Course contents:

1. The Structure of Matter
2. Quantum Mechanical Principles
3. Applications of Quantum Mechanics
4. The H Atom
5. The Covalent Bond
6. Atomic Spectroscopy
7. Molecular Spectroscopy
8. Intermolecular Forces
9. Solid State
10. Transport Properties
11. Partition Functions
12. Laws and Theories of Kinetics

Course Responsibilities

Bi-Weekly Discussions  5
Weekly Assignments  10  20%
Mid-sem Exams  2  40%
Final Exam  1  40%

Weekly Assignments
These assignments are intended for you to work at home. These will contain both questions and problems related to the course material. These are to be submitted as specified. Late assignments will not be accepted.

Bi-weekly Discussions
These discussions are intended to start a dialogue among the students, and between the students and the instructor. These are intended to improve the self-study capabilities of the students and also to stimulate interest in Physical Chemistry. The instructor will be at hand to lead the discussion and to moderate. The topics for discussion will be announced one week in advance. The instructor will clarify difficult concepts and derivations. We shall draw straws to decide who will present the material at the beginning of each discussion period. Attendance will be taken. Students are urged to form teams of two for the discussions (during the first class). This will enhance interaction between students and each one can help the other.

Mid-Sem and Final Examinations
The mid-sem examinations will carry 20% weightage each and the final exam will have 40% weightage. The remaining 20% will be for the weekly assignments. While mid-sems will include the material covered till one week before the actual date of the examination, the final will cover the entire course material. The final exam will be the ACS standard examination. Any one wishing to take a make-up exam will have to produce a valid exemption note from a qualified Physician, explaining why the student can't take the examination on the scheduled date and time. Make-up examinations may not be given without such a note. First Mid-Sem, March 2, 9.30 am; Second Mid-Sem, April 6, 9.30 am and Final Exam is to be announced.

Grading
The final grade in the course will primarily depend on the overall performance in the course such as participation in discussions, completing the assignments, and performance in the written examinations.
Assignment #1 Due February 9, 12 noon
1. Derive an expression for e/m, as described in J. J. Thomson's cathode ray experiments.
2. Derive the average energy of an ensemble of oscillators using Boltzmann distribution and Planck's equation.
3. Define energy density, emissive power of a black body and Wien's displacement law.
4. Derive the relation between the energy density and the temperature of a black body.
5. Write the photoelectric equation and what is the effect of intensity on the photoelectrons emitted?
6. Derive Bohr's equation and then derive Ritz's formula from it.
7. Write the wave equation and convert it to Schrödinger's equation using de Broglie relation.
8. Do problems 19.1; 19.2; 19.9; 19.10; 19.11 and 19.15.

Assignment #2 Due February 16, 12 noon
1. Discuss the interpretation of the wave function.
2. Write operators for position, momentum, total kinetic energy, and total energy.
3. Write wave functions, and energy functions of particle in a box, harmonic oscillator, rigid rotor and hydrogen atom.
4. Define commutator, hermitian operator, linear operator, eigen function, eigen value, Laplacian operator, and Hamiltonian operator.
5. Explain the mathematical basis for the uncertainty principle.
6. Explain why electrons do not spring into the nucleus, using particle in a box model.

Assignment #3 Due February 23, 12 noon
1. Write the radial equation for hydrogen atom.
2. Draw the wave functions and radial distribution functions for 1S, 2S, and 3S states.
3. Explain the trend in the ionization energies of rare gases.
4. Do problems 22.1, and 22.11

First Mid-Sem, March 2nd 9.30 am.

Assignment #4 Due March 8, 12 noon
1. Write the electronic configuration of carbon atom. Discuss the valence bond model for methane. Describe how the atomic orbitals can be combined to form hybrid orbitals to give a tetrahedral shape for methane.
2. Discuss the valence bond model for the hydrogen atom. Discuss the contributions of the ionic structures to the resonance hybrid.
3. State and describe the variation theorem. How is it useful in the quantum mechanical descriptions of multi-electron systems?
4. What is the overlap integral? How can it be used to determine the directional character of the covalent bond?
5. Define the four quantum numbers of a multi-electron system. Give the equations describing the quantization of the angular momenta. What are the allowed values of these quantum numbers?

Assignment #5 Due on March 15, 12 noon
1. Derive Beer's law and define absorbance, transmittance and molar absorption coefficient.
2. Define all the quantum numbers of multi-electron atoms. Give equations which govern the corresponding angular momenta.
3. What is a term symbol? Write term symbols for the atoms O, F, N and Cl.
4. Derive the equation that relates the total angular momentum of an atom and its magnetic moment.
5. Explain the terms gyromagnetic ratio, Zeeman effect, and Bohr magneton?
6. How many NMR signals are to be expected for ethanol and why?
7. Do problems 24.1, 24.5, 24.9, 24.13a, 24.15. Sections that are not in the syllabus:
   20.4; Derivation in 21.5.2 but the remaining is included; 21.6.2-21.7.2; derivation in 21.8 not included but the remaining discussion is included; 22.2.1; 23.12-16.

Assignment #6 Due on March 29, 12 noon
1. Write the energy changes accompanying a molecule undergoing rotational-vibrational transitions. Use the quantum numbers v and J.
2. Write the various vibrational modes of carbon dioxide and nitrous oxide. Why is the Q branch allowed for carbon dioxide while it is forbidden for HCl?
3. Do problems 25.1 and 25.4. Sections 25.11-25.16 not in syllabus.

Second Mid-Sem, April 6, 9.30 am.
Assignment # 7       Due on April, 12 noon
1. Derive an expression for the interaction energy between two dipoles.
2. Explain what is the dispersion energy.
3. Derive van der Waals constants a and b, using the expression for the intermolecular forces.
4. What is excluded volume?
5. What is Lennard-Jones Potential?
6. Explain why the boiling point of methanol is much greater than fluoromethane?
   Section 26.3 not in syllabus.
8. Explain why Xe has a higher boiling point than He.

Assignment # 8       Due on April 19, 12 noon
1. Sketch the unit cells of simple cube, body centered cube, face centered cube and a hexagonal close packed unit cell.
2. Draw the unit cells of rutile, zinc blende, CsCl, NaCl and wurzite.
3. State the radius ratio rules and explain why it may not work in every case.
4. Describe the powder diffraction method of Debye-Scherrer.
5. Do problems 27.2, 27.4, 27.5, 27.10, and 27.15.
   Chapter 28 is not in syllabus.

Assignment # 9       Due on April 26, 12 noon
1. Derive the equation for the general transport and the thermal conductivity of a gas.
2. Derive the equation for the collision number.
3. Describe how Avagadro's number may be estimated from van der Waals 'b'.
4. Do problems 30.1a,d, 30.3, 30.5, and 30.7. Chapter 31 is not in syllabus.

Assignment # 10      Due on May 3, 12 noon
1. Define the order, rate constant, rate and overall order of a chemical reaction.
2. How are the stoichiometric coefficients related to the order of an elementary reaction?
3. Derive the rate expressions for a first order and for a second order reaction.
4. Do problems 32.4, 32.7, 32.8, 32.11, 32.13, 32.16, and 32.26.
5. Explain the concept of activation energy and write the Arrhenius equation.
6. Derive the expression for the rate constant using the collision theory and the theory of absolute reaction rates.
7. Compare the collision theory with the theory of absolute reaction rates.
8. Do problems, 33.1, 33.2, 33.3, and 33.8. Chapters 34 and 35 are not in syllabus.

Final Exam (TBA)