranteed *at least a grade in the B-range.*

Tentative Course Outline

Here's a brief and tentative outline of the topics we will cover this term. There may be supplemental readings distributed throughout the term. The sequence of topics is tentative and I'll give you updated schedules along the way.

1. The Foundation
   (a) Properties of waves
   (b) From the classical to quantum world
   (c) Wave equations
2. Atoms and Atomic Structure
   (a) Hydrogen: atomic orbitals
   (b) Helium: adding another electron is trouble
   (c) Beyond helium: approximations and trends
   (d) Periodicity & atomic spectroscopy: exciting atoms
3. Molecules
   (a) Transitions: translation, rotation, and vibration, oh my!
   (b) Chemical bonding: from atomic to molecular orbitals
   (c) Spectroscopy: using transitions to talk to molecules
4. The Solid State
   (a) From molecules to solids
   (b) Solid state structures
   (c) Diffraction: communicating with solids
   (d) Structure-property relationship in solids

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Independent Projects

This project is intended to be a fun introduction to independent thinking and research. Students may work in pairs on projects. The object is for you to propose a question and investigate the answer. Several possible projects are suggested here; you are encouraged to develop your own ideas.

Most any topic related to the material covered in Physical Chemistry I and II is acceptable, as long as the instructor approves it in advance. By **Wednesday, February 17 (at the latest)**, you should submit your topic for approval. A 2–3 page proposal, with at least 3 primary (not web) references, is due **Friday, March 11**. This document is 15% of the project grade. More details about the proposal format will be distributed in class. **Each research team is required to meet with me before the proposal submission deadline.**

The last four lab sessions will be dedicated to project work. In addition, you will time throughout the semester to work in the laboratory on your project, so do not wait until the end of the semester to begin. Please be aware that projects are limited by equipment and supply availability.

An 8–10 page paper (written individually) is due **Friday, May 6** (our final class day). You will also make a presentation to the class on that day. Additional information on the paper and presentation will be discussed in class.

Grades will be assigned on the basis of presentation, creativity, effort, completeness, relevance, and evidence that you have learned something new. Actual results are much less important than explanations and analyses. A few suggestions are listed below.

Extensions of existing laboratory experiments:

1. Kinetics of bromination of deuterated acetone
2. Kinetics of the halogenation of acetone with a different halogen or catalyst
3. Further characterization of biodiesel, biodiesel of other oils
4. Further exploration of the phase diagram of binary or ternary system, using DSC or other techniques
5. Other applications of bomb calormietry

"New" laboratory experiments:

1. Studies of the physical properties of macromolecules, micelles, polymers
2. Ternary phase diagrams (from Sime text)
3. Monomer/dimer equilibrium (from Sime text)
4. Study of oscillating chemical reactions
5. Enzyme kinetics or other kinetics experiments, including using NMR spectroscopy
6. Kinetics of photochromic substances
7. pKa of a weak acid
8. A P-Chem experiment that interests you, such as one from "Experiments in Physical Chemistry" by Garland et al. (available on reserve) or other texts (see me for those)
9. A P-Chem experiment that interests you form a recent issue of *J. Chem. Ed* (available on-line, talk to me for possible suggestions)

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Laboratory Information and Organization

In addition to information on the course syllabus I have compiled this document to outline some organizational features of Physical Chemistry Laboraotry.

- Due to the heavy use of instrumentation in the laboratory component of the course, all lab work will be performed in teams of 2 (3 if necessary). Student groups are expected to work as a team to complete each assigned experiment and independent project. If issues with an individual's participation in a team arises, please see me as soon as possible.
- **All written reports are to be completed individually**. The format for each experimental report is detailed in the lab manual. Full reports should follow the format outlined in introductory material in the manual and is modeled after a chemistry journal article. Summary reports do not have a formal format, but should be constructed to the same standards in terms of writing style, data analysis, and data presentation.
- There is no set schedule to complete the experiments. You are responsible for completing the seven experiments outlined in the manual by Tuesday, March 22 (at the latest). This format should give you time to work on other experiments and/or your project during "downtimes".

  You may complete the experiments in any order, but take note of the following:

  - Some experiments will require an entire lab period to complete and some can be done in a shorter amount of time. Details of suggested time requirements for each experiment are listed in the table on the back.
  - Several experiments require a specific piece of equipment that can only be used by a single group. In this case, sign-up sheets will be available and groups will be required to sign up in advance to use these instruments.
  - Some experiments allow synthesis and product analysis to be completed in different weeks, while others require immediate analysis.

  You are expected to use your time productively, allowing for additional work on your projects during the semester. Students in previous semesters have requested additional time to complete project work, beyond the last weeks of the semester. By working smart you should have ample time during the semester to begin project work, which can then be completed during the last four weeks of lab. The last four lab meetings are reserved for project work.
- Teams are required to check-out with me each week to discuss laboratory progress. A short summary form will be submitted at the end of lab each week to report on work done in lab during the current session and a brief plan for the next meeting. These forms will also serve to inform me of the completion of an experiment for the purposes of lab report submission (see the syllabus for information on lab report due dates).
- Teams are required to meet with me before the project proposal deadline (Friday, March 6) to discuss details of their proposal. I also suggest meeting with me before the February 18 topic deadline if you need help identifying a project.

Experiment	Minimum Suggested Time Required	Notes
1 (Week 1)	1 lab meeting	product needs to be washed and dry before analysis
1 (Week 2)	1 lab meeting	bomb calorimeter sign-up required (1 team per week)
2	1 lab meeting	see me for spectrophotometers, multiple available
3	1 h (analysis = 30 min)	only one plate reader available, sign-up for time
4	1 lab meeting	DSC sign-up required (1 team per week)
5	1 lab meeting	multiple spectrophotometers available, sign-up suggested
6	1–1.5 hours	Synthsis/characteriztion separate, one spectrofluorometer available
7	1 hour	IR use required, can be done by multiple groups in a week

Formal Lab Report Grading Rubric

The format for formal lab reports is described in detail in the laboratory manual. There are additional materials posted on the course website to assist you in writing formal laboratory reports.

	4 – Exceptional	3 – Admirable	2 – Acceptable	1 – Poor	0 - Substandard	Score
Abstract	Clear, concise, and thorough summary including context, important results, and conclusions.	Refers to most of the major points, but some minor details are missing or not clearly explained	Misses one of more major parts of the results, context, or conclusions	Missing several majors aspects and merely repeats information from the introduction	None or unrelated	___X 2
Introduction	A cohesive, well-written summary (including all relevant chemistry) of the background material pertinent to the experiment with appropriate references. Places the purpose of the experiment in context.	Is nearly complete but does not provide context for minor points. Contains relevant information but fails to provide background for one aspect of the experiment, or certain information is not cohesive.	Certain major introductory points are missing (ex: background, theory, chemistry, context, etc.) or explanations are unclear and confusing. References are used properly.	Very little background information is provided and/or information is incorrect. No references are provided.	None or unrelated	___X 2
Experimental	Contains details on how the experiment was performed and the procedures followed. Written in the correct tense and omits information that can be assumed by peers (trained chemists)	Narrative includes most important experimental details but is missing one or more relevant pieces of information.	Missing several experimental details or some incorrect statements.	Several important experimental details are missing. Narrative is incorrect, illogical, or copied directly from the lab manual. Written in the incorrect tense.	None or unrelated	___
Results (Presentation of results, figures and tables)	All figures, graphs, and tables are numbered with appropriate captions. All tables, figures, etc. are explicitly mentioned in the text. Relevant experimental data are presented which are used in the discussion.	All figures, graphs, and tables are correctly drawn, but some have minor problems that could be still be improved. All data and associated figures, etc. are mentioned in the text. Most relevant data present.	Most figures, graphs, and tables are included, but some important or required features are missing. Certain data reported are not mentioned in the text or are missing. Captions are not descriptive or incomplete.	Figures, graphs, and tables are poorly constructed; have missing titles, captions or numbers. Certain data reported are not mentioned in the text. Important data missing.	None or unrelated	___X 2

Overriding criterion: If any portion of the report is identified as not being original and/or not done by the student, the paper will receive a zero and academic dishonesty charges will be filed.

	4 – Exceptional	3 – Admirable	2 – Acceptable	1 – Poor	0 - Substandard	Score
Discussion/ Conclusions	Demonstrates a logical, coherent working knowledge and understanding of important experimental concepts, forms appropriate conclusions based on interpretations of results, includes applications of and improvements in the experiment, references collected data and analysis, refers to the literature when appropriate, and demonstrates accountability by providing justification for any errors. Address all specific points or questions posed in the lab manual.	Demonstrates an understanding of the majority of important experimental concepts, forms conclusions based on results and/or analysis but either lacks proper interpretation, suggests inappropriate improvements in the experiment, refers to the literature insufficiently, or lacks overall justification of error. Address most of the specific points or questions posed in the lab manual.	While some of the results have been correctly interpreted and discussed, partial but incomplete understanding of results is still evident. Student fails to make one or two connections to underlying theory. Address some of the specific points or questions posed in the lab manual.	Does not demonstrate an understanding of the important experimental concepts, forms inaccurate conclusions, suggests inappropriate improvements in the experiment, refers to the literature insufficiently, and lacks overall justification of error. Address none of the specific points or questions posed in the lab manual.	None or unrelated	___ X 2
References	All sources (information and graphics) are accurately documented in ACS format.	All sources are accurately documented, but a few are not in ACS format. Some sources are not accurately documented.	All sources are accurately documented, but many are not in ACS format. Most sources are not directly cited in the text.	All sources are accurately documented but not directly cited in the text.	Sources are not documented nor directly cited in the text.	___
Overall Style and Organization	Appropriate as a piece of scientific writing. Words were chosen carefully and appropriately. Sentence structure was clear and easy to follow. Evidence the report was edited by the author to improve clarity and readability.	Minimal awkward phrasing or word choices. Report is easy to read and constructed properly. Evidence of editing.	Many passages are phrased poorly, contained awkward word choices, or many long sentences. Narrative is disorganized in many places. Tense not appropriate or not in agreement in several places.	Poorly organized narrative with frequent awkward phrases and poor word choices. Sentences are too long or short. Lacks cohesion, style and fluidity. Many instances of verb tenses not agreeing. No evidence of editing.	Incorrect format, style and organization.	___ X 2
Mechanics (grammar, spelling, etc.)	From a technical standpoint, the paper is free of spelling, punctuation, and grammatical errors	Less than three grammatical and/or spelling errors	Multiple grammatical and/or spelling errors.	Frequent spelling and grammatical errors. Visit to Writing Center strongly encouraged.	Extreme technical errors. Visit to Writing Center strongly encouraged.	___

Summary Lab Report Grading Rubric

Unlike formal lab reports, summary reports do not need to follow a particular format. However, they must be constructed to the same standards in terms of writing style, data analysis, and data presentation. Please be sure to address specific points or questions raised in the lab manual.

	4 – Exceptional	3 – Admirable	2 – Acceptable	1 – Poor	0 - Substandard	Score
Data and Analysis	Presented in a clear manner. Data tables and figures are constructed correctly. Raw data is not included. Important calculations are demonstrated. Error analysis included when appropriate.	Is nearly complete, but missing important table, figures, or calculations. Some tables/figure unclear or contain too much information (ex: raw data). Error analysis is present by incomplete.	Missing important data or analysis to support discussion. Tables or figures are missing/incomplete. Error analysis is incomplete and/or incorrect. Raw data is presented in addition to other figures/tables.	Missing several major results and/or analyses. No tables or figures. Only raw data included. No evidence of data analysis.	None or unrelated	X 2
Discussion	Written clearly and in the appropriate style. Data is used to support claims Addresses all the points and/or questions posed in the laboratory manual. Critical analysis of results is included. Comparison to literature results included when appropriate.	Written clearly but the style is not appropriate in some passages. Data is used to support claims. Addresses most of the questions/points raised in the lab manual. Analysis of results is present but lacks clarity. Some literature comparison is included.	Discussion is not clear and does not use data to support claims. Omits several points/questions posed in the lab manual. Minimal comparison to literature results.	Very little discussion of results and data is not used as support. Discussion is unclear and/or disorganized. Does not address points/questions posed in the lab manual. No comparison to literature results.	None or unrelated	X 2
Mechanics (grammar, spelling, etc.)	From a technical standpoint, the paper is free of spelling, punctuation, and grammatical errors	Less than three grammatical and/or spelling errors	Multiple grammatical and/or spelling errors.	Frequent spelling and grammatical errors. Visit to Writing Center strongly encouraged.	Extreme technical errors	
Overall Style and Organization	Appropriate as a piece of scientific writing. Report organized to tell the "story" of the experiments. References included when necessary.	Minimal awkward phrasing or word choices. Organization makes points clear but could be improved. References cited when appropriate.	Writing contains awkward phrases and word choices Disorganized in many places. Tense not appropriate or not in agreement in several places. Missing some references when necessary.	Poorly organized with frequent awkward phrases and poor word choices. Lacks cohesion, style and fluidity. Many instances of verb tenses not agreeing. No references included when required to cite sources.	Little evidence of any effort to construct a summary report.	

Overriding criterion: If any portion of the report is identified as not being original and/or not done by the student, the paper will receive a zero and academic dishonesty charges will be filed.