Course No.	Course Name	L-T-P-Credits
CY 407	**Quantum Chemistry**	**4-0-0: 04**
Prerequisite: NIL		

Course Objectives: The main objective of the course is to provide basic knowledge of quantum mechanics. The course is planned to present to the students the relevance of quantum mechanics in Chemistry by showing the exactly solvable problems and approximated methods in detail. The course also demonstrates the solution of H-atom and the application of the for bigger atomic/molecular systems to enter into quantum chemistry.

Course Outcomes: After successful completion of the course, students will be able to:

1. Understand the basic postulates of quantum mechanics
2. Learn the operator algebra and its relevance to quantum mechanics
3. Understand the exact solution of particle in 1-d, 2-d and 3-d box and its application to chemistry problems
4. Understand the exact solution of harmonic oscillator its application to chemistry problems
5. Understand the exact solution of rigid rotator its application to chemistry problems
6. Understand the exact solution of H-atom
7. Learn the approximate methods of quantum chemistry and how to go beyond H-atom
8. Understand molecular Hamiltonian, Potential energy, and molecular Schroedinger equation to setup
9. Learn the basic idea of ab initio calculations, basis set, Hartree-Fock and higher level calculations

SYLLABUS

Module	**Contents**	**Hours**
I	**Introduction** Failure of classical mechanics; Planck's quantum theory; wave-particle duality, uncertainty principle; postulates of quantum mechanics; Operators in quantum mechanics, eigenvalues and eigenfunction; wave function-orthogonality and normalization theorems.	10
II	**Schrödinger wave equation and its applications** Applications of Schrödinger wave equation: free particle-particle in a one dimensional box, particle in a three dimensional cubic, particle in a ring. Classical and quantum mechanical treatment to one dimensional harmonic oscillator, quantum mechanical tunnelling; rigid rotator as a model for a rotating diatomic molecule. Angular momentum: Spin and orbital angular momentum	16
III	**Hydrogen and hydrogen like atoms** Solving of Schrodinger equation for the H-atom (or H-like species), separation of relative coordinates, radial solution, probability and radial	06

	distribution function, angular solution, representation of orbitals, degeneracy, orbital and spin angular momentum. L-S and j-j couplings.	
IV	**Approximation methods** Variation theorem, linear variation functions. Time independent Perturbation theory for non degenerate and degenerate systems (first order only); application of variation method and perturbation theory to the Helium atom. Antisymmetry principle, Slater determinant, term symbol and spectroscopic states.	06
V	**Bonding** Born-Oppenheimer approximation, Hellmann–Feynmann theorem and its applications. Molecular orbital (MO) and Valence bond (VB) theories, application to diatomic molecules such as, H_2, H_2^+, N_2, O_2, and CO; Application of projection operator in bonding (e.g. H_2O, NH_3). Huckel molecular orbital theory: Postulates, application to ethylene, butadiene, and benzene, extended Huckel theory and its applications to some simple molecules. Hartree–Fock theory of closed shell electronic configurations of atoms and molecules; Coulomb and exchange integrals, Koopman's theorem.	10

Essential Readings:

1. I. N. Levine, "Quantum Chemistry", Prentice Hall, 7th Edition, 2016.
2. D. A. McQuarrie, "Quantum Mechanics", Viva Student Edition, 2016.

Supplementary Readings:

1. P. W. Atkins and R. S. Friedman, "Molecular Quantum Mechanics", Oxford University Press, 5th Edition, 2012.
2. A. K. Chandra, "Introductory Quantum Chemistry", Tata McGraw-Hill Education, 4th Edition, 2017.
3. J. L. Powell and B. Crasemann, "Quantum Mechanics", Dover Publications, 2015