

CHM5440 - Physical Chemistry II

Winter 2004

Instructor: Alexander V. Benderskii 73 Chemistry
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Lectures: Mon, Tue, Wed, Fri 9:35-10:30 AM, 1109 Science Hall
Office hours: Tue, Wed 10:30-11:30 AM

Text: Physical Chemistry, by R. J. Silbey and R. A. Alberty (3rd Edition).

Topics covered by the course: Quantum mechanics (Ch. 9); atomic structure (Ch. 10); molecular structure (Ch. 11); rotational and vibrational spectroscopy (Ch. 13); electronic spectroscopy (Ch. 14); kinetic theory of gases (Ch. 17); chemical kinetics (Ch. 18). The emphasis will be made on the *fundamental physical principles* that form a unified base for understanding chemistry and spectroscopy.

- ◆ The reading assignments must be completed BEFORE each lecture.
- ◆ There will be surprise 15 min. quizzes during the lectures (approximately 10 through the semester) that will contribute to the final grade. At the end, two lowest quiz scores may be dropped.
- ◆ ***The last day to drop the class is Friday Feb. 13, 2004.***
- ◆ There will be 3 midterm exams (1 hr each) and a final exam (2.5 hrs).
- ◆ *All exams and quizzes will be closed-book.*
- ◆ All exam dates are **final**, permission (with legitimate excuse) must be obtained **24 hours before** the date and time of the exam.
- ◆ All homework assignments must be turned in on time, which will be announced.
- ◆ Zero grade (0 pts) will be assigned if an exam/quiz is missed or a homework assignment is not turned in on time.
- ◆ **Grading:** Homework: 15%
Quizzes: 10%
Midterm exams: 50%
Final exam: 25%

There will be no curve grading. The final grade will be determined based on an absolute

Grading Scale:

93-100%	A
88-92%	A-
84-87%	B+
80-83%	B
77-79%	B-
73-76%	C+
69-72%	C
66-68%	C-
63-65%	D+
60-62%	D
57-59%	D-
<56%	E

CHM 5440 Course syllabus:

Week	Date	Topics	Reading assignments
1	1/12	Introduction to the course. Math review	
	1/13	Classical mechanics: a deterministic theory. Failures of classical mechanics.	9.1
	1/14	The wave-particle duality. The de Broglie wavelength. The Heisenberg Uncertainty Principle. The wavefunction.	9.1 - 9.3
	1/16	The Schrodinger equation.	9.14, 9.3
2	1/19	No class (University holiday)	
	1/20	Particle in a 1D box: <i>quantization</i> of energy	9.6
	1/21	Operators	9.4, 9.5
	1/23	Postulates of Quantum Mechanics	9.13, 9.5
3	1/26	Particle in 2D and 3D box: <i>degeneracy</i>	9.7
	1/27	Tunneling	9.15
	1/28	Vibrational motion: Harmonic Oscillator	9.9
	1/30	Quantum-mechanical Harmonic Oscillator	9.10
4	2/2	Commutator and the uncertainty principle. The superposition principle.	9.4, 9.5, 9.8
	2/3	Rotational motion: classical description	9.11
	2/4	Rotational motion in 2D: particle on a ring.. <i>Review</i>	9.11, 9.12
	2/6	<i>Exam I</i>	
5	2/9	Rotational motion in 3D. Angular momentum.	9.11, 9.12
	2/10	Hydrogen atom: the Schrodinger equation	10.1, 10.15
	2/11	Hydrogen atom: energy levels, spectra	10.1, 10.2
	2/13	Hydrogen atom: wavefunctions <i>Last day to drop class</i>	10.3
6	2/16	Hydrogen atom: expectation values of physical observables.	10.3, 10.4
	2/17	Variational Method	10.6
	2/18	Helium Atom	10.7
	2/20	Electron spin. Pauli Exclusion Principle	10.5, 10.8
7	2/23	Multi-electron atoms: the Aufbau Principle and the periodic table	10.10, 10.11
	2/24	Atomic spectroscopy	10.12, 10.13
	2/25	Atomic spectroscopy	10.13, 10.14
	2/27	Quantum Chemistry. The SCF Hatree-Fock Method	10.9
8	3/1	Diatomic molecules: the Born-Oppenheimer Approximation	11.1
	3/2	The hydrogen molecular ion H_2^+	11.2
	3/3	Electronic states and energies of H_2^+ . <i>Review</i>	11.3
	3/5	<i>Exam II</i>	
9	3/8	MO description of the hydrogen molecule	11.4
	3/9	Electron configuration of homonuclear diatomics	11.5
	3/10	Polyatomic molecules: Valence bond method	11.6
	3/12	Polyatomic molecules: Huckel MO theory The band theory of solids: metals, semiconductors, insulators	11.7 11.11

	3/15 - 3/20	Spring Recess	
10	3/22	Spectroscopy: an introduction	13.1, 13.2
	3/23	Rotational spectra of diatomics	13.3, 13.4
	3/24	Vibrational spectra of diatomics	13.6
	3/26	Vibration-rotation spectra	13.7
11	3/29	Vibrations of polyatomic molecules	13.8
	3/30	Electronic spectroscopy of diatomics	14.1 - 14.4
	3/31	Electronic spectroscopy of diatomics	14.3, 14.5
	4/2	Photochemistry and chemical dynamics	14.8, 19.10
12	4/5	Kinetic theory of gases: the Maxwell distribution	17.1 - 17.3
	4/6	Collisions of the gas-phase molecules. Pressure. Mean free path	17.5 - 17.8
	4/7	Transport phenomena: diffusion and viscosity. <i>Review</i>	17.10, 17.11
	4/9	<i>Exam III</i>	
13	4/12	Chemical kinetics: reaction rates	18.1, 18.2
	4/13	Order of reactions.	18.2
	4/14	Reversible reactions and the detailed balance principle	18.3, 18.5, 18.8
	4/16	Consecutive reactions and kinetic schemes	18.4
14	4/19	Reaction mechanisms	18.7
	4/20	Temperature dependence of the reaction rates	18.6
	4/21	Bimolecular reactions	18.9
	4/23	Chain reactions	18.11, 18.12
15	4/26	<i>Course Review</i>	
	4/30	<i>Final Exam</i>	