20MSC503T					Physical Chemistry-I					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
3	0	0	0	3	25	50	25	--	--	100

COURSE OBJECTIVES (04)

- To familiarize the students with concepts of thermodynamics and thermodynamic properties of macroscopic systems
- To understand the theories of reaction kinetics and factors affecting reaction kinetics
- To understand the basic principles of electrochemistry, inter-phase and their applications,
- To understand the concepts of, surface chemistry and various surface phenomenon and their applications

Unit 1 Classical Thermodynamics **10 h**

Third law, thermodynamics, need for it, Nernst heat theorem and other forms of stating the third law. Thermodynamic quantities at absolute zero, apparent exceptions to the third law - thermodynamics of systems of variable composition, partial molar properties, chemical potential, relationship between partial molar quantities, Gibbs Duhem equation and its applications (the experimental determination of partial molar properties not included)- thermodynamic properties of real gases, fugacity concept, calculation of fugacity of real gas, activity and activity coefficient, concept, definition, standard states and experimental determinations of activity and activity coefficient of electrolytes.

Unit 2 Chemical Kinetics **12 h**

Kinetics of complex reactions, Simultaneous reactions - opposing, parallel and consecutive reactions, the steady state approximation, Temperature dependence and Arrhenius law, theories of reaction rates- collision theory, transition state theory RRK and RRKM theories potential energy surfaces, reaction coordinates, reaction probabilities, kinetic isotope effects, factors determining reaction rates in solution, solvent dielectric constant and ionic strength. Chain reactions - linear reactions, branching chains - explosion limits; Rice–Herzfeld scheme; kinetics of free radical polymerization reactions. Enzyme catalysis - rates of enzyme catalysed reactions - effect of substrate concentration, pH and temperature - determination of Michael's parameters, Lineweaver-Burk and Eadie plots Salt effects. Photochemical reactions. Ultrafast reactions

Unit 3- Electrochemistry **12 h**

Ion transport in solution - migration, convection and diffusion -Fick's laws of diffusion conduction - ion-solvent interaction: Born model and Born equation, enthalpy of ion-solvent interaction and its calculation, Eley-Evan model, solvation number and methods for determination of solvation number, ion association: Bjerrum equation, fraction of ions associated, ion association constant; influence of ionic atmosphere on the conductivity of electrolytes-The Debye Huckel-Onsager equation for the equivalent conductivity of electrolytes - experimental verification of the equation - conductivity at high field and at high frequency - conductivity of non-aqueous solutions-effect of ion association on conductivity. The electrode-electrolyte interface-electrical double layer-electro capillary phenomena, Lippmann equation - the Helmholtz- Perrin - Guoy-Chapmann and Stern models, electro kinetic phenomena relation between current and rate of electrode reaction, current-overpotential relationship, Tafel equation and its importance Tiselius method of separation of protons of proteins - membrane potential.

Unit 4- Surface Chemistry **10 h**

Surface Phenomena, Gibbs adsorption isotherm, types of adsorption isotherms, solid-liquid interfaces, contact angle and wetting, solid-gas interface, physisorption and chemisorption, Freundlich, derivation of Langmuir and BET isotherms, surface area determination. Kinetics of surface reactions involving adsorbed species, Langmuir-Hinshelwood mechanism, Langmuir-Rideal mechanism, Rideal-Eley mechanism, Surface Films, Langmuir-Blodgett films, self-assembled mono layers, membranes/bilayers, collapse pressure, surface area and mechanism of heterogeneous catalysis, phase transfer catalysis.

Max. 44 h

COURSE OUTCOMES (06)

On completion of the course, student will be able to

CO1 - Apply the concepts of thermodynamic to understand the thermodynamic properties of macroscopic systems

CO2 – Interpret reaction rates and propose reaction mechanism with the help of concepts of chemical kinetics

CO3- Articulate the factors determining reaction rates and concept of catalysis-chemical reaction

CO4- Acquire knowledge about theories of surface chemistry and their applications.

CO5- Understand the fundamental concept about surface phenomenon and catalysis.

CO6- Analyse and apply the principles of electrochemistry in real world problems.

TEXT/REFERENCE BOOKS

1. P. W. Atkins, Physical Chemistry, Oxford University Press, 6thEdn., (1998).
2. D. McQuarie, and J. D. Simmen, Physical Chemistry, University Science, 1stEdn., (1998).
3. S. Glasstone, Thermodynamics for Chemists, Affiliated East West Press, (1965).
4. P.W. Atkins, Physical Chemistry, Oxford University Press, 6th Edn., 1998.
5. K. J. Laidler, Chemical Kinetics, Harper and Row Publishers, 3rd Edn., 1987.
6. J. O. M. Bockris and A. K. N. Reddy, Modern Electrochemistry, Plenum Press, 1970

END SEMESTER EXAMINATION QUESTION PAPER PATTERN

Max. Marks: 100 **Exam Duration: 3 h**

Part A/Question: 3 Questions from each unit, each carrying 3 marks	36 Marks
Part B/Question: 2 Questions from each unit, each carrying 8 marks	64 Marks