University of Wisconsin-Madison
Chemistry 562 Physical Chemistry
Syllabus Spring 2018

Chemistry 562 is the second course of a two-semester sequence on physical chemistry at the advanced undergraduate level. It is most often taken by advanced chemistry and chemical engineering majors, but it is also highly appropriate for other science and engineering interests, *e.g.,* biochemistry, physics, or materials science. It is also taken by graduate students in a variety of science and engineering fields. Chemistry 562 is a three credit course for all these categories of students, based on the three 50 minute lectures per week. The structure of the course presumes a sound background in chemistry and physics and, because the course uses calculus, previous course work in that area. The course is mathematically flavored with an emphasis on physical models, particularly their development and manipulation. It is assumed that students taking this course already have a background in chemical thermodynamics and other aspects of macroscopic physical chemistry, either from taking Chemistry 561, the first half of the sequence, or from similar course work in other departments. The subjects of Chemistry 562 are (1) the quantum mechanical description of atomic and molecular structure, (2) high-resolution gas phase molecular spectroscopy (primarily atoms and diatomic molecules), and (3) the use of quantum statistical mechanics to compute the thermodynamic properties of gases (mainly atoms and diatomic molecules). We will begin by describing the origins of quantum mechanical concepts and theory in the early twentieth century. This will be followed by study of the time independent Schrodinger Equation (the most fundamental basis of quantum wave mechanics) and related mathematical ideas, particularly the concepts of eigenfunctions and eigenvalues. Examples will include the particle in a box, the harmonic oscillator, angular momentum in quantum mechanics, and the hydrogen atom. Infrared, Raman, microwave, and ultraviolet-visible spectroscopy of gas phase molecules, especially diatomic molecules, will be covered. The quantum mechanical description of atomic structure of many-electron atoms and of small diatomic molecules will be explained, with emphasis on the mathematical basis for understanding the nature of the chemical bond using molecular orbital theory. Finally an introduction to statistical mechanics will be given to establish the connection between the quantum mechanical description of atoms and molecules and the thermodynamic description of bulk gases.

Course Information

Meeting Times and Location: Lectures meets MWF 8:50 to 9:50 AM in 1315 Chemistry; discussion times depend on section

Course Designations: Advanced level; physical science breadth; counts as L&S credit

Instructional mode: face-to-face

Course website: https://learnuw.wisc.edu/

How Credit hours are met: This 3-credit class meets each week for three 50-minute lectures and one 50-minute discussion. Over the course of the semester, students are expected to do at least 135 hours of learning activities, which includes class attendance, reading, studying, preparation, problem sets, and other learning activities.

Official Course Description: Molecular theory: quantum chemistry, molecular structure and spectra, statistical mechanics, selected topics in the molecular theory of matter in bulk.

Requisites: CHEM 561 or 565 or CBE 310; PHYS 202 or 208

Staff

Professor: R. Claude Woods, rcwoods@wisc.edu, 4337 Chemistry Building, available by appointment

Teaching Assistants: Schuyler Kain, skain@wisc.edu and Matisha Dorman, dorman3@wisc.edu. Office hours will be announced near the start of the semester.

There are four different discussion sections at different hours (one hour per week for each section) that will be similar in content and structure. Students should attend the one in which they are enrolled unless there are unavoidable special circumstances, in which case the student affected should contact Professor Woods.

Learning Objectives

1. Develop a basic understanding of the way in which quantum mechanical theory is used to describe the microscopic behavior of atoms and molecules in chemistry and their interaction with electromagnetic radiation. This includes the photon concept, the quantization of energy and angular momentum, the wave-particle duality, the uncertainty principle, and the need to use probabilities in describing outcomes of experiments.
2. Achieve proficiency in solving numerical problems in quantum theory and spectroscopy, including the use of the fundamental constants of nature to convert between various units, *e.g.,* converting photon descriptions between wave length, wave number frequency, Hertz frequency, momentum, or energies in J, kJ/mol, eV, Hartrees, *etc*.
3. Learn to solve for and interpret the eigenfunctions and eigenvalues of the time independent Schrodinger Equation for the most important simple quantum mechanical systems: the one and three dimensional particle in a box and harmonic oscillators, the angular momentum problem, the hydrogen-like atom, the helium and second row atoms, the hydrogen molecule ion, the

hydrogen molecule, other first and second row homonuclear diatomics, and the vibrational-rotational motion of diatomic molecules.

4. Understand the assignment and analysis of the rotational (microwave), vibration-rotational (infrared), and electronic-vibrational-rotational (UV-visible) spectroscopy of gas phase diatomic molecules.
5. Derive the basic expressions for calculating thermodynamic functions (enthalpy, entropy, Gibbs free energy, equilibrium constants, etc.) from equilibrium statistical thermodynamics and use them to calculate these macroscopic properties from spectroscopic and quantum chemical data in simple cases.

Textbook

Text: Atkins, Peter, and de Paula, Julio, **Physical Chemistry,** Volume 2, 10th edition, W. H. Freeman and Co. The textbook covers substantially the same material as will be covered in the lectures, but the order of presentation and the emphasis on topics will be different in the lectures. There is also a single volume hard-bound version of this text, but all the chapters that are covered in Chemistry 562 are contained in Volume 2. The 8th or 9th editions will serve equally well for the purposes of this course.

Policies and Procedures

Lectures: Attendance at lectures is important, as lecture notes will not be posted. The lectures will define what the course is, and it will be practically impossible to keep up without faithful attendance. You are responsible for all material covered in class.

Problem Sets: Problems will be graded, and solutions to all problems will be distributed and placed on the course web page. You should be prepared to discuss the problems in your discussion section. We encourage you to discuss the problems with each other, but you must hand in and take responsibility for your own solutions. It is permissible for groups of two or three students to work together on the problem set, but final turned in work must be done by each student individually. Problem set grades will be used in calculation of final grades, as discussed below.

Discussion: You will meet with your teaching assistant for a discussion period each week. This is a time to discuss the lecture material and problem sets. Attendance at the discussion sections is expected and is highly important to success in this course. The teaching assistants will also have scheduled office hours each week for optional help for students. Professor Woods is also available for individual student help on an appointment basis.

Calculator: There will be considerable emphasis on numerical calculations and unit conversions on the homework and examinations. Therefore a good scientific calculator will be required and **must be brought to all tests**.

Grading: There will be two tests during the semester and one final examination that will count as much as both tests combined. All the tests will be heavily influenced by the problem sets, so that mastery of the problems will be essential for doing well on the tests. There will be numerical grades on each test that will be added for a final total at the end of the semester. Each test will also have a letter grade to give students an idea of where they stand. Final letter grades will be assigned at the end of the semester by the professor in consultation with the teaching assistant. There is no pre-determined numerical score that is required for an A or any other letter grade. In no case will the final assigned letter grades be in a different order than the final numerical point totals. The point distribution for the final course grade is as follows:

First mid-term	100
Second mid-term	100
Final examination	200
Problem set total	50
Grand total	450

Course website: Learn@UW will be used for posting problem sets, problem set answers, announcements, handouts, grades, and other material pertinent to this course. Lecture notes will only be provided to students with approved unavoidable absences from lecture.