COURSE OUTLINE (Chapters of Atkins are indicated, and tentative time requirements are indicated. This outline is subject to modification as the semester progresses)

Unit 0 *- Introduction (August 25, 1 lecture)*

I. Preliminaries
   A. Overview of Physical Chemistry
   B. Dimensions and Units (Appendix 1)
   C. Mathematical Review (Appendix 2)

II. Review of Classical Mechanics (Appendix 3)
   A. Specifying the State of the System
   B. Newton's Law
   C. Rotational Motion
   D. Harmonic Motion in 1-D
   E. Summary of Classical Physics

Unit I *- Quantum Theory: Introduction and Principles (Chapter 8,6 lectures)*

I. Failures of Classical Physics
   A. Breakdown of the Equipartition Theorem
   B. Spectral Distribution of Black-Body Radiation
   C. Line Spectra of Atoms
   D. Photoelectric Effect
   E. Diffraction of Electrons (de Broglie equation)

III. Quantum Picture
   A. Specifying the State of the System (wave functions)
   B. QM Principles (operators, expect values)

Unit II *- Quantum Mechanical Applications (Chapter 9, 3 lectures)*

I. Translational motion
   A. Particle in Free Space
   B. Particle in 1-D Box
   C. Particle in 2-D Box
   D. Particle in 3-D Box

II. Vibrational Motion
   A. 1-D Harmonic Oscillator

III. Rotational Motion and Angular Momentum
   A. The Two-Particle Rigid Rotor (angular momentum)

IV. Tunneling

Unit III *- Atomic Structure and Spectra (Chapter 10, 6 lectures)*

I. The Hydrogenlike Atom
   A. Clues from Line Spectra
   B. Clues from Scattering Expts
   C. QM of Hydrogenic Atom

II. Many Electron Atoms
   A. The Orbital Approximation
   B. Spin
   C. Penetration and Shielding
   D. Aufbau Principle
   E. Periodicity of Ionization Energies
   F. Numerical Computations of Many Electron Atomic Orbitals

III. Spectra of Many-Electron Atoms (briefly)

Unit IV *- Molecular Structure (Chapter 11, 7 lectures)*

I. The Hydrogen Molecule-ion
   A. Born-Oppenheimer Approximation
   B. The Molecular Orbital Approximation

II. Diatomic Molecules
   A. Hydrogen and Helium
   B. Period 2 Diatomics
   C. Heteronuclear Diatomics
   D. The Variation Principle
   E. Hybridization

III. Polyatomic Molecules
   A. Water
   B. Hybridization in Polyatomics
   C. Highly Conjugated Systems - Huckel
   D. Advanced Computations

IV. Molecular Symmetry (Chapter 12 , 2 lectures)
   A. Symmetry Elements and Operations
   B. Symmetry Classes of Molecules
   C. Consequences of Symmetry

Unit V *- Spectroscopy (Chapters 13, 14, & 15 ,5 lectures)*

I. General Features of Spectroscopy
   A. Experimental Techniques
   B. Intensity of Spectral Lines
   C. Line Widths

II. Pure Rotational Spectra

III. High Resolution Vibrational Spectra (w/ rotational fine structure)

IV. Vibrational Spectra of Polyatomics

V. Raman Spectra

VI. Electronic Spectra of Molecules (diatomic)

VII. Lambert-Beer Law

VIII. Magnetic Resonance Spectra

Unit VI *- Statistical Mechanics (Chapter 16 & 17, 7 lectures)*

I. Introduction
   A. Microscopic and Macroscopic Worlds
   B. Microstates
   C. Binomial Theorem
   D. Statistical Definition of Entropy
   E. Energy Considerations
   F. Macroscopic Systems- the Boltzmann Distribution Law
   G. Sample Calculation for Rotation of a Diatomic
   H. Detailed Derivation of Boltzmann Law

II. The Machinery of Statistical Mechanics
   A. Connection of Partition Function with Thermodynamics
   B. Evaluation of Partition Function
   C. Total Translational Partition Function - Perfect Gas
   D. Thermodynamics of an Ideal Monatomic Gas
   E. Rotational Partition Function
   F. Vibrational Partition Function