

**UNIVERSITY OF WASHINGTON
DEPARTMENT OF CHEMISTRY**

Chemistry 455, Autumn 2003

http://depts.washington.edu/chemcrs/

Instructor:

Professor Thomas Engel
Bagley 214, 685-2330, engel@chem.washington.edu

Grader

Catherine Cooksey (ccooksey@u.washington.edu)

Office Hours:

Thomas Engel: Mon 1:30-2:20, CHB 339; Wed 2:00-3:00, BAG 319; and Fri 10:30 - 11:20 CHB 439.

Catherine Cooksey: Tuesdays 10:00 - 11:00, Bagley 2

Text:

Chem 455: Quantum Chemistry and Spectroscopy T. Engel (OUGL Copy Center)

Additional texts on reserve in the Chemistry Library

Peter Atkins, *Physical Chemistry*, 7th edition

D. A. McQuarrie and J. D. Simon, *Physical Chemistry, a Molecular Approach*

Lectures:

M, W, F, 9:30-10:20, Bagley 154

Discussion/Tutorial:

Th, 9:30-10:20, Bagley 154

Course Objectives: In this course, we will study quantum mechanics and its major applications in chemistry. The applications include the electronic structure of atoms and the chemical bond.

APPROXIMATE LECTURE AND READING SCHEDULE (Omit supplemental Sections in text)

Day	Week	Reading	Day	Week	Reading
M	Sept 29	Chapters 1-2: From Classical to Quantum Mechanics, The Schrödinger Equation	M	Nov 10	Chapter 10: Multielectron Atoms
W			W		
F			F		
M	Oct 6	Chapter 3-4: The Postulates, Using Quantum Mechanics on Simple Systems	M	Nov 17	Chapter 11: Atomic Spectroscopy
W			W		
F			F		
M	Oct 13	Chapter 5-6: Particle in the Box and the Real World, Commuting and Noncommuting Operators	M	Nov 24	Chapter 12-13: Chemical Bonding in Diatomic Molecules
W			W		
F			F		
M	Oct 20	Chapters 7: A Quantum Mechanical Model for the Vibration and Rotation of Molecules	M	Dec 1	2nd Exam Chapter 14: Molecular Shapes and Energy Levels for Polyatomic Molecules
W			W		
F			F		
M	Oct 27	1st Exam Chapter 8: Vibrational and Rotational Spectroscopy of Diatomics	M	Dec 8	Last day of classes
W			W		
F			F		
M	Nov 3	Chapter 9: The Hydrogen Atom	Final Exam: Tues, Dec 16, 8:30-10:20 a.m.		
W					
F					

— OVER —

CLASS SESSIONS

The material indicated in the class schedule will be discussed in the lecture. Discussion is a two-way street. It would be great if you bring up concepts you didn't understand, material you think needs more discussion, and topics you want to talk about in the lectures. Please ask lots of questions in class and in the office hours to help you get the most from this course! Because the best time to discuss these issues is when they are covered in lecture, you will get a lot more out of the course if you are up to date in your reading and problem solving.

PROBLEM SOLVING

In order to learn how to use the concepts we will be dealing with, it's important to work problems. You will practice this in the discussion sessions and by working on homework assignments. Feel free to work on the homework with others, but make sure you have understood the problem and its solution.

HOMEWORK ASSIGNMENTS

Homework problems are assigned each lecture day and are posted on the course web site. They are due at 3:30 p.m. the following lecture day. You can hand them in after the lecture or put them in my mailbox (#15). Late submissions will not be accepted. The assignments will be graded by giving half the weekly points on the basis of how much of the assignment was finished. The other half will be based on the rigorous grading of one of the problems each week. If you have worked 20 minutes on a problem and don't see how to solve it, see me in an office hour or email me for a hint. It's a good idea to make a photocopy of your homework for study purposes, because it takes a while to get the graded papers back to you.

EXAMS AND COURSE GRADING

There will be two hourly exams and a two-hour final exam, as indicated on the schedule. Final grades are based on the total number of points obtained on the exams and the homework.

2 midterm exams	200 points
homework assignments	100 points
final exam	<u>200 points</u>
	500 points