

Class Web Site: <http://www.uwosh.edu/facstaff/gutow/physical-chemistry-1>

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 Chemistry*, 9th Edition
Barrante, *Applied Mathematics for Physical Chemistry*, 3rd edition.
Chemistry 370 Lab Manual Fall 2011

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 9:10-10:10 (HS 208); *Lab (HS-428):* M 1:50 - 5:10 (sec 1), T 1:20-4:30 (sec 2).

Office Hours: Dr. Gutow (HS-412): MF 10:20-11:20 TTh 9-10, W 1:50-2:50 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 assignments will be worth 25 pts each. 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.

A randomly selected "discussion" or "exercise" question will be graded out of 5 pts. A randomly selected "problem" will be graded out of 10 pts. The remainder of each homework will be graded as attempted/not attempted out of an additional 10 pts. Discussion of the homework with your classmates and instructor are encouraged. If you are 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 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 x 5 pts =	50 pts
Graded Homework:	10 x 25 pts =	250 pts
Exams:	3 x 200 pts =	600 pts
Lab	300 pts	<u>300 pts</u>
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/facstaff/gutow>, or by following the direct link at the top of the syllabus. Problem sets and answer keys will be password protected. If you are registered for the class you will be able to use your campus e-mail login to access the password protected parts of the site.

SYMBOLIC MATH PACKAGES: The open source SAGE math package is available on the [Chem SAGE Server](#) or can be downloaded from the [SAGEmath web site](#) and installed on your personal computer. Information on user accounts on the Chem SAGE Server will be provided in class. MAPLE™ is available on the computers in the open access labs in Halsey.

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.

Lecture and Homework Schedule:

Topic (text sections)	Lectures	Homework Due*
I. Thermodynamics & Statistical Mechanics 1 (Energy)		
Properties of Gases (1.x, 20.1-20.3)	9/7, 9/9, 9/12	9/14
The First Law (2.1-2.2, 15.1-15.3)	9/14, 9/16, 9/19, 9/21, 9/23	9/19, 9/26
Heat Capacity, Work & Enthalpy (2.3-2.5, 16.2-16.4)	9/26, 9/28, 9/30, 10/3	9/30, 10/5
Review	10/5	
Exam 1 (Unit I)	October 6 or 7, 2011 (Th or F)	TBD
II. Thermodynamics & Statistical Mechanics 2 (Entropy)		
Adiabatic Processes & State Functions (2.6 - 2.12)	10/10, 10/12	10/14
Entropy and Ensembles (3.1-3.2b, 15.4-15.7, 16.7, 3.2c-3.4)	10/14, 10/17, 10/19, 10/21, 10/24	10/21
Free Energies and the Fundamental Equation (3.5, 16.1, 3.6-3.9)	10/26, 10/28, 10/31, 11/2, 11/4	10/31, 11/7
Review	11/7	
Exam 2 (Unit II)	November 8 or 9, 2011 (T or W)	TBD
III. Mixtures and Equilibria		
Simple Mixtures (5.1-5.5, 5.10-5.13)	11/11, 11/14, 11/16, 11/18	11/21
Equilibrium and E-Chem (6.1-6.2, 16.8, 6.3-6.9)	11/18, 11/21, <i>Thanksgiving</i> , 11/28, 11/30, 12/2	12/5
Molecular Interactions (17.1-17.10)	12/5, 12/7, 12/9, 12/12	12/14
Review	12/14	
Exam 3 (Unit III)	December 15 or 16, 2011 (Th or F)	TBD

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

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 included in the lab manual. 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. Formal laboratory reports: 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. **You will be required to use proper ACS formatting for your references this semester (examples are given immediately below).** 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.
 - *Journal Article:* Ref#. Authors *Journal Title* **Year**, volume, pages.
 1. Maniero, A. M.; Acioli, P. H.; Silva, G. M. e.; Gargano, R. *Chemical Physics Letters* **2010**, *490*, 123-126.
 - *Book Section:* Ref#. Authors *In Book Title*; Editors, Ed.; Publisher: City, Year; pages.
 1. Hiatt, R. In *Organic Peroxides*; Swern, D., Ed.; Wiley-Interscience: New York, 1971; Vol. 2, p 1-151.
 - *Book:* Ref#. Authors *Book Title*; Publisher: City, Year; pages.
 1. Adamson, A. W. *Physical Chemistry of Surfaces*; 5 ed.; John Wiley & Sons: New York, 1990; p 7-11.
 - *Web Reference:* Ref#. Authors, *Title* **Year**, Link accessed Date.
 1. Gutow, J. H. *Dr. Gutow's Atomic Orbital Viewer* **2006**, http://www.uwosh.edu/faculty_staff/gutow/Orbitals/CI/CI_AOs.shtml accessed Jan. 14, 2011.
2. Feature article for a newsmagazine: 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. Poster presentation: 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. Sample calculations and error analysis are not to be part of the article but should be turned in for grading.
4. Oral report: Over the course of the semester groups of students will work to prepare a 10

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™ should be used as visual aids.

5. Peer Review: 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. Is the formatting correct (margins, figure and table numbers and format, reference format, etc.)?
6. 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?
7. 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 SciFinder™ or another database 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 one week 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. **In an effort to save trees and facilitate reviews we will be using an experimental web site. Turn in a single electronic copy of each report to this web site before class.** Detailed instructions will be provided in class. Reviews of classmates' reports are worth 2 points each.

Reports are due before 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.

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

allotted 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, formulae 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 x 5 =	30	pre-laboratory preparation
6 x 5 =	30	laboratory notes
6 x 2 =	12	reviews of reports
6 x 20 =	120	laboratory reports (one is a poster, one is article)
1 x 10 =	10	oral report
1 x 10 =	10	statistical mechanics worksheet
	<u>78</u>	<u>final exam</u>
	300	points total

Lab Schedule:

		Week Due			
Week of	Project	Written	Review	Rewrite	Oral
9/12	Library Assignment	9/19 (Data Sheet)	-	-	-
9/19	Real and Ideal Gases	-	-	-	-
9/26	Real and Ideal Gases (continued)	10/3 (formal)	10/10	10/17	10/17
Rotate through 2 labs (Heat of Combustion, Solution Calorimetry)					
10/3	Comb/Sol'n	-	-	-	-
10/10	Comb/Sol'n (continued)	10/17 (formal)	10/24	10/31	10/31
10/17	Sol'n/Comb	-	-	-	-
10/24	Sol'n/Comb (continued)	10/31 (poster)	-	-	11/14
Rotate through 2 labs (Partial Molar Volume, Refractometry and Viscometry)					
10/31	Statistical Mechanics Worksheet	-	-	-	-
11/7	PMV/RV	-	-	-	-
11/14	PMV/PMV	11/21 (formal)	11/28	12/5	12/5
11/21	<i>RV/PMV</i>	11/28 (article)			
11/28	Electrochemistry	-	-	-	-
12/5	Electrochemistry (continued)	12/12 (formal)	-	-	-
12/12	90 min Lab Exam (exact time to be arranged)				

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 -Ideal -van der Waals -Virial Expansion	Pure Gases Gas Mixtures To simplify thermodynamic models
Kinetic Molecular Theory	Gases (molecular speeds and energies), Collision cross section
Quantum Mechanics	Particle-on-a-line, Particle-in-a-box Allowed energies (Translation, Rotation, Vibration, Electronic) Boltzmann Distribution (most random distribution)
Classical Thermodynamics -fugacity/activity -Maxwell Relations -Colligative Properties	Reaction enthalpies, entropies and free energies ($\Delta H, \Delta S, \Delta G$) Constant pressure (isobaric) phenomena Constant temperature (isothermal) phenomena Heat engines (adiabatic versus isothermal processes) Equilibria (Phase, Electrochemical, Chemical) Physical changes (phase) Mixtures (F_p, B_p , 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
Surfaces	Surface tension, surface pressure

Lab Report Grading Sheet on next page.

Formal Report Grading Sheet

Skill Level Indicators: **N** Novice: requires explicit guidance of instructor
 I Intermediate: performs with minimal guidance
 A Advanced: exhibits independence; may modify protocols to new conditions, instruct others
 ne No Expectation in this area

<i>CATEGORY AND CRITERIA</i>	<i>N/I/A</i>	<i>POINTS</i>
Performance of Experiment (N needs list of steps to follow; I plans steps from a general description; A uses the literature to develop procedure)		-----
Prelab (contains: outline of procedures, complete reagent table, complete equipment table, calculations for making solutions. A complete, I tables and procedures mostly complete or complete, N substantial parts missing)		/5
Notebook		
Record data accurately (I numbers recorded; A additional observations)		
Record procedures followed (N none; I minimal; A work could be reproduced from notes)		/5
Report		
Abstract: system studied; method used; important results		/1
Introduction: what experiment will tell us (-0.5); balanced equations for reactions (-0.5); what's known (-0.5); theoretical background/basis (-0.5)		/2
Experimental: reagents (-0.5); equipment specifications/name (-0.5); procedures followed (only refers to text -1.5, N)		/2
Results: data is complete; prose connects and explains progression between pieces of data; data displayed as table or graph when appropriate		/2
Discussion: significance of experiment (-1); comparison to literature; answers to text questions (-1); discussion of error sources (-1/2)		/2
Grammar & Report Format Deductions		
Spelling/grammar (some errors -1, many -2, unreadable -3); vocabulary(-0.5); tense consistency(-0.5) not using passive voice(-1/2)		
Organize material into standard sections (minor problems -1/2, major problems -1, N)		
Margins ~1", if too big or too small (-0.5), missing page numbers (-0.5) (not perfect N)		
Equations: not properly numbered (-0.5), complete description including definition of variables (some missing -1/2, many missing -1, most -1.5)		
Figures and Tables: not properly numbered (-0.5), captions missing (-1), captions incomplete or misplaced (-0.5), labeling errors (axes, headings, units, up to -1)		
References: missing superscript reference numbers in text (-0.5), not numbered in order of use in text (-0.5), not in ACS format (-0.5), not complete (-0.5)		
Data Analysis & Interpretation		
Performs algebraic calculations: includes equations; units (-1/2); sample calculations (-1); accuracy (up to -4)		/4
Graphs data (N simple graph, I regression/curve fitting)		/2
Uses computer simulations/molecular modeling		
Assessment of Reliability of Results		
Estimates error in measurements (N gives sources of error (-2), I propagates errors--includes equations, sample calculations (-2))		/3.5
Significant digits		/0.5
Literature Search		
Finds appropriate references (provide abstract)		/0.5
Compares literature results with own		/0.5
Report overall N/I/A and point total		/20

Poster Grading Sheet

Presenter Names: _____

Follows Experimental Protocols (N/I/A)

Prelab (N/I/A) _____ of 5 pts.

Notebook (N/I/A) _____ of 5 pts.

Visual Presentation/Format (2 pts). Score: _____

Format (2 pts)

Title/author list (0.5 pt). Score: _____

Text/Poster Size (1 pt). Score _____

References in appropriate format and with links when possible (0.5 pt). Score: _____

Grammar/Spelling/Content (5 pts). Score: _____

Calculations(6 pts). Score _____

(from handed in notebook pages and presented data)

Error Analysis (4 pts). Score _____

(from handed in notebook pages and as displayed on poster)

Literature Search (1 pts)

Compares Results with literature (0.5). Score: _____

Finds Valid Reference (0.5). Score: _____

Total for Poster (of 20 pts): _____