
CHEM 542 PHYSICAL CHEMISTRY II

Quantum Mechanics, Atomic and Molecular Structure, and Spectroscopy

Syllabus and Class Schedule

Course Description	Chemistry 542, the second course in a 2-semester sequence of physical chemistry, provides an introduction to quantum mechanics, atomic and molecular structure, spectroscopy, and statistical mechanics. (3 credit hours)
Prerequisites	Completion of CHEM 111, 112, 321, 331, and 332 with a C or better, CHEM 541.
Instructor	Lisa Lever, Ph.D. Office: Smith 409 Office hours: M 10:00-11:00, TTH 9:30-10:30 and T 1:00-3:00 and by appointment email: llever@uscupstate.edu website: http://faculty.uscupstate.edu/llever/ Phone: 503-5713
Texts and Calculator	<i>Physical Chemistry Thermodynamics, Structure, and Change</i> , 10th Edition, Peter Atkins and Julio de Paula, W. H. Freeman. (required) <i>Student's Solutions Manual for Physical Chemistry: Thermodynamics, Structure, and Change</i> , Charles Trapp, Marshall Cady, and Carmen Giunta. (on library reserve) A scientific calculator will be needed for exams, homework, and classroom work. Bring your calculator and textbook to class every day.
Attendance	Class attendance and participation is expected of all students. Attendance will be checked each class period. Students are responsible for getting class notes and information for any missed classes.

Lecture	We will focus on problem solving and active learning activities in class. For class time to be most effective, students should read the relevant material in the textbook and work assigned homework prior to class.
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Homework	Homework problems will be assigned for practice in applying concepts and developing problem solving skills. Where appropriate, problems should be solved using Excel or Mathcad. You should attempt problems on your own first before consulting the solutions manual or other sources. You are encouraged to discuss problems with other students and the instructor. Graded homework assignments should represent your own work and understanding. You should show all your work. Your method for solving the problem is more important than getting the correct numerical answer!
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Tests	<p>Three tests will be given during the semester. If you have to be absent on the day of a test, notify the instructor as soon as possible. An opportunity to make up a missed test will be given only for an unavoidable absence.</p> <p>Test 1 Thursday, Feb. 9 Test 2 Tuesday, Mar. 14 Test 3 Thursday, Apr. 13</p>
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Final Exam	<p>Thursday, Apr. 27, 11:30-2:30</p> <p>The final exam will be cumulative. The score on the final exam may be used to substitute for the lowest test grade or one missed test.</p>
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Grades	<p>The course grade will be calculated as follows:</p> <table><tr><td>Class participation and homework</td><td>20%</td></tr><tr><td>Tests</td><td>55%</td></tr><tr><td>Final exam</td><td>25%.</td></tr></table> <p>Grading scale: A ≥ 90 > B+ ≥ 87 > B ≥ 80 > C+ ≥ 77 > C ≥ 70 > D+ ≥ 67 > D ≥ 60 > F</p>	Class participation and homework	20%	Tests	55%	Final exam	25%.
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Internet

Class and homework assignments and course web links will be posted on the instructor's web site at:

<http://faculty.uscupstate.edu/llever/>

Class handouts, lecture notes, homework and test keys, and grades will be posted on Blackboard:

<https://blackboard.sc.edu/>

Technology

Lectures will meet in the active learning classroom, LIBR 238. Students are encouraged to bring USB drives, smartphones, tablets, and/or laptops to be able to display and/or save your work. These devices are to be used for class work only during class time.

Learning Goals

Students will apply the concepts of quantum mechanics in this course to the study of atoms and molecules. Specifically students will

- Describe the experimental evidence that led to the development of quantum theory.
 - Apply the principles of quantum theory to calculate the properties of atoms and molecules in motion.
 - Apply quantum mechanics to study the electronic structure of atoms and molecules and their spectra.
 - Describe the physical insights that result from mathematical derivations.
 - Solve chemically relevant problems using advanced mathematical methods and symbolic mathematical and computational software.
 - Communicate course concepts through class discussions/presentations.
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Disability Statement

USC Upstate supports the ongoing development of an accessible university that embraces diversity through educational programming, services, resources, and facilities that are usable by all members of the campus community. In keeping with University policy, any student with a disability who requests academic accommodations should contact Disability Services at 503-5199 to arrange an appointment with a Disability Services staff member. Students are encouraged to seek an appointment as early in the semester as possible, as accommodations are not provided retroactively.

Chemistry 542 Tentative Schedule

Date			Topic	Read before class
Jan.	10	T	Electromagnetic radiation, blackbody radiation	Foundations Topic C, Ch. 7 Topic 7A
	12	Th	Origins of quantum mechanics	
	17	T	Schrödinger equation and the wavefunction	Ch. 7 Topic 7B
	19	Th	Principles of quantum mechanics	Ch. 7 Topic 7C
	24	T	Translational motion	Ch. 8 Topic 8A
	26	Th	Vibrational motion	Ch. 8 Topic 8B
	31	T	Rotational motion	Ch. 8 Topic 8C
Feb.	2	Th	Angular momentum	
	7	T	Hydrogenic atoms	Ch. 9 Topic 9A
	9	Th	Test 1 (Ch. 7 & 8)	
	14	T	Multielectron atoms	Ch. 9 Topic 9B
	16	Th	Atomic spectra	Ch. 9 Topic 9C
	21	T	Molecular structure, valence bond & MO theory	Ch. 10 Topics 10A & 10B
	23	Th	Diatomic molecules	Ch. 10 Topics 10C & 10D
	28	T	Polyatomic molecules	Ch. 10 Topic 10E
Mar.	2	Th	Hückel approximation, computational approaches	
	7	T	Spring Break	
	9	Th		
	14	T		
	16	Th	Symmetry elements and point groups	Ch. 11 Topics 11A & 11B
	17	F	<i>Last day to withdraw from course</i>	
	21	T	Character tables	
	23	Th	Applications of symmetry	Ch. 11 Topic 11C
	28	T	Molecular spectroscopy	Ch. 12 Topic 12A
	30	Th	Molecular rotation and rotational spectroscopy	Ch. 12 Topics 12B & 12C
Apr.	4	T	Vibrational spectroscopy of diatomics	Ch. 12 Topic 12D
	6	Th	Vibrational spectroscopy of polyatomics	Ch. 12 Topic 12E
	11	T	Electronic spectroscopy	Ch. 13 Topic 13A
	13	Th	Test 3 (Ch. 11 & 12)	
	18	T	Decay of excited states	Ch. 13 Topic 13B & C
	20	Th	Statistical thermodynamics/Wrap up	
	27	Th	Final exam 11:30-2:30	

This is a tentative syllabus, and the instructor reserves the right to make adjustments in the syllabus and schedule as necessary.