Subject Code : P8CH3

CORE COURSE III - PHYSICAL CHEMISTRY I

UNIT – I

1. Group theory - Concepts

Elements of group theory – definition – group multiplication tables – conjugate classes, conjugate and normal subgroups – symmetry elements and operations – point groups – assignment of point groups to molecules, - Matrix representation of geometric transformation and point groups – reducible and irreducible representations– properties of irreducible representation – construction of character tables – bases for irreducible representation – direct product – symmetry adapted linear combinations – projection operators.

UNIT - II

2. Quantum Chemistry – I

Inadequacy of classical mechanics, Black body radiation, Planck's quantum concept, Photoelectric effect. Bohr's theory of hydrogen atom :Hydrogen spectra, Wave-particle dualism, Uncertainty principle, Inadequacy of old quantum theory.

Schrödinger equation, Postulatory basis of quantum mechanics. Operator algebra: operator, linear and hermitian, eigen functions and eigen values, angular momentum operator, commutation relations, related theorems.

Applications of wave mechanics to simple systems – particle in a box, one and three-dimensional, distortion of the box and Jahn-Teller effect, quantum numbers, zero-point energy, orthogonalisation and normality, finite potential barrier – tunneling.

UNIT – III

3. Chemical Kinetics- I

Theories of reaction rate – Absolute reaction rate theory (ARRT) - Significance of reaction co-ordinate – Potential energy surfaces – Kinetic isotope effect – Molecular dynamics – Marcus theory of electron transfer processes.

Principle of microscopic reversibility - Steady–state approximation – Chain reactions: thermal and photochemical reactions between hydrogen and halogens - Explosions and hydrogen – oxygen reactions.

UNIT – IV

4. Molecular Thermodynamics - I

Calculation of Thermodynamic probability of a system – Difference between thermodynamic probability and statistical probability – Ergodic hypothesis –Derivation of Boltzman distribution equation – physical significance of partition function- translational, rotational, vibrational and electronic partition functions – Quantum statistics – Bose – Einstein and

Fermi – Dirac distribution equations – comparison of B.E and F.D statistics with Boltzman statistics – Concept of Negative Kelvin Temperature.

Relationships between partition function and thermodynamic properties such as E, H, Cp, Cv, P. Derivation of PV=RT, Molecular interpretation of entropy- Derivation of S=klnW- Establishment of analogous nature of S= klnW to ds= dq_{rev}/T. Calculation of S, A, G etc., from partition functions– calculation of equilibrium constants for very simple reactions.

UNIT – V

Fast reaction techniques: Introduction, flow methods (continuous and stopped flow methods)- Relaxation methods (T and P jump methods) – Pulse techniques (pulse radiolysis, flash photolysis, Shock tube method)- molecular beam method – lifetime method.

Photochemistry and Radiation Chemistry:

Photophysical processes electronically excited molecules Jablonski diagram – Stern-Volmer equation and its applications – experimental techniques in photochemistry – chemical actinometers –lasers and their applications.

Radiation Chemistry

Differences between radiation chemistry and photochemistry – sources of high energy radiation and interaction with matter – radiolysis of water, solvated electrons – Definition of G value – Curie –Linear energy transfer LET and Rad – Scavenging techniques- use of dosimetry and dosimeters in radiation chemistry- application of radiation chemistry.

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