

Course Overview: Physical chemists and physicists make extensive use of mathematical models to describe natural phenomena. There is an underlying assumption 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.

Required Texts: Atkins & de Paula, *Physical Chemistry*, 7th Edition

Barrante, *Applied Mathematics for Physical Chemistry*, 2nd edition.

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

Lectures: 10:20-11:20 MWF (HS 367)

Office Hours: Dr. Gutow (HS-412): MWF 8:30-9:30, T 9-10. Dr. Matsuno (HS-409): MW 2-3, Th 8-9, F 12-1. 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 ungraded exercises to be worked and one graded problem (10 pts each) provided by the professor. Numerical answers will be provided for the exercises so that you may check your work. Treat the graded exercise as an open book, take-home quiz, which can be discussed with the instructor but not classmates. The lowest three scores will be dropped when calculating your grade. The goal of the graded homework is to provide a measure of individual student mastery of problems and skills that are too involved to be included on an exam. Please do not collaborate on these graded problems. You are encouraged to work together on all other homework and exercises.

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 100 points (plus 10 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.

Grading:	Critical Thinking Exercises:	10 x 5 pts =	50 pts
	Graded Homework:	10 x 10 pts =	100 pts
	Exams:	3 x 100 pts =	<u>300 pts</u>
	Total:		450 pts

The total points necessary to receive a particular grade are listed below. The instructor reserves the right to change the point total downward.

A: 405 AB: 383 B: 360 BC: 333 C: 311 CD: 284 D: 248 F: <248

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:

- 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.

Class Schedule:

Chapter	Lectures	Homework Due*
I. Classical Thermodynamics		
1: Properties of Gases	1/31, 2/2	2/7
2: The First Law: the concepts	2/4, 2/7, 2/9, 2/11	2/14
3: The First Law: the machinery	2/14, 2/16, 2/18	2/21
4: The Second Law: the concepts	2/21, 2/23, (2/25)	2/28
5: The second Law: the machinery	2/25, 2/28, 3/2	3/4
Review/lab oral report	3/4	
Exam 1 (Unit I)	Monday, March 7, 2005	
II. Statistical Thermodynamics		
Introduction to quantum mechanics	3/9	3/21
19: Statistical Thermodynamics: the concepts	3/11	3/21
<i>Spring Break 3/12 - 3/20</i>		
19. Statistical Thermodynamics the concepts (continued)	3/21	3/28
20: Statistical Thermodynamics: the machinery	3/23, 3/25	3/28
6: Physical transformation of pure substance	3/28, 3/30	4/4
7: The properties of simple mixtures	4/1, 4/4, 4/6	4/8
Review/lab oral report	4/8	
Exam 2 (Unit II)	Monday, April 11, 2005	
III. Equilibrium and Transport		
9: Chemical Equilibrium	4/13	4/18
10: Equilibrium electrochemistry	4/15, 4/18, 4/20	4/22
24: Molecules in motion	4/22, 4/25, 4/27	4/29
22: Macromolecules	4/29, 5/2, 5/4	5/6
28: Processes at Solid Surface	5/6, 5/9	not due
Review/lab oral report	5/11	
Exam 3 (Unit III)	Friday, May 13, 2005	

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

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 web site is: pchems05. The password will be supplied the first day of class.

TEXTS: The following books are on reserve 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

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.

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)
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 -fugacity/activity -Maxwell Relations -Colligative Properties -Phase rule	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 (surface phenomena) -Electrochemical -Chemical Physical changes (phase) Mixtures Fp, Bp, vapor pressure and Osmotic pressure changes Donan membrane equilibria
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
Kinetics	Adsorption isotherms