

Chemistry 309 - Physical Chemistry I
Fall 2007

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Office Hours: I am usually in my office by 9:00 A.M. and stay at least until 6:00. Please feel free to stop by for help at any time. If I cannot help you immediately, I will make an appointment for you to come by later, on the same day if possible. If I am not in my office you can reach me by e-mail or by phone for an appointment.

Prerequisites: Chemistry 141, Math 212 and Physics 132, 133 or 134. Chem 317, Math 235 (Calculus III) and Math 240 (Differential Equations), while not required, are strongly recommended.

Text:

Required: Peter Atkins and Julio DePaula, Physical Chemistry, Eighth Edition, W. H. Freeman, New York, 2006

Recommended: Physical Chemistry requires a lot of mathematics. You should have a solid command of your introductory calculus. Many of you will need to refer to your calculus book for help with differentiation and integration. In addition, we will be using mathematics beyond Math 211-212. In each case I will teach you the necessary math, but many of you will find it useful to have a reference available. The bookstore or online booksellers carry two inexpensive series that you may find helpful. They are the Schaum Outline Series, which includes volumes on Calculus, Differential Equations, Partial Differential Equations, Linear Algebra, and Advanced (Multivariable) Calculus, and the Essentials Series, which includes three volumes on Calculus, two on Differential Equations, and one on Linear Algebra. At the very least you should have either your book from Mathematics 211-212 or the Schaum Outline volume on Calculus.

Tentative Course Schedule: During our two semesters, we will be attempting to answer two very broad questions. The first is "What controls a chemical reaction?" This can include such diverse questions as where an equilibrium lies and what happens to the energy introduced into a molecule during a reaction. The second is "What makes some states of matter stable and others reactive?" It subsumes other questions like, "What causes some reactions to occur while others don't?" Alternatively, we could ask "What governs the stability of mixtures?" As we explore these questions in the course of our two semesters, we will be following a grand circle. We will begin with macroscopic treatments of chemical phenomena, using the tools and postulates of Equilibrium Thermodynamics. Toward the end of the semester we continue with macroscopic physical chemistry, but will turn to matter in a state of change, the

study of Chemical Kinetics. At the beginning of the second semester we will turn to the microscopic world of atomic particles, atoms and molecules, which is ruled by Quantum Mechanics. We will then develop tools to take the results of Quantum Mechanics and use them to understand molecular spectroscopy, the interaction of molecules with light. Finally if time allows, we will use statistical methods to apply the results of quantum mechanics to a microscopic theory of chemical reactions, Chemical Dynamics.

Our tentative course schedule for the first semester is:

Lecture	Date	Chapter	Topic
1	8/27	Ch. 1.1	Review Syllabus; General Description of Physical Chemistry; Systems; Types of Variables
2	8/29	Ch. 1.2	State Variables; Zeroth Law of Thermodynamics; Ideal Gas Equation of State
3-4	8/31-9/3	Ch. 1.3-1.4	Real Gases; Critical Point; Equations of State for Real Gases; Introduction to Math for P-Chem
5-6	9/5 - 9/7	Ch. 2.1-2.3	Work; State Functions; Path Functions; Reversibility; First Law of Thermodynamics
7-8	9/10-9/12	Ch. 2.4, 2.10, 2.11	Heat; Non p-V work; Canonical Variables; Formal Definition of State Functions; Perfect Differentials
	9/14		Rosh Hashana – No Class
9	9/17	Ch. 2.4, 2.5	Calorimetry; Heat Capacity; Molecular Basis of Heat Capacity
10	9/19	Ch. 2.5 – 2.12, Further information 2.2.	Enthalpy; $C_p - C_v$; Joule Experiment; Joule-Thompson Experiment
11	9/21	Further	Adiabatic Processes

		information 2.1	
12	9/24	Ch. 2.7-2.9	Thermochemistry; Kirchoff's Law
	9/26		Test One
13	9/28	Ch. 3.1-3.2	Carnot Cycle; Discovery of Entropy
14	10/1	Ch. 3.3	Entropy; Entropy Calculations; Second Law of Thermodynamics
15	10/3	Ch. 3.4	Temperature Dependence of Entropy; Third Law of Thermodynamics; Debye Extrapolation; Statistical Approaches to Entropy; Standard Third Law Entropy; Entropy of Reaction
16	10/5	Ch. 3.5-3.6	Gibbs Energy; Hemholtz Energy; Physical Meaning of Gibbs and Hemholtz Energies
17	10/8	Ch. 3.7, 3.8	Fundamental Equation of Thermodynamics; Maxwell Relations; Thermodynamic Square
18	10/10	Ch. 3.9	Thermodynamic Equations of State; Pressure Dependence of Free Energy; Chemical Potential
19	10/12	Lecture Notes	Reduction of Partial Derivatives
	10/13-10/16		Fall Break
20	10/17	Further information 3.2, 4.1, 4.3	Chemical Potentials of Real Gases - The Fugacity; Phase Diagrams
21-22	10/19-	Ch. 4.2,	Thermodynamic Treatment of Phase Boundaries;

	10/22	4.4-4.7	Derivation of the Clausius-Clapeyron Equation; First and Second Order Phase Transitions
23	10/24	Ch. 5.1-5.2	Partial Molar Quantities; Thermodynamics of Mixing
24	10/26	Ch. 5.3-5.4	Chemical Potential of Liquids; Chemical Potential of Ideal Liquid Mixtures; Henry's Law; Raoult's Law; Thermodynamics of Ideal Solutions
	10/29		Test Two (This test will cover material only up to lecture 23 on 10/24.)
25	10/31	Ch. 5.6-8.8	Chemical Potentials of Real Solutions; Activities
26	11/2	Ch. 5.9	Ionic Activities; Mean Activity Coefficient; Debye-Huckel Equation
27	11/5	Ch. 5.5, 6.2	Fractional Distillation; Boiling Point Elevation; Osmotic Pressure, Gibbs Phase Rule
28	11/7	Ch. 7.1-7.2	Reaction Gibbs Function; Extent of Reaction; Reaction Gibbs Function and Equilibrium Constants
29	11/9	Ch. 7.2	Chemical Equilibria in Real Gases and Solutions
30	11/12	Ch. 7.3-7.4	Temperature Dependence of K; Pressure Dependence of Equilibria; Le Chatelier's Principle
31	11/14	Ch. 22.2	Introduction to Kinetics; Rate of Reaction; Simple Rate Laws; Order of Reaction
32 - 33	11/16-11/19	Ch 22.1, Ch 22.3-22.4	Determination of Rate Laws; Integral Rate Equations; Half Lives; Rate of Approach to Equilibrium
	11/21-11/25		Thanksgiving Break

34-35	11/26- 11/28	Ch. 23.1- 23.2,	Chain Reactions
	11/30		Test Three
36-37	12/3-12/5	22.6-22.8	Mechanisms and Rates Laws
38	12/7	Ch. 22.5	Temperature Dependence of Reaction Rates
	12/14 or 12/17		Final Exam 9:00 A.M. to 12:00 Noon 12/14or 2:00 P.M. to 5:00 P.M. 12/17 or self-scheduled between December 10 and December 13th.

Next semester we will be covering atomic and molecular structure, spectroscopy, statistical thermodynamics, and advanced topics in kinetics.

Tentative Test Schedule

There will be three hour exams and a final exam. The final exam can be taken at 9:00 A.M. on Friday, December 14th, at 2:00 P.M. on Monday, December 17th, or can be self scheduled between December 10th and December 14th. If you choose to self-schedule the exam, you may either take the exam in the P-Chem lab, or must make your own arrangements for a place to take the exam, and must make arrangements with me at least two days before you plan to take the exam. The final exam will be cumulative. The three one hour exams are tentatively scheduled for September 26th, October 29th and November 30th. Tests will cover all material up to the day of the exam.

Notebook

This semester you will be given the option of keeping a double entry notebook on your reading. The notebook must be a bound notebook, with each page divided vertically in half. On the left-hand side you are to summarize what you have read in a given section of the text, while on the right hand side you are to write a response consisting of questions, comments or ideas that arise from the reading. I will grade this notebook at the end of the semester. The notebook grade will be based on completeness (did you do all the chapters?), on the accuracy and clarity of your summaries, and on the thoughtfulness of your responses. Up to 3.5 points of extra credit added to your final grade can be earned for completion of the notebook.

Grading

Homework, the one hour exams, a final exam and the laboratory will be the basis for the course grade. The weighting for each of these components is as follows:

Homework:	10%
Three One Hour Tests:	45%
Final Exam:	20%
Laboratory:	25%

The grades for each of the one hour exams and the final exam will be based on a modified curve. This means that a traditional bell curve grading distribution will be my lower limit. If, for example, on examining the papers which would correspond to a C on the tradition curve, I feel that they are B work I will modify the curve to reflect this. I have no objection to assigning all A's if everyone does excellent work.

Homework

Regular completion of homework problems is essential in mastering physical chemistry. This is especially true since it will take time and practice for you to translate mathematical expressions into physical and chemical intuition.

Each homework assignment will be a selection of problems from Atkins and DePaula. You are to attempt to complete all problems. After you have completed a problem or worked until no further progress is possible, having worked at least 20 minutes on the problem, compare your results with at least one other person in the class, and try to work it out together. If this fails, look up the answer in the solution manual on reserve in the library. Then mark on your homework report the problem number, the time spent, the person you consulted with and whether the problem was worked correctly.

Homework reports and homework will be due each Monday at the beginning of class. Every one who attempts all problems for the week and turns in their homework report on time will receive full credit. Late reports will not be accepted. It is particularly important that you be completely frank about whether or not you have successfully completed a problem: it won't hurt your grade and it may be my only clue that you need help.

Collaboration on the problems from Atkins and DePaula is strongly encouraged. A group of three to four people working together and discussing both the lecture materials and the problems together is often ideal. Talking through material is an excellent way to improve your comprehension or to zero in on areas in need of clarification. However, each of you knows how she or he works best and you should work in the way that you are most comfortable.

Attendance

You are expected to attend class. You are responsible for all material covered in class. If you miss a lab for what I deem a valid reason (illness, etc.), I will try to arrange for you to make up the lab. However, anyone who misses a lab without an excuse will be given a zero for that exercise, and will not be given an opportunity to make up the lab. No test makeups will be given. A missed test will count zero unless you are excused for a valid reason. I will determine the validity of the excuse. If you miss a test but are excused, the next test will count double. Please let me know if you have advance knowledge of missing a test or a lab.

Honor Code

The Richmond College and Westhampton College Honor Codes are very special and have the full support of this department. You will be expected to sign an honor pledge on each test We expect that behavior in this class will be consistent with this code. However, collaboration on homework is allowed and encouraged.