

COURSE-3 PHYSICAL CHEMISTRY-I

Block-1

A brief resume of black body radiation, Planck's law of radiation, wave particle duality of material particles, de broglie equation, Heisenberg uncertainty principle. Wave equation progressive and stationary waves, schrodinger wave equation, eigen values and eigen functions; well behaved functions. Concept of operators(operator and operand)- Algebra of operators, commutative and non commutative operators, linear operator. Laplacan operator, Hamiltonian operator, Hermitian operator, angular momentum operator, postulates of quantum mechanics.

Block-2

Molecularity and stoichiometry of reactions, determination of order of reaction (zero order, first order and second order) with respect to reactant and total order of reaction. Complex reactions- parallel consecutive and reversible reactions. Theories of reaction rates: collision theory and limitations activated complex theory and its application to reactions in solution. Energy of activation, other activation parameters-determinations and their significance. Lindemann theory of uni molecular reactions. Factors affecting the order of reaction – primary and secondary salt effects. Effects of dielectric constant, pressure and volume on the rate of reaction.

Block-3

A brief resume of laws of thermodynamics (combined form of 1 and 2nd laws), entropy as a measure of unavailable energy, concept of fugacity and free energy, entropy and free energy changes and spontaneity of processes. Variation of free energy with T and P, Maxwell's relations, thermodynamics equations of states, limitations of Vant Hoff's equation. Nerst heat theorems and its applications. Third law of thermodynamics, determination of absolute entropies. Application of thermodynamics: Entropy and free energy of mixing, partial molar quantities, partial molar volume and free energy (chemicals potential), their significance and determinations (slope and intercept methods). Gibbs – Duhem and Duhem-Margules equations.

Block-4

Consequences of light absorption. Laws of photochemistry-Grothus-Draper law, Stark-Einstein law. Quantum yield, determination of quantum yield, actinometers.

The Jablask diagram and its significance. Photochemical reactions: The photochemical rate law. Kinetics of photochemical reactions. Kinetics of Hydrogen-Chlorine, Hydrogen-Bromine reactions. Kinetics of decomposition of HI. Energy transfer in photochemical reaction. Photosensitization and quenching. Fluorescence and Phosphorescence. Quenching of fluorescence. Chemiluminescence. The oscillator strength. The geometry of excited states, the laser and maser.

Reference books

1. Chandra, A. K. Introduction to Quantum Chemistry 3rd Ed. *Tata McGraw Hill, New Delhi, 1988.*
2. Prasad, R. K. Quantum Chemistry, *New Age International Publications, New Delhi, 1997.*
3. Walter, Kimball and Eyring, Quantum Chemistry, *John-Wiley, New York. 1961.*
4. Barrow, G. M. Physical Chemistry, *McGraw Hill, New York, 1996.*
5. Maron and Lando, Fundamentals of Physical Chemistry,
6. Atkins, P. W. Physical Chemistry, 4th Ed, *ELBS, London, 1990.*