CLUSTERUNIVERSITYSRINAGAR

SYLLABUS (FYUP UNDERNEP 2022)

Offered by Department of Chemistry

Semester 6th (Major Course)

Title: Advanced Topics in Physical Chemistry

Course Code: UGCHM22J603 **Max. Marks: 150**
Credits: 6 (Theory:4, Practical:2) **Theory External: 80;Min Marks: 32**
Contact Hrs: 120 (Theory: 60, Practical: 60) **Theory Internal (Continuous Assessment): 20 Marks, Min. Marks: 08**
Practical Experimental Basis=30, Min. Marks: 12
Practical Experimental (Continuous assessment)=20,Min.Marks:08

Course Objectives:

- To understand the origin of quantum mechanics and strangeness in quantum mechanical formulation.
- To understand Schrodinger equation and apply the quantum mechanical formulation for evaluating some atomic and molecular properties.
- Understand basics of spectroscopy and its power to understand structure and reactivity of molecules

Course Outcomes: On completion of the course, the student should be able to:

- Appreciate the importance of transition from classical to quantum mechanics for understanding atomic/molecular world.
- Apply quantum mechanical formulations to simple systems so as to distinguish between the quantum results from the expected classical ones.
- Understand and interpret the rotational, vibrational and electronic spectra of simple molecules under the realm of quantum mechanics

UNIT1: An introduction to Quantum Chemistry (15 Hrs)

Limitation of Classical mechanics: Blackbody radiation, photoelectric effect, heat capacity of solids and atomic spectra. Wave-particle duality: de-Broglie equation.

Operators: Elementary concept of operators, Algebra, Rules for setting operators (position and linear momentum), eigenfunctions and eigenvalues, Hamiltonian operator, Linear and Hermitian operators, Physical interpretation of wave function, Orthogonality and Normalization of wave function.

Schrodinger's wave equation and it's importance. Postulates of quantum mechanics. Solution of schrodinger wave equation for particle in one-dimensional box.

UNIT2: Molecular Spectroscopy (15 Hrs)

Interaction of electromagnetic radiation with atoms and molecules. Line width of the peaks and peak broadening

Rotational spectroscopy: Moment of inertia, classification of molecules on the basis of moment of inertia. Energy of a rigid diatomic rotor, selection rules for rotational transitions. Rotational spectrum of heterodiatomic molecule. Determination of bond length. Relative population of rotational levels intensity of sepctral lines.

Vibrational Spectroscopy: Classical and quantum mechanical (qualitative) treatment of simple harmonic oscillator, selection rules for vibrational transition, pure vibrational spectrum of a diatomic molecule, determination of force constant, relation of force constant with bond length and bond energy, Vibrational degrees of freedom.

UNIT3: Surface Chemistry (15 Hrs)

Liquid Surface: Surface tension, the pressure difference across curved surfaces (Laplace equation), vapor pressure of droplets (Kelvin equation). Thermodynamics of Interfaces: Surface excess and it's relation with surface tension, Gibbs adsorption isotherm.

Surfactants: Introduction, types, cmc and micellization, factors affecting cmc.

Solid surfaces: Adsorption at solid surfaces, adsorption isotherms; Freundlich and Langmuir adsorption isotherm,

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

UNIT4: Chemical Kinetics (15 Hrs)

Theories of chemical kinetics: Simple collision theory based on hard sphere model, estimation of rate constants of atomic reactions. Activated complex theory of reaction rates (Thermodynamic formulation). Comparison with collision theory.

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

Kinetics of Solution Phase Reactions: Effect of solvent on reaction rates (diffusion controlled reactions), Ionic Reactions; single & double sphere models of ionic reactions, the effect of ionic strength.

Practicals (2 Credits- 60 Hrs) (Any 05)

a) Investigation of the variation of viscosity with concentration of a liquid and determination of it's unknown concentration.

b) Determination of the radius of a molecule by viscosity measurement.

c) Determination of cmc of any surfactant.

d) Kinetic investigation of acid-catalyzed hydrolysis of an ester (titrimetry or conductometry) to; i) establish the order of reaction with respect to the ester and ii) to establish the role of the nature of acid over its catalytic performance.

e) To validate the Beer-Lambert law.

f) Determine the wavelength of maximum absorption (λ_{max}) of any two two compounds (like $KMnO_4$, $K_2Cr_2O_7$, $CuSO_4$)

g) Determination of the unknown concentration of a compound spectrophotometrically.

In addition to this and in-order to understand the genesis of the quantum mechanics, the students should be exposed to online videos demonstrating the early development of quantum mechanics.

SUGGESTEDREADING:

a) Physical Chemistry- A Molecular Approach - D. A. McQuarie & J. D. Simon, University Science Books, 1997.

b) Quantum Chemistry - Ira. N. Levine, 7th Edition, Pearson, 2009.

c) Principles of Physical Chemistry; B.R. Puri, L.R. Sharma and L.S. Pathania; 47th Edn.,Vishal Pubs & Co, 2017.

d) Quantum Chemistry, R. K. Prasad, 2nd Edition, New Age Publishers, 2001.

e) Fundamentals of Molecular Spectrsocopy; C.N.Banwell, E.M.Mc Cash; 4th edn; Tata McGrawHill; 1994.

f) Quantum Chemistry and Spectroscopy, 2018, by Thomas Engel, Philip Reid, Pearson Publications.

g) Physical Chemistry, 2017, by David W. Ball, Cengage India Private Limited, second Edition.

h) Physical Chemistry; T. Engel, P. Reid,; 3rdEdn., Pearson India, 2013. 9.

i) A Textbook of Physical Chemistry, Thermodynamics and Chemical Equilibrium (SI Units) - Vol. 2; K.L Kapoor; 6 thEdn, McGraw Hill Education, 2019.