OC H 403 : PHYSICAL CHEMISTRY

COURSE OUTCOME:

- To understand the theoretical basis of catalysis, corrosion and various complex reactions which find relevance in biological processes and are of industrial importance.
- The students are introduced to the modern techniques developed for the practical applications of these concepts in different areas of science and technology.
- This course will enable the students to handle issues related to corrosion in the day to day life and in industrial reactors;enzyme mediated reactions in biochemistry, biotechnology and pharmaceutical chemistry etc.

UNIT-I: Catalysis **[15hours]**

Catalysis: Homogeneous Catalysis–equilibrium and steady state treatments, activation energies of catalysed reactions. Acid - base catalysis (general and specific), protolytic and prototropic mechanisms, catalytic activity and acid strength measurements. Kinetics of enzyme catalysed mechanisms – Michaelis – Menten mechanism. Effect of pH, temperature and inhibitors. 6hrs.

Acidity functions: Hammett acidity function, Zucker–Hammett hypothesis, and Bunnett hypothesis. 2hrs

Surface Chemistry: A review of adsorption isotherms, uni- and bi- molecular reactions. Multilayer adsorption: BET equation – application in surface area determination. Harkin – Jura equation and application. Semiconductor catalysis, n- & p- type. Mechanism of surface reactions. Langmuir – Hinshelwood and Langmuir Rideal mechanisms. 7hrs

UNIT – II **[15 hours]**

Chemical Kinetics:

Composite reactions: Rate equation for composite reaction mechanisms (simultaneous and consecutive reactions, steady state treatment, rate determining steps and microscopic reversibility), Chain reactions (hydrogen-halogen reactions with comparison). Auto catalytic reactions (Hydrogen-Oxygen reaction) and Oscillatory reactions. 6hrs.

Reactions in solution: Solvent effects on the reaction rates, Factors determining reaction rates in solution, reaction between ions (effect of dielectric constant and ionic strength), substitution and correlation effects (Hammet and Taft equations-linear free energy relations.) Ion-dipole and dipole-dipole reactions (Pre exp factors and influence of ionic strength) and diffusion controlled reactions. 4 hrs.

Fast reactions-Introduction, Study of fast reactions by-flow, relaxation, molecular beam, and spectroscopic and analytical methods. 3hrs.

Theory of reaction rates- Temperature dependence and the Arrhenius theory of reaction rates, collision theory of bimolecular reactions, its importance and limitations. Introduction to transition state theory. 2hrs.

UNIT-III **[15hours]**

Electrochemistry of solutions: Ionic atmosphere-introduction, derivation and its effect on thetheory of conductivity. Walden`s rule. Debye-Huckel limiting law (DHL), its modification and verification. Bjerrum theory of ion association, triple ion formation and its significance. 4hrs.

Corrosion: Introduction, Importance and principles, Forms of corrosion (Galvanic, Atmospheric, stress, microbial and soil). Techniques of Corrosion rate measurement (instrumental and non-instrumental). EMF series &Galvanic series and their limitations. Thermodynamics (Pourbaix diagram). Concept of mixed potential theory and its importance in terms of Kinetics (Tafel and Evans diagram), effect of oxidizer and passivity of corrosion. Protection against corrosion (Design improvement, Anodic and cathodic protection, inhibitors, coating). 6 hrs.

Analytical Applications of Electrochemistry -Principles and Applications of Polarography, Cyclic voltammetry, Coulometry, Amperometry and chrono systems. 5hrs.

REFERENCES

1. Chemical Kinetics, K. J. Laidler, Pearson Education, Anand Sons(India) 3rd ed., 2008.
2. Fundamentals of Chemical Kinetics, M.R.Wright, Harwood Publishing, Chichesrer, 1999.
3. Kinetics & Mechanisms of Chemical Transformations, J Rajaram & J C Kuriacose, Macmillan, Delhi,42007.
4. Chemical &Electrochemical Energy Systems, R. Narayan & B. Viswanathan (University Press), 1998.
5. Industrial Electrochemistry, D. Peltcher & F. C. Walsh (Chapman & Hall)1990.
6. Principles and Applications of Electrochemistry–Crow (Chapman hall, New York) 2014
7. An Introduction to metallic corrosion and its prevention-Raj Narayan (Oxford-IBH, New Delhi), 1983.
8. Electrochemistry and Corrosion Science-Nebtor Ferez (Springer Pvt.Ltd.), Delhi, 2010.
9. Instrumental Methds of Chemical Analysis, Kudesia Sawhney, Pragati Prakasha(Meerut).

OC S 404 : SPECTROSCOPY AND ANALYTICAL TECHNIQUES

COURSE OUTCOME:

- Students will learn the basic principles and applications of ESR Spectroscopy, NQR Spectroscopy,
- Students can be familiarising with Mossbauer Spectroscopy, Photoelectron spectroscopy, Atomic absorption Spectroscopy, Emission Spectroscopy, Molecular Luminescence Spectroscopy and Light Scattering methods.
- The students will also trained in the field of Ion Exchange Chromatography, Exclusion Chromatography and Thermal methods
- Overall students can solve the problems related to spectroscopy

UNIT- I: **[12 Hours]**

Electron Spin Resonance Spectroscopy: Basic principles, hyperfine couplings, the 'g' values, factors affecting 'g' values, isotropic and anisotropic hyperfine coupling constants, Zero Field splitting and Kramer's degeneracy. Measurement techniques and Applications to simple inorganic and organic free radicals and to inorganic complexes.

NQR Spectroscopy: Quadrupolar nuclei, electric field gradient, nuclear quadrupole coupling constants, energies of quadrupolar transitions, effect of magnetic field. Applications.

Mössbauer Spectroscopy: The Mössbauer effect, chemical isomer shifts, quadrupole interactions, measurement techniques and spectrum display, application to the study of Fe^{2+} and Fe^{3+} compounds, Sn^{2+} and Sn^{4+} compounds(nature of M-L bond, coordination number and structure), detection of oxidation states and inequivalent Mössbauer atoms.