GAYATRI VIDYA PARISHAD
COLLEGE FOR DEGREE AND PG COURSES (AUTONOMOUS)
Affiliated to Andhra University | | Accredited by NAAC and NBA
VISAKHAPATNAM

DEPARTMENT OF ORGANIC CHEMISTRY

M.Sc. (PREVIOUS) CHEMISTRY SYLLABUS
SEMESTER-II
PAPER-I: GENERAL CHEMISTRY-II
(Effective from the admitted batch of 2022-2023)

Credits: 4		**Theory: 4 Hours**
Max Marks: 100	**External: 80**	**Internal: 20**

Course Outcomes (COs)/Course Specific Outcomes (CSOs):
Upon completion of the course the students will be able to:

CO 1: To know the concepts of classical and quantum mechanics of Wave equation.
CO 2: To solve the simple quantum mechanical problems such as simple harmonic oscillator, particle in a 1Dbox, rigid rotor, H atom etc.
CO 3: To solve wave equation of hydrogen atom and calculate energy and wave functions of perturbation theory.
CO 4: To calculate energy and wave functions of variation theory and its applications.
CO 5: To learn the Valence bond, LCAO approximation and the electronic transitions in the hydrogen molecule.

Course learning outcome (LOs):
Upon completion of the course the student will be able

LO 1: To learn the quantum mechanics methods for electron in the atom, ion and molecules.
LO 2: To acquire knowledge of molecular in one dimensional box, three-dimensional box and to solve wave equation problems.
LO 3: To acquire knowledge of molecular symmetry and group theory and to solve chemical problems.
LO 4: To develop the knowledge and learn the concept of tunneling, simple harmonic oscillator, rigid wave functions of electron in the atom.
LO 5: To derive the valence-hybridization-covalent bond-calculation of ionic and covalent bond contributions in hydrogen molecule.

Unit-I **[12 Hours]**

Wave equation – interpretation of wave function–properties of wave function–normalization and orthogonalization, operators–linear and non-linear commutators of operators.
Postulates of quantum mechanics, setting up of operators observables–Hermitian operator – Eigen values of Hermitian operator.

Unit-II **[12 Hours]**

Wave mechanics of simple systems with constant potential energy, particle in one dimensional box–factors influencing colour–the concept of tunneling.
Particle in a three-dimensional box, rigid rotor, wave mechanics of systems with variable potential energy-simple harmonic oscillator.

UNIT-III **[12 Hours]**

Hydrogen atom-solution of R(r), θ (θ) and Φ (ϕ) equations-probability density in orbitals-shapes of orbitals.

Perturbation theory- time independent perturbation (only first order perturbation is to be dealt with)–application to ground state energy of hydrogen and helium atom.

UNIT –IV **[12 Hours]**

Variation principle-applications to hydrogen and helium atoms-calculation of zero-point energy of harmonic oscillator-many electron atom- Comparison between Perturbation and variation theorems.

Hartee-Fock self-consistent field method and introductory concepts of Density functional theory (DFT).

UNIT-V **[12 Hours]**

Valence bond approach-directed valence-hybridization-covalent bond-calculation of ionic and covalent bond contributions in hydrogen molecule.

Molecular orbital theory – LCAO approximation – hydrogen molecule ion – hydrogen molecule (fundamental concepts only) – The electronic transitions in the hydrogen molecule.

Text Books:

1. Introductory Quantum Chemistry, A.K. Chandra, 4th Edition, Tata McGraw Hill, New Delhi (2006).

2. Quantum Chemistry and Spectroscopy, M.S. Pathania, Vishal Publishing Co., New Delhi (1981).

3. Quantum Chemistry, H. Eyring, J. Walter and G. Kimball, John Wiely & Sons, New York, (1944)

4. Fundamentals of Quantum Chemistry, R. Anantharaman, Macmillan Publishers India Ltd.,

New Delhi (2000)

5. Quantum Chemistry, Ira N. Levine, 7th Edition, Pearson, New Delhi, (2013)4. Group Theory and its Applications to Chemistry, K. V. Raman, Tata McGraw – Hill Publishing Company Ltd., New Delhi.

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