Course No: PGCHM17C103

Title: Physical Chemistry (04 Credits)

Max. Marks: *100* ***Course Duration:*** *64 Contact hours*

Continuous Assessment: 20 *End Term Assessment: 80*

Unit-I Quantum Chemistry (16 Contact hours)

Exact quantum mechanical results: Time-independent and time-dependent Schrodinger equation. Postulates of quantum mechanics. Operator concept, quantum mechanical operators in Cartesian and Spherical polar co-ordinate systems, some properties of quantum mechanical operators. Review of particle in a box problem. The solution of problems of harmonic oscillator & the rigid rotator. Tunneling effect. Born-Oppenheimer approximation. Solution of the Hydrogen-like atom problem, radial and angular wave functions.

Unit-II Surface Chemistry (16 Contact hours)

Liquid Surface: Pressure difference across curved surfaces (Laplace equation), vapor pressure of droplets (Kelvin equation), Capillary condensation. **Thermodynamics of Interfaces:** Surface excess, surface tension and thermodynamic parameters, Gibbs adsorption isotherm.

Solid liquid interface: Contact angle, young's equation, wetting, Wetting as contact angle phenomena.

Solid surfaces: Adsorption at solid surfaces, adsorption models; Langmuir adsorption isotherm, BET adsorption isotherm and its use in estimation of surface area. Adsorption on porous solids.

Unit-III Chemical kinetics-I (16 Contact hours)

Theories of Chemical Reactions: Activated complex theory of reaction rates, statistical & thermodynamic formulations, comparison with collision theory. Theories of unimolecular reactions (Lindman, Hinshelwood), Introduction to potential energy surfaces.

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

Chain reactions: Explosive reactions, Polymerization reactions (free radical, cationic and anionic)

Unit-IV Chemical kinetics-II **(16 Contact hours)**

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

Reactions in solution: Diffusion controlled reactions (partial & full microscopic diffusion control), Ionic Reactions; Single & double sphere models of ionic reactions.

Enzyme catalyzed Reactions: Kinetics of enzyme catalyzed reactions, Effect of substrate concentration, temperature and pH. Enzyme inhibition.

Structure Reactivity Relationships: Quadratic Free-Energy Relationships (QFER), Hammet and Taft relationships.

Books Recommended:

1. Physical Chemistry –P. W. Atkins, 9th Edition, ELBS , Oxford, 2009
2. Physical Chemistry- A Molecular Approach - D. A. McQuarie & J. D. Simon, University Science Books, 1997.
3. Introduction to Quantum chemistry - A. K. Chandra, TataMcGraw Hill, 1997.
4. Quantum Chemistry - Ira. N. Levine, 7th Edition, Pearson, 2009.
5. Quantum Chemistry, R. K. Prasad, 2nd Edition, New Age Publishers, 2001.
6. Physics and Chemistry of Interfaces, H-J, Butt, K. Graf and M. Kappl, 2nd Edition, Wiley-VCH Verlag Gmbh and Co. KGaA, 2006.
7. Physical Chemistry of Surfaces, A. W. Adamson and A. P. Gast, 6th Edition, John Wiley and Sons, Inc. 1997.
8. Chemical Kinetics, K. J. Laidler, 3rd Edition, Pearson, 1987.
9. Chemical Kinetics and Reaction Dynamics, Paul L. Houston, Dover Publications, INC., Mineola, New York, 2001.
10. Chemical Kinetics and Dynamics, J. I. Steinfeld, J. S. Francisco, W.L. Hase, Prentice Hall, 1989.
11. Chemical Kinetics and Catalysis, R.I. Masel, Wiley, 2001
12. Chemical Kinetics: From Molecular Structure to Chemical Reactivity, Luis G Arnaut, Sebastiao Jose Formosinho, Hugh Burrows, Elsevier, 2007.