**CHEM 3750-3760 - PHYSICAL CHEMISTRY**

**Textbook:** PRINCIPLES OF PHYSICAL CHEMISTRY by Raff, 2001, Harcourt-Brace.

**Prerequisites:**  Physics and Calculus; Pre- or Corequisites: CHEM 3710,
CHEM 3510-3511, CHEM 2220-2221; Corequisite: CHEM 3780-3790

**Reference**

**Books:** 1. Margenan and Murphy, "The Mathematics of Physics and Chemistry", Van Nostrand, Princeton (1956).

 2. Hanna M., "Quantum Mechanics in Chemistry", 2nd Ed., Benjamin, NY (1969).

 3. Moore, "Physical Chemistry", 4th Ed., Prentice Hall (1972).

 4. Levine, "Physical Chemistry", McGraw Hill, NJ (1978).

 5. Atkins, P., "Physical Chemistry", Freeman, SF (1978).

 6. Barrow, "Physical Chemistry", McGraw Hill, NY (1979).

Outline of the course

 I. Thermodynamics

 1. Introduction

 2. First law of thermodynamics

 Work, internal energy, heat

 Equation of gases

 Thermochemistry

 3. Second law of thermodynamics

 Carnot heat engine

 Entropy

 Criteria of chemical equilibrium

 Exact differentials and maxwell relations

 Free energy

 Calorimetric methods

 4. Third law of thermodynamics

 5. Phase equilibrium

 Phase rule

 One component systems

 Clapeyron equation

 Multiple component systems

 Colligative properties of solutions

 6. Chemical equilibrium

 Equilibrium constants

 Free energy of formation

 Temperature effects

 7. Electrochemical cells

 Units, etc.

 Potentiometric determination

 Cells (convention)

 Thermodynamics of cells

 Equilibrium of biochemical reactions

 II. Quantum Chemistry

 8. Classical quantum chemistry

 Heat capacity

 Photoelectric effects

 Line spectra

 Bohr's theory of hydrogen atom

 9. Operators. Schrödinger equation

 Wave function

 Postulates

 10. Some simple systems

 Particle in a box

 Harmonic oscillator

 The rigid rotor angular momentum

 11. Hydrogen atom

 Quantum numbers

 Spring electrons

 Pauli exclusion principle

 12. Approximate methods

 Variational principle

 Purturbation theory

 13. Symmetry

 14. Molecular electron structure

 H2+

 Homodiatomic molecule

 Electronegativity

 Intermolecular forces

 15. Molecular spectroscopy

 Rotational

 Vib-rotational

 Electronic

 16. Magnetic resonance spectroscopy

III. Chemical Kinetics

 17. Kinetic theory of gases

 Pressure of a gas

 Velocities distribution

 Average velocities

 Collision number

 Transport phenomena

 18. Kinetics I

 Basic relationships

 Temperature effect

 19. Kinetics II

 Theories of chemical kinetics

 Collision theory

 Transition state theory

 Unimolecular reactions

 20. Kinetics III liquid phase

 Diffusion controlled reactions

 Acid-base catalysis

 Enzyme catalysis

 21. Photochemistry

 Intramolecular processes

 Quantum yields

 22. Irreversible processes in solution

 Viscosity

 Conductivity

 Electric mobility

 23. Statistical mechanics