Chemistry 342
Quantum Mechanics and Spectroscopy
(Physical Chemistry II)
Spring, 2006

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Office Hours: Tu 2: 00 – 4:00
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by appointment

322 MYBK
TuTh 10:50 -12:05
WebCT page: http://webct.cofc.edu/webct/public/home.pl

Required Text: 1. Physical Chemistry, 7th Edition
Peter Atkins and Julio de Paula
W. H. Freeman and Company, 2002

Course Expectations:
Chemistry 342 is the second course in a two-course sequence in physical chemistry. The purpose of this course is to give you the foundations of quantum mechanics and spectroscopy.

A few comments regarding this course:

1. Math skills are essential. *
2. You will perform better if you can recall concepts learned in physics.
3. Concepts learned in freshman chemistry will be revisited in this course, so an understanding of those concepts will help you do well.
4. Reading the text will assist you in understanding and familiarizing yourself with the "lingo" of physical chemistry.
5. Performing the exercises at the end of the chapters will greatly facilitate solving the homework problems.

*CHEM342 is a math intensive course. Although the math used is not much more complex than that in 341, many of the concepts we cover *will* be new to you. Although the requirements for CHEM342 do not include a course on differential equations, you WILL see them used in this course. There is no requirement that you ***solve*** these kinds of equations, however you will need to be familiar with ***how*** they are used in the realm of physical chemistry.

Grading:
The final course grade will be based on your performance on problem sets, hour exams and the final using the formula below:

Problem sets	200 points
Hour exams (3 at 200 points each)	600 points
Final exam	200 points

(To be given on ***Tuesday May 2 from 9-11 am***)
ACS final exam will be given during the scheduled final exam period.

Exams will be given in class. The dates of these exams will be announced approximately two weeks prior to the exam. **There will be NO make up exams given.** If you are ill and cannot make it to class on the announced exam day, you must present a college accepted excuse. If you miss two exams, you will fail the course.

Grading Scale:	920 – 1000	A	700 – 750	C
	870 – 910	B+	600 – 690	D
	800 – 860	B	$\leq$ 590	F
	760 – 790	C+		

Problem Sets:
Problem sets will be assigned periodically during the semester and will comprise 20% of your final grade. It is up to you to make sure that you understand the assigned problems. You are welcome to work on these problems with a small group of students, but you must turn in your own solutions. These exercises are key to learning the course material and those who *understand* them will do well on the exams! Problem sets will normally be due at the start of class one week after they are assigned. Late problem sets will NOT be accepted.

Homework problems are listed in the lecture outline. The problem in **bold** will be solved by using the guidelines below and will be the only problem graded.

Guidelines for problem solving:

1. **Begin the problem on a separate sheet of paper.** Start with a clear statement of the problem in writing. DO NOT simply copy the problem from the text, *but state it in your own words*. Your solution should show clearly the strategy used in your problem solving.

2. Each step should be a logical consequence of the previous steps.

3. **Solve equations algebraically for the desired result. DO NOT insert numbers until the algebra is finished.** Avoid calculating intermediate numerical results that are not needed. **All numbers MUST have units.** Keep track of your units and show your conversion factors. Answers without units are meaningless. Keep track of significant figures in your mathematical results.

4. Finish each problem with a concluding sentence. How does it relate to the original question asked? What things did you learn from this problem, an application of a theory, a sense of the

magnitude of a quantity, a math "trick", etc.? Make sure you mention at least one "big" picture thing that you learned. Use this statement to bring yourself to a new level of understanding about physical chemistry and/or the problem. Think about the implication of the answer to the science. What does that tell you about the size or direction of the effect being illustrated by the problem, etc.? This reflection is important—**The time when you can learn the most from a problem is after you have the solution in hand!**

Detailed answer keys will be distributed to you on the day the homework assignment is due.

The Honor Code
The Honor Code of the College of Charleston specifically forbids:

Lying: knowingly furnishing false information, orally or in writing, including but not limited to deceit or efforts to deceive relating to academic work, to information legitimately sought by an official or employee of the College, and to testimony before individuals authorized to inquire or investigate conduct; lying also includes the fraudulent use of identification cards.
Cheating: the actual giving or receiving of unauthorized, dishonest assistance that might give one student an unfair advantage over another in the performance of any assigned, graded academic work, inside or outside of the classroom, and by any means whatsoever, including but not limited to fraud, duress, deception, theft, talking, making signs, gestures, copying, unauthorized reuse of previously graded work, unauthorized use or possession of study aids, memoranda, books, data, or other information.
Attempted cheating: a willful act designed to accomplish cheating, but falling short of that goal.
Stealing: the unauthorized taking or appropriating of property from the College or from another member of the college community. Note also that stealing includes unauthorized copying of and unauthorized access to computer software.
Attempted stealing: a willful act designed to accomplish stealing, but falling short of that goal.
Plagiarism:

- The verbatim repetition, without acknowledgement, of the writings of another author. All significant phrases, clauses, or passages, taken directly from source material must be enclosed in quotation marks and acknowledged either in the text itself or in footnotes/endnotes.
- Borrowing without acknowledging the source.
- Paraphrasing the thoughts of another writer without acknowledgement.
- Allowing any other person or organization to prepare work which one then submits as his/her own.

Penalties for Violations of the Honor Code
Penalties for violations of the Honor Code range up to and include expulsion from the

College. Attempted cheating, attempted stealing, and the knowing possession of stolen property shall be subject to the same punishment as the other offenses. Because the potential penalties for an Honor Code violation are extremely serious, all students should be thoroughly familiar with the above definitions and be guided by them.

CHEM442-Physical Chemistry II
Quantum Mechanics and Spectroscopy
Course Outline: Spring, 2006

Topic	Reading Assignment	Homework Assignment
Intro to quantum theory Failures of classical mechanics Wave-particle duality Schroediger equation Born interpretation Principles of quantum mechanics Wavefunction Uncertainty principle	**Ch. 11**	Problems **7,** 16, 19 and 20
Quantum theory: the basics Translational motion Particle in a box Vibrational motion Harmonic oscillator Rotational motion Rigid rotor Approximation methods	**Ch. 12**	Problems 22, 25, 27**, 29**
Exam 1: Tuesday, January 31 **Chapters 11 & 12**		
Atomic Structure & Spectra The hydrogen atom Atomic orbitals Spectroscopic selection rules Many-electron atoms Spectra of complex atoms Spin orbit coupling Singlet and triplet states Term symbols	**Ch. 13**	Problems 5, 7, **20,** 26
Molecular Structure Born-Oppenheimer approximation Valence bond theory Molecular orbital theory Huckel approximation	**Ch. 14**	Exercises 10b, 13b, 14b **Problem 13**
Exam II: Tuesday February 28 **Chapters 13 & 14**		

Topic	Reading Assignment	Homework Assignment
Spectroscopy I Rotation Rotational Raman Vibration Vibrational Raman Polyatomic molecules IR Vibrational Raman	**Ch. 16**	Problems 3, 5, 14, **29**
Spectroscopy II Electronic transitions Fluorescence and phosphorescence Lasers Photoelectron spectroscopy	**Ch. 17**	Problems 11, 13**, 21**, 22
Spectroscopy III Magentic resonance NMR ESR	**Ch. 18**	Problems 2, 10, 21, **22**
Exam III: Thursday April 20 **Chapters 16, 17, & 18**		