Chemistry 412
Physical Chemistry: Quantum Mechanics and Spectroscopy

General Information

Instructor:	Dr. Kimberly Lawler-Sagarin
Contact Info:	SC 218, x 3202, ksagarin@elmhurst.edu
Text:	*Quantum Chemistry & Spectroscopy* by T. Engel, 2nd edition (Required) *Applied Mathematics for Physical Chemistry* by J. R. Barrante, 3rd edition (Required) *Student's Solutions Manual for Quantum Chemistry & Spectroscopy* (Optional, recommended)
Class Meetings:	MWF 9:15am-10:20am Schaible Science 236
Office hours:	M 2-3pm, Tu 11am-noon, W 2:30-3:30pm, other times by appointment *These are subject to change. My regular office hours will begin week 2.* *Finals week: there will be a review session in the afternoon of reading day and office hours will be by appointment.*
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 quantum theory and spectroscopy 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 atoms, chemical bonding, and atomic and molecular spectroscopy grounded in the fundamentals of quantum theory;
2. be able to apply the concepts, methods and techniques of quantum chemistry to simple chemical systems and make predictions for these systems;
3. be able to use molecular symmetry as an aid for solving problems related to chemical bonding and molecular spectroscopy;
4. have the ability to use simple physical systems as models for understanding more complex systems;
5. 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 quantum mechanics and spectroscopy;
    - ability to approach unfamiliar physical problems and identify what conceptual and factual background information is needed to solve 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;

6. acquire a basic vocabulary relating to computational chemistry, appreciate both the power and limitations of this type of chemistry, and be able to interpret routine computational results in the chemical literature.

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

- Exams (3): 140 points each (420 total) = 42%
- Final exam: 160 points (ACS quantum/spectroscopy exam) = 16%
- Homework Problem Sets, Endurance Problems, Computational Assignments and In-class Problems: 420 points = 42%
- Instructor Evaluation: used to decide borderline cases (within 2% 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, 62% = C, 50% = 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 84% 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 (i.e. a passing average).
3. Turn in and receive grades for at least 80% of the problem sets and "endurance problems".
4. Attend and arrive on time to 90% of the in-class problem days
5. Turn in **all** computational assignments.

Failing to meet one or more of these requirements will result in a student not being graded on 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. For example, failing the final, skipping an excessive number of homework assignments, skipping a computational assignment, or repeatedly arriving late to in-class problem days 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.

Structure and Assignments

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

- interactive lecture
- in-class problems
- homework help
- discussion/questions from the readings and problem sets

Homework Problem Sets

Problem sets will be assigned and collected approximately weekly. Typically, 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 to 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 unless stated otherwise, though I may offer a grace period until after seminar on Wednesdays. 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 to redo the problem two times. For these problems, which will be marked, you will be graded out of 10 points on your first attempt, or out of 8 on your second.

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 guidelines 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 due on Friday will generally be graded by the following Monday.

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). 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.

Computational Chemistry Assignments

Several computational chemistry exercises will be assigned. These will utilize the computational chemistry programs CAChe, Spartan, and some on-line tools. CAChe is available in SC 209 on the PC machines, and Spartan is available on just a few computers - you need to borrow a software key to run this program. We have a site license for CAChe. If you would like a copy of CAChe for your own computer, you may obtain a copy of the software and access code from Dr. Losey or Dr. Sagarin. The access code must be updated yearly, typically in October.

Computational assignments will vary in structure and in the tools required.

Overall Homework/in-class Point Structure

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

- In-class Problems = 8 × 5 pts = 40 pts
- Endurance Problems = 5 × 10 pts = 50 pts
- Problem Sets = 12 × 20 pts (avg.) = 240 pts
- Computational Assignments = 5 × 20 (avg.) = 100 pts

A maximum of 420 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 420 points or will be scaled up to 420 points. The above estimates a total of 430 points.

Collaboration

Working in groups on the homework is not prohibited; in fact, it is strongly 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 five "flexible" Late Certificates. Each certificate is good for turning in one assignment one "class day" late. A class day is any MWF in which the college is holding class. Late certificates may be combined and are good for any type of assignment, including a missed in-class assignment. They should be saved until you really need them!

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.

"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 80% 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. **There are NO exceptions.**

Exams

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.**

The final exam will be the ACS Physical Chemistry - Quantum Mechanics exam. Our exam is scheduled for the Friday of finals' week, December 18th, at 8:00 a.m. 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. The time limit for the final is 1 hour, 40 minutes.

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 2% of next highest grade).

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 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. Because of this, I ask that you arrange to have or do the following:

- Web access, either through your home/dorm or by arranging 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/

Tentative Lecture Schedule:

Physical chemistry is a very large subject and we won't be able to cover every topic in detail. The following tables are guides indicating approximately how much time we will spend on each chapter and topic and the scheduling of assignments and exams. We may deviate substantially from this schedule, spending more time on subjects as needed. Chemistry 412 will be directed toward the study of quantum mechanics, spectroscopy, chemical bonding and symmetry. 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.	Topics
1	M	Aug. 31	0	Class Intro, Math Review
	W	Sept. 2	1	Failures of classical physics
	F	Sept. 4	1	Failures (con't), wave-particle duality
2	M	Sept. 7	*	No Class - Labor Day!
	W	Sept. 9	2	A few principles of quantum mechanics
	F	Sept. 11	3	Principles (con't), Quantum mechanical postulates
3	M	Sept. 14	3/4	Principles and postulates (con't), the particle in a box problem
	W	Sept. 16	4	The particle in a box problem (con't)
	F	Sept. 18	4/5	2D boxes, some variations on the box problem
4	M	Sept. 21	5	Heisenberg's Uncertainly Principle
	W	Sept. 23	5	The particle in a box and the real world
	F	Sept. 25	6	Stern-Gerlach, commutation relations
5	M	Sept. 28	16	Introduction to group theory
	W	Sept. 30	16	Symmetry operations and point groups
	F	Oct. 2	-	**exam 1**
6	M	Oct. 5	16	Assigning point groups
	W	Oct. 7	16	Working with character tables
	F	Oct. 9	16	Applications of group theory
7	M	Oct. 12	*	No Class - Fall Recess!
	W	Oct. 14	7	Rotation in two and three dimensions
	F	Oct. 16	7	Harmonic oscillator
8	M	Oct. 19	8	Introduction to spectroscopy
	W	Oct. 21	8	Rotational spectroscopy
	F	Oct. 23	8	Vibrational spectroscopy
9	M	Oct. 26	9	The hydrogen atom
	W	Oct. 28	10	Many-electron atoms, orbital approximation, Pauli
	F	Oct. 30	-	**exam 2**
10	M	Nov. 2	10	Many-electron atoms, term symbols
	W	Nov. 4	10	Variational principle, Hartree-Fock SCF
	F	Nov. 6	11	Lasers
11	M	Nov. 9	lec	Perturbation theory
	W	Nov. 11	lec	Perturbation theory (con't)
	F	Nov. 13	12	Molecular orbital theory - H_2
12	M	Nov. 16	12	Molecular orbital theory - diatomics
	W	Nov. 18	13	Molecular orbital theory - polyatomics
	F	Nov. 20	13	Simple Hückel Theory
13	M	Nov. 23	13	Variations on Hückel Theory
	W	Nov. 25	14	Electronic spectroscopy of molecules, absorption
	F	Nov. 27	*	No Class - Thanksgiving Break!
14	M	Nov. 30	14	More on electronic spectroscopy, fluorescence and phosphorescence
	W	Dec. 2	15	Computational chemistry - ab initio vs. semi-empirical
	F	Dec. 4	15	Computational chemistry - reliability of models
15	M	Dec. 7	15	More on computational chemistry
	W	Dec. 9	15	Computational chemistry - real world problems
	-	Dec. 11	-	**exam 3**
16	M	Dec. 14	*	No Classes - Reading Day
	W	Dec. 16		
	F	Dec. 18		**Final Exam 8:00 am**

Table 1: Tentative Topics Schedule - Chemistry 412 - Spring 2009

Week #	Day	Date	Text Chpt.	Assignments Due	Exams/In-class
1	M	Aug. 31	0		in-class
	W	Sept. 2	1		
	F	Sept. 4	1		
2	M	Sept. 7	*		No Class - Labor Day!
	W	Sept. 9	2	problem set 1	
	F	Sept. 11	3	endurance 1	
3	M	Sept. 14	3/4		
	W	Sept. 16	4	problem set 2	
	F	Sept. 18	4/5	endurance 2	
4	M	Sept. 21	5		
	W	Sept. 23	5	problem set 3	
	F	Sept. 25	6		
5	M	Sept. 28	16	problem set 4	
	W	Sept. 30	16		
	F	Oct. 2	16		**exam 1**
6	M	Oct. 5	16		
	W	Oct. 7	16	problem set 5	
	F	Oct. 9	16	comp 1	
7	M	Oct. 12	*		No Class - Fall Recess!
	W	Oct. 14	7	problem set 6	
	F	Oct. 16	7	endurance 3	
8	M	Oct. 19	8		
	W	Oct. 21	8	problem set 7	
	F	Oct. 23	8	comp 2	
9	M	Oct. 26	9		
	W	Oct. 28	10	problem set 8	
	F	Oct. 30	-		**exam 2**
10	M	Nov. 2	10		
	W	Nov. 4	10	problem set 9	
	F	Nov. 6	11	endurance 4	
11	M	Nov. 9	lec		
	W	Nov. 11	lec	problem set 10	
	F	Nov. 13	12	endurance 5	
12	M	Nov. 16	12		
	W	Nov. 18	13		
	F	Nov. 20	13	comp 3	
13	M	Nov. 23	13		
	W	Nov. 25	14	problem set 11	
	F	Nov. 27	*		No Class - Thanksgiving Break!
14	M	Nov. 30	14		
	W	Dec. 2	15	comp 4	
	F	Dec. 4	15		
15	M	Dec. 7	15	problem set 12	
	W	Dec. 9	15	comp 5	
	F	Dec. 11	-		**exam 3**
16	M	Dec. 14	*		.....No Classes - Reading Day
	W	Dec. 16	-		
	F	Dec. 18	-		**Final Exam 8:00 am**

Table 2: Tentative Text/Assignment Schedule - Chemistry 412 - Fall 2009