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.

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

Office Hours: Dr. Gutow (HS-412): MWF 11:30-12:30, TTh 10:30-11:30 or by appointment.

Reading Assignments and Homework will cover a week or two and will have parts due at the beginning of each class meeting. Assignments will not be accepted late, but some of your lowest scores will be dropped.

> **Reading Assignments** will come primarily from the textbook. Other sources will be used as necessary.
>
> **Homework** will be due for each class and consist of three sections of one or more questions each. The first two sections will focus on material we will be discussing during the class meeting for which the assignment is completed.
>
> > **Critical Thinking Exercises/Discussion Questions:** The questions are 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.
> >
> > **Practice Exercises**: These will come primarily from the exercises section at the end of the chapter. The goal is to help you figure out what you need to ask about in class.
> >
> > **Problems:** These problems will be a little more challenging and based on material discussed in the previous class.

Exams: There will be 220 available points on each exam. However, exams will be scored out of 200 points (20 pts of extra credit distributed throughout the exam). 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:

Homework & in class worksheets:		25%
Exams:	3 x 200 pts	50%
Lab:		25%
Total:		100%

Grade Cutoffs: A/A- > 87%, B+/B/B- > 77%, C+/C/C- > 67%, D+/D > 60%, F ≤ 60%. The cutoffs will not be adjusted upwards, but the instructor reserves the right to lower them.

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 login to access the password protected parts of the site.

CLASS DISCUSSION LIST: A private Google group has been set up for this class. Registering for the class adds you to the group. This e-mail discussion group will be used by the instructor to distribute notices and links to assignments. You should use this group to ask questions of fellow students. The instructor monitors the list and will try to address any unanswered questions after 48 hours. If you want to access the group on the web the direct link is: https://groups.google.com/forum/#!forum/uwo_chem370f12

SYMBOLIC MATH PACKAGES: These can help you do algebra and calculus. 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 Schedule:

Topic (text sections)	Lectures
I. Thermodynamics & Statistical Mechanics 1 (Energy)	
Properties of Gases (1.x, 20.1-20.3)	9/5, 9/7, 9/10
The First Law (2.1-2.2, 15.1-15.3)	9/12, 9/14, 9/17, 9/19, 9/21
Heat Capacity, Work & Enthalpy (2.3-2.5, 16.2-16.4)	9/24, 9/26, 9/28, 10/1
Review	10/3
Exam 1 (Unit I)	**October 4 or 5, 2012 (Th or F)**
II. Thermodynamics & Statistical Mechanics 2 (Entropy)	
Adiabatic Processes & State Functions (2.6 - 2.12)	10/8, 10/10
Entropy and Ensembles (3.1-3.2b, 15.4-15.7, 16.7, 3.2c-3.4)	10/12, 10/15, 10/17, 10/19, 10/22
Free Energies and the Fundamental Equation (3.5, 16.1, 3.6-3.9)	10/24, 10/26, 10/29, 10/31, 11/2
Review	11/5
Exam 2 (Unit II)	**November 6 or 7, 2012 (T or W)**
III. Mixtures and Equilibria	
Simple Mixtures (5.1-5.5, 5.10-5.13)	11/9, 11/12, 11/14, 11/16
Equilibrium and E-Chem (6.1-6.2, 16.8, 6.3-6.9)	11/16. 11/19, *Thanksgiving,* 11/26, 11/28, 11/30
Molecular Interactions (17.1-17.10)	12/3, 12/5, 12/17, 12/10
Review	12/12
Exam 3 (Unit III)	**December 13 or 14, 2012 (Th or F)**

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 will be handed out separately in class and 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 and which computer they are on. 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/Cl/Cl_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. 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. Error analysis is not to be part of the poster 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. Computer projections should be used as visual aids.
5. Peer Review: All articles published in the literature are reviewed by anonymous

reviewers. Articles 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 rubric 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, page numbers, double spaced, figure and table numbers and format, reference format...)?
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 SciFinder™ title, abstract and reference page 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 <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. **<u>In an effort to save trees and facilitate reviews you will be turning in the reports electronically to TWO web sites. You must upload a copy to the class D2L dropbox and one to the experimental P-chem report web site. Turn in a single electronic copy of your report to each web site before class.</u>** Detailed instructions will be provided in class. Reviews of classmates' reports are worth 2 points each.

Reports are due <u>before</u> 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, 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 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
	78	final exam
	300	points total

Lab Schedule:

		Week Due			
Week of	**Project**	**Written**	**Review**	**Rewrite**	**Oral**
9/10	Library Assignment	9/17 (Data Sheet)	-	-	-
9/17	Real and Ideal Gases	-	-	-	-
9/24	Real and Ideal Gases (continued)	10/1 (formal)	10/8	10/15	10/15
Rotate through 2 labs (Heat of Combustion, Solution Calorimetry)					
10/1	Comb/Sol'n	-	-	-	-
10/8	Comb/Sol'n (continued)	10/15 (formal)	10/22	10/29	10/29
10/15	Sol'n/Comb	-	-	-	-
10/22	Sol'n/Comb (continued)	10/29 (article)	-	-	11/12
Rotate through 2 labs (Partial Molar Volume, Refractometry and Viscometry)					
10/29	Statistical Mechanics Worksheet	-	-	-	-
11/5	PMV/RV	-	-	-	-
11/12	PMV/PMV	11/19(formal)	11/26	12/3	12/3
11/19	*RV/PMV*	11/26 (poster)			
11/26	Electrochemistry	-	-	-	-
12/3	Electrochemistry (continued)	12/10(formal)	-	-	-
12/10	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 (ΔH,ΔS, ΔG) Constant pressure (isobaric) phenomena Constant temperature (isothermal) phenomena 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
Surfaces	Surface tension, surface pressure

Lab Report Grading Rubric on next page.

by Jonathan Gutow — last modified Aug 21, 2012 08:03 AM
Printing Instructions
8.5" x 11" printing is best at 60% scale in landscape orientation
Student Name
Course
Experiment
Prelab Score
0.0
Notebook Score
0.0
Assessment Summary

Mastery Summary

Prelab Quality
N - significant omissions in tables and procedures
I - tables and procedures mostly complete or complete
A - tables and procedures complete and additional useful information included

Performance of Lab
N: Novice - needs list of steps to follow
I: Intermediate - plans steps from a general description
A: Advanced - uses the literature to develop procedure

Notebook Quality
N - data missing
I - numbers recorded
A - additional observations

Report Quality
N - significant omissions or errors in one or more sections, major formatting errors, serious readability problems.
I - few omissions or errors, no significant formatting errors, most grammar correct.
A - only minor omissions or errors, no significant formatting errors, none or minor grammatical issues.

Grade

Report Sections

Abstract (of 1)
An excellent abstract will be less than 250 words and contain: what was studied; what techniques were used; what conclusions were reached; key quantitative results.

Introduction (of 2)
An excellent introduction will contain: what is already known about what was studied; theoretical background/basis for the experiment; balanced equations for any chemical reactions; what the experiment will tell us; and is written such that the reader is likely to want to read the report.

Experimental (of 2)
An excellent experimental section will contain: procedures followed in enough detail to be reproduced; equipment specifications (model and manufacturer at a minimum) for all but glassware; reagents and their specifications (manufacturer/source at minimum); and the experimental will be written as what was done not a recipe (it should be in past tense, passive voice).

Results (of 2)
An excellent results section will contain: prose connecting and explaining the progression between pieces of data; a complete set of data displayed in tables or graphs as appropriate; tables and graphs should be numbered properly and referred to in the text; conclusions do not belong in this section, although it is reasonable to point out key features of the data that may be important in reaching conclusions; primarily in past-tense and passive voice, except when referring to data the reader is looking at in this results section.

Discussion (of 2)
An excellent discussion/conclusion section will contain: conclusions drawn from the results; a statement of the significance of the experiment or conclusions; comparison to literature results; answers to any questions in the lab handout; discussion of error sources; discussion of quality of results based on the errors.

Analysis and Interpretation

Algebraic Calculations (of 4)
Equations for all calculations in logical order with all variables defined. Units on graphed and tabulated data. Sample calculations in notebook. Numerical calculations may be performed using computers, but what was done must be accurately recorded. Calculations accurate.

Graphing Data or Simulations (of 2)
Good graphs will have axes with appropriate labels (including units), data will be displayed with error bars, and symbols or line styles will be used to differentiate data sets and fits. Use of simulations is rated as follows: N - follows explicit instructions; I - performs with minimal guidance; A - modifies simulation protocols for new situations.

Errors and Significant Digits (of 4)
Accurately propagates errors, includes equations used, sample calculations in notes. Just giving sources of errors or estimates of measurement errors(-2). Any errors in significant digits (-1/2).

Literature Search (of 1)
Finds a closely related reference. Provides evidence of a literature search in the form of the SciFinder title, abstract and reference page for the closely related reference. Compares the results of experiment with literature values (may be from text or good database rather than the literature search reference).

Grammar, Spelling and Formatting Deductions

General Formatting
Papers with these errors will be returned without grading and a late penalty will be deducted until a corrected paper is turned in.
Margins ~1". Page numbers required. Must be double spaced.

Grammar, Spelling and Organization
some errors (-1); many (-2); unreadable (-3); vocabulary(-0.5); tense consistency(-0.5);not using passive voice(-0.5); organize material into standard sections (minor problems -0.5, major problems -1)

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)

Equations
not properly numbered (-0.5), complete description including definition of variables (some missing -0.5, many missing -1, most -1.5)

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)

Report only total
0.0
Marked Report
No file