

CHEM 482: Physical Chemistry II

Fall 2007

MWF 10:00-10:50 in 403 Day Hall

Instructor: Prof. Christopher Fecko
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Office Hours: Wednesday 2-3 pm
Thursday 2-3 pm
or by appointment

Course Description

We will explore the theories and applications of quantum chemistry, spectroscopy and statistical thermodynamics. By the end of this course, an active participant should be able to:

- outline the principles of quantum mechanics, with particular emphasis on those aspects that distinguish this theory from classical physics
- describe the internal structure and energetic properties of atoms and molecules
- explain how atomic and molecular parameters, such as bond lengths and binding energies, can be derived from various spectroscopic measurements
- describe how statistical thermodynamics relates the macroscopic properties of a bulk material to the energetic properties of individual component molecules
- solve theoretical and numerical problems related to the topics described in the four previous course goals at the level of the assigned homework

Prerequisites

CHEM 481 (PHYS 116, PHYS 117 and MATH 383)

Textbook

Physical Chemistry, 8th Edition, Volume 2
by Peter Atkins and Julio de Paula

Class Schedule (approximate)

Chapter 8	Quantum theory: introduction and principles	Aug 22, 24, 27, 29, 31(q)
Chapter 9	Quantum theory: techniques and applications	Sept 5, 7, 10, 12, 14(q), 17
Chapter 10	Atomic structure and atomic spectra	Sept 19, 21, 24, 26 (q), 28
Midterm 1	October 5	
Chapter 11	Molecular structure	Oct 1, 3, 8, 10, 15, 17 (q)
Chapter 13	Molecular spectroscopy 1: rotational and vibrational spectra	Oct 22, 24, 26, 29, 31
Chapter 14	Molecular spectroscopy 2: electronic transitions	Nov 2 (q), 5, 7, 9, 12
Midterm 2	November 19	
Chapter 16	Statistical thermodynamics 1: the concepts	Nov 14, 16, 26, 28
Chapter 17	Statistical thermodynamics 2: the applications (partial)	Nov 30, Dec 3, 5 (q)

Reading and Assignments

Lectures for this course will be based on the material in Atkins' textbook according to the approximate schedule listed above. To get the most out of each lecture, I encourage you to read the text before coming to class. Lectures may include supplemental material that is not included in the text. Unless otherwise noted, you are responsible for the material covered in the chapters as well as the material covered in class.

Although it is most important to understand the conceptual basis of the topics we cover in this course, it is also essential that you are able to apply the concepts by solving mathematical problems. For most students, the ability to solve problems quickly (as is required on quizzes or exams) requires much practice. As we begin each chapter, I will suggest a set of problems that cover the important material and should help you adequately prepare for exams. The assignments will not be collected, so it is up to you to determine how many problems to complete.

Examinations and Grading

Quizzes: There will be six short (10-15 min) quizzes given during class time, scheduled for Aug 31, Sept 14, 26, Oct 17, Nov 2 and Dec 5. I will drop your lowest quiz score when computing your final quiz grade. The quizzes will not be offered at any alternate time, and missed quizzes will receive a score of 0.

Midterm Exams: There will be two 50 minute exams during class time on October 5 and November 19. If you cannot take a midterm at the scheduled time, contact me at least 2 weeks in advance of the exam, and I will consider giving you an exam a day or two early. Exam make-ups will only be permitted in extreme circumstances that are documented by a written explanation. Exams offered at alternate times may be oral exams.

Final Exam: There will be a final, cumulative exam on Friday, December 14 at 8:00 am. It will include a short section on material covered after the second midterm, as well as a cumulative section covering the entire semester.

Quizzes and exams may contain conceptual, theoretical and numerical problems. I will provide a table of integrals and the values of numerical constants that are necessary to complete the problems. I will also provide many of the equations that are needed (taken directly from the text with no further definitions or explanations).

Final Grade: Your final grade will be determined by your average quiz grade (30%), midterm exam grades (20% each) and final exam grade (30%).

Honor Code

(Policy adopted by the faculty of the Department of Chemistry on September 9, 1977)

“Since all graded work (including homework to be collected, quizzes, papers, mid-term examinations, final examinations, research proposals, laboratory results and reports, etc.) may be used in the determination of academic progress, no collaboration on this work is permitted unless the instructor explicitly indicates that some specific degree of collaboration is allowed. This statement is not intended to discourage students from studying together or work together on assignments which are not to be collected.”