Please go to Dr. Salter's syllabus on the following web page
http://www.cs.moravian.edu/~csalter/ch332syl.html
The below has been copied for archival purposes.

SYLLABUS

Course: CH 332 Physical Chemistry II
Semester: Spring, 2011

Professor: Carl Salter
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Required Text: *A Guided Inquiry to Quantum Chemistry* by Tricia Shepard and Alex Grushow, in beta release for testing

Optional Texts: P. W. Atkins, *Physical Chemistry*, 6th Ed. Freeman, 1998
Rodney J. Sime, *Physical Chemistry: Methods, Techniques, and Experiments* Saunders College Publishing, 1990

Physical chemistry is the application of physics and mathematics to chemical systems. Physical chemistry is therefore a demanding interdisciplinary subject, requiring a working knowledge of calculus, mechanics, and chemistry.

Catalog Description: States of matter, chemical thermodynamics, theory of solutions, chemical equilibria, electrochemistry, chemical kinetics, elementary quantum theory. Problems and laboratory reinforce theoretical discussion. *Prerequisites*: Chemistry 220.2 or 222, Mathematics 171, and Physics 112. Three 50-minute periods, one 50-minute problem session, one three-hour laboratory.

Lecture: You will receive copies of my lecture notes throughout the course of the semester. These notes plus the textbook should allow you to solve homework problems on your own. Because you have already received the lecture notes, the **lecture periods will usually be group problem-solving sessions** involving the POGIL exercises from the *Guided Inquiry* workbook. The critical thinking questions are worked in class by your group. Your team work must **work together** on these questions, so that every member of the team agrees with the team answer. There will also be some group assignments which don't come from the workbook.

Homework sets including computer projects will be due approximately each week. The homework assignments include the **exercises** at the end of each activity--**not the critical thinking questions**.

It is crucial that you **keep up with assignments**. If you have struggled with a problem and no solution is in sight, please call me or come by my office. It is much easier for both of us if you deal with these problems immediately. When I took physical chemistry, I saw my professor about twice each day. There is simply too much information to absorb by yourself; you need to "talk out" these new ideas with someone: if not me, then a classmate.

You should plan to **work all the exercises** in *A Guided Inquiry to QC*. This workbook is **not** a textbook; it is not a complete description of the course content. My lecture notes should help you, but you should also read the textbook by Atkins, which has both exercises and problems at the end of each chapter. The **exercises** are relatively simple "plug and chug" calculations that are based directly on the text. (The problems at the end of the chapter are more difficult.) While you are studying the text, you should look at the exercises. You should read **all the exercises** at the end of each chapter in Atkins because they closely follow the presentation of the text, and therefore aid comprehension of the material. If you really want to learn from the Atkins book, try to work **about half of the exercises at the end of the chapter.** That will get you ready for my tests!

Tentative Schedule: Our goal this semester is to cover introductory quantum theory and its applications to chemistry.

Atomic and Molecular Energies
Electronic Structure of Atoms
Electronic Structure of Molecules
The Distribution of Energy States
Spectroscopy

Atkins Material
Quantum Theory Chapter 11 2,4,5,6,9,10,16
Quantum Theory Chapter 12 2,3,4,12,14,15
Atomic Structure Chapter 13 3,4,7,9,10,11,14
Molecular Structure Chapter 14 2,3,5,6,10,11,14

Evaluation: Twelve tests will be given; they will be given on the following Thursdays: January 27, February 3, 10, 17, and 24, March 4, 17, 24, and 31, April 7, 14, and 21. These quizzes are scheduled for every Thursday except the Thursday of the week after Easter. The two lowest test grades will be dropped from your average; however, you may only drop tests that you actually take. **An unexcused absence from a test will result in a grade of zero which cannot be dropped.** Each test will contain a bonus question; points from the bonus question may be retained in your average even if the test grade is dropped. Tests can be picked up in Lou Ann's office on the day that it is taken. Return the tests to Lou Ann.

The Final Exam is scheduled for Wednesday May 4 at 8:30 am. You may bring with you one sheet of paper with written notes.

Homework sets including computer projects will be due at the end of each week. See the schedule of topics for assigned problems. By the way, these are the <u>problems</u> at the end of each chapter, not the exercises. You should attempt <u>all the exercises</u> at the end of each chapter because they closely follow the presentation of the text, and therefore aid comprehension of the material. No homework may be submitted after 5 pm, Friday April 29, the last day of class.

Lab reports are an important part of this course. Lab reports for each lab experiment will be due one week after the completion the experiment. You must turn in all lab reports to receive a passing grade in the course. Unacceptable lab reports will not be accepted! You will be required to resubmit an unacceptable lab report. You are required to work with your lab partner--the two of you must read and evaluate lab reports before they are turned in to me. An extensive list of online advice about lab report format, style, and content is available on my web site. The lab report evaluation form is also on my web site. During the semester there will be lab report writing workshops during lecture--it is crucial that you bring writing assignments to class on those days. No resubmitted lab reports will be accepted after 5 pm, Monday May 2, two days before the final exam.

Attendance: Three unexcused absences results in failure of the course. After two unexcused absences you and your advosor will receive an email notice. Absences may be excused by a written doctor's slip or an email from an athletic coach or college trip organizer (a planned absence). Students are required to complete missed material immediately after their return from any absence. For planned absences such as travel for a college event, students are expected to complete missed material before the absence occurs.

The final grade will be determined as follows:

Comprehensive Final exam 20%

Homework and computer projects 15%

Tests 40%
(N.B. Because of the bonus points, it is possible to earn up to 50% from the tests.)

Lab reports 25%

It is within the instructor's purview to apply qualitative judgment in determining grades for an assignment or for the course.
Students who wish to request accommodations in this class for a disability should contact Mr. Joe Kempfer, Assistant Director of Learning Services for Disability Support, 1307 Main Street (extension 1510). Accommodations cannot be provided until authorization is received from the office of Learning Services.

Laboratory

The laboratory course gives you the opportunity to measure physical and chemical constants. I will emphasize the importance of statistics in determining how precisely you have measured these constants. In fact, the early experiments are designed to teach you the use of statistics in evaluating experimental data.

Some form of eye protection, either plastic glasses or goggles, is required whenever you are in lab, except when you are working at the computer. There are no restrictions on the clothing you wear in lab. You may work in the lab at night, but you must not work alone! The person in the lab with you does not have to be a member of the physical chemistry class.

You will find that I do not provide detailed lab handouts that tell you exactly how to do an experiment. In the lab you will find general information about the goal of the experiment, but it is up to you to decide how to do your experiment. And it is your experiment; you should have the pleasure of deciding how you want to do it. If I tell you how to do the experiment, you won't have as much fun because you'll be trying to get results that please me. All I care about is that you design an experiment that really measures what you want to measure, and that you estimate the precision of your measurement. Of course, I'll be there whenever you want to talk to me about your experiment. And in that regard, let me warn you that I am very opinionated and hold very definite ideas about the way things should be done in the lab. This is an inevitable consequence of spending fifteen years of my life doing chemical research. My job is to use my experience to help you avoid bad ideas and mistakes. Nevertheless, if you believe an idea you have is right, don't drop it just because I say it's wrong. Stick with it until you understand why it is wrong, or until you can prove to me that it is right.

You should keep some organized record of the work you do in lab, but I want you to decide how you want to do that; I am not going to grade your personal notebook. I will from time to time call you into my office and ask you to answer questions about your lab work; you can bring in your notebook and refer to it during these interviews. Therefore you need to record information in your notebook so that several weeks later you will be able to look at it and know what you did in the lab. By the way, you do not need to write down a detailed experimental procedure in the notebook; instead, refer to the lab textbook where you found the procedure. If you modify the procedure or apparatus, be sure to record that.

Guidelines for Homework Assignments

Begin each problem on a separate sheet of paper. Start each problem with a clear statement of the problem. At each point in your solution explain your strategy. It is critical that you explain ***WHY*** you are approaching a problem in a particular way and ***WHY*** you have done each step in your solution.

Intermediate steps should be logical consequences of previous steps. If you are going to divide by two and/or move a term from on side of the equation to the other it is sufficient to write the new expression on the line below the previous expression without comment. Nontrivial steps require an explanation. If two adjacent expressions are equal, they should be connected by an equal sign (=). If two adjacent expressions are NOT equal DO NOT connect them with an equal sign.

Equations cannot materialize out of thin air. If you use an equation from the text, your notes, another reference you must document it. For example, Eq. (27) Ch. 1 Atkins; Integral 967, CRC Math Tables, Copyright 1984; or class notes 9/27/98. This is just like using references in a paper or lab report. In addition to documenting where an integral came from you need to show any steps necessary to get the integral in your homework to look like the integral in the math table.

Solve equations algebraically for the desired result. DO NOT insert numbers until the algebra is finished.
Avoid calculating intermediate numerical results that are not needed.

All numbers should have units! Keep track of your units and show your conversion factors.
Answers without units are meaningless. Keep track of significant figures in your numerical results.

If at anytime I cannot follow your work I quit grading that problem. Once I get to the second problem on a set that I can't follow, I quit grading your entire set and you get a zero on any ungraded problems.

Finish each problem with a concluding sentence. What is the final result? Does it make sense? (If the result is absurb, find out the cause of the error.) How does it relates to the original question asked? What things did you learn from this problem, an application of a theory, a sense of the magnitude of a quantity, a math "trick", etc.? Make sure you mention at least one "big" picture thing that you learned. You may also mention useful problem-solving details which were illustrated. Use this statement to bring yourself to a new level of understanding about physical chemistry and/or the problem. Think about the implication of the answer to the science. What does that tell you about the size or direction of the effect being illustrated by the problem, etc.? This reflection is important—**The time when you can learn the most from a problem is after you have the solution in hand!**

In many problems you are communicating with a reader using the languages of mathematics and physics to explain chemistry. It is your job to use the language in a clear and precise manner to demonstrate your mastery of a problem. Remember the "reader" may be you reviewing for an exam!

Grading System for Homework Assignments

To make grading easy each problem will be graded on a 10 point scale. Your homework assignments will be graded in two parts. In the first part you earn up to 7 points by attempting each problem and working it to a successful mathematical and physical result. The final 3 points are based on your written comments during the solution and your reflection at the end of the problem. 30% of your homework is based on your writing!

You probably need to become familiar with this system before you are comfortable with it. For the first three homework assignments you will turn in your problems, I will grade them and return them to you promptly, at which time you can rewrite the homework to improve on the **written part** of the problems. I will then regrade your homework. After the third homework set you will not have a chance to improve your grade by rewriting.

Lab Reports

GENERAL RULES: Lab reports should be produced on a laser printer or ink-jet printer; they must be printed on one side of the page and the text must be double-spaced. To the greatest extent possible condense data and numerical results into tables for easy reading. Tables of data or numerical results are single-spaced and should be produced using the wordprocessor's table routine; columns must be labeled and units specified. Graphs and other figures should be made conveniently small and placed in the text as close as possible to their first mention in the report. Make sure that axes are labeled and units are specified. All figures should have a caption. Take care to use correct superscripts and subscripts when writing chemical and algebraic formulas. All but the simplest mathematical equations should be created using the wordprocessor's equation editor. If you place a chemical structure from ChemDraw into the document, make sure that the image is appropriately sized. All pages of the lab report should be numbered except the cover sheet. The page bearing the title and abstract is page number 1. The final page of your report should contain "Literature Cited".

Place a cover sheet on top of the report. The cover sheet should bear a title for the experiment, The name of the course, your name, the name of your lab partner, and the date that the experiment was carried out in the laboratory. The title of the experiment should also appear at the top of the first page. Do not place your name or your lab partner's name on any numbered page of the lab report.

Have your lab partner read your complete lab report and fill out the evaluation form. Read the evaluation and decide if you want to make changes to your report. Then turn in the report and the evaluation form.

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REPORT SECTIONS: I strongly suggest the following outline for your lab reports, although for some experiments certain sections may not be needed. When writing the lab report, remember that the important ideas to communicate are the results of your measurements, the analysis of the data, and the conclusions you can draw based on your results. Many of the sections of the lab report, especially data analysis and sample calculations, will help you think about your results. When you include a section, label it!

Experiment Title that is descriptive of what you studied or the goal of the experiment
Name
Name of Lab Partners
Date submitted

Abstract: A brief paragraph on the question your experiment attempts to answer, and the important results (numerical results) and conclusions you have made from the experiment. Other students should be able to read your abstract and decide whether they are interested in the rest of the report. The abstract DOES NOT contain a description of the experiment or background information behind the experiment.
Abstracts that begin with "The purpose of this experiment was ..." or "We did this experiment to find out ..." are usually inappropriate. These sentences belong in the Introduction. A good starting sentence for an abstract is "Our investigation of [ ] revealed that ..." That start leads directly to results and conclusions.

Introduction: A few brief paragraphs on the reasons for doing the experiment. What is the question about Nature that you hope to answer? Why is the question important? Discuss what you already know and what you hope to learn. Any theory or prior experiment that is related to the current question should be discussed here. This is where you should place important background information.
If the molecule under study is big or unusual, like azulene, this is the place to insert a chemical structure from ChemDraw.
If you are investigating a particular physical equation, such as the Nernst equation, insert it in the introduction using the equation editor in Word.

Experimental Method: A brief outline of how the measurements are made. In many cases a nice drawing of the apparatus will be helpful. You should not describe in detail how the experiment was performed; instead, reference the source of your procedure.

Raw Data: A presentation of the measurements you made during the experiment. A table or graph will usually help the reader absorb the data. Place several sets of data on one graph for easy comparison. Show all the data you took. If you reject some of the data from further analysis, explain why.

Data Analysis: Describe the method of analyzing the data that you used to determine any physical or chemical constants. Be sure to include a sample calculation so that others can follow your calculation. If you used a computer program, be sure to mention which program you used. If you wrote the program, include a copy in an appendix to your report.
Never present the numerical results of a least-squares fit without an accompanying graph; the fit function should be graphed as a line and the experimental data should be plotted as individual points.
Never copy the entire output of an Excel regression into a Word document without editing it to remove the unneeded words and statistics. You are better off formating the results in Word as a

Word table, or creating a new Table in Word. All tables must conform to ACS style: no vertical rules!

Error Analysis: Determine the 95% confidence limits of the physical or chemical constant you found during the data analysis. Compare your constants with the literature values and determine the accuracies (percent error). Did the correct answer fall within the confidence limits you computed? If not, why not?
This is the appropriate place to discuss determinate sources of error; that is, errors that could have thrown your value off either too high or too low. Generally, if the accepted value is outside your 95% confidence limits, then your experiment suffers from some determinate source of error, and you should attempt to find out what it is. Usually a few careful control experiments will help you track down the source of error. But you can't wait until you write your report to do that! You've got to think about it while you apparatus is ready!

Conclusions: Bear in mind that your conclusions are the most important part of the report. You do an experiment to answer a question about Nature. The answer to the question should be the focus of your conclusion. The preliminary sections of the report simply provide the reader with the background needed to accept your answer. ANSWER THE QUESTION!

A good way to organize your conclusion is to create a Toulmin analysis of your argument. Be explicit about your claims, your warrant, and your data (or grounds). The discussion of your data will be clearer if you refer directly to tables, charts, pictures, observations, or graphs that appear earlier in the lab report. You first job is to make sure that readers will understand your claims and the reasons for your claims.

In addition, use the conclusion to think about the physical and chemical implications of your results. When you believe your results answer the question put to Nature, you should try to understand the physical and chemical meaning of your answer: Does the structure of the molecule under study explain the result? In other words, why did you get the answer that you got? Mention other questions that remain unanswered, and propose further experiments that could answer them. Could you do the same experiment on a different compound, or a different experiment on the same compound, that would answer other questions? Many bad lab reports are written because students don't think about the meaning of their results.

A Common Pitfall: The "Quality of the Data" Conclusion. Your conclusion should not say that you got "perfect" data or good data or acceptable data or bad data. The goal of the experiment is to answer a question about Nature, not to obtain "perfect" data. Getting "perfect" data is impossible! Getting "perfect" data or even good data does not make you a scientist. You are a scientist when you ask questions about Nature and design experiments to answer them. Many students misuse their conclusion in an attempt to explain why their data are bad or untrustworthy, so that they can avoid answering the question put to Nature. This will not be permitted!
Random error exists in all experimental data -- multiple measurements and signal averaging will slowly remove random error from your results. Much more insidious is determinate error -- the way to find out if determinate error exists is to run little control experiments throughout the

course of the experiment. Ask yourself at every stage of the experiment, "Does this make sense? Can I believe these results?"

Data that are so "bad" that they do not answer the question will not be accepted. If an experiment is incapable of producing data good enough to answer the question, you must find out why. Therefore, you must repeat an experiment until it answers the question put to Nature, or until you understand why it cannot.

Literature Cited: Be sure to cite the sources of your lab procedure, your data analysis, and any chemical information that you mention in the introduction and conclusion. I am particularly looking for citations to related information you got from physical chemistry textbooks, physical chemistry laboratory textbooks, and articles in the Journal of Chemical Education. As a general rule you should follow the citation conventions that you see in the Journal of Chemical Education. Be aware that these conventions will surely be different from those you had to use in earlier writing classes. Consult the ACS Style Guide or ask me if you have questions!

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MATTERS OF STYLE: Write your report so that your intended audience is other physical chemistry students. This shouldn't be hard, since you will probably read a few old lab reports before you do the experiment, and remember that your lab partner must read your report.

Sime has some good recommendations on matters of continuity and style, tense, voice, grammar, numbers, and proofreading. Here's a quick summary:

Introduce tables and figures with one or two descriptive sentences above their location in the report. Use the text below the table or figure to describe its meaning and significance.

Conjunctive Adverbs such as "above all", "rather", "therefore", and "however" will help your reader connect sentences and ideas. Sime has more examples.

Keep your language simple. Try to use short, common words and simple phrases. Avoid fancy words and fuzzy phrases. Sime has many examples of fancy words/phrases and simple alternatives; here are just a few:

FANCY	SIMPLE
ascertain	find out
endeavor	try
modification	change
utilize	use
due to the fact that	because
on account of	because

in order that	so
it is obvious that	obviously

Report your work in the Past Tense.

Use the passive voice throughout your description of the experimental procedure.

"10 mls of the NaOH solution were pipetted into the test tube and shaken until a precipitate formed. The preciptate was collected by filtration on ashless filter paper." Notice that we avoid "I did this" and "then we did that"; after three or four sentences of that stuff, you get this "sing-song" sound to the report that is difficult to read.

Watch out for dangling participles.

Passive voice descriptions of experimental procedures can become infected with dangling participles.

"Using a 10 ml pipette, NaOH solution was added." It's a dangling particple because the solution cannot use a pipette!

Switch to a prepositional phrase, or, on some occasions when clarity demands, switch to the active voice.

"10 ml of NaOH solution were added with a pipette." OR "Using a 10 ml pipette, we added NaOH solution."

Report published results and accepted theories in the Present Tense.

"The voltage of electrochemical cells is predicted by the Nernst equation."

"Ethanol is a more polar solvent than hexane."

"The Nernst equation describes the relationship between cell voltage and chemical concentrations."

"Substitution reactions on primary halides take place *via* the S_N2 mechanism."

Report your conclusions in the Present Tense.

"Our results show that NaOH is a stronger base than NH_3."

"We found that azulene's heat of combustion is higher than that predicted using simple bond energies."

"Our results indicate that the unknown is iron sulfate."

"We believe that the hgher temperatures resulting from the malfunctioning temperature controller caused the product to decompose."

Use the active voice during the introduction and conclusion.

Transitive verbs will help you out of the passive voice trap: "Our results indicate ..."; "My experiments show ..." "Our control experiment proved ..." These are stronger, clearer sentences that make for better reading. (I have no objection to personal pronouns in your lab reports; there's nothing wrong with an occasional "I" or "we". CS)

Proofread a paper copy. Try reading the paper out loud.

Summarized from Rodney J. Sime, *Physical Chemistry: Methods, Techniques, and Experiments*, Saunders College Publishing, 1990. Chapter 8, pages 165-175.

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CRAZY EXCERPTS: Try to avoid writing nonsense such as these examples of logical slips and brilliant bull, which are taken from real p chem lab reports. I've included the comments I wrote in the margin of the report:

Means testing [of chloride percentage] is used to determine if the [unknown] sample is the same as the known ...
Means testing cannot prove that two substances are identical. Two different chemical compounds could have the same chloride percentage.

... it was evident that our temperature readings were higher than expected.
By how much? Don't leave your reader hanging by leaving out a crucial detail.
... we can attribute this systematic error to improper thermometer calibration.
Any assumption such as this should be tested independently. Check the thermometer in an ice bath and in boiling water. See the note above about Error Analysis!

Raw Data
weight of hydrochloric acid = 0.734 g
I know you didn't weigh out the hydrochloric acid solution! That can't be "raw data"!
moles HCl = 0.20 moles
Watch out for zeros and sig figs! 0.734 g HCl = 0.0201 mole HCl

Heat capacity assumes ideal gas behavior as well as a reversible gas.
How do you shift gears on an ideal gas? Processes are reversible, not gases!

CO_2's trigonal planar configuration ...
Carbon dioxide is linear. Check your Gen Chem book!

Raw Data

trial	mass	volume	calculated molecular weight
1	.0912 g	37.14 ml	60.34 g/mole
2	.1018	42.33	59.09
3	.1008	45.45	54.49

The volume of a gas sample will be proportional to its mass. In the calculation of molecular weight, we divide by volume. Therefore the third molecular weight value is low because the volume is too large.

... acetone could have inhibited vapor molecules from displacing water in the burette, thus resulting in a volume for the third trial that was too low.

The volume's too large, not too small! Your explanation is meaningless!

Raw Data

trial	barometric pressure	temperature
1	745.74 mm Hg	20.6 C
2	745.74	20.6 C
3	745.74	20.6 C

... temperature and barometric pressure were closely watched during the experiment. They remained approximately constant through all trials performed.

Why did you say "approximately"? They never changed at all!

Possible causes of error in this experiment were variations in the barometric pressure, the temperature, ...

What variations? Your data denies the existence of changes in temperature and pressure. You are contradicting yourself.

Error Analysis

The percent error in this experiment was quite large. It was calculated as follows: % error = [(26.69 - 17.74)/26.69] x 100% = 33.53%. However, it is hard to say how accurate this experiment can be. There exists no value with which to compare our experimental value.

You have just contradicted yourself; percent error **is** a measure of accuracy.

All three trials fell within the 95% confidence limit.

Completely unsurprising! The important question is, does the accepted literature value fall with in the the confidence limits.

The reason for the large variance is because the trial is so far off from the actual molecular weight, due to a high standard deviation.

Statistical nonsense! Variance is just the square of the standard deviation, so if one is high, the other will be too. This statement confuses accuracy and precision--it suggests that bad accuracy causes bad precision.

... the average of the three trials differed from the accepted value by only 3.56%. However, when you take a closer look, the results from sample 3 should disturb you. It differs by 9.33% from the mean.

Whoa! Why did you switch from comparing against the accepted value to comparing against the mean?

This shows that the results from the other two trials are good enough to save the combined results.
Statistical nonsense! Results cannot "save" other results. Many repetitions of an experiment allow random errors to cancel out when the average is computed. That's not salvation!

... because the reciprocal of temperature is taken, a small error in the temperature means a huge error in the reciprocal.
Sounds like what you need is a big error in temperature so you'll get a small error in the reciprocal!

In retrospect, we shouldn't have been so zealous to get as many points on the graph. We should have had fewer points ... More actual points would fall on the best straight line in this case.
Great idea! You should probably have gotten just two points, so that they will both fall exactly on the best straight line!

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