SYLLABUS

PHYSICAL CHEMISTRY    CH3520    SPRING, 2004

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Office Hours: by Appointment


GRADING:

<table>
<thead>
<tr>
<th>Exam Type</th>
<th>Points</th>
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</thead>
<tbody>
<tr>
<td>Hour Exam I</td>
<td>100</td>
</tr>
<tr>
<td>Hour Exam II</td>
<td>100</td>
</tr>
<tr>
<td>Final Exam</td>
<td>200</td>
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<td>Total</td>
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COURSE OUTLINE:

1. Chemical Kinetics (Chapter 17)
   a. The basic rate laws, complex versus elementary reactions
   b. The integrated rate equations
   c. The kinetics of opposing, sequential and parallel reactions
   d. The experimental determination of rate equations
   e. Rates and mechanisms of complex reactions
   f. The temperature dependence of reaction rates
   g. Chain reactions
   h. Catalysis
   i. Enzyme catalyzed reactions; the Michaelis-Menten equation

2. Quantum Mechanics (Chapter 18)
   a. Origin of Quantum Mechanics
   b. Nature of microscopic particles
   c. The Bohr Atom
   d. Operators and the postulates of quantum mechanics
   e. Translational motion: the particle in the box
   f. Vibrational motion: the harmonic oscillator
   g. Rotational motion: the rigid rotor
   h. Perturbation theory and variational theory
   i. Properties of Hermitian operators
3. Atoms (Chapter 19)
   a. The quantum mechanical solution for the hydrogen atom
   b. Angular momentum and electron spin
   c. The helium atom
   d. Pauli exclusion principle, antisymmetry of electrons
   e. The total orbital and spin angular momentum in atoms
   f. Many electron atoms: their wave functions and electronic states
   g. The Hartree-Fock method
   h. The configuration-interaction method

4. Molecular Structure (Chapter 20)
   a. Characteristic geometries and properties of polyatomic molecules
   b. The Hamiltonian for diatomic molecules; the Born-Oppenheimer approximation
   c. The vibration and rotation of diatomic molecules
   d. The \( \text{H}_2^+ \) molecule and molecular orbitals
   e. The \( \text{H}_2 \) molecule
   f. Molecular orbital method for diatomic molecules
   g. Hybrid orbitals
   h. Molecular orbital structure of simple polyatomic molecules
   i. The valence bond method
   j. The theoretical prediction of molecular properties
   k. Advanced quantum methods: the Hartree-Fock, CI, MP, CC and DFT methods.
   l. Semi-empirical and force field methods

5. Molecular Spectroscopy (Chapter 21)
   a. The nature of electromagnetic radiation
   b. The Beer-Lambert law and selection rules
   c. Rotational and vibrational spectra of diatomic molecules
   d. Group theory
   e. Rotational and vibrational spectra of polyatomic molecules
   f. IR and Raman spectroscopy
   g. UV-vis spectroscopy of electronic states

6. Statistical Thermodynamics (Chapter 22)
   a. Thermodynamic probability
   b. The Maxwell-Boltzmann distribution
   c. The partition function
   d. The statistical mechanical determination of energy, enthalpy, entropy, free energies and heat capacities
   e. Translational, vibrational, rotational and electronic contributions
   f. The direct summation method
There is no predefined scale for the grades on exams. After each exam, the breaks for the grades will be given. Re-grades for any exam must be requested within one week after the return of the exam.

All students will be required to take the final exam that will include all topics covered during the semester. The standard ACS exam in quantum chemistry will be included in the final exam.

Practice problems from the textbook will be assigned during the course. Although these will not be collected or graded, it is recommended that you solve as many as possible to gain experience with the kind of problems that will be on the exams.

An unexcused absence will be an automatic zero on the exam. If you have a valid reason to be absent from an exam as for a field trip, job interview, athletic event, etc., notify the instructor prior to the exam. If an unanticipated problem makes it impossible to attend the exam, notify the instructor as soon as possible. An extended delay will be considered to be an unexcused absence.