20CY106 PHYSICAL CHEMISTRY - 2

Hours Per Week :

L	T	P	C
3	1	-	4

Course Description and Objectives:

This course is an introduction to quantum mechanics for *use* by chemists. Topics include particles and waves, wave mechanics, semi-classical quantum mechanics, perturbation theory, molecular orbital theory. Also, it involves developing an understanding of quantum mechanical principles, and applying these principles to master the underlying concepts of electronic structure for atoms and molecules along with rotational, vibrational, and electronic spectroscopy. It helps to understand the different types of adsorption isotherms, and difference between macromolecules, colloids, micelles. Besides, this course deals with the nuclear chemistry in understanding the macroscopic observables associated with nuclear change and the microscopic or chemists view of nuclear change.

Course Outcomes:

Upon completion of the course, the student will be able to achieve the following outcomes:

COs	Course Outcomes
1.	Understand the basic principles and concepts of quantum mechanics and describe single and multi-electron atoms with the independent particle model.
2.	Analyze the various concepts of phase equilibrium components such as degree of the freedom and phase rule to interpret various phase diagrams.
3.	Apply concept of molecular interactions to study various spectroscopic methods.
4.	Distinguish various types of adsorption isotherm and study the different characteristics of macromolecules, colloids, micelles and vesicles.
5.	Apply the concept of nuclear reactions such as Fission and Fusion to various applications of materials.

Unit – I:

Quantum Chemistry:

Review of classical mechanics, Wave-particle duality and Uncertainty principle, Postulates of quantum mechanics,Operator algebra. Properties of Hermitian operators, Eigenvalue problem. Commutators and Uncertainty Principle,Elementary applications of quantum mechanics,unbound motion in one dimension. Tunnelling. Bound motion, particle-in-a-box (1D & 3D), harmonic oscillator and rigid rotor, Angular momentum algebra- Hydrogen atom.

Unit - II:

Phase Diagram and Phase Equilibria:

Phase rule, Derivation of phase rule, Thermodynamic and Phase Equilibria; One Component System Phase Diagrams; Two Component System Phase Diagrams: Binary eutectic, azeotropic, Intermediate compounds, Solid solution, Liquid immiscibility.

Unit - III :

Molecular Spectroscopy:

Interaction of radiation with matter, Selection rules. Line width and line shapes.

Rotational, vibrational and rotational-vibrational spectroscopy of diatomic molecules, Selection rules, Rotational energy levels of polyatomic molecules. Applications, Polyatomic molecular vibrations. Local and normal modes, Infrared spectroscopy, selection rules, Rotational and vibrational Raman Spectroscopy and selection rules.

Franck-Condon principle, Electronic spectroscopy. Selection rules. Resonance Raman transitions and application. Principles of Mossbauer spectroscopy.

Unit – IV:

Adsorption, Macromolecules and Aggregates:

Physisorption, Chemisorpton, Types of adsorption, Adsorption Isotherm (Langmuir-Freundlich isotherm), BET analysis, Mean molar mass, Laser light scattering, Ultracentrifugation, Electrophoresis, viscosity, Colloids, Micelles, Surface films (Self Assembly), biological membranes, Impact on nanoscience: Nanofabrication with self-assembly monolayer.

Unit – V:

Nuclear Chemistry:

Structure of atomic nucleus - Radioactivity: Determination of half-life, radioactive decay kinetics, parent-daughter decay-growth relationships, nuclear reactions

Nuclear power reactors – Nuclear fission and fusion, types of nuclear power reactors, basic features and components of a nuclear power reactor.

Applications of Radioisotopes: Physico-chemical, and analytical applications ^{14}C dating. Medical, agricultural and industrial applications of isotopes. Health and safety aspects.

Text Books:

1. Atkins, P. W. & Paula, J. de Atkins' Physical Chemistry, 10th Edition, Oxford University Press
2. R, West, Solid State Chemistry and its Applications, john Wiley & Sons, 1984 (Reprint Edition)
3. McQuarrie, D. A. & Simons, J. D. Physical Chemistry: A Molecular Approach, Viva Press

Reference Books:

1. Gileady, Physical Electrochemistry, Fundamental, Techniques and Applications, Wiley-VCH – 2011
2. J. Bard and L. R. Faulkner, Electrochemical Methods: Fundamentals and Applications, 2nd Edition, Wiley 2001
3. Puri, Sharma, and Pathania, Principles of Physical Chemistry
4. Kapoor K.L, A Text Book of Physical Chemistry, McGraw Hill India.
5. Levine, I. N. Physical Chemistry, 6th Edition, McGraw-Hill India.
6. Castellan, G. W. Physical Chemistry, Narosa