B.Sc. III Paper III

Physical Chemistry –

Unit I
(Introductory Quantum Mechanics, Spectroscopy, Physical Properties & Molecular Structure)

I Introductory 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 Broglie's hypothesis, the Heisenberg's uncertainty principle, Hamiltonian operator.

II *Spectroscopy*

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

III Physical Properties and Molecular Structure:

Optical activity, polarization - (Clausius – Mossotti equation), orientation of dipoles in an electric field, dipole moment, induced dipole moment, measurement of dipole moment-temperature method and refractivity method, dipole moment and structure of molecules, magnetic properties-paramagnetism, diamagnetism and ferromagnetics.

Unit II

IV Elementary Quantum Mechanics

Schrodinger wave equation and its importance, physical interpretation of the wave function, postulates of quantum mechanics, particle in a one dimensional box.

Schrodinger 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.

Molecular orbital theory, basic ideas – criteria for forming M.O from A.O., construction of M.O's by LCAO – H_2^+ ion, calculation of energy levels from wave functions, physical picture of bonding and antibonding wave functions, concept of σ, σ^*, π, π^* orbitals and their characteristics. Hybrid orbitals – sp, sp^2, sp^3; calculation of coefficients of A.O's used in sp and sp^2 hybrid orbitals.

Introduction to valence bond model of H_2, comparison of M.O. and V.B. models.

Unit III
(Spectsroscopy)

V Rotational Spectrum:

Diatomic molecules: Energy levels of a rigid rotor (semi-classical principles), selection rules, spectral intensity, distribution using population distribution (Maxwell-Boltzmann distribution) determination of bond length, qualitative description of non-rigid 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 anharmonic 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, selection rules.

Electronic Spectrum: Concept of potential energy curves for bonding and antibonding molecular orbitals, qualitative description of selection rules and Franck-Condon principle.

Qualitative description of σ, π and n M.O., their energy levels and the respective transitions.

Unit IV

(Photochemistry, Solutions, Dilute Solutions and Colligative Properties)

VI Photochemistry:

Interaction of radiation with matter, difference between thermal and photochemical processes. Laws of photochemistry: Grothus – Drapper law, Stark – Einstein law, Jablonski diagram depicting various processes occurring in the excited state, qualitative description of fluorescence, phosphorescence, non-radiative processes (internal conversion, intersystem crossing), quantum yield, photosensitized reactions – energy transfer processes (simple examples).

Solutions, Dilute Solutions and Colligative Properties:

Ideal and non-ideal solutions, methods of expressing concentrations 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 from osmotic pressure. Elevation of boiling point and depression of freezing, Thermodynamic derivation of relation between molecular weight and elevation in boiling point and depression in freezing point. Experimental me0thods for determining various colligative properties.

Abnormal molar mass, degree of dissociation and association of solutes.