Programme: M. Sc. Part-II (Chemistry)
Title of the Course: Quantum Chemistry and Statistical Thermodynamics
Course Code: PCC-501
Number of Credits:03 **Effective from AY:** 2019-20

Prerequisites for the course:	Should have studied the courses PCC-401, PCC-402 and PCO-401. Should have basic knowledge of Physical Chemistry.	No. of lectures
Course Objectives:	To introduce quantum chemistry so of the advance topics. To introduce various concepts statistical thermodynamics.	
Course Outcomes:	Students should be in a position to understand various concepts of quantum chemistry viz. the wave function and applications. Students should be in a position to understand various concepts in statistical thermodynamics viz. the partition function and applications.	
Content:	1. **Quantum Chemistry** 1.1 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, quantisation, Eigen values and Eigen functions. 1.2 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. 1.3 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. 1.4 VB and MO theory, Huckel 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 Huckel Theory to ethylene, butadiene and benzene molecules.	18 hours
	2. Statistical Thermodynamics 2.1 The language of statistical thermodynamics: Probability, ensemble, macrostate, 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. 2.2 Translational, Rotational, Vibrational and Electronic Partition functions for diatomic molecules. Relation between thermodynamic functions and partition functions and their statistical interpretations. Equilibrium constants from partition	18 hours

	function. 2.3 Law of Equipartition energy. Theories of specific heat of solids. Comparison between Einstein and Debye theories. 2.4 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/ tutorials /assignments/ presentations/ self-study or a combination of these could also be used. Sessions shall be interactive in nature to enable peer group learning.	
Text Books/ Reference Books	1. P.W. Atkins & J. De. Paulo, *Atkins' Physical Chemistry,* Oxford Univ. Press, 2007, 8th Ed. 2. I. N. Levine, *Quantum Chemistry*, Prentice-Hall, New Delhi, 1995, 4th Ed 3. A.K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw Hill, New Delhi, 1992. 4. R. McWeeny, *Coulson's Valence*, ELBS, Britain, 1979. 5. M.C. Gupta, *Statistical Thermodynamics*, Wiley Eastern, New Delhi, 1990. 6. K. Huang, *Statistical Mechanics*, Wiley India, 2nd Ed. 7. H. Metiu, *Physical Chemistry, Statistical Mechanics,* Taylor & Francis, New York, 2006.	