

# Chemistry 411

## Physical Chemistry

### Syllabus - Fall 2007

#### General Information

**Instructor:** Dr. Kimberly Lawler-Sagarin  
**Office:** SC 218 **Phone:** x 3202  
**e-mail:** ksagarin@elmhurst.edu  
**Text:** *Thermodynamics, Statistical Thermodynamics, and Kinetics* by Engel and Reid, 1st ed (Req.)  
*Applied Mathematics for Physical Chemistry* by J. R. Barrante, 3rd edition (Req.)  
*Quantum Chemistry & Spectroscopy* by T. Engel, 1st edition (Req./Rec.)  
**Materials:** Laboratory Notebook (any brand, however, it should be  
quad ruled and designed for this purpose)  
Scientific Calculator (bring to all class meetings)  
**Class Meetings:** MWF 9:15 a.m. - 10:20 p.m. Schiabe Science 236/209  
**Lab Meetings:** Th 1:00 - 5:00 p.m. Schiabe Science 209/237  
**Office hours:** M 2-3 p.m., W 1:30-3:30 p.m., F 1:30-2:30 p.m. and 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): 110 points each = 33%
- Final Exam: 200 points = 20%
- Homework Problem Sets, Endurance Problems, Directed Reading Assignments, Computer/Computational Assignments and In-class Problems: 320 points = 32%
- Laboratory Component = 150 points = 15%
- Instructor Evaluation: used to decide borderline cases (within 2.5% 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 86% = A, 74% = B, 60% = C, 48% = D scale. This means if you receive an overall percentage of 86.00% and complete all course requirements, you will get an A. If you have an overall percentage of 85% 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.

Failing to meet one or more of these requirements will result in a student 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, you may expect at least a one-grade penalty for each requirement which is not fulfilled. 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 grade lower 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
- discussion/questions from directed reading questions

Laboratory activities, policies and assignments are discussed in the Laboratory Syllabus for Chemistry 411.

### Homework Problem Sets

Problem sets will be assigned and collected approximately weekly. They will be due Wednesdays at the beginning of class.

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 about 10-26 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.** Homework and assignments are 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 will assign "suggested problems" which will not be collected and graded. These problems will be available on the web site. It is particularly recommended that you work through these problems in addition to the regular homework. Homework solutions will also be available on the course web site.

## 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". This is a problem which you will generally have the opportunity to "redo" until it is complete and correct. In general, this problem will be a longer and more involved problem than regular homework problems. Endurance problems will be due on most Fridays.

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 and will be graded primarily on effort (i.e. a serious attempt = full credit). Attendance is required for credit. 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 informally decide to use part of a class period for an in-class exercise without advance notice. These will not involve the assignment of points, but you will be held responsible for the material discussed.

## Computer Assignments

Several computational chemistry and other computer based activities will be assigned. These will utilize CAChe, our new computational program Spartan, and some on-line tools. Assignments will be in the form of worksheets. Due dates will be announced. Points will vary but a approximately 40 points are predicted for this category.

## Overall Assignment Point Structure

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

- In-class problems = 8 (usually Fridays)  $\times$  5 pts = 40 pts
- Endurance problems = 6  $\times$  10 pts = 60 pts
- Computational assignments = (varies) = 40 pts
- Problem Sets = 11  $\times$  17 pts (avg.) = 187 pts estimated

A maximum of 320 points may be accumulated by a student. The above estimates The actual points possible in each of these categories may vary, but the combined total possible will be *at least* 320 points, or will be scaled up to 320 points. The above estimates a total of 327 points, but the actual points may vary.

## 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 411 are also required to abide by the Physical Chemistry honesty policy (will be handed out in class and will be available on the course web site).

## 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 assignments 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)

Certificates are as follows:

### **Late Homework Problem Sets**

- One certificate will allow you to turn in a problem set 1 day late (1 weekday, by 5 p.m. the NEXT weekday).
- One certificate will allow you to turn in a problem set 1 week late. Use of the one-week late certificate will generally mean the students will occasionally have access to the key or the graded work of others. Thus, a student with an unused week-late certificate will be able to turn in a corrected problem set to be graded again the last week of class.

### **Missed In-class Assignments**

- One certificate will allow you to make up an in-class problem (by turning in the worksheet or problems with 1 week) for full credit.

### **Late Endurance Problems**

- One certificate will allow you one free redo on an endurance problem. This is essentially a one week late certificate. This allows you to skip a redo and turn it in the following week for the same credit, or to turn in your first attempt on the second attempt due date for full credit.

### **Flex Certificate**

- One certificate will allow you to turn in a problem set, endurance problem or lab assignment 1 day late (1 weekday, by 5 p.m. the NEXT weekday).

### **“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. You will not receive homework points for the late assignment, but it will be counted toward the homework completion course requirement (completing 70% of assigned work) and will be considered in the instructor evaluation. Homework assignments in this course are challenging and frequent, so it is essential to stay caught up with current material.

### **Exams**

There will be three 65 minute midterm exams. Each exam may include lecture and laboratory 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.

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. All such instances will require documentation before a make-up exam will be given.

The final exam will be comprehensive and is scheduled for Friday, December 14th, 8:00a.m. Students also enrolled in Advanced Inorganic, or with another exam conflict, can arrange to take the final at another time, should they choose to, however the exam will be offered at the scheduled time as well.

### **Instructor Evaluation**

Instructor evaluation will be based on classroom attendance, effort on homework, laboratory performance, overall improvement and/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 based on a positive evaluation in any three of the following: 1) regular attendance (>90%) 2) your laboratory grade is one or more grades higher than your lecture grade (this one counts as two of the three needed) 3) excellent effort on homework (ALL assignments turned in with at least 90% of the problems attempted.) 4) improvement on exams throughout the semester (> 20 point improvement) 5) consistently good progress (no bombed exams) or 6) 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.

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

The course web site will be the primary means of distributing homework and exam solution keys, suggested problems, examination and lab 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 facilitate e-mail and grading communication. Because of this, I ask that you arrange to have or do the following:

- Web access, either through home/dorm or arrange your schedule to accommodate some time in one of the on-campus labs each week.
- If you will primarily be using your own computer, obtain Acrobat reader or another pdf display program. Acrobat Reader can be downloaded for free from Adobe (<http://www.adobe.com/>). Most on-campus computers should have this. (Many of the documents I will distribute will be in "pdf" format, hence the requirement.)
- An e-mail account which you check frequently. Accounts are available for free to all Elmhurst College students from Academic Computing Labs, but you are free to use any address you like.

The 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 and we won't be able to cover every topic in detail. The following is a guide indicating approximately how much time we will spend on each chapter. We may deviate substantially from this schedule, spending more time on subjects as needed. Chemistry 411 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. The topics of kinetics and surface science topics will be introduced in the laboratory much earlier than in class as many of our labs will address these issues.

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 are subject to change.

Week #	Day	Date	Text Chpt.	Assignments Due	Exams/In-class
1	M	Aug. 27	1		in-class
	W	Aug. 29	2		
	F	Aug. 31	2		
2	M	Sept. 3	-		No Class - Labor Day!
	W	Sept. 5	3	homework 1	
	F	Sept. 7	3		
3	M	Sept. 10	4		in-class
	W	Sept. 12	4	homework 2	
	F	Sept. 14	5	endurance 1	
4	M	Sept. 17	5		exam 1
	W	Sept. 19	5	homework 3	
	F	Sept. 21	-		
5	M	Sept. 24	5		in-class
	W	Sept. 26	6	homework 4	
	F	Sept. 28	6	endurance 2	
6	M	Oct. 1	6		in-class
	W	Oct. 3	7	homework 5	
	F	Oct. 5	7	endurance 3	
7	M	Oct. 8	-		No Class - Fall Recess!
	W	Oct. 10	8		
	F	Oct. 12	8	endurance 4	
8	M	Oct. 15	8		in-class
	W	Oct. 17	9	homework 6	
	F	Oct. 19	9		
9	M	Oct. 22	10		in-class
	W	Oct. 24	12	homework 7	
	F	Oct. 26	12		
10	M	Oct. 29	13		exam 2
	W	Oct. 31	13	homework 8	
	F	Nov. 2	-		
11	M	Nov. 5	13		in-class
	W	Nov. 7	14		
	F	Nov. 9	14	endurance 5	
12	M	Nov. 12	15		in-class
	W	Nov. 14	15	homework 9	
	F	Nov. 16	15	problem 7	
13	M	Nov. 19	16		in-class
	W	Nov. 21	18	homework 10	
	F	Nov. 23	-	No Class - Thanksgiving Break!	
14	M	Nov. 26	18		in-class
	W	Nov. 28	18		
	F	Nov. 30	19	endurance 6	
15	M	Dec. 3	19	homework 11	exam 3
	W	Dec. 5	19	All Redos Due	
	F	Dec. 7	-		
16	M	Dec. 10	-	Review Session - Reading Day!	Final Exam 8:00 am
	F	Dec. 14	-		

Table 1: Tentative Schedule - Chemistry 411 - Spring 2006