Chem 336 Physical Chemistry III

Catalog Data:	Chem 336 Physical Chemistry III (3-0-3) The topics include introduction to quantum mechanics, model quantum mechanical systems, atomic structure and spectra, introduction to chemical bonding and molecular spectroscopy.
Textbook:	Physical Chemistry, 9th ed. P. Atkins, Freeman & Co. New York, 2010
Chapters to be Covered:	7, 8, 9, 10, 12, 13
Reference:	None
Coordinator	Dr. L. Krasnoperov, Professor, Chemistry.
Course Objective:	The course is designed to introduce students to basic concepts in quantum mechanics, chemical bonding and spectroscopy
Prerequisites by Topic:	Functions of two and several variables Partial derivatives Integrals Differential equations Classical mechanics Electricity and magnetism Basic chemical principles
Topics:	1. Origins of quantum mechanics and the failure of classical mechanics. Black-body radiation. Planck's constant. Heat capacities of solids and diatomic molecules. Atomic and molecular spectra. $\Delta E=h\nu$ The photoelectric effect. The wave-particle duality. De Broglie wavelength. The wavefunction. The Born interpretation. The time dependent and time independent Schroedinger equations. Finite motion. Normalization. Quantization. Operators, eigenfunctions and eigenvalues. Hamiltonian. Hermitian operators. Superpositions. Average (expectation) values. The Heisenberg uncertainty principle. Commutators. (2 weeks). 2. Applications of quantum mechanics to model systems. Free translational motion. Particle in a 1D

box. Zero point energy. Motion in 2 and more dimensions. Separation of variables. Degeneracy. Potential barrier. Tunneling. Transmission probability. Above-the-barrier reflection. Vibrational motion. Linear (harmonic) oscillator. Rotational motion. 2D rotation. Particle on a ring. Angular momentum. 3D rotation. The vector model. Spin. (2 weeks).

3. Atomic structure and spectra. Hydrogen and hydrogenlike atoms. Ritz combination principle. Hamiltonian. Separation of variables. The radial solutions. Bound states. Atomic orbitals. Shells and subshells. s,p and d orbitals. Spectroscopic transitions and selection rules. The structure of many-electron atoms. The orbital approximation. The helium atom. The Pauli principle. The Slater determinant. Penetration and shielding. The Aufbau (building-up) principle. Hund's maximum multiplicity rule. Ionization energies and electron affinities. Self-consistent field. Quantum defects. Rydberg states. Singlet and triplet states. Spin-orbit coupling and fine structure. Term symbols and selection rules. (2 weeks).

4. Molecular structure. The Born-Oppenheimer approximation. Valence-bond theory. Diatomic molecules. Polyatomic molecules. Hybridization. Molecular orbital theory. The hydrogen molecule ion. MO-LCAO-molecular orbital as linear combination of atomic orbitals. Bonding and antibonding orbitals. Homonuclear diatomic molecules. σ and π orbitals. The overlap integral. Electronic structure. Bond order. Heteronuclear diatomic molecules. Bond polarity. Electronegativity. The variation principle. Zero overlap approximation. MO for polyatomic molecules. MO LCAO. The Huckel approximation. Ethene and frontier orbitals. Butadiene. Benzene and aromaticity. Computational chemistry. The Hartree-Fock equation. Semi-empirical and ab initio methods. CNDO. Density functional theory. (2 weeks)

5. Molecular spectroscopy 1. Transition moments. Selection rules. Rotational spectra. Moments of inertia. Rotational energy levels. Spherical rotors. Symmetric top rotors. Linear rotors. Degeneracies. Stark effect. Rotational transitions. Rotational selection rules. Rotational spectra. Rotational Raman spectra. Nuclear statistics and rotational states. Vibration of diatomic molecules. Harmonic approximation. Vibrational spectra. Selection rules. Anharmonicity. Vibrational-rotational spectra. Vibrational Raman spectra. Vibrations of polyatomic molecules. Normal modes. Infrared absorption spectra of polyatomic molecules. Vibrational Raman spectra of polyatomic molecules. (2 weeks)

6. Molecular spectroscopy 2. Electronic transitions. Beer-Lambert law. Electronic spectra of diatomic molecules. Selection rules. Vibrational structure. Frank-Condon principle. Rotational structure. Electronic spectra of polyatomic molecules. Electronically excited states. Fluorescence and phosphorescence. Photodissociation. Predissociation. (2 weeks)

Laboratory Projects: None

Course Schedule: 3 hours lecture weekly

Prepared by: Dr. Lev Krasnoperov, January 18, 2013

Grading:	**Hour Exam 1** **(after approx. 4 - 5 weeks)**	**200**
	Hour Exam 2 **(after approx. 8 - 9 weeks)**	**200**
	Final Exam	**300**
	Homeworks[a)] **(via Quizzes)**	**220**
	Attendance	**80**

	Total:	**1000**

Grade determination. Scores less than 45% of the total normally result in F. Scores larger than 85% of total always result in A. The distribution of the grades between these benchmarks as well as the F and A boundaries depend on the overall performance of the class.

[a)]Homework grades will be given based on THREE quizzes 110 pts each, 35 min, two problems similar to those from the homework assignments, with different numerical data, TWO BEST quizzes will be taken into account (homework grades will be assigned contingent submission of all homework assignments).

The NJIT honor code will be upheld and any violations will be brought to the immediate attention of the Dean of Students.
Students will be consulted with by the instructor and must agree to any modifications or deviations from the syllabus throughout of the semester.

Prepared: **Dr. Lev Krasnoperov**

Date: **January 18, 2013**

CHEM 336, Physical Chemistry III
Spring 2012
Atkins, 9th Edition

Homework is due two weeks later after the assignment. The date of the assignment of the first homework is the first lecture. Adjustment due to delay caused by class cancellations or other reasons that cannot be foreseen are possible.

Homework assignments:

Homework

#1	**Exercises: 7.1a, 7.7a, 7.10a, 7.11a, 7.13a, 7.14a, 7.15a, 7.17a** **Problems: 7.5, 7.7, 7.9** **Theoretical problems: 7.15, 7.17, 7.21, 7.23**
#2	**Exercises: 8.1a, 8.3a, 8.4a, 8.11a, 8.12a, 8.14a, 8.20a, 8.21a** **Problems: 8.1, 8.3** **Theoretical problems: 8.11, 8.13, 8.15, 8.21, 8.29**
#3	**Exercises: 9.1a, 9.3a, 9.9a, 9.11a, 9.14a, 9.16a, 9.19a, 9.23a, 9.27a** **Problems: 9.3, 9.11** **Theoretical problems: 9.17, 9.19, 9.25**
#4	**Exercises: 10.1a, 10.3a, 10.4a, 10.5a, 10.6a, 10.8a, 10.9a, 10.10a, 10.11a, 10.13a, 10.16a, 10.17a** **Problems: 10.9** **Theoretical problems: 10.17, 10.19**
#5	**Exercises: 12.1a, 12.2a, 12.3a, 12.5a, 12.10a, 12.13a, 12.15a, 12.20a, 12.23a, 12.24a, 12.25a, 12.26a** **Problems: 12.5, 12.9**
#6	**Exercises: 13.1a, 13.4a, 13.5a, 13.9a, 13.10a, 13.11a, 13.12a, 13.15a, 13.17a** **Problems: 13.1, 13.13**