

CHE 371: Kinetics and Thermodynamics Fall 2008

Class Meetings: Lecture: M, T, W, F 9:00 AM, Olin 103
Laboratory: T, W 1:30-5:20 PM, R 2:30-6:20 PM

Instructor: Prof. Amanda Nienow, Nobel 106C, 933-7327, anienow@gustavus.edu
Office Hours: T/W 10:30 or By appointment (not on campus Mon and Thurs PM)

Laboratory Instructors: Prof. Amanda Nienow (see above)
Prof. Steve Miller, Nobel 107B, 933-7321, smiller3@gustavus.edu

Textbook: Donald A. McQuarrie and John D. Simon, *Physical Chemistry: A Molecular Approach*. Sausalito, CA: University Science Books, 1997.

Website: http://homepages.gac.edu/~anienow/CHE-371a/che_371.html

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. In this table the topics are listed by chapter in McQuarrie and Simon... Quantum Mechanics = Review; Ch 16 = Properties of Gases, Ch 17 = Boltzmann Factor and Partition Functions, Ch 18 = Partition Function and Ideal Gases, Ch 19-21 = The Laws of Thermodynamics, Ch 22 = Helmholtz and Gibbs Energies, Ch 23 = Phase Equilibria, Ch 24-25 = Solutions, Ch 26 = Chemical Equilibrium, Ch 28 = Kinetics.

Table of Topics and Events for CHE 371

Dates	Topics/Chapter	Items of Interest
Sept 2-5	Quantum Mechanics/Review	
Sept 8-12	Chapter 16	
Sept 15-19	Chapter 17	
Sept 22-26	Chapter 18	
Sept 29-Oct 3	Chapter 19	Exam 1: Sept 30 (Ch16-18, QM)
Oct 6-10	Chapter 19	Nobel Conference: Oct 7-8
Oct 13-17	Chapters 19 and 20	
Oct 20-24	Chapters 20 and 21	Reading Days: Oct 20-21
Oct 27-31	Chapter 22	
Nov 3-7	Chapter 23	Exam 2: Nov 4 (Ch 19-22)
Nov 10-14	Chapters 24 and 25	
Nov 17-21	Chapter 26	
Nov 24-28	N/A	Exam 3: Nov 25 (Ch 23-26)
Dec 1-12	Chapter 28, Kinetics	
Final Exam	Cumulative: QM, Ch 16-28	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:

$$(155/165)*0.2 + (260/300)*0.4 + (417/500)*0.2 + (135/150)*0.2 = 0.882 \text{ or } 88.2\%$$

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 (~11) homework sets due throughout the semester. These problem sets are generally due on Tuesdays. 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	Quantum Mechanics	9/9
2	Ch 16	9/16
3	Ch 17	9/23
4	Ch 18	9/30
5	Ch 19	10/14
6	Ch 20, Ch 21	10/28
7	Ch 22	11/4
8	Ch 23	11/11
9	Ch 24, Ch 25	11/18
10	Ch 26	11/25
11	Kinetics (Ch 27/28/+)	12/12

2. Exams and Quizzes:

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

Exam 1: QM, Ch 16-18 of McQuarrie and Simon, Tuesday Sept 30, 2008

Exam 2: Ch 19-22 of McQuarrie and Simon, Tuesday Nov 4, 2008

Exam 3: Ch 23-26 of McQuarrie and Simon, Tuesday Nov 25, 2008

Final Exam: Cumulative (QM, Ch 16-28) with emphasis on kinetics, 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 three laboratory sections on Tuesday, Wednesday and Thursday afternoons starting at 1:30 PM (T, W) and 2:30 PM (R). Note: The laboratory instructor for the Thursday course is Dr. Steve Miller. 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.

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 the Fridays before each week of rotation. These pre-lab sessions will be held in class and there will be four 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.

Tentative Lab Schedule

Dates(s)	Investigation	Report Due
Sept 2-4	Intro to P Chem Lab	N/A
Sept 9-11	Computational Study of the Heats of Formation and Combustion of Hydrocarbons – WebMO Review	Sept 19
Sept 16-Oct 16 (4 Weeks)	Bomb Calorimetry and Determination of Resonance Energy of Benzene	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 7-9	Nobel Conference: No Lab	N/A
Oct 21-23	Reading Days: No Lab	N/A
Oct 28 -Nov 6 (2 Weeks)	Computational and Experimental Study of the Isomerization in N,N-dimethylacetamide (DMA)	Nov 14
Nov 11-Dec 11 (4 Weeks)	Independent Projects	Dec 12
Nov 25	Thanksgiving Break: No Lab	N/A

Tentative Prelab Sessions: Prelab sessions will be held on 9/12, 9/19, 9/26, and 10/10 for the four rotating labs. Prelab lecture for the DMA lab will be held 10/27.

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 particular piece of work in question to referral to the honor board depending on the circumstances.

Accommodations:

If you have a physical, psychiatric/emotional, medical, or learning disability that may have an effect on your ability to complete assigned course work, please let me know. I will provide assistance and accommodations upon receiving verification from Laurie Bickett in the Academic Advising Center. The Gustavus Adolphus College policies on this matter can be found at www.gustavus.edu/oncampus/advising/disability.cfm.