COURSE SYLLABUS: CH3520 PHYSICAL CHEMISTRY
SPRING, 2007

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Office Hours: by Appointment (arrange via email)


Physical Chemistry, CH3520, covers the fundamental theories and experiments underlying modern chemistry, in particular modern spectroscopy and structural analyses. A major part of this course is the development of problem solving skills. This chemistry and these problem solving skills underlie all science and engineering disciplines. A large component of this course is problem oriented, beginning in your pre-lecture reading of your text (with worked examples) and the assigned homework problems. The interplay of experiment and theory is emphasized. Lecture will guide you through the important material, help with difficult concepts, and apply principles in the problems solved. Your problem solving skills are further exercised and perfected as you work the assigned, end-of-chapter problems. Finally, these skills are tested on the quizzes, the mid-term exams and the final exam.

COURSE OUTLINE:

1. Quantum Mechanics (Chapter 18)
   (HWP*: 7, 10, 13, 15, 17, 20, 22, 23, 27, 32, 33, 34, 36, 40, 41, 43, 45, 48, 50, 53, 55, 58, 59)
   a. Origin of quantum mechanics (18.1-18.2)
   b. Nature of microscopic particles and the Bohr Atom (18.3-18.6)
   c. The Schrodinger equation (18.7 and Hand-out)
   d. The particle in a box and degeneracy (18.8-18.10)
   e. Operators and the postulates of quantum mechanics (18.11 and Hand-out)
   f. Vibrational motion: the harmonic oscillator (18.12-18.13)
   g. Rotational motion: the rigid rotor (18.14)
   h. Perturbation theory and variational theory, approximation methods (18.15)

2. Atoms (Chapter 19)  (HWP: 4, 8, 9, 14, 16, 17, 23, 26, 27, 31, 33, 36, 38, 39, 50)
   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

* HWP = assigned home work problems
3. Molecular Structure (Chapter 20) (HWP: 21, 25, 26, 29, 30, 31)
   a. Characteristic geometries and properties of polyatomic molecules
   b. The Hamiltonian for diatomic molecules; the Born-Oppenheimer approx.
   c. The vibration and rotation of diatomic molecules
   d. The $H_2^+$ molecule and molecular orbitals
   e. The $H_2$ 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 HF, CI, MP, CC and DFT methods.
   l. Semi-empirical and force field methods

4. Molecular Spectroscopy (Chapter 21) (HWP: 1, 2, 3, 4, 7, 8, 20, 36, 37, 38, 39, 47, 49, 50, 51, 52, 53, 54 (omit c & d), 105, 123, 124, 125)
   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 (see Hand-outs)
   e. Rotational and vibrational spectra of polyatomic molecules
   f. Prediction and calculation of IR and Raman spectra (see Hand-outs)
   g. UV-visible spectroscopy of electronic states

5. Statistical Thermodynamics (Chapter 22) (HWP: )
   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

GRADING:

<table>
<thead>
<tr>
<th>Component</th>
<th>Points</th>
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<tbody>
<tr>
<td>Hour Exam I</td>
<td>100</td>
</tr>
<tr>
<td>Hour Exam II</td>
<td>100</td>
</tr>
<tr>
<td>Quizzes</td>
<td>50</td>
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<tr>
<td>Extra Credit</td>
<td>variable</td>
</tr>
<tr>
<td>Final Exam</td>
<td>200</td>
</tr>
<tr>
<td>Total</td>
<td>450</td>
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On exam weeks, there will be class the day of the exam, but no class on Friday after the exam.

Extra-credit problems may be assigned (e.g. Harmonic Oscillator Calculation). Practice problems from the textbook are assigned above (see "HWP:"), and others may be discussed during the course. Although these will not be collected or graded, it is recommended that you solve these to test your understanding of the material and to gain experience with the kind of problems that will be on the exams.
CH3520 SYLLABUS: Grading (continued)

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.

EXAM POLICIES

Preparing for the Exam

NO MAKE-UPS for missed exams. Plan on taking the exam at the assigned times. If you have a valid reason to be absent from an exam (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 an exam, notify the instructor as soon as possible. An extended delay will be considered to be an unexcused absence. An unexcused absence will be an automatic zero for that exam. Excused absences result in the average of your other midterm exams being awarded for the missed exam.

Excused/Unexcused Absences:

- Granted by the Office of Student Affairs. If you know that you will have an official university excused absence on exam day (university athletic event or religious holiday), you are required to make arrangements as early as possible in advance of the exam date.
- Examples of excused absences granted in the past include serious illness (medical excuse required) or a death in the family. Excuses may be documented through the Office of Student Affairs.
- Examples that are NOT excused: travel home or to attend a social event.

Taking the Exam:

- One 3x5 equation card (on Final – two 3x5 equation cards)
- Come on-time and seat yourself promptly in proper test seating arrangement.
- Bring only allowed items. Do NOT bring cell phones, CD players, iPods, earphones, or other electronic devices.

After Exam – Tracking Your Score

- Exam Scores (individual and cumulative) will be posted on WebCT.
- Answer Keys will be provided after each exam.

Academic Dishonesty

Academic integrity is expected. Any violations will result in a 0 for the course and a recommendation of expulsion from MTU. Policies and procedures are in “Academic Integrity at MTU – A Guide for Students and Faculty.” Specific violations: copying from another’s work or exam, allowing copying from your work or an exam, or facilitation of any academic dishonesty.
CH3520 SYLLABUS (continued)

MTU ADA Statement
MTU complies with all federal and state laws and regulations regarding discrimination, including the Americans with Disabilities Act of 1990 (ADA). If you have a disability and need a reasonable accommodation for equal access to education or services at MTU, please call Dr. Gloria Melton, Dean of Students, at 7-2212. For other concerns about discrimination, you may contact your advisor, department head/chair, or the Affirmative Action Office.

WebCT Information
The WebCT site for CH3520 can be accessed at http://courses.mtu.edu/
Enter your WebCT User ID, your WebCT password, and then click on “login.” You will see the list of courses for which you are enrolled. Click on CH3520.

There is a course Gradebook within WebCT, where you may track your grades. Periodically examine this gradebook for accuracy, and report any discrepancies to me.

This Syllabus may be found on the WebCT site for this course.