M.Sc.I –Paper III **Second Semester**

PHYSICAL CHEMISTRY **Marks:80**

I. Quantum Chemistry: ***50 Hrs.***

A: Introduction to exact quantum Mechanical Results:
The Schrodinger equation and the postulates of quantum mechanica. Discussion of solution of the Schrodinger equation to the some medel system *viz.* particle in abox, the harmonic oscillator, the rigid rotor, the hydrogen atom.

B: Approximate methods:
The variation theorem, linear variation principle. Perturbation theory (first order and non- degenerate). Simple application of variation method and perturbation theory.

C: Angular Momentum:
Ordinary angular momentum, eigenfuctions for angular momentum, eigenvalues of angular momentum.

D: Electronic structure of atom:
Electronic configuration, Russell-Saunders term and coupling schemes, Slater-Condon parameter, term separation energy of p^n configuration, term separation energy for the d^n configuration, magnetic effects: spin-orbit coupling and Zeeman splitting.

E: Molecular Orbital Theory:
Huckel theory of conjugated system, bond order and charge density calculation. Application to ethylene, butadiene etc. Introduction to extended Huckel theory.

F: Unifying Principal:
Electromagnetic radiation, interaction of electromagnetic radiation with matter-absorption, emission, transmission, reflection, refraction, dispersion, polarization and scattering. Uncertainty relation and natural line width and natural line broadening, transition probability, results of the time dependent perturbation theory, transition moment, selection rules, intensity of spectral line, born-Oppenheimer approximation, rotational, vibrational and electronic enery level.

II. Thermodynamics: ***40 Hrs.***

A: Classical Thermodynamics:
Brief resume of concepts of low of thermodynamics, free energy, chemical potential and entropy. Partial molar quantities and their physical significance. Concepts of fugacityand determination of fugacity.

Application of phase rule to three component system, second order phase transition.

B: Statistical Thermodynamics:

Concepts of distribution, thermodynamic probability and most probable distribution. Ensemble averaging. Canonical, grand canonical and microcanonical ensembles, corresponding distribution law (usingLgrang"s methods of undetermined multipliers.)

Partition fuctions- translational, rotational, vibrational and electronic parttion fution,calculation of thermodynamic propertiesin the term of partition function. Application ofpartition function. Heat capacity behavior of solid- chemical equilibrium and equilibrium constant in the term of partition function.

C: Non Equilibrium Thermodynamics:

Thermodynamic criteria for non – equillibrium stat, etropy production and entropy flow, entropy balance equation for different irreversible processes (e.g. heat flow , chemoical reaction etc.) transformation of generalized fluxed and forces, non equilibrium stationary states, phenomenological equation, microscopic reversibility and Onager's reciprocity relation, electrokinetic phenomena, diffusion, electric conduction, irreversible thermodynamics for biological system, coupled reaction .