Chemistry 413
Physical Chemistry: Thermodynamics, Kinetics and Statistical Mechanics
Syllabus - Spring 2012

General Information

Instructor: Dr. Kimberly Lawler-Sagarin **Phone:** x 3202
Office: SC 218 **e-mail:** ksagarin@elmhurst.edu

Text: *Thermodynamics, Statistical Thermodynamics, and Kinetics* by Engel and Reid, 2nd ed (Req.)
Applied Mathematics for Physical Chemistry by J. R. Barrante, 3nd edition (Req.)
Quantum Chemistry & Spectroscopy by T. Engel, 2nd edition (Req./Rec.)

Materials: Laboratory Notebook (any brand, however, it should be quad ruled)
Jump drive for working on data analysis during laboratory time (Rec.)
Scientific Calculator (bring to all class meetings)

Class Meetings: MWF 9:15 a.m. - 10:20 p.m. Schiable Science 209

Lab Meetings: T 1:00 - 5:00 p.m. Schiable Science 237

Office hours: W 11:30-12:30, Th 1:30-3:00 p.m., F 10:30-11:30 p.m., other times as arranged

Web Site: http://www.elmhurst.edu/˜ ksagarin/pchem/

Goals of the Course

The major goals for this course are centered around acquiring a conceptual understanding of thermodynamics, chemical kinetics and statistical thermodynamics and developing your ability to apply these and related concepts to solve chemical problems. Some specific goals are listed here. You are encouraged to consider and discuss with me how these might apply to your chosen career/life path. Students completing this course will:

1. Develop more sophisticated mental models of chemical and physical change, grounded in the fundamentals of thermodynamics;
2. Be able to apply the concepts, methods and techniques of thermodynamics to chemical systems and make predictions for these systems;
3. Have the ability to use simple physical systems as models for understanding more complex systems;
4. Appreciate the role of kinetic studies in chemistry and across the physical and life sciences;
5. Be able to derive rate laws for simple chemical processes from proposed mechanisms and design kinetic experiments to test the validity of these mechanisms;
6. Appreciate the role of statistical mechanics in linking microscopic systems with macroscopic thermodynamic properties;
7. Use statistical thermodynamics to calculate thermodynamic properties for simple chemical systems;
8. Acquire specific skills necessary for future work in science or science-related areas, whether it be in this course, other advanced courses, graduate school, medical or business professions or the industrial laboratory. Specifically, the student will acquire or continue to enhance his/her:
    - Facility with computer spreadsheets and graphics, for transforming raw data into quantities of conceptual or theoretical interest;
    - Capacity to "do" algebra efficiently and accurately;
    - Ability to use calculus with confidence and apply these concepts to problems in thermodynamics and chemical kinetics;
    - Ability to approach unfamiliar physical problems and identify what conceptual and factual background information is needed to solve the the problem;

- Ability to simplify physical problems by making physically reasonable, justifiable and testable assumptions;
- Critical analytic thinking and logical reasoning skills which are of great value in formal scientific research and most other areas of life.

Grading

As your instructor, my goal is to help and encourage you to learn. All students learn differently, thus I try to utilize a broad range of methods and assignments. This means that there will be a lot of different opportunities for you to apply the concepts we will be investigating this semester. Correspondingly, there are many different ways to earn points and demonstrate your understanding of the material in this course.

Grades on all assignments will be given in points. Points in all categories will be approximately equivalent. Each category will be weighted as stated below.

Breakdown

- Lecture Exams (3): 100 points each = 30%
- Quizzes: 60 points total = 6%
- Final Exam: 160 points = 16%
- Homework Problem Sets, Endurance Problems and In-class Problems: 300 points = 30%
- Laboratory Component = 180 points = 18%
- Instructor Evaluation: used to decide borderline cases (within 1% of next highest grade)

Grading Scale

The grading scale will depend in part on my assessment of the difficulty of exams and the final. The grading scale for students completing all course requirements will not be raised above the following scale:

A	92%
A-	90%
B+	86%
B	76%
B-	72%
C+	70%
C	64%
C-	60%
D+	58%
D	52%

This means if you receive an overall percentage of 92.00% and complete all course requirements, you will get an A. If you have an overall percentage of 86% and you have completed all course requirements, you will be guaranteed *at least* a B+.

Course Requirements

To be graded on the grading scale defined above, you must complete all the course requirements listed below:

1. Pass the final exam
2. Receive at least a 40% *combined average* on the three midterm exams
3. Turn in and receive grades for at least 80% of the problem sets and "endurance problems".
4. Turn in all laboratory reports and analyses.

5. Receive a passing grade in both the lecture and laboratory portions of the course (410 points in lecture, 93.6 points in lab).

In the unlikely even that a student does not meet one or more of these requirements, that student will not be graded by the grading scale described in the previous section. Grades in these cases are determined on an individual basis and are at the instructor's discretion. In general, at least a one-grade penalty for each requirement which is not fulfilled is imposed. Thus, failing the final, skipping an excessive number of homework assignments, not turning in a lab report, skipping an excessive number of in-class assignments may result in a lower grade than the number of points you have accumulated would otherwise indicate.

Completing homework assignments is considered **essential** for success in this course.

Students who are conscientious about completing homework typically have no trouble earning a high grade in physical chemistry.

College Policies

College policies on incompletes/drops/unauthorized withdrawals will be followed. Also, **read carefully** the Code of Academic Integrity and the Student Rights and Responsibilities section of the current Student Handbook (E Book) to understand College policies regarding plagiarism, cheating, non-discrimination, and policies regarding privacy with regard to student records. All such policies will be strictly enforced.

If you have a diagnosed disability or believe that you have a disability that might require reasonable accommodations for academic instruction please contact the Disability Services Provider (630) 617-3753. It is your responsibility to initiate a request for services from DSP and to provide appropriate verification of disability. Upon disclosure of a disability verified by DSP, any reasonable accommodation will be made.

Lecture Class Structure and Assignments

Each regular class meeting will be composed of some combination of the following activities:

- interactive lecture
- in-class problems
- discussion/questions from problem sets

Laboratory activities, policies and assignments are discussed in the Laboratory Syllabus for Chemistry 413.

Homework Problem Sets

Problem sets will be assigned and collected approximately weekly. They will generally be due **Wednesdays at 3:30 p.m.**

Each problem statement should be written out, with full solutions following (this makes it easier for me to provide feedback, for you to interpret that feedback, and for you to use the problem sets to study later). Show all your work for mathematical problems. **NO** credit will be given for problems if work is not shown. Final answers should include correct units, answers without units will be considered incorrect. Please put your name at the top of your assignment and staple all pages together.

Each problem set will be worth variable (10-28) points. Problems will generally be worth 2 or 4 points each, though more extensive problems may be assigned more points. You will receive one half the points for *seriously* attempting each problem. The remaining points will be assigned based on successful completion of the problem. **One point will be taken off if problem statements aren't included in your assignment.** Although these assignments are due at 3:30 p.m., other assignments will be due at the **beginning** of class. Please see the section entitled "Policy for Late or Missed Assignments" for additional information.

In addition to assigned homework which will be collected and graded, I suggest you work through the color-coded problems in the text with full answers available in the students' solutions manual in addition to the regular homework. Specific recommendations will be made prior to each exam. Homework solutions will be available on Blackboard.

Endurance Problems

Problem solving skills are very important to professional chemists. Unlike homework problems which can be put aside unfinished, problems encountered in chemical research can't just be turned in partially finished. This is true in industry and medical related professions as well as the academic research environment. To develop your problem solving skills, we will have several *endurance problems*. An *endurance problem* is an in-depth problem consisting of several related tasks. You will have the opportunity to "redo" each endurance problem until it is complete and correct.

Each "endurance problem" will be worth 10 points.

The "redo" system works as follows:

1. Original Due date: Turn in first attempt
   - if acceptable → 10 points (you're done!)
   - if an attempt was made but the problem is not complete and correct → "redo"
2. 1 week after original due date: Turn in redo 1
   - if acceptable → 8 points (you're done!)
   - if an attempt was made but the problem is not complete and correct → "redo"
3. 2 weeks after original due date: Turn in redo 2
   - if acceptable → 6 points (you're done!)
   - if an attempt was made but the problem is not complete and correct → problem is graded out of 6 points.
4. If no attempt or only a cursory attempt is made to redo the problem, you will receive a zero. There is a maximum of three submissions of each problem.

Once in a while, such a problem may be assigned without the opportunity for a redo. For these problems, which will be marked, you will be graded out of 10 points on your first attempt.

Overall Format: The problem statement should be included with each endurance problem. Your solution should be written out, showing all work (including unit conversions). A running commentary on your reasoning and strategy should accompany your assignment. All sources should be listed (i.e. the textbook, other textbooks, journal articles, etc.) and all assumptions must be clearly stated (and "reality checked", if appropriate). Please put your name at the top and staple all pages together. Failure to follow these guideline will result in an automatic redo and point deduction.

For redos: start a new page labeled "Redo 1" or "Redo 2" and staple this to the original problem. Turn the whole package in. Endurance problems will generally be graded by the end of the following day.

Please note that these may accumulate, so try not put these off until the last minute. You may have as many as three to turn in at once. Endurance problems and re-submissions will generally be accepted only on their due dates.

In-class Problems

Some class periods will be devoted to in-class problems. In-class problem days may include class discussions and problem presentation by group members. These exercises will be worth 5 points. On-time attendance is

required for full credit. These will not be announced in advance. If you miss one of these days, you may use a late certificate to make up the assignment and the missed points. To avoid using a late certificate, advance arrangements should be made if you know you are going to miss class for an excused absence (due to an order from the US Military, or if you are officially representing the College). Extreme unforeseen circumstances such as serious illness or a death in the immediate family will also be considered excused absences, though these may require documentation. Minor common inconveniences such as vehicular trouble, parking, etc, will require a late certificate.

Some in-class problems may take more time than allotted and you will be asked to complete the assignment by the next class period. Occasionally, I may use a small portion of a class period for an in-class exercise. This will not involve the assignment of points, but you will be held responsible for the material discussed.

Overall Assignment Point Structure

A rough estimate of the points possible in each of these homework assignment categories is provided below:

- In-class problems = 6 × 5 pts = 30 pts
- Endurance problems = 5 × 10 pts = 50 pts
- Problem Sets = 12 × 16-20 pts (avg.) = 220 pts estimated

A maximum of 300 points may be accumulated by a student. The actual points possible in each of these categories may vary, but the combined total possible will be *at least* 300 points, or your accumulated points will be scaled up to an equivalent percentage score out of a total possible of 300 points. The above is an approximate breakdown on points among the various types of assingments, but this is only an estimate.

Collaboration

Working in groups on the homework is not prohibited, in fact, it is encouraged. Group work can greatly facilitate your understanding of a subject. However, the work you present **must be your own**. *This includes all excel-type spreadsheets, graphics, computational assignments, and laboratory data.* Do not simply copy the answers from a classmate or copy a problem solution directly from a solutions manual. These activities are considered cheating, will not help you develop the problem-solving skills necessary for success in physical chemistry, and will be dealt with in accordance with college policies.

Again, working in groups on the homework is encouraged. However, to develop your problem solving skills and improve test performance, I advise you to attempt homework problems on your own before getting help from classmates. Once you have tried the problems on your own, you are in a good position to discuss approaches and strategies with one another.

College policies on academic honesty will be followed. Please **read carefully** the Code of Academic Integrity and the Student Rights and Responsibilities section of the current Student Handbook (E Book) to understand College policies regarding this issue. Please also see the Policy on Academic Honesty adopted by Elmhurst's Division of Natural Sciences (http://www.elmhurst.edu/ earls/honestypolicy.html). This is available as a link from the pchem web site. Students in Chemistry 412 and 413 are also required to abide by the Physical Chemistry honesty policy. Two copies will be handed out in class, one for you to sign and return and one to keep for reference. A copy of the policy is also available on the course web site. Violations of the Physical Chemistry Honesty Policy may result in failing the course.

Policy for Late or Missed Assignments

Because everyone has a bad week, gets sick, or just runs behind, you will get a series of "Late Assignment Certificates". **Late homework or endurance problems will NOT be accepted for regular grading unless accompanied by a certificate**, or the assignment is postponed for the entire class. Exceptions to

this policy will only be made in the case of serious (and documented) illness or tragedy. (See: "What if I run out of certificates?" below)

You will receive four "flexible" late certificates. Each certificate is good for turning in one **lecture** assignment one "class day" late. A class day is any MWF in which the college is holding class. Late certificates may be combined, should be saved until you really need them and are good for any type of assignment, including a missed in-class assignment.

A student with three or more unused late certificates at the end of the term may choose to redo (for full credit) any ONE assignment. The chosen assignment may be a problem set, an endurance problem, an in-class assignment or a computational assignment.

The late policy for the laboratory is described in the Laboratory Syllabus.

"What if I run out of certificates?"

If you run out of certificates for routine mishaps and delays and have to miss any additional assignment(s), you may turn in the assignment(s) at the end of the semester. These assignments will be counted toward the homework completion course requirement (completing 80% of assigned work), and will be considered in the instructor evaluation. Additionally, the instructor may choose to award partial points for completing these assignments, but in no case will this exceed 40% of the score the assignment would have earned if it was turned in on time. It is the student's responsibility to turn in the homework for consideration. Points may be awarded at the instructor's discretion based on extenuating circumstances, quality of the assignment (grade it would have received if turned in on time) and other factors. Homework assignments in this course are challenging and frequent, so it is essential to stay caught up with current material. **Please do NOT fall behind. There will be no exceptions to this policy.**

Quizzes

This term of physical chemistry builds on knowledge and skills you learned in your prior chemistry courses. In particular, all students should already have a working knowledge of gas laws, basic thermodynamics and basic kinetics. To fully understand the advanced concepts addressed in physical chemistry, we must build up from this very sound foundation. To that end, we do review these concepts and will have some homework problems designed to reinforce this material. Occasional quizzes will stress basic concepts in this foundational material as well as fundamental new concepts and basic problem solving. Quizzes will generally be given during laboratory time. Notecards will not be allowed on quizzes.

Exams

Midterm exams will primarily focus on advanced physical chemistry concepts and problem solving. Students may bring to the exam one 4"x6" index card in their own writing containing equations and other material they choose. As stated above, no such card is allowed for quizzes.

There will be three midterm exams. Each exam may include lecture material, any previous homework and in-class assignments, assigned material in the text as well as any additional reading or activities assigned. You are responsible for the assigned reading in the text regardless of whether that material has been discussed in lecture. No exams will be dropped. It is your responsibility to be aware of scheduled exam dates and any rescheduled exams.

I will grant permission to make up an exam if the absence is due to any of the following: (1) serious illness; (2) an order from the US Military; (3) officially representing the College; (4) death in the immediate family. Students producing the required documentation in a timely manner will be allowed to take a make-up exam. **Students with an unauthorized absence on an exam day will be able to make up the exam with a 20% point penalty. Students showing up unprepared for an exam (no notecard) must take the exam with no notecard.**

Individual students may request to take the exam at another time during finals week if that better fits

into their finals week schedules, however, the class final exam time will not be moved. Individual students requesting an alternate time are encouraged to coordinate with others in the same situation. The approval of alternate times is at the discretion of the instructor.

Instructor Evaluation

Instructor evaluation will be based on classroom attendance, attitude, effort on homework, improvement or consistently good progress and my evaluation of your understanding of the material in the course. This will be used to decide borderline cases. If you are on the borderline between two grades, you may be bumped up to the higher grade if you attend and arrive on time to 95% of class meetings, have not skipped assignments and you meet any one of the following additional requirements: 1) excellent effort on homework (all assignments turned in with at least 80% of the problems attempted on each, 90% or better overall score.) 2) improvement on exams throughout the semester ($>$ 25 point improvement) 3) consistently good progress (no bombed exams) or 4) if it is the opinion of the instructor that you understand the material better than your exams indicate. Note these criteria will only be used in borderline cases (within 1% of next highest grade).

Computer Software, E-mail and Web Access, etc.

The course web site will be the primary means of distributing homework assignments, exam study guides, laboratory help sheets, and many other handouts. Assignment sheets will be handed out in class, but will be available on the web site if you must miss class for some reason. I will make available links to web tutorials and other on-line resources throughout the year. We will also use the blackboard course management system to distribute solution keys, grades and facilitate e-mail communication. You must have regular Internet access, e-mail access and a pdf reader to access course materials. I will also put an announcement feed on the website.

The recently renovated course web site is: http://www.elmhurst.edu/~ksagarin/pchem/

> *A theory is the more impressive the greater the simplicity of its premises, the more different kinds of things it relates, and the more extended its area of applicability. Therefore the deep impression that classical thermodynamics made upon me. It is the only physical theory of universal content which I am convinced will never be overthrown, within the framework of applicability of its basic concepts.* (A. Einstein).

Tentative Lecture Schedule:

Physical chemistry is a very large subject ranging from microscopic to macroscopic physical and chemical phenomena. Unfortunately, we will will not be able to address every cover every topic in detail. Instead, this course is designed as a survey of classical and modern physical chemistry with an emphasis in problem solving.

The following is a guide indicating approximately how much time we will spend on each topic. We may deviate substantially from this schedule, spending more or less time on subjects as needed. Chemistry 413 will be directed toward the study of gases and molecular interactions, thermodynamics, phase diagrams, kinetics and statistical thermodynamics. We will also study some surface science topics in the lab.

Exams may be rescheduled in the event of a severe deviation from the schedule or in the case of exam conflicts for a majority of the students. (Please bring these to my attention as soon as possible.) Rescheduled exams will be announced at least one week prior to the new exam date. Homework assignment due dates, endurance problem due dates and in-class problem days are subject to change.

Week #	Day	Date	Text Chpt.	Topics
1	M	Jan. 30	1	Introduction, math review
	W	Feb. 1	1	Thermodynamics definitions, gas law review
	F	Feb. 3	2	*q, w* and U, What is work? Heat? First Law
2	M	Feb. 6	2	Heat capacity, enthalpy, adiabatic expansions
	W	Feb. 8	3	Fun math with state functions, T & P dependence of U, H
	F	Feb. 10	3/4	More math with state functions, thermochemistry
3	M	Feb. 13	4	Review Hess's Law, temperature dependence of reaction enthalpy
	W	Feb. 15	5	Spontaneous change: statistical/thermodynamic definitions
	F	Feb. 17	5	Calculating absolute entropy from primary data
4	M	Feb. 20	5	Calculating entropy changes
	W	Feb. 22	5	Gibbs and Helmholtz energy
	F	Feb. 24	6	Properties of G and U
5	M	Feb. 27	6	Partial molar quantities, chemical potential
	W	Feb. 29	6	Equilibrium
	F	Mar. 2	*	**exam 1**
6	M	Mar. 5	7	Real gases, compression factor, equations of state
	W	Mar. 7	8	Chemical potential and phase transformations
	F	Mar. 9	8	Phase diagrams of pure substances, Clapeyron equation
7	M	Mar. 12	8	Phase boundary calculations, Ehrenfest classification
	W	Mar. 14	9	Two and three component phase diagrams
	F	Mar. 16	9	Ideal and real solutions
8	M	Mar. 19	-	No Class - Spring Break!
	W	Mar. 21	-	No Class - Spring Break!
	F	Mar. 23	-	No Class - Spring Break!
9	M	Mar. 26	9	Activities, different standard states
	W	Mar. 28	12	Intro to statistical mechanics: basic probability theory
	F	Apr. 30	13	Microstates and configurations, Boltzmann distribution
10	M	Apr. 2	14	Canonical ensemble, molecular partition functions
	W	Apr. 4	14	Individual partition functions (trans, rot, vib, electronic)
	F	Apr. 6	-	No Class - Easter Break!
11	M	Apr. 9	14	Individual partition functions (continued)
	W	Apr. 11	*	**exam 2**
	F	Apr. 13	15	Statistical thermodynamics
12	M	Apr. 16	16	Kinetic theory of gases, Maxwell's distribution
	W	Apr. 18	16/17	Collisions, effusion, diffusion and viscosity
	F	Apr. 20	18	Basic kinetics review
13	M	Apr. 23	18	Kinetic mechanisms
	W	Apr. 25	19	Deriving complex kinetic mechanisms
	F	Apr. 27	19	Kinetics of chain reactions, explosions
14	M	May 30	18	Reaction dynamics, activation and diffusion controlled rxns
	W	May 2	18	Activated complex and transition state theory
	F	May 4	19	Advanced concepts in kinetics
15	M	May 7	19	Heterogeneous catalysis, photochemical reactions
	W	May 9	19	Photochemical reactions (con't)
	F	May 11	*	**exam 3**
16	M	May 14	-	Optional review class sometime this week.
	W	May 16	-	
	F	May 18	*	Final Exam 8:00 am

Table 1: Tentative Schedule - Chemistry 413 - Spring 2012

Week #	Day	Date	Text Chpt.	Assignments Due	Exams & Quizzes
1	M	Jan. 30	1		in-class
	W	Feb. 1	1		
	F	Feb. 3	2	homework 1	
2	M	Feb. 6	2		
	W	Feb. 8	3	homework 2	
	F	Feb. 10	3/4	problem 1	
3	M	Feb. 13	4		quiz Tues. 2/14
	W	Feb. 15	5	homework 3	
	F	Feb. 17	5		
4	M	Feb. 20	5		quiz Tues. 2/21
	W	Feb. 22	5		
	F	Feb. 24	6	problem 2	
5	M	Feb. 27	6		
	W	Feb. 29	6	homework 4	
	F	Mar. 2	*		**exam 1**
6	M	Mar. 5	6		
	W	Mar. 7	7	homework 5	
	F	Mar. 9	8		
7	M	Mar. 12	8		quiz Tues. 3/13
	W	Mar. 14	8	homework 6	
	F	Mar. 16	9	problem 3	
9	M	Mar. 19	-		*No Class - Spring Break!*
	W	Mar. 21	-		*No Class - Spring Break!*
	F	Apr. 23	-		*No Class - Spring Break!*
8	M	Mar. 26	9		
	W	Mar. 28	9	homework 7	
	F	Mar. 30	12	problem 4	
10	M	Apr. 2	13		quiz Tues. 4/3
	W	Apr. 4	14	homework 8	
	F	Apr. 6			*No Class - Easter Break!*
11	M	Apr. 9	14		
	W	Apr. 11	*		**exam 2**
	F	Apr. 13	15		
12	M	Apr. 16	16		
	W	Apr. 18	16/17	homework 9	
	F	Apr. 20	18		
13	M	Apr. 23	18		quiz Tues. 4/24
	W	Apr. 25	18	homework 10	
	F	Apr. 27	19	problem 5	
14	M	Apr. 30	19		quiz Tues. 5/1
	W	May 2	18	homework 11	
	F	May 4	18		
15	M	May 7	19	homework 12	
	W	May 9	19	All Redos Due	
	F	May 11	*		**exam 3**
16	M	May 14	-	Optional review class sometime this week.	
	W	May 16	-		
	F	May 18	*		Final Exam 8:00 am

Table 2: Tentative Schedule - Chemistry 413 - Spring 2012