KFT 331/3 - Physical Chemistry III

Course Objectives:

1) To introduce the theoretical aspects of chemical kinetics and the applications.
2) To introduce the fundamentals of quantum mechanics and to apply quantum mechanics to simple systems.
3) To introduce the fundamentals of statistical thermodynamics and to derive the thermodynamics functions in terms of the partition functions.

Topic	**Content**	**Number of lecture hours**	**Expected outcome – upon completion of this course, the student should be able to:**
1. The Mechanisms of Elementary Processes	• The kinetic theory of collisions • Equilibrium and rate of reaction • Statistical mechanics of chemical equilibrium • The transition-state theory • Applications of the theory of absolute reaction rates • The thermodynamical formulation of reaction rates	9	• Understand the concept of hard-sphere collision theory. • Explain the terms: collision density, collision cross-section and collision frequency factor. • Explain how partition functions can be obtained for the different types of molecular motion: translational, vibrational, rotational and electronic. • Derive the transition-state theory equation, namely the Eyring equation. • Derive the thermodynamic parameters for activation.
2. Elementary Gas-Phase Reactions	• Unimolecular reactions	2	• Explain the Lindemann-Hinshelwood mechanism.
3. Reactions in Solution	• Factors determining reaction rates in solution	2	• Discuss solvent effects on reaction rates, including ionic-strength effect. • Express the kinetic salt effect in terms of the variation of the rate constant of a reaction between ions with the ionic strength of the solution.

Topic	Content	Number of lecture hours	Expected outcome – upon completion of this course, the student should be able to:
4. Catalysis	• Acid-base catalysis • Enzyme catalysis	3	• Discuss the principles of catalysis, especially catalysis by acids, bases and by enzymes. • Derive the Michaelis-Menten equation. • Apply the Lineweaver-Burk plot for the analysis of an enzyme-catalysed reaction that proceeds by Michaelis-Menten mechanism and the significance of the intercept and the slope.
5. Photochemistry	• The Grotthus-Draper law • The Einstein-Stark law of photochemical equivalence • Photochemical reactions • Photosensitization	2	• Explain the basic principles of photochemical reactions.
6. Quantum Chemistry	• Postulates • Well-behaved wavefunctions • Hermitian operators • Eigenfunctions and normalization • Schroedinger equation • Heisenberg uncertainty principle • Quantum mechanics of simple systems: particle in a box and harmonic oscillator	10	• Understand the postulates that formulate the modern quantum theory. • Ascertain whether an operator is Hermitian or otherwise. • Understand the Heisenberg uncertainty principle which expresses a fundamental difference between measurement of classical and quantum systems. • Formulate and solve the Schroedinger equation for the particle in a box problem. • Formulate the Schroedinger equation for the harmonic oscillator. • Calculate the energy in wavenumber and wavelength corresponding to a spectral transition between two energy levels. • Determine the degree of degeneracy of an energy level for two-dimensional and three-dimensional systems.

Topic	Content	Number of lecture hours	Expected outcome – upon completion of this course, the student should be able to:
7. Statistical Thermodynamics	• Microscopic states • Boltzmann distribution • Molecular partition functions for ideal gases: translational, rotational, vibrational and electronic • Thermodynamic quantities from partition functions • Calculation of equilibrium constants for reactions of ideal gases	8	• Derive the Boltzmann distribution • Know the definition of molecular partition function. • Write the partition functions for different types of molecular motions. • Derive and calculate thermodynamic quantities from partition functions. • Use the partition functions to calculate equilibrium constants.
TOTAL		**36**	