20MSC508T					Physical Chemistry-II					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
3	0	0	0	3	25	50	25	--	--	100

COURSE OBJECTIVES (-04)

- Conceptualize the fundamental principles of the properties of matter, energy quantization, its application,
- To develop the fundamental understanding about the classical and statistical models of thermodynamics.
- To acquire knowledge about concepts of photochemistry and photochemical processes
- Understand the symmetry properties of molecules and application of group theory in understanding the molecular properties based on symmetry.

Unit I Quantum Chemistry **12 h**

The failures of classical physics, Bohr's quantum theory, Wave particle duality, Operator algebra, Linear and Hermitian operators, Quantum mechanical postulates, Schrodinger equation for a particle in one and three dimensional boxes, Rigid rotator and simple harmonic oscillator, Schrodinger equation for hydrogen atom and its solution-Derivation of Eigen function and Eigen value for hydrogen atom. Term symbols, LS and JJ coupling. The origin of electronic quantum numbers and physical significance - radial probability density-significance of magnetic quantum number with respect to angular momentum. Hydrogen molecule ion and hydrogen molecule-Pauli's exclusion principle. Born Oppenheimer approximation, Mulliken designation of molecular orbitals. MO theory of bonding, MO treatment of H-bonded systems, ethylene, butadiene and benzene. Approximation methods: Perturbation and variation method, wave functions for many electron atoms – Hartree-Fock SCF method, Slater orbital

Unit 2 Statistical Thermodynamics **10 h**

Statistical view of entropy. Laws of thermodynamics from statistical considerations. Molecular view of temperature and heat capacity. Derivation of Maxwell Boltzmann distribution law – partition functions and their calculation. Expressions for thermodynamic quantities in terms of partition functions-translational, rotational, vibrational and electronic contributions to the thermodynamic properties of perfect gases, Intermolecular forces in imperfect gases. Thermodynamic quantities in terms of partition functions. Statistical mechanics of simple gases and solids. Kinetic theory of gases. Equilibrium constant, mean energies and heat capacities in terms of partition functions. Bose-Einstein and Fermi-Dirac statistics. Use of Statistical Thermodynamics in understanding molecular interaction in liquids.

Unit 3 Photochemistry **10 h**

Absorption and emission of radiation, Franck Condon principle decay of electronically excited states, Jablonski diagram, radiative and non-radiative processes, fluorescence and phosphorescence, spin-forbidden radiative transitions, inter conversion and intersystem crossing. Theory of energy transfer - resonance and exchange mechanism, triplet-triplet annihilation, photosensitization and quenching. Spontaneous and induced emissions. Einstein transition probability-inversion of population - laser and masers. Flash photolysis: Chemi and thermo luminescence.

Unit 4 Group Theory **12 h**

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 group, reducible and irreducible representations, construction of character tables, bases for irreducible representation, direct product, symmetry adapted linear combinations, projection operators. Orthogonality theorem - its consequences. Symmetry aspects of molecular orbital theory, planar π-systems, symmetry factoring of Huckel determinants, solving it for energy and MOs for ethylene and 1,4-butadiene, sigma bonding in AXn molecules, hybridization, tetrahedral, octahedral, square planner, trigonal planar, linear, trigonalbipyramidal systems, hybrid orbitals as linear combination of AOs, electronic spectra, selection rule, polarization electron dipole transition, electronic transitions in formaldehyde, butadiene, configuration interaction, symmetry types of normal molecules, symmetry coordinates, selection rules for fundamental vibrational transition.

Max. 44 h

COURSE OUTCOMES (06)

On completion of the course, student will be able to

CO1- Understand the properties of matter and the wave-particle duality

CO2 - Apply statistical models to understand the thermodynamic properties of macroscopic systems

CO3 - apply the concept of quantization of energy and its modes

CO4- Investigate the photochemical processes and apply of principles of photochemistry to real life phenomenon

CO5-Relate symmetry of the molecules to their properties

CO6-Apply group theory and character table to analyse the molecular properties

TEXT/REFERENCE BOOKS

1. A. K. Chandra, Introductory Quantum Chemistry, Tata McGraw Hill, 1994
2. C. McClelland, Statistical Thermodynamics, Chapman and Hall, (1973).
3. F. A. Cotton, Chemical Applications of Group Theory, Wiley Eastern, 1991.
4. L. K. Nash, Elements of Classical and Statistical Thermodynamics, Addison-Wesley, (1970).
5. K. K. Rohatgi - Mukerjee, Fundamentals of Photochemistry, Wiley (1992).

END SEMESTER EXAMINATION QUESTION PAPER PATTERN

Max. Marks: 100	**Exam Duration: 3 h**
Part A/Question: 3 Questions from each unit, each carrying 3 marks	36 Marks
Part B/Question: 2 Questions from each unit, each carrying 8 marks	64 Marks