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: Cooksy, *Physical Chemistry* (2 volume set, *Thermodynamics* and *Quantum Mechanics*).

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 10:20-11:20, TTh 9:30-10:30 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 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:	_	<u>25%</u>
Total:		100%

Grade Cutoffs: A/A- > 87%, B+/B/B- > 77%, C+/C/C- > 67%, D+/D > 60%, $F \le 60\%$. 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/d/forum/uwo_chem370f13.

SYMBOLIC MATH PACKAGES: These can help you do algebra and calculus. The open source SAGE math package is available on the <u>Chem SAGE Server</u>, on the computers in P-Chem lab and can be downloaded from the <u>SAGEmath web site</u> and installed on your personal computer. Information on user accounts on the Chem SAGE Server will be provided in class. MAPLETM 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:

<u>Topic</u> (text sections: VOLUME.CHAPTER)	<u>Lectures</u>
I. Statistical Mecha	anics of Gases
Intro/Historical Background (T.1)	9/4
Intro to quantum and statistical mechanics (T.2)	9/6, 9/9, 9/11, 9/13
Partitioning energy (T.3)	9/16, 9/18, 9/21, 9/23
Molecular Interactions (T.4, Q.10 Q.12)	9/25, 9/27, 9/30
Review	10/2
Exam 1 (Unit I)	October 3 or 4, 2013 (Th or F)
II. Thermodynamics & S	tatistical Mechanics
Heat Capacities (T.7)	10/7, 10/9, 10/11, 10/14
First Law (T.8)	10/16, 10/18, 10/21, 10/23
Second Law, Third Law and Mixing (T.9)	10/25, 10/28, 10/30, 11/1
Review	11/4
Exam 2 (Unit II)	November 5 or 6, 2013 (T or W)
III. Thermodynamics of Equilibrium	ria, Mixtures and Reactions
Phase Transitions (T.10)	11/8, 11/11, 11/13, 11/15
Solutions (T.11)	11/18, 11/20, 11/22, 11/25
Reactions (T.12)	12/2, 12/4, 12/6, 12/9
Review	12/11
Exam 3 (Unit III)	December 12 or 13, 2013 (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 Lewis 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. The equipment list only needs to list equipment. However, you must try to make it complete. The list should contain every piece of glassware and equipment you think you will need. This includes, for example, pipets, spatulas, sensors, D/A interfaces and computers.

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. <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. **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.
 - o 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. <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. 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. 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. <u>Peer Review:</u> 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 including a comparison with the literature, 10 points on calculations including error analysis, 1 point for literature search. 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 SciFinderTM 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 SciFinderTM 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 P-chem report web site. Turn in an electronic copy of your report to each web site before class. Detailed instructions will be provided in class. Reviews of classmates' reports are worth 2 points each.</u>

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.

Chemistry 370: Physical Chemistry I Dr. Jonathan Gutow

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Syllabus Fall 2013

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 x 20 = 120 laboratory reports (includes posters and article)

 $1 \times 10 = 10$ oral report

 $1 \times 10 = 10$ statistical mechanics worksheet

78 <u>final exam</u> 300 points total

Lab Schedule:

			Week Due	2	
Week of	Project	Written	Review	Rewrite	Oral
9/9	Library Assignment	9/16 (Data Sheet)	-	-	-
9/16	Real and Ideal Gases	-	-	-	-
9/23	Real and Ideal Gases (continued)	9/30 (formal)	10/7	10/14	10/14
9/30	Statistical Mechanics Worksheet	-	-	-	-
	Rotate through 2 labs (Heat of	Combustion, Soluti	ion Calorim	etry)	
10/7	Comb/Sol'n	-	-	-	-
10/14	Comb/Sol'n (continued)	10/21 (formal)	10/28	11/4	11/4
10/21	Sol'n/Comb	-	-	-	-
10/28	Sol'n/Comb (continued)	11/4 (poster)	-	-	11/18
R	otate through 2 labs (Partial Molar	Volume, Refracton	netry and Vi	iscometry)	
11/4	PMV/RV	-	-	-	-
11/11	PMV/PMV	11/18(formal)	11/25	12/2	12/2
11/18	RV/PMV	11/25 (poster)			
11/25	Electrochemistry	-	-	-	-
12/2	Electrochemistry (continued)	12/9(article)	-	-	-
12/9	90 min Lab Ex	cam (exact time to b	e 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	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
	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

Lab Report Grading Rubric on next page.

sources; discussion of quality of results based on

the errors.

8

questions in the lab handout; discussion of error

be from text or good database rather than the

literature search reference); answers to any

appropriate; tables and graphs statement of the significance of the experiment or properly and referred to in the conclusions; comparison to literature results (may

aining the progression between An excellent discussion/conclusion section will

Discussion (of 2)

plete set of data displayed in contain: conclusions drawn from the results; a

Mastery Summary

Performance of Lab		A: Advanced - uses t
Prelab Quality N - significant omissions in tables and procedures	I - tables and procedures mostly complete or complete	information included

Assessment Summary

Notebook Score

Bomb Calorimetry

Experiment Chem 370

Prelab Score

5.0

Student Name

Cal O. Rimetry

ns steps from a general description the literature to develop procedure st of steps to follow

N - significant omissions or errors in one or more sections, Report Quality

A - additional observations

 I - numbers recorded Notebook Quality N - data missing

I - few omissions or errors, no significant formatting errors,

major formatting errors, serious readability problems.

g

Report Sections

			Results (of 2)
Abetmort (of 1)	Introduction (of 9)	Experimental (of 2)	An excellent results section will contain: prose
An occollant obstract	.dictaco Ilim acito	An excellent experimental section will contain:	An excellent experimental section will contain: connecting and explaining the progression between
will be less than 250	what is already brown about what		procedures followed in enough detail to be pieces of data; a complete set of data displayed in
Will be less than 200	What is all early brown about what	reproduced; equipment specifications (model	reproduced; equipment specifications (model tables or graphs as appropriate; tables and graphs
words and contain.	was studied, theoretical		should be numbered properly and referred to in the
tochricus studied, wild	hologod oggations for one obomitol		text; conclusions do not belong in this section,
recrimques were used,	balanced equations for any crientifical	treaming were used, basalice defaults for any creaming the manufacturer/source at minimum); and the	although it is reasonable to point out key features
wild coliciusions were	in one in written each that the moder	reactions, what the experiment will tell experimental will be written as what was done of the data that may be important in reaching	of the data that may be important in reaching
	us, and is written such that the reader	not a recipe (it should be in past tense, passive	not a recipe (it should be in past tense, passive conclusions; primarily in past-tense and passive
quantitative results.	is likely to want to read the report.	voice).	voice, except when referring to data the reader is
			looking at in this results section.

Grade

Analysis and Interpretation Graphing Data or Simulations (of 2)

N

8

Sample calculations in notebook. Numerical calculations may be performed using computers, but what was done variables defined. Units on graphed and tabulated data.

Equations for all calculations in logical order with all

Algebraic Calculations (of 4)

must be accurately recorded. Calculations accurate.

search in the form of the SciFinder Finds a closely related reference. Provides evidence of a literature Literature Search (of 1)

equations used, sample calculations in

errors in significant digits (-1/2).

Accurately propagates errors, includes

Errors and Significant Digits (of 4)

title, abstract and reference page for the closely related reference. References notes. Just giving sources of errors or estimates of measurement errors(-2). Any

Grammar, Spelling and Formatting Deductions

Equations

,		
Papers with these errors will be	Grammar, Spelling and Organization	Figures and Tables
returned without grading and a late	returned without grading and a late some errors (-1); many (-2); unreadable (-3);	not properly numbered (-0.5), c
penalty will be deducted until a	vocabulary(-0.5); tense consistency(-0.5);not using passive missing (-1), captions incomple	missing (-1), captions incomple
corrected paper is turned in.	voice(-0.5); organize material into standard sections (minor misplaced (-0.5), labeling errors	misplaced (-0.5), labeling errors
Margins ~1". Page numbers	problems -0.5, major problems -1)	headings, units, up to -1)
required. Must be double spaced.		

General Formatting

Φ	some errors (-1); many (-2); unreadable (-3);	not properly numbered (-0.5), captions not properly numbered (-0.5),	not properly numbered (-0.5),
	vocabulary(-0.5); tense consistency(-0.5); not using passive missing (-1), captions incomplete or complete description including	missing (-1), captions incomplete or	complete description including
	voice(-0.5); organize material into standard sections (minor misplaced (-0.5); labeling errors (axes, definition of variables (some m	misplaced (-0.5), labeling errors (axes,	definition of variables (some m
	problems -0.5, major problems -1)	headings, units, up to -1)	-0.5, many missing -1, most -1

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) tion of variables (some missing many missing -1, most -1.5) plete description including

No file