BACHELORS WITH CHEMISTRY AS MAJOR
6th SEMESTER

CHM622J3: CHEMISTRY _ ADVANCED CONCEPTS IN PHYSICAL CHEMISTRY

CREDITS: THEORY-4, PRACTICALS-2

THEORY (4 CREDITS: 60 HOURS)

Course Objectives:

- *To introduce the concepts of fast reactions and kinetic investigations of fast reactions.*
- *To make students to understand the reason for need and role of solvent and solvent characteristics on the kinetics of solution phase reactions.*
- *To introduce the basic concepts of enzyme kinetics*
- *To introduce students to basic concepts of statistical thermodynamics and learn how to use of concepts for estimation of thermodynamic parameters of simple systems.*
- *To introduce the basic concepts of X-Ray crystallography and interpretation of the X-Ray diffractograms*

Learning outcomes:

- *Students shall learn what are fast reactions and how the kinetic investigations are carried out for such reactions.*
- *Students will learn about the ways a solvent shall affect the kinetics of reactions in solution*
- *Students shall appreciate the difference between the solution and gas phase reactions*
- *Learn how to use the activated complex theory for the estimation of rate constants for gas phase, solution phase and surface reactions.*
- *Students shall understand how reaction kinetics of ionic reactions can be changed through use of salt addition and solvent change*
- *Students shall learn the basic concepts of statistical thermodynamics and how to use these concepts for the estimation of thermodynamic parameters of simple systems*
- *Students learn the basic concepts of X-Ray crystallography and how to interpret X-Ray diffractograms of simple crystalline solids*

Unit-I: Advanced Chemical Kinetics (15 hours)

Kinetics of Fast Reactions: General features of fast reactions, study of fast reactions by flow method, relaxation method and flash photolysis.

Theories of Chemical Reactions: Potential energy surfaces, Activated complex theory of reaction rates, statistical & thermodynamic formulations, comparison with collision theory.

Kinetics of Solution Phase Reactions: Effect of solvent on reaction rates, Diffusion controlled reactions (partial & full microscopic diffusion control), Ionic Reactions; Single & double sphere models of ionic reactions, the effect of ionic strength.

Unit-II: Catalysis (15 hours)

Heterogenous Catalysis: Kinetics of Surface Reactions, Unimolecular & bimolecular surface reactions [Langmuir-Hinshelwood & Langmuir- Riedel mechanism], classical & statistical treatments.

Enzyme Catalysis: Introduction to enzyme-catalyzed reactions, Michaelis-Menton equation, effect of temperature and pH. Enzyme inhibition.

Specially Catalysed Reactions: Fischer-Tropsch process, Haber-Bosch process, Photocatalysis, reactions, Photocatalytic breakdown of water.

Unit-III: Statistical Thermodynamics (15 hours)

Basics of Probability theory: Probability, Fundamental counting principle, Permutations, Configurations, Concept of distribution, thermodynamic probability and most probable distribution. Sterling approximation.

Distribution Laws: Boltzmann, Bose-Einstein and Fermi- Dirac distribution laws (Derivation and their comparison).

Partition function: Meaning & its significance, Translational, rotational, vibrational and electronic partition functions. Relation between partition function and thermodynamic functions.

Application to Chemical Systems: Calculation of thermodynamic properties in terms of partition functions, and application to ideal monoatomic & diatomic gases. Equilibrium constant in terms of partition function.

Unit-IV: X-Ray Diffraction of solids (15 hours)

Laws of Crystallography, Lattice Planes and Miller indices; Interplanar distance, Bragg equation, Debye-Scherrer method of X-ray structural analysis of crystals, Systematic absences, identification of cubic unit cells from systematic absences in diffraction pattern. Structure factor and its relation to intensity. Calculation of structure factor for Rock salt, and cesium chloride structures.

Books Recommended:

1) Physical Chemistry –P. W. Atkins, 9th Edition, ELBS , Oxford, 2009.

2) Elements of Physical Chemistry, Peter Atkins and Julio de Paula, 7th Edition, Oxford University Press, 2016.
3) Physical Chemistry, Concepts and Models, Volume II, Nabakumar Bera, Subhasree Ghosh, Paulami Ghosh, Techno world.
4) Atkins' Physical Chemistry, Peter Atkins, Julio de Paula & James Keeler, 11th Edition, Oxford University Press, 2018.
5) Chemical Kinetics, K. J. Laidler, 3rd Edition, Pearson, 1987.
6) Chemical Kinetics and Reaction Dynamics, Paul L. Houston, Dover Publications, INC., Mineola, New York, 2001.
7) Chemical Kinetics and Dynamics, J. I. Steinfeld, J. S. Francisco, W.L. Hase, Prentice Hall, 1989
8) Chemical Kinetics and Catalysis, R.I. Masel, Wiley, 2001
9) Chemical Kinetics: From Molecular Structure to Chemical Reactivity, Luis G Arnaut, Sebastiao Jose Formosinho, Hugh Burrows, Elsevier, 2007.
10) An Introduction to Chemical Thermodynamics, R. P. Rastogi and R. R Misra, 6th Edition, Vikas Publishing House Pvt. Ltd. 2018.
11) A systematic Approach to Statistical Thermodynamics, Vakil Poddar, Pragati Prakashan, 2019.
12) Statistical Thermodynamics, M.C.Gupta, New Age International, 1993.
13) Chemical Thermodynamics, Classical, Statistical, and Irrevrsible, Pearson, 2013.
14) Solid State Chemistry and its Applications, West, Wiley, 2014. 5.
15) The Physical Chemistry of Solids, Borg, Biens, Academic press, 1992.

PRACTICALS (2 CREDITS: 60 HOURS)

1. Kinetic investigations of $MgCO_3$-HCl reaction to;
    i. Estimate rate of the reaction
    ii. Determine effect of particle size of $MgCO_3$ on the rate of reaction
2. Kinetic investigations over any one of the two clock reactions viz. Hydrogen peroxide-Iodide or Persulphate-iodide reactions;
    a) Estimation of the rate of reaction
    b) Effect of concentration and hence estimation of the order of reaction
    c) Effect of the catalyst over the rate of reaction
    d) Effect of the surface area of the catalyst over the rate of reaction
    e) Effect of the ionic strength over the kinetics of the reaction
3. Kinetic investigations of acid-catalysed hydrolysis of an ester (Titrimetry or /conductometry) to;
    a) Establish the order of reaction with respect to the ester
    b) To establish the role of the nature of acid over its catalytic performance

BOOKS RECOMMENDED:

1. Practical Physical Chemistry, Findley, Kitchener, Longman, 1977.
2. Advanced Practical Physical Chemistry, Yadav, Goel Pub, 1994.
3. Experiments in Physical Chemistry, 5th ed., Schoemaker et al, MGH, 1989.
4. Advanced Physical Chemistry Experiments, J. N. Gurtu, and Amit Gurtu, Pragati Prakashan, 2017.