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Dr. Jonathan Gutow

Class Web Site: http://www.uwosh.edu/faculty_staff/gutow/Chem_370_F08/P-Chem_Home.html

Course Overview: Physical chemists and physicists make extensive use of mathematical models to describe natural phenomena. The underlying assumption is that the universe has an organization that can be expressed as a function of certain parameters. This semester we will concentrate on developing the models that describe the bulk thermodynamic and equilibrium properties of matter. We will make the connection between the microscopic (molecular level) properties of substances and these bulk properties using results from quantum mechanics.

You should be able to use these models to predict the behavior of matter. This means both estimating the range in which a measurement will fall and solving mathematical story problems, using approximations where valid. A summary list of the models and the types of systems to which you should be able to apply them is at the end of this syllabus.

Laboratory experiments will illustrate concepts being discussed in lecture and familiarize you with many of the tools used by physical chemists. The tools you will learn to apply include the chemical literature; written and oral communication; mathematical functions; error analysis; and mechanical and electronic equipment such as vacuum pumps and computers.

Required Texts: Atkins & de Paula, Physical Chemisty, 8th Edition

Barrante, Applied Mathematics for Physical Chemistry, 3rd edition.

Required Equipment: bound duplicating laboratory notebook, pen (for writing in lab notebook), scientific calculator and goggles.

Prerequisites: three semesters of calculus (Calc III may be concurrent), two semesters of calculus based physics (second semester may be concurrent).

Class times: Lectures: MWF 10:20-11:20 (HS 310); Lab: W 1:50 - 5:10 (sec 1, HS-428), Th 1:20 4:30 (sec 2, HS-428).

Office Hours: Dr. Gutow (HS-412): M 3-4, TTh 9:10-10:10, WF 8:30-9:30 or by appointment.

Reading Assignments: A study sheet will be distributed approximately weekly, listing the specific reading assignments.

Critical Thinking Exercises: Short assignments designed to help you learn how to use the textbook and other reference sources to prepare for class. For example, you might be asked to find definitions, compare two models and explain when it is appropriate to use each or work through some 'what if' calculations. Some in-class group worksheets will also be used. In general a group of these will be handed out with the reading and homework assignments. Each exercise is to be finished for a specific class. Since the primary goal of these exercises is to help you learn how to prepare for class the majority of these assignments will be given out during the early part of the semester. A copy is due at the beginning of the class for which they are assigned. They will be graded on a pass/fail basis and are worth 5 points each. Up to 50 points may be received for these exercises. A minimum of twelve such assignments will be given during the semester. You are encouraged to discuss these assignments with your classmates as well as the instructor.

Homework: Homework will be distributed with the reading and critical thinking assignments. Homework will consist of "discussion" and "exercise" questions, which are straightforward practice with definitions and equations, plus "problem" questions, which require more involved application of concepts and problem solving. The "discussion" and "exercise" questions will be graded as attempted/not attempted out of 5 pts total. The "problems" will be graded out of 20 pts total. Discussion of the homework with your classmates and instructor are encouraged. If you are

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having trouble with particular types of problems try additional questions of a similar type. Numerical answers to many of the "exercises" and "problems" are available in the textbook appendices. Detailed solutions to most "problems" will be provided on the class web site two days

after the homework due date. The best 10 out of 12 homeworks will count for your grade. Doing

ALL the homework is the best way to prepare for exams in this class.

Homework is due in class on the day specified when handed out. Late homework will be marked down 10%/day. No homework will be accepted after the detailed answer key has been posted on the class website two days after the due date.

Exams: There will be three exams worth 200 points (plus 20 pts extra credit). The exams will be written to be completed in one hour, but you will be given unlimited time. The first two exams will be administered in the testing center and the last exam will be administered in a classroom at a time to be arranged. The material requires that exams be cumulative, but primary emphasis will be on the chapters covered since the previous exam. The goal of this course is not to memorize formulas, but to learn how to use models to make predictions. You will be provided with an equation sheet for each exam consisting of the fundamental equations of each model. Additionally, you will be allowed to bring a 3" x 5" card of *handwritten* notes to the exam. There will also be a 90 minute laboratory exam (see the lab section of the syllabus for more details).

Grading:

Critical Thinking Exercises:	$10 \times 5 \text{ pts} =$	50 pts
Graded Homework:	$10 \times 25 \text{ pts} =$	250 pts
Exams:	$3 \times 200 \text{ pts} =$	600 pts
Lab	300 pts	300 pts
Total:		1200 pts

Additional Resources:

WEB RESOURCES: This syllabus, copies of homework assignments and answer keys will be available at the course web site. The course web site may be accessed by starting at the instructor's home page: http://www.uwosh.edu/faculty_staff/gutow/. Problem sets and answer keys will be password protected. The username for login into the protected part of the web site is: chem370F08. The password will be supplied the first day of class.

TEXTS: The following books are on reserve in in the Halsey Resource Center (HS-289). You may find it useful to see difficult concepts described a number of ways. Homework assignments will suggest sections of these texts to look at for additional help.

Barrante, *Applied Mathematics for Physical Chemistry* QD455.3.M3 B37. A good review of chemical applications of graphing and calculus.

Barrow, *Physical Chemistry*. Contains good descriptions of statistical mechanics without detailed quantum mechanics.

Warren, *The Physical Basis of Chemistry*, QD475.P47. This book has nice simplified, but accurate, descriptions of many of the quantum, spectroscopic and thermodynamic concepts we will discuss.

Nash, *Elements of Statistical Thermodynamics*, QC311.5.N3. This is a little pamphlet that very lucidly develops the underlying concepts of Statistical Thermodynamics.

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Lecture and Homework Schedule:

Chapter	<u>Lectures</u>	<u>Homework Due</u> *	
I. Classical Thermodynamics			
1: Properties of Gases	9/3, 9/5	9/10	
2: The First Law	9/8 - 9/22	9/17, 9/24	
3: The Second Law: the concepts	9/24-10/3	9/29, 10/6	
Review	10/6		
Exam 1 (Unit I)	Wednesday, October 8, 2008	1	
II. Stati	stical Thermodynamics		
Introduction to quantum mechanics	10/10		
16: Statistical Thermodynamics:	10/13, 10/15	10/17	
the concepts			
17: Statistical Thermodynamics:	10/17, 10/20	10/22	
the machinery			
4: Physical transformation of pure substance	10/22, 10/24	10/27	
5: The properties of simple mixtures	10/27 - 10/31	11/3	
Review	11/3		
Exam 2 (Unit II)	Wednesday, November 5, 2008	1	
III. Equilibrium and Transport			
7: Chemical Equilibrium	11/7-11/14	11/17	
21: Molecules in motion	11/17-11/21	11/24	
24: Macromolecules	11/24, 12/1, 12/3	12/5	
25: Processes at Solid Surface	12/5, 12/8	not due	
Review	12/10		
Exam 3 (Unit III)	Friday, December 12, 2008	1	

^{*}The homework will generally be handed out during the first lecture on each chapter.

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Laboratory

Laboratory Notebooks: Notebooks should be records of everything a scientist does. They are used as legal evidence that an experiment was performed in patent claims and are often referred to by other scientists working on related experiments. Entries should be made in permanent ink. *Notes from pre-lab lectures should not be recorded in your notebook*, but all calculations and data analysis should be. A minimum checklist of what should be in your notebook is available on the class web site. Pages should be numbered consecutively and a table of contents included. Date each page as it is used and start a new page on each day; do not tear out pages, simply draw a line through errors. Lab notebooks will be checked each day and initialed by your instructor. You will turn in your duplicate pages for grading with each lab report.

Pre-lab preparation: Read the description of the experiment and any additional assignment. The experiments are not described as a list of steps to be followed, so careful reading and reflection before lab will be required to develop a plan for the project.

In your notebook record a brief outline of the procedure you expect to follow and construct two tables of information: 1) reagents; 2) equipment. In the reagents table write the chemical name, chemical formula, a drawing of the structure, the state in which it will be found (solid, liquid, gas, or in solution), and hazard information from the Material Safety Data Sheet(s), which are available online or in the stockroom. If solutions are to be prepared, calculate the amounts needed. Each row in the equipment table should contain the property to be measured, the equipment used for the measurement, and the sample(s) that will be measured.

During lab: Procedures actually followed should be described in your laboratory notebook. Do not rely on a summary written before the lab, although you may just note deviations from your planned procedure. List lab partners. Include all experimental observations, data and calculations; you should tape in computer printouts and spectra (cut or fold to fit). If data is stored in computer files accurately record the data file names. Goggles and appropriate clothing (no sandals or shorts) must be worn at all times. Failure to wear safety goggles may result in ejection from lab and an F in the course.

Lab Reports: Because scientists use many formats for communicating information, we will practice a variety of report styles this semester.

- 1. <u>Formal laboratory reports</u>: Your reports should be written as if for publication in *The Journal of Physical Chemistry*. Assume that your readers have studied physical chemistry but are not familiar with your handouts. A sample lab report is available on the class web site. Additional recommendations on word choice, grammar, reference format, notation and nomenclature may be found in *The ACS Style Guide*, J. S. Dodd, Ed. (QD8.5.A25) which is on reserve in the Halsey Resource Center.
- 2. <u>Feature article for a newsmagazine</u>: This is aimed at the general public so should connect the experiment to more common experiences. The length should be two to three typewritten pages plus one or two figures or graphs. Sample calculations and error analysis are not to be part of the article but should be attached for grading.
- 3. <u>Poster presentation</u>: This is the way most scientific work is communicated at meetings. Posters must be eye-catching and informative. Keep text to a minimum. You must have: a title, author's name, an introduction, a body (consisting mostly of tables and figures with appropriate captions), a conclusion and references.
- 4. Oral report: Over the course of the semester groups of students will work to prepare a 10

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minute presentation on one laboratory. The instructor will assign a topic and a date for the oral presentation for each group. Each group member will present a part of the report (Introduction, Experimental, Results/Discussion) The time limit means it will be a summary of the material in a formal report. Overhead transparencies or PowerPoint^a should be used as visual aids.

5. <u>Peer Review</u>: All articles published in the literature are reviewed by anonymous reviewers. They are only published after the reviewers are satisfied that they are accurate, well written and a new contribution to the scientific body of knowledge. Most articles are rewritten at least once in response to reviewers' comments. Often additional experiments are also done. You will review two of your peers' formal lab reports for each formal report that is due and rewrite your reports based on the reviews returned to you.

Students may discuss the write-up and calculations with each other but every student must turn in an individual report. Reports must be typed or computer word processed. Use of computers for data plotting and analysis is encouraged as is reference to the chemical literature for accepted values.

Reports will be graded as follows: 9 points on writing, 10 points on calculations including error analysis, 1 point for literature search/comparison with the literature. A copy of the grading cover sheet for formal reports is attached to this syllabus. The criteria are:

- 1. Does the report contain all the sections (abstract, introduction, experimental method, results, discussion)? Is the information logically distributed among the sections?
- 2. Is sufficient information given in experimental methods for another physical chemistry student to repeat the experiment without referring to your handouts?
- 3. Have all the discussion questions been answered?
- 4. Are the spelling and grammar correct? Is verb tense consistent (present or past)? In general past is appropriate unless referring to data presented in the report. Is the voice correct? Most scientific articles are in the passive voice. For example: instead of, "we did the experiment three times," write, "the experiment was done three times." Note that the implied "by " is left out.
- 5. Are the equations used in calculations included? Are there any errors in the calculations? Are the significant figures carried correctly? Are the error estimates reasonable?
- 6. Was a literature search performed? Is a copy of the title/author/abstract found in the search attached. You may use the references supplied in handouts or the text for actual comparison, but you must perform a literature search using SciFinderTM and provide at least one abstract found this way from an appropriate reference.

The reviews will be due the lab day after the reports were originally due. You may rewrite reports based on the reviews. If you turn in the rewritten report within <u>one week</u> of getting the reviews, the grade will be recalculated as the mean average of the original and rewritten reports. A copy of one of your reports, the best, will be kept for your student portfolio. Thus you should rewrite at least one report. Turn in **three** copies of the initial version of your formal reports and **two** copies of rewritten reports with the original graded version attached. Reviews of classmates' reports are worth 2 points each.

Reports are due in class the week following completion of the project. Late reports will be marked down 10%/day. Incomplete reports will be returned and the late penalty assessed.

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Laboratory Exam: There will be a 90 minute final exam based on work done in lab. You will be able to refer to your textbooks, lab reports, and lab notebooks on the exam. The 90 minutes alloted for the exam will not be enough to figure out what you did from your text and your lab reports. You will only have enough time to use them as references to get constants, formuli and relationships correct. You will need to review your laboratory reports and correct any mistakes you made in order to do well on this exam. You will also be responsible for material from the prelabs and assigned reading. Two non-graded problem sets will be distributed during the semester to assist your preparation for the exam.

Grading:

10 library worksheet

 $6 \times 5 = 30$ pre-laboratory preparation

 $6 \times 5 = 30$ laboratory notes $6 \times 2 = 12$ reviews of reports

 $6 \times 20 = 120$ laboratory reports (one is a poster)

 $1 \times 10 = 10$ oral report

 $1 \times 10 = 10$ statistical mechanics worksheet

78 final exam

300 points total

Lab Schedule:

Week of	Project	Written	Review	Rewrite	Oral
9/1	Library Assignment	9/8 (Data Sheet)	-	-	-
9/8	Real and Ideal Gases	-	-	-	-
9/15	Real and Ideal Gases (continued)	9/22 (formal)	9/29	10/6	10/6
Rotate through 2 labs (Heat of combustion, Solution Calorimetry)					
9/22	Comb/Sol'n	-	-	-	-
9/29	Comb/Sol'n	10/13 (formal)	10/20	10/27	10/27
10/6	Sol'n/Comb	-	-	-	-
10/13	Statistical Mechanics Worksheet	10/13	-	-	-
10/20	Sol'n/Comb	10/27 (article)	-	-	11/10
Rotate through 2 labs (Partial Molar Volume, Refractometry and Viscometry)					
10/27	PMV/RV	-	-	-	-
11/3	PMV/PMV	11/10 (formal)	11/10	11/17	-
11/10	RV/PMV	11/17 (poster)	-	-	12/1
11/17	Electrochemistry	-	-	-	-
11/24	no laboratory	-	-	-	-
12/1	Electrochemistry (continued)	12/8 (formal)	-	-	-
12/8 90 min Lab Exam (exact time to be arranged)					

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Assessment of Learning: As part of the department's assessment of its majors program, evidence will be added to your portfolios to demonstrate your ability to do a number of things.

From Lecture:

- 1. describe the structure and composition of matter;
- 2. apply theoretical and mechanistic principles to the study of chemical systems employing both qualitative and quantitative approaches;
- 3. use theories of microscopic properties to explain macroscopic behavior;
- 4. explain the role of energy in determining the structure and reactivity of molecules;
- 5. use mathematical representations of physical phenomena.

From Lab:

- 1. read and follow experimental protocols;
- 2. properly set up and safely manipulate laboratory equipment;
- 3. plan and execute experiments, including the use of the chemical literature;
- 4. maintain accurate records of experimental work;
- 5. analyze data statistically and assess reliability of results;
- 6. prepare effective written scientific reports;
- 7. use mathematical representations of physical phenomena;
- 8. use and understand modern instrumentation;
- 9. use computers for chemical applications;
- 10. retrieve specific information from the chemical literature;
- 11. work cooperatively in problem solving situations.

Models you will learn to apply:

Models	Be able to apply to
Gas Laws	Pure Gases
-Ideal	Gas Mixtures
-van der Waals	To simplify thermodynamic models
-Virial Expansion	
Kinetic Molecular Theory	Gases (molecular speeds and energies)
Quantum Mechanics	Particle-on-a-line, Particle-in-a-box, Particle-on-a-ring
	Allowed energies (Translation, Rotation, Vibration, Electronic)
	Boltzmann Distribution (most random distribution)
Classical Thermodynamics	Reaction enthalpies, entropies and free energies ($\Delta H, \Delta S, \Delta G$)
-fugacity/activity	Constant pressure (isobaric) phenomena
-Maxwell Relations	Constant temperature (isothermal) phenomena
-Colligative Properties	Heat engines (adiabatic versus isothermal processes)
	Equilibria (Phase, Electrochemical, Chemical)
	Physical changes (phase)
	Mixtures (Fp, Bp, vapor pressure and Osmotic pressure changes)
Statistical Thermodynamics	Heat capacities (C_p versus C_v)
	Entropy of matter
	Equilibria
	Chemical reactions
	Physical changes
	Classical thermodynamics
Transport	Diffusion, Viscosity, Sedimentation, Electrochemistry, Electrophoresis
Surfaces	Adsorption isotherms

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ASSESSMENT GOAL #2 Laboratory Report Cover Sheet

Student:	
Course:	Semester/Year:
Skill Level Indicators N Novice: requires explicit guidance of instructor I Intermediate: performs with minimal guidance A Advanced: exhibits independence; may modify pro ne No Expectation in this area number in parentheses indicates maximum deduction Performance of experiment N I A	
Follow experimental protocols (N needs list of s	teps to follow; I plans steps from a general description; A
uses the literature to develop procedure)	
Laboratory Notebooks N I A /	5
Record data accurately (I numbers recorded; A a	additional observations)
Record procedures followed (N none; I minima	l; A work could be reproduced from notes)
Laboratory Report N I A/ 9	
Spelling/grammar (some -1, many -2, unreadable (-1/2)	e -3); vocabulary (-1/2); tense consistency (-1/2); voice passive
Organize material into standard sections (minor	problems -1/2, major problems -1)
Abstract: system studied; method used; importa	nt results (-1 if absent, no other deductions)
Introduction: what experiment will tell us (-1);	balanced equations for chemical reactions (-1)
Experimental: reagents (-1/2); equipment specification (-2, N)	fications/name (-1/2); procedures followed (only refers to text
Results: data is complete; displayed as table or	graph when appropriate (up to -1)
Discussion: significance of experiment (-1)); comparison to literature; answers to text questions (-1);
discussion of error sources (-1/2)	
Equations: complete description including defined in the complete description in the complet	nition of variables (some missing -1/2, many missing -1, most
References: complete; correct format	
Data Analysis and Interpretation N I A	_/6
Performs algebraic calculations: includes equations	ions;units (-1/2); sample calculations (-1); accuracy (up to -4)
Graphs data (N simple graph, I regression/curve	fitting) (up to -2 if missing)
Uses computer simulations/molecular modeling	
Assess reliability of results N I A/4	
Estimates error in measurements (N gives source	es of error (-2), I propagates errors
includes equations, sample calculations (-2))	
Significant digits (-1/2)	
Literature Search N I A / 1	
Finds appropriate references (provide abstract) (-1)
Compares literature results with own (-1)	