Name of the Programme: M. Sc -I (Physical Chemistry)

Course Code: CHP-501 **Title of the course:** Quantum Chemistry and Statistical Thermodynamics

Number of Credits: 04

Effective from AY: 2022-23

Prerequisites for the course:	Students should have studied physical chemistry courses at M.Sc. Chemistry in semester I	
Course Objective:	1. Introduction of various concepts of quantum chemistry. 2. To introduce various concepts of statistical thermodynamics.	
Content	**1. Quantum Chemistry** a. The origin of quantum mechanics: Planck's quantum theory, wave particle duality, uncertainty principle concept of wave function, the Born interpretation of wave function. Normalization and orthogonalizations, quantization, Eigen values and Eigen functions. b. Postulates of quantum mechanics; Schrödinger equation for free particle, particle in a box, degeneracy. Quantum mechanical operators and their properties, commutation relations, Hamiltonian and Laplacian operators, Harmonic oscillators, Angular momentum, Ladder Operators. c. Approximate methods, Schrödinger equation, its importance and limitations, Born-Oppenheimer approximation, Anti-symmetric wave functions and Slater determinants (many electron system e.g. He atom), Exclusion and Aufbau principle, Variation method, Linear Variation Principle, Perturbation theory (first order non-degenerate) and their applications to simple systems. d. MO theory, Hückel MO theory, Bond-order, Charge density matrix, Unification of HMO and VB theory, their applications in spectroscopy and chemical reactivity, electron density forces and their role in chemical bonding. Hybridization and valence MOs of H_2O, NH_3 and CH_4. Application of Hückel Theory to ethylene, butadiene and benzene molecules.	No of hours 34
	2. Statistical Thermodynamics a. The language of statistical thermodynamics: Probability, ensemble, microstate, degeneracy, permutations and combinations. Configuration and weights, the dominant configuration. The Boltzmann distribution. The molecular partition function: its interpretation and its relation to uniform energy levels. b. Translational, Rotational, Vibrational and Electronic Partition functions for diatomic molecules. Relation between	26

	thermodynamic functions and partition functions and their statistical interpretations. Equilibrium constants from partition function. c. Law of Equipartition energy. Theories of specific heat of solids. Comparison between Einstein and Debye theories. d. Concept of symmetric and antisymmetric wave functions. Ortho and para hydrogens. Quantum Statistics: Fermi-Dirac (FD)and Bose-Einstein (BE) statistics. Comparison between MB, FD and BE Statistics.	
Pedagogy	Mainly lectures and tutorials. Seminars / term papers /assignments / presentations / self-study or a combination of some of these can also be used. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning.	
References / Readings	1. P. W. Atkins and J. D. Paula, Physical Chemistry, 8th Ed., Oxford University Press, New Delhi. 2007 2. G. M. Barrow, Physical Chemistry, 5th Ed., Tata McGraw Hill, New Delhi. 2016. 3. M.C. Gupta, Statistical Thermodynamics, Wiley Eastern, New Delhi. 1990 4. I. N. Levine, Quantum Chemistry, 7th Ed., Prentice-Hall, New Delhi. 1999 5. H. Metiu, Physical Chemistry, Statistical Mechanics, Taylor & Francis, New York , 2006	
Course outcomes:	1. Students should be in a position to understand and explain various concepts of quantum chemistry viz. the wave function and applications. 2. Students should be able to explain various concepts in statistical thermodynamics viz. the partition function and applications. 3. Students will be able to explain postulates of quantum mechanics. 4. Students will be able to explain law of equipartition energy.	