

Chemistry 358

Spring 2006

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Text: **Physical Chemistry: A Molecular Approach** McQuarrie & Simon
Office hours: Mon. & Wed. 12:00-2:00 & Tues 11:00-12:30 and by appointment.
(I may not be sitting in my office, but I will be somewhere on the 4th floor.)

"Let us remember, please, that the search for the constitution of the world is one of the greatest and noblest problems presented by nature."
-- Galileo

"In so far as quantum mechanics is correct, chemical questions are problems in applied mathematics." -- Eyring, Walter & Kimball, 1944

I think I can safely say that nobody understands quantum mechanics.

--R. Feynman

"A scientist is someone whose curiosity survives education's assaults on it."-- Sir Hermann Bondi

"If you get confused, logic out your dilemma." -- Picker X-Ray Corp. Digital Printer Manual, 1966

Welcome to Chemistry 358 for the Spring of 2006. The aim of this course is to present and develop the principles of physical chemistry emphasizing those areas of critical importance to understanding the underlying principles of all modern science. Reading, writing and problem assignments are an essential part of the course; they should be undertaken in a timely and serious manner.

The study Quantum Mechanics and the related fields of spectroscopy and kinetics/dynamics will be emphasized. Although quantum mechanics is often viewed as an esoteric subject only of interest to theoretical physicists, it is the theory that permits us to understand many of the properties of matter that we observe every day, such as why glass is transparent and why copper conducts electricity and Styrofoam doesn't. Quantum technology is the technology of the present and of the future. Devices such as lasers, medical imaging devices like MRI and PET, and the atomic clocks that make the GPS possible, all depend on the quantum nature of matter. Quantum mechanics will drive cutting-edge technology for years to come.

Course Objectives:

- 1) To demonstrate mastery of the fundamental concepts of physical chemistry, including: quantum mechanics, spectroscopy and chemical kinetics, by both descriptive and quantitative means.
- 2) To learn and reinforce logical strategies for solving quantitative problems.
- 3) To gain insight into the ever-expanding role of chemistry within the context of society, medicine, materials and environment.
- 4) To learn the essentials of maintaining a laboratory logbook containing an accurate, concise, and complete record of all laboratory observations, results, calculations, conclusions, notes, etc.
- 5) To improve your ability to correctly compose and write a scientific report containing the following components:
 - a) scientific accuracy
 - b) logical development and presentation
 - c) proper writing style (grammar, spelling and sentence structure)
 - d) appropriate format
 - e) clear and concise data presentation.
- 6) To show proficiency in the use of computers to collect, analyze, interpret, and present scientific data.

Course structure:

The course will be composed of both classroom and laboratory activities and instruction. These are tightly integrated components of the course and demands a significant commitment in time, and energy as well as a comprehensive understanding of your required previous coursework in chemistry, physics and math. Students are responsible for knowing material in the assigned reading, problems, labs, and lectures. Working problems, studying and understanding the material are keys to doing well. It is assumed that the students are familiar with the background material in Chemistry, Physics and Mathematics. While I am glad to help you in reviewing these topics, it is your responsibility to make up any weaknesses or deficiencies you might have. Much of the course material involves a high degree of conceptual understanding (not simple memorization), so adequate preparation and study are essential. It is **not** sufficient to learn the material from the lecture alone - you should read and think about the topics covered **before** attending lecture. If you still can't get a problem or concept, please see me for help. We will cover much detailed and difficult material this semester, so our pace must be geared toward those who are prepared to learn. In homework and exams be neat, box answers, show your work and units (partial credit will be given).

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

- Interactive lectures
- In-class problems
- Discussion/questions from readings and problem sets

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

- Interactive lectures
- Experiment design and procedure
- Data analysis techniques

Homework:

Relevant chapters and web materials should be read prior to class (assigned weekly) to assist you in preparation for contributing to classroom discussions, articulating your understanding of the material, and to help rapidly identify topics which you may find particularly difficult. Problems, both web based and at the end of each chapter, will be assigned on a weekly basis. Problem sets **will be** collected and graded. Informal writing assignments (once or twice a week) will be graded on a scale of 0 to 3. These assignments are designed to help you understand the material and to lead you through the basic steps of writing the final, formal lab report due at the end of each module. **LATE** assignments will **NOT** be accepted.

Lab Reports:

The report for each lab will vary and the grading criteria will be handed out prior to the relevant lab. For the first three reports, you will be required to review and edit another student's report as well as write your own. Thus, 3 due dates are required for each of these reports. You will first turn in a completed draft of your report. I will then assign a reviewer for your draft; you will review another student's draft. The reviewer will have 2-3 days to go over the report and prepare written comments prior to returning it to me. I will then give it back to you to either incorporate the suggestions of the reviewer or explain why you have not. You will have one week for the rewrite. You must turn in the first draft, reviewer's comments and the final draft. Each **day late**, at any step of the process, will result in a **10% reduction** of final score. You will also have the opportunity to revise (and resubmit within one week for a higher grade) up to two of your reports after I have graded them. The first one must be revised and you may select any other one for revision.

Grading Criteria:

Lab Reports	5 - Reports due	20 % of final grade
Laboratory technique and participation		5% of final grade
Midterm Exams (2)		40% of final grade
Final Exam		20% of final grade
Problem Sets		15% of final grade

Grading Scale:

A	90 - 100 %	B	80 - 89 %	C	70 - 79 %
D	60 - 69 %	F	≤ 59 %		

Chapters	Topic	Week
Chapt. 1	The Need for Quantum Theory	1 Jan 9
Chapt. 2 & MC A	The Classical Wave Equation & Complex Numbers	1 Jan 11 & 13
Chapt. 3 & MC B	PIB and Probabilty	2 Jan 18 & 20
Chapt. 3 & MC B	PIB and Probabilty	3 Jan 23
Chapt. 4 & MC C	Postulates of QM and Vectors	3 Jan 25 & 27
Chapt. 5 & MC D	Harmonic Oscillator	4 Jan. 30, & Feb 1
Chapt. 5	Rigid Rotator	5 Feb 3 & 6
Chapt. 1 -5	Review	5 Feb. 8
Chapt. 1 -5	Midterm Exam I	5 Feb. 10
Chapt. 6 & MC E	Hydrogen Atom & Determinants	6 Feb 13, 15 & 17
Chapt. 7	Variational & Perturbational Techniques	7 Feb. 20 & 22
Chapt. 8	Multielectron Atoms	7 Feb. 24
Chapt. 8	Multielectron Atoms	8 Feb. 27
Chapt. 9	Diatomoc Bonding	8 March 1 & 3
Chapt. 11	Computational Quantum Chemistry	9 March 6 & 8
Chapt. 12 & MC F	Group Theory & Matrices	9 March 10
Chapt. 12 & MC F	Group Theory & Matrices	10 March 13
Chapt. 1-9 & 11-12	Review	10 March 15
Chapt. 1-9 & 11-1	Midterm Exam II	10 March 17
	Spring Break	11 March 20-24
Chapt. 13	Molecular Spectroscopy	12 March 27 - 31
Chapt. 27	Kinetic Theory of Gases	13 April 3
	Assessment Day No Class	13 April 5
Chapt. 27	Kinetic Theory of Gases	13 April 7
Chapt. 28	Kinetics I	14 April 10 - 14
Chapt. 29	Kinetics II	15 April 17 - 21
All	Questions and Review	16 April 24 - 28
All	Final Exam 10:15 – 12:15	May 2