CHE 371: Kinetics and Thermodynamics
Fall 2011

Class Meetings: Lecture: M, T, W, F 9:00 AM, Nobel 222
Laboratory: T, W 1:30-5:20 PM, Nobel 107

Instructor: Prof. Amanda Nienow, Nobel 106A, 933-7327, anienow@gustavus.edu
Office Hours: By appointment

Textbook: Peter Atkins, Julio de Paula, and Ronald Friedman. *Quanta, Matter and Change: A molecular approach to physical chemistry.* W.H. Freeman and Company, New York, 2009.

Other Required Materials: Gustavus Adolphus College, *Physical Chemistry Laboratory Manual* (available only through the campus bookstore); laboratory notebook, calculator, goggles

Website: We will use Moodle for this course.

Course Overview:
Physical chemistry is the quantitative interpretation of the macroscopic properties of matter informed by a detailed understanding at the atomic and molecular level. Physical chemistry is an exciting field with important connections to topics as diverse as protein folding to the ozone hole to rational drug design and to organic synthesis. Thermodynamics is a subject that quantifies the stability of macroscopic systems, the flow of energy between macroscopic systems, and the ensuing transformations that occur. Physical chemistry unifies the laws of thermodynamics that predict the likelihood of chemical transformations, chemical kinetics that indicate how fast a chemical transformation will occur, and adds the insights gained at a molecular level to make solid predictions of the chemistry of matter. In this course, we will study the application of thermodynamics and kinetics to chemical systems providing an important foundation for the understanding of chemical and biochemical systems.

Attendance Policy:
Class: The material presented in this course can be abstract and mathematically challenging, and seeing it in class will be helpful to your understanding. With that said, I understand that we are all busy adults, and that there may be an occasion on which you need to miss class. Please take your education responsibly and attend class regularly. Also grant me the courtesy of informing me of planned absences in advance. Excessive and regular absences will lead to a drop in your grade (5-10 absences) or an automatic failure (10 or more absences).

Lab: To get credit for laboratory assignments, you **must** be present. I will make exceptions to this rule only for emergencies and illness. If this need arises, please inform me as soon as possible.

Course Topics:
This course will cover the Properties of Gases, Statistical Mechanics, the Laws of Thermodynamics, Phase and Chemical Equilibria, Solution Chemistry, and Kinetics. I will attempt to include some chemical and/or biochemical examples throughout the course. The table below outlines the timeframe for our discussions; note that this schedule IS SUBJECT TO CHANGE!

TENTATIVE Table of Topics and Events for CHE 371

Dates	**Topics**	**Items of Interest**
Sept 6-9	Quantum Mechanics/Review	
Sept 12-16	Statistical Thermodynamics; Ch 13	**Quiz: Take Home, QM/Ch 13**
Sept 19-23	First Law of Thermodynamics; Ch 14	
Sept 26-30	First Law of Thermodynamics; Ch 14	
Oct 3-7	First and Second Law of Thermodynamics; Chs 14 & 15	**Nobel Conference**: Oct 4-5
Oct 10-14	Second Law of Thermodynamics; Ch 15	
Oct 17-21	Second Law of Thermodynamics; Ch 15	
Oct 24-28	Exam and DMA Pre-lab lecture	**Reading Days**: Oct 24-25 **Exam 1: Oct 26, Ch 14-15**
Oct 31-Nov 4	Physical Equilibra, Ch 16	
Nov 7-11	Physical Equilibra, Ch 16	
Nov 14-18	Chemical Equilibra, Ch 17	
Nov 21-25	Equilibra Review and Exam	**Exam 2: Nov 22, Ch 16 and 17** **Thanksgiving Break**: Nov 23-27
Nov 28- Dec 2	Molecular Motion and Kinetics (Parts of Ch 18-21)	
Dec 5-9	Molecular Motion and Kinetics (Parts of Ch 18-21)	
Dec 12-14	Molecular Motion and Kinetics (Parts of Ch 18-21)	**Exam 3: Dec 14, Chs 18-21**
Final Exam	Cumulative: QM, Ch 13-21	**TBA**

Grading:
Your course grade will be based on an absolute scale for four sections of the course: homework (20%), exams (40%), laboratory (20%), and the final exam (20%). Remember that you can not compare the weight of a homework assignment directly to the weight of a laboratory assignment as they are in different categories! (See grade for Student Example below).

Grading Itemization:
Homework, Quizzes, and Review Presentation: 165 pts (20%)
Exams (3 @ 100 pts each): 300 pts (40%)
Laboratory (Reports, Notebooks, Project)*: ~500 pts (20%)
Final Exam: 150 pts (20%)
* You **must** pass the laboratory portion of this class to receive a passing grade in the course.

Calculation of Grade for Student Example:
(155/165)*0.2 + (260/300)*0.4 + (417/500)*0.2 + (135/150)*0.2 = 0.882 or 88.2%

Absolute exam grading scale: Grade ranges for final grades, expressed as a percentage are:

	B+ 86 – 88.9 %	C+ 76 – 78.9 %	D+ 66 – 68.9 %
A 93 - 100 %	B 82 – 85.9 %	C 72 – 75.9 %	D 60 – 65.9 %
A- 89 – 92.9 %	B- 79 – 81.9 %	C- 69 – 71.9 %	F 0 – 59.9 %

The absolute grading scale ensures that students have some sense of where they stand with respect to grades throughout the course, and may help encourage group studying without a sense that people are competing with each other.

Lab: To get credit for laboratory assignments, you **must** be present. I will make exceptions to this rule only for emergencies and illness. If this need arises, please inform me as soon as possible.

Graded Items:

1. Problem Sets

Working problems is essential to the mastery of the material in physical chemistry. In this course, there will be several homework sets due throughout the semester. The assignments will be designed to keep you current with the course material and provide insight into the types of problems which you are most likely to see on quizzes and exams. Also, note that HW is a significant contributor to your course grade (20%–the same as the final exam!). It is very much in your best interest to complete the assignments and understand the material covered in them!

These problem sets are *generally* due on Thursdays. I am available during office hours and may hold semi-regular homework sessions if desired. The tentative due dates for these assignments are below.

Homework #	Topic	Due Date
1	Ch 8	9/22
2	Ch 14	9/29
3	Ch 14/15	10/20
4	Ch 16	11/10
5	Ch 16/17	**MON** 11/21
6	Ch 18/19	12/8
7	20/21	12/14

2. Exams and Quizzes:

There is currently one scheduled quiz – a take home quiz given on Wed 9/14 and due Thurs 9/15 by 10:30 am. The quiz will cover Quantum Mechanics and Chapter 13 of Atkins, de Paula and Friedman.

There will be three term exams and a final exam. These exams are *tentatively* scheduled:

Exam 1: Chapters 8, 14, and 15 of Atkins, de Paula and Friedman, Wed, Oct 26, 2011
Exam 2: Chapters 16-17 of Atkins, de Paula and Friedman, Tues, Nov 22, 2011
Exam 3: Chapters 18-21 of Atkins, de Paula and Friedman, Wed, Dec 14, 2011
Final Exam: Cumulative (QM, Ch 8, 13-21) TBA

Students must arrange **in advance** to take an exam at any other than the scheduled time, and may do so only for a valid health or school-related activity. Exams missed without pre-arrangement are entered as zero credit and cannot be made up.

3. Laboratory:

Experimentation plays an integral role in the course. The laboratory offers the opportunity to put your conceptual understanding of the subject to work. There will be two laboratory sections on Tuesday and Wednesday afternoons starting at 1:30 PM (T, W). Each investigation will require careful preparation including preparing your notebook and reading the material in the handout as well as any literature articles required for the investigation. One of the goals for the laboratory sections is to help you learn to work together as a group – both in the lab and in writing a report. Thus, the majority of the lab reports will be written as a group. Choose your group carefully at the beginning of the semester – you will want to work with others with similar work ethics, schedules, and interest levels. Once the groups have been determined, there will be some role assignment within the groups to ensure even work loads throughout the semester.

Due to the nature of the physical chemistry lab (i.e., high dependence on instrumentation), part of the laboratory portion of the course will be a rotation of labs. In this rotation, there will be four different experiments each week. You will be assigned a group and over a period of four weeks, you will complete all of the investigations. This rotation-style laboratory session can cause some confusion as the labs can not all be directly related to current course material and there is only one instructor and one TA per session. To overcome some of this confusion, we will have extended pre-lab sessions on some of the Fridays before the week of rotation. These pre-lab sessions will be held in class and there will be two simultaneous pre-lab groups run by either the instructors or lab TAs. These group sessions may consist of lecture, small group activities (i.e., pre-lab assignments), and/or quiet time to plan a procedure or complete necessary calculations.

Careful record keeping in a laboratory notebook is critical to this laboratory work. Your notebook should be bound with consecutively numbered pages. Each page should be dated, and a table of contents should be kept at the front of the book. Notes on the operation of instruments, summaries of the experiments, and observations made in lab must be noted in pen. Spectra, and other data, can be taped or pasted into the book. Results, in the form of tables where applicable, and any related calculations, should be included. *It is your responsibility to get your notebook checked by the lab TAs* when you are finished with an entry for a specific lab (probably during the NEXT lab period).

A brief but carefully written report will be turned in at the beginning of class on the Friday of the week following completion of an investigation, giving you ~ 8 days to complete the report. There will be 5% penalty per day late. The word processed report will include a brief summary of the goals of the investigation, carefully tabulated experimental data (including any spectra or other raw electronic data), analysis, and responses to questions. This will be discussed in detail in the first lab session and in the lab manual.

Tentative Lab Schedule

Dates(s)	Investigation	Report Due
Sept 6 & 7	Intro to P Chem Lab	N/A
Sept 13 & 14	Computational Study of the Heats of Formation and Combustion of Hydrocarbons – WebMO Review	In lab: Sept 20 or 21
Sept 19-Oct 21 (4 Weeks)	Bomb Calorimetry and Determination of Resonance Energy of Benzene	In class on Friday following the end of each lab session (~1 week after lab)
	Determination of the Heat of Vaporization of Various Liquids	
	Solution Kinetics of an Organic Reaction	
	Kinetics of a Diffusion Controlled Reaction as Measured by Fluorescence Spectroscopy	
Oct 4 & 5	Nobel Conference: No Lab	N/A
Oct 24-25	Reading Days: No Lab	N/A
Oct 31 -Nov 11 (2 Weeks)	Computational and Experimental Study of the Isomerization in N,N-dimethylacetamide (DMA)	In lab: Nov 15 or 16
Nov 14-Dec 14 (4 Weeks)	Independent Projects: Proposal Due Nov 29 or 30 Presentation and Report Due Dec 13 or 14	In lab: Dec 13 or 14
Nov 23-27	Thanksgiving Break: No Lab	N/A

Tentative Prelab Sessions: Due to the varied schedule of the lab investigations, prelab lectures will occasionally be held during a Friday lecture period. Tentatively, these sessions are scheduled for 9/16 and 9/23 for the four rotating labs and 10/28 for the DMA lab.

Gustavus Honor Code:
Gustavus has adopted an honor code. Each of you is required to abide by the following pledge: "As a community of scholars, the faculty and students of Gustavus Adolphus College have formulated an academic honesty policy and honor code system, which is printed in the Academic Bulletin and in the Gustavus Guide. As a student at Gustavus Adolphus College I agree to uphold the honor code. This means that I will abide by the academic honesty policy, and abide by decisions of the joint student/faculty Honor Board." Pledge: “On my honor, I pledge that I have not given, received, or tolerated others use of unauthorized aid in completing this work.”
In physical chemistry you will work together on problems in study groups and you will work together in laboratory but you will still be required to turn in work that is **solely** your own. On exams you will not receive any assistance and will add the following pledge: "On my honor, I pledge that I have not given, received, or tolerated others' use of unauthorized aid in completing this work." The penalty for not adhering to the honor code will range from taking a zero on the work in question to referral to the honor board depending on the circumstances.

Accommodations:
Gustavus Adolphus College is committed to ensuring the full participation of all students in its programs. If you have a documented disability (or you think you may have a disability of any nature) and need reasonable academic accommodation to participate in class, take tests or benefit from the College’s services, then you should speak with the Disability Services Coordinator, for a confidential discussion of your needs and appropriate plans. Course requirements cannot be waived, but reasonable accommodations may be provided based on disability documentation and course outcomes. Accommodations cannot be made retroactively; therefore, to maximize your academic success at Gustavus, please contact Disability Services as early as possible. Disability Services (https://gustavus.edu/advising/disability/) is located in the Advising and Counseling Center.