

SEMISTER –II

Code: 202103	Title : Physical Chemistry	Credits : 4
Objectives: - 1. Explain the concept of activation energy and its effects on the rates of chemical reactions. 2. Apply the tools to derive the rate law and its mechanism 3. To explain the influence of different parameters on rate of reactions 4. To explain concept of quantum chemistry , operators , oscillators and numerical. 5. Apply the basic principles of the major spectroscopes, including Raman, ESR, Mossbauer, NMR.		
Paper -I		60 Hours
Unit I	Quantum Chemistry:- The Schrodinger equation, particle in a one dimensional box, Eigen values and Eigen functions, operators, properties of quantum mechanical operators, Hermitian, Linear, Ladder, Hamiltonian and angular momentum operators. Particle in three dimensional box, harmonic oscillator, rigid rotator and numericals.	15 Lectures
Unit II	Chemical Kinetics and Molecular Reaction Dynamics :- 1. Elementary Reactions in Solution:- Solvent Effects on reaction rates, Reactions between ions- influence of solvent Dielectric constant, influence of ionic strength, Linear free energy relationships Enzyme action 2. Kinetics of reactions catalyzed by enzymes -Michaelis-Menten analysis, Lineweaver-Burk and Eadie Analyses. 3. Inhibition of Enzyme action: Competitive, Noncompetitive and Uncompetitive Inhibition. Effect of pH, Enzyme activation by metal ions, Regulatory enzymes. 4. Kinetics of reactions in the Solid State:- Factors affecting reactions in solids Rate laws for reactions in solid: The parabolic rate law, The first order rate Law, the contracting sphere rate law, Contracting area rate law, some examples of kinetic studies.	15 Lectures
Unit III	Quantum Chemistry:- Term symbols and selection rules, spin-orbital coupling, the variation theorem, nondegenerate perturbation theory and applications. Huckel molecular orbital theory of conjugated systems, application to ethylene, butadiene, cyclopropenyl radical , cyclobutadiene and benzene, numericals.	15 Lectures
Unit IV	Molecular Spectroscopy:- 1. Raman Spectroscopy:- Introduction, Rotational Raman spectra, Vibrational Raman Spectra, polarization of light and Raman effect, structure elucidation from combined Raman and IR spectroscopy, applications in structure elucidation. 2. Electronic spectroscopy of molecules:- Born – Oppenheimer approximation, electronic spectra of diatomic molecules, vibrational coarse structure, rotational fine structure dissociation energy and dissociation products, electronic structure of diatomic molecules, molecular photoelectron spectroscopy, application. 3. ESR and Mossbauer spectroscopy applications.	15 Lectures

	4. Principles of NMR : - Chemical applications of PMR in structure elucidation.	
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Reference Books :

1. Quantum Chemistry : Ira N. Levine
2. Quantum Chemistry : R.K. Prasad
3. Quantum Chemistry : B.K. Sen
4. Introduction to Molecular Photo-chemistry : C.H.J. Wells
5. Atkin's Physical Chemistry : Peter Atkins
6. Physical Chemistry : G.K. Vemulapalli.
7. Fundamentals of molecular spectroscopy : C.N. Banewell and E.Mc. Cash (Fourth edition).
8. K.J. Laidler and J.H. Meiser, Physical Chemistry, 2nd Ed., CBS Publishers and Distributors, New Delhi, 1999.
9. Principles of Chemical Kinetics, 2nd Ed., James E. House, ELSEVIER, 2007.