OC H 413: PHYSICAL CHEMISTRY

Course Outcome

- To understand the theoretical basis of catalysis, corrosion, various complex reactions which find relevance in biological processes and are of industrial importance and photochemical aspects of chemical reactions.
- 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 catalytic reactions, corrosion in the day to day life and in industrial reactors; enzyme mediated reactions in biochemistry, biotechnology, pharmaceutical chemistry, electronic spectroscopy and different category of photochemical reactions etc.

UNIT-I **[12 Hours]**

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. Semiconductor catalysis, n- & p- type. Industrial applications of catalysis.

Surface Chemistry: A review of adsorption isotherms, Langmuir and Freundlich isotherms-derivation. Multilayer adsorption: BET equation–derivation, application in surface area determination. Harkin–Jura equation and application.

Mechanism of surface reactions. Langmuir-Hinshelwood & Langmuir Rideal mechanisms.

UNIT-II **[12 Hours]**

Composite reactions: Rate equation and derivation of rate constants simultaneous and consecutive reactions, steady state treatment, rate determining steps, Chain reactions (hydrogen-halogen reactions with comparison, derivation of rate equation for H_2-Br_2). Auto catalytic reactions (Hydrogen-Oxygen reaction), explosion limits and Oscillatory reactions.

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).

Fast reactions: Introduction, Study of fast reactions by-flow, relaxation (T&P jump methods).

UNIT-III **[12 Hours]**

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

Corrosion: Introduction, Principles, and classification. Techniques of corrosion rate measurement (instrumental and non-instrumental). Thermodynamics (Pourbaix diagram). Concept of mixed potential theory and its importance in terms of Kinetics (Tafel and Evans diagram), passivity of

corrosion. Protection against corrosion (Design improvement, Anodic and cathodic protection, inhibitors, coating).

Unit-IV **[12 Hours]**

Photochemistry: Introduction to photochemistry. Determination of quantum yield- Actinometry. Frank-Condon principle and its implications in predicting shapes of absorption and emission spectra. Effect of solute solvent interactions on electronic spectra-spectral shifts. Physicochemical properties of electronically excited molecules-excited state dipole moments, acidity constants. Flash photolysis technique.

Photochemical kinetics of unimolecular and bimolecular processes. Quenching-collisions in the gas phase and in solution (Stern-Volmer equation). Photoisomerization, photo Fries rearrangement and Norrish type cleavage reactions with specific examples.

References

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3. Kinetics & Mechanisms of Chemical Transformations, J. Rajaram& J. C. Kuriacose, Macmillan (2007).
4. Chemical &Electrochemical Energy Systems, R. Narayan & B. Viswanathan, University Press (1998).
5. Industrial Electrochemistry, D. Peltcherand, F. C. Walsh, Chapman & Hall (1990).
6. Principles and Applications of Electrochemistry, D. R. Crow, Chapman Hall (2014).
7. An Introduction to metallic corrosion and its prevention, Raj Narayan, Oxford-IBH (1983).
8. Electrochemistry and Corrosion Science, Nebtor Ferez, Springer (2010).
9. Instrumental Methods of Chemical Analysis, H. Kaur, Pragati Prakashana (2018).
10. Fundamentals of Photochemistry, K. K. Rohatgi-Mukherjee, New Age Bangalore (2000).
11. Physical Chemistry, 7th edn., P. W. Atkins, Oxford University Press (2002).
12. Photochemistry, 2nd edn., Gurdeep Raj, Goel Publishing House (1991).
13. Photochemistry, Carol E. Wayne and Richard P. Wayne, Oxford University Press (1996).