MJD Govt. College Taranagar (Churu) Department of Chemistry B.Sc.-III (Syllabus) PHYSICAL CHEMISTRY PAPER-III

Unit-I

Elementary Quantum Mechanics

Black-body radiation, Planck's radiation law, photoelectric effect, heat capacity of solids, Bohr's model of hydrogen atom (no derivation) and its defects, Compton effect.

De Brogile hypothesis, Heisenberg's uncertainty principle, Sinusoidal wave equation, Hamiitonian operator, Schrodinger wave equation and its importance, physical interpretation of the wave function, postulates of quantum mechanics, particle in a one dimensional box. Schrödinger wave equation for H-atom, separation into three equations (without derivation), quantum numbers and their importance, hydrogen like wave functions, radial wave functions, angular wave functions.

Unit-II

Molecular orbital theory, basic ideas-criteria for forming. M.O from A.O,

construction of M.O's by LCAO,H2

+ ion, calculation of energy levels from 'wave

functions, physical picture of bonding: and antibonding wave functions, concept of s, s *, p, p * orbitals and their characteristics. Hybrid orbitals-sp, sp2, sp3, calculation of coefficients of A.O's used in these hybrid orbitals.

Introduction to valence bond model of H2, comparison of M. O. and V. B. models.

Unit-Ill

Spectroscopy

Introduction: electromagnetic radiation, regions of the spectrum, basic features of different spectrometers, statement of the Born-Oppenheimer approximation, degrees of freedom.

Rotational Spectrum

Diatomic molecules, Energy levels of arigid rotator (semi-classical principles), selection rules, spectral intensity, distribution using population distribution (Maxwell-Boltzmann distribution) determination of bond length, qualitative description of nonrigid rotor, isotope effect.

Vibrational spectrum

Infrared spectrum: Energy levels of simple harmonic oscillator, selection rules,

pure vibrational spectrum, intensity, determination of force constant and qualitative relation of force constant and bond energies, effect of an harmonic motion and isotope on the spectrum, idea of vibrational frequencies of different functional groups.

Raman Spectrum concept of polarizability, pure rotational and pure vibrational Raman spectra of diatomic molecules, selction rules.

Unit – IV

Thermodynamics -ll

Second law of Thermodynamics :Need for the law, different statements of the law. Carnot cycle and its efficiency, Carnot theorem. Thermodynamic scale of temperature.

Concept of entropy: Entropy as a statement function, entropy as a function of V & T, entropy as a function of P & T, entropy change in physical change, Clausius inequality, entropy as a criteria of spontaneity and equilibrium. Entropy change in ideal gases and mixing of gases.

Third Law of Thermodynamics :Nernst heat theorem, statement and concept of residual entropy, evaluation of absolute entropy from heat capacity data. Gibbs and Helmholtz functions; Gibbs function (G) and Helmholtz function (A) as thermodynamic quantities, A & G as criteria for thermodynamic equilibrium and spontaneity, their advantages over entropy change. Variation of G with A and P, V and T.

Unit-V

Solutions, Dilute Solutions and Colligative Properties

Ideal and non-ideaf solutions, method of expressing concentration of solutions, activity and activity coefficient.

Dilute solution, colligative properties, Raoult's law, relative lowering of vapour pressure, molecular weight determination. Osmosis, law of osmotic pressure and its measurement, determination of molecular weight form osmotic pressure. Elevation of boiling point and depression in freezing point. Expdwmental methods for determining various colligative properties. Abnormal molar mass, depree of dissociation and association of solutes.