**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