

Course Title: Physical Chemistry-

Course Code: CH-380

Credit Hours: 3-1

Pre-requisite: Nil

Course Objectives

1. This course will provide the students with an extensive theoretical knowledge about different kinetic theories of gases, chemical thermodynamics and their applications, chemical kinetics of third order reactions as well as the comparison between classical and quantum mechanics.

Contents

2.

Chemical Kinetics. Integrated rate laws: Third order reactions with same and different initial concentrations of reactants. Effect of temperature on the reaction rate.

Elementary and complex reactions: opposing, parallel, consecutive bimolecular reactions and chain reactions. Steady state approximation, Lindemann's theory of unimolecular reactions. Bimolecular collision theory, transition state theory, kinetics of thermal and photochemical reactions.

Quantum Chemistry. Limitation of classical mechanics, Wave and particle nature of matter, de Broglie's equation, Heisenberg's uncertainty principle. Schrodinger wave equation and its solution for particle in 1-dimensional and 3-dimensional boxes. Concept of quantization of energy, introduction to spectroscopy of molecules, spectra of hydrogen and hydrogen like atoms.

Electrochemistry: An introduction to electrochemistry, chemical reactions and redox potentials, electrochemical cells and types of electrodes. Nernst's equation and its application. Predicting reactions, stability of oxidation states, cell potential and

potential, transference number. Ions in aqueous solution. Ionic activity and Debye Hückel thermodynamics. Theory of metallic conduction. Electrode potential, liquid junction theory.

Thermoelectric Materials. Introduction. Basis. Waste heat estimate. Conversions.

Phononic contribution. Electronic contribution. Grain boundaries affect.

6 Practical

- a. Determination of partial molar quantities.
- b. Determination of free energy changes, standard free energies.
- c. Determination of heat of solution, ionic reactions and other experiments
 - Determination of molecular weight of a polymer by viscosity method. from thermochemistry.

- d. Precipitation value of electrolytes.
- e. Measurement of IR spectra of simple compound and their interpretation.
- f. Determination of percentage composition of KMnO_4 - $\text{K}_2\text{Cr}_2\text{O}_7$ in given solution by spectrometry.
- g. Evaluation of pKa value an indicator by spectrometric method.
- h. Synthesis of metal oxide nanoparticles and their characterization using IR and XRD techniques.

7. Course Outcomes
 - a. On successful completion of the course the student will be able to:
 - b. Explain the behavior of gases while using kinetic molecular theory.
 - c. Explain several thermodynamic quantities and their applications in Chemistry.
 - d. Explain the chemical kinetics of third order reaction with effect of different reaction conditions.
 - e. Use fundamental concepts of quantum mechanics to solve different problems in Chemistry

8. Text Books
 - a. Alberty, R. A., Robert J.S. and Moufígi G. B. ”
Physical Chemistry . 4th ed, John Wiley and Sons (2004).
 - b. McQuarrie, D. A., Physical Chemistry; A Molecular approach, Viva Books Pvt.Limited, 2008.

9. Recommended Books (Theory)
 - a. Ball, D W., Physical Chemistry 1st ed., Brooks/Cole Co. Inc. (2003).
 - b. Smith, E. Brain, Basic Chemical Thermodynamics 5th ed., Imperial College Press(2004).
 - c. Chorkendorff, I. and Niemantsverdríet, J.W.
Concept of Modern Catalysis and Kinetics 1st ed., John Wiley and Sons (2003).
 - d. Espenson, J. H. Chemical Kinetics and Reaction Mechanism 2nd ed., McGraw Hill(2002).

10. Recommended Books (Practicle)
 - a. David P. Experiments in Physical Chemistry 5th ed. (1989).
 - b. Shoemaker C.W., Nibler G.J.W. and Christian G.D. ”
Analytical Chemistry 6th ed.(2004).
 - c. James A.M. and Prichard F.E. ” Practical Physical Chemis