

# Chemistry 357, Physical Chemistry I

Fall 2013

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Instructor: Professor William D. Price

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Classroom: Science Bldg 465 MWF 11:00 – 11:50 & M 12:00 – 1:50

Text: **Physical Chemistry: A Molecular Approach** McQuarrie & Simon

Office hours: TWF from noon – 1:00 pm. and by appointment.

(I may not be sitting in my office, but I will be somewhere on the 4<sup>th</sup> floor.)

Welcome to Chemistry 357 for the Fall of 2013. 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.

**Catalog Description:** A systematic study of physical chemistry. (4 credit hours. PR: C or better in all of the following: CHM 212, PHY 211 and MTH 230)

## 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 demand 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

## Ground Rules/ Student Behavior:

- 1) ATTENDANCE is not mandatory, however quizzes make up a significant portion of your final grade and cannot be made up at a later time or date.
- 2) EXAMS AND QUIZZES are graded and may be scaled, depending on the relative difficulty, to yield a normal distribution.
- 3) EXAMS: Exams will typically have both in-class and take-home components. You are responsible for lecture and assignments up to the time of the exam. Pay close attention to the lecture. I will stress what I believe is important. Normally questions will be on material covered since the last exam, but the nature of the subject is such that the knowledge needed for an exam is cumulative from the beginning of the course. It must, therefore, be assumed that you are conversant with earlier material. In answering any non-multiple-choice problem, giving only the final answer is not sufficient. Unless you show in detail how you got your answer you may get little or no credit. Showing intermediate work allows me to give you part credit even though your final answer may be incorrect. On the other hand, irrelevant formulas may detract from your answer. Please endeavor to keep your work as readable as possible. While it is understood that you are working under a time limit, I cannot give credit unless I can follow the logic of your solution.
- 4) ABSENCE FROM HOUR EXAM: If you miss an exam you must obtain an excused absence from the Dean of Student Affairs (BOG Policy AA-13). If you know ahead of time that you cannot make the exam, you may communicate with me **before** the exam about scheduling a makeup without obtaining an official university excused absence.

- 5) CELL PHONES must be in silent mode while in the classroom. Cell phones (or any other electronic devices other than calculators) are not permitted to be used or handled, in any way, during exams. Cell phones should not be visible while taking an exam.
- 6) HOMEWORK PROBLEMS 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.
- 7) 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.
- 8) ACADEMIC DISHONESTY will be treated as described by Marshall BOG Policy AA-12 (<http://www.marshall.edu/president/Board/Policies/MUBOG AA-12 Academic Dishonesty.pdf>)
- 9) STUDENTS WITH DISABILITIES: All possible accommodations will be made. See <http://www.marshall.edu/disabled>.
- 10) ALL UNIVERSITY POLICIES will be followed in this course; these may be reviewed at the following web site: [http://www.marshall.edu/academic-affairs/?page\\_id=802](http://www.marshall.edu/academic-affairs/?page_id=802).
- 11) MAKE-UP WORK: All quizzes or exams missed due to an excused absence (*vida supra*) **will** be made up on Wednesday Dec 4, 2013 between the hours of 12 and 2 pm. If you are planning on making up work on this make-up day you **must** let me know by email by 4 pm Monday, Dec 2, 2013.

#### Grading Criteria:

Lab Reports	5 - Reports due	30 % of final grade
Laboratory technique and participation		5% of final grade
Midterm Exams (2)		30% 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	<b>1</b> Aug 26
Chapt. 2 & MC A	The Classical Wave Equation & Complex Numbers	<b>1</b> Aug 28 & 30
Chapt. 3 & MC B	PIB and Probabilty	<b>2</b> Sept 4 & 6
Chapt. 3 & MC B	PIB and Probabilty	<b>3</b> Sept 11 & 13
Chapt. 4 & MC C	Postulates of QM and Vectors	<b>4</b> Sept 16 - 20
Chapt. 5 & MC D	Harmonic Oscillator	<b>5</b> Sept 23 & 25
Chapt. 5	Rigid Rotator	<b>5 &amp; 6</b> Sept 27 & 30
Chapt. 1 –5	Review	<b>6</b> Oct 2
<b>Chapt. 1 –5</b>	<b>Midterm Exam I</b>	<b>6</b> Oct 4
Chapt. 6 & MC E	Hydrogen Atom & Determinants	<b>7</b> Oct 7 - 11
Chapt. 7	Variational & Perturbational Techniques	<b>8</b> Oct 14 - 18
Chapt. 8	Multielectron Atoms	<b>9</b> Oct 21 - 25
Chapt. 9	Diatomoc Bonding	<b>10</b> Oct 28 – Nov 1
Chapt. 1-9	Review	<b>11</b> Nov 4 & 6
<b>Chapt. 1-9</b>	<b>Midterm Exam II</b>	<b>11</b> Nov 8
Chapt. 11	Computational Quantum Chemistry	<b>12</b> Nov 11 - 15
Chapt. 13	Molecular Spectroscopy	<b>13</b> Nov 18 - 22
	Thanksgiving Break	<b>14</b> Nov 25 - 29
	Special Topics	<b>15</b> Dec 2 - 5
<b>All</b>	<b>Final Exam Due</b>	<b>Dec 10</b>

