

3128 807 TCU  
TJHO 320 30110 809

**PAPER-IV(C)**  
**QUANTUM MECHANICS AND**  
**PHOTOCHEMISTRY**

**Time: 3 Hrs.**

**M.M. 100**

**Note: The paper will be divided into THREE sections.**

**Section-A :** Ten questions (short type answer) two from each Unit will be asked. Each question will be of one mark and the candidates are required to attempt all questions. **Total 10 marks**

**Section-B :** Five questions (answer not exceeding 250 words) one from each Unit with internal choice will be asked and the candidates are required to attempt all questions. Each question will be of 10 marks. **Total 50 marks**

**Section-C :** Four questions may be in parts covering all the five Units (answer not exceeding 500 words) will be asked. The candidates are required to attempt any TWO questions. Each question will be of 20 marks. **Total 40 marks**

**UNIT-I**

Experimental foundation of quantum theory, mathematical techniques, postulates of quantum theory and consequences of the postulates, Heisenberg principle of uncertainty, angular momentum, eigen values.

Solution of the Schrodinger equation for some simple systems - Particle in a box, rigid rotator, harmonic oscillator and the hydrogen atom.

Approximate methods - Variation principle and perturbation theory, time dependent perturbations.

**UNIT-II**

Group theory and symmetry properties - Definition of group, symmetry operation and point groups, representation of group characters, reducible representation, relationship of group, group characters and reducible representation.

Huckel molecular orbital theory and its applications to organic chemistry-simple molecular orbital calculations, calculation of electron densities, bond order and free valence.

Ligand field theory of the free atom, the atom in complex, energy level diagrams, magnetic and spectral properties of complexes.

**UNIT-III**

Laws of photochemistry, units and dimensions, types of electronic transitions, charge transfer transitions, potential energy diagram, Franck-Condon principle, crossing of potential energy surfaces, geometry of some electronically excited molecules.

Types of photophysical pathways, radiation less transitions, internal conversion (IC) and intersystem crossing (ISC), fluorescence emission and structure, triplet states and phosphorescence emission, delayed fluorescence.

#### UNIT-IV

Stern-Volmer equation, excimer and excited state, quenching by added substances, charge transfer mechanism, quenching by oxygen, nitric oxide, paramagnetic metal ions and triplet energy states, intramolecular energy transfer, energy transfer processes in rare earth chelates and coordination compounds, fast multi step migration of excitation energy.

Classification of photochemical reactions, rate constants and lifetimes of reacting energy states, effect of light intensity on the rate of photochemical reaction, photofragmentation, isomerization and other rearrangement reactions.

#### UNIT-V

Light sources and their standardization, actinometry, chemical actinometry, measurement of emission characteristics, fluorescence, phosphorescence and chemiluminescence, techniques for study of transient species in photochemical reactions, laser and photochemical reactions.

Origin of life, mutagenic effects of radiation, photosynthesis, photoelectrochemistry of excited state redox reactions, solar energy conversion and storage.

#### Books Recommended :

1. Basic Quantum Chemistry by Leon, Wiley (1965)
2. Quantum Chemistry, R.K. Prasad

3. Photochemistry, J.G. Cavert and J.N. Pitts, Wiley (1966)
4. Molecular Photochemistry, N.J. Turro, Benjamin (1966)
5. Fundamentals of Photochemistry, K.K. Rohatgi-Mukherjee, New Age
6. Photochemistry, R.P. Wayne, Butterworth, (1970)
7. Quantum Chemistry, I. Levine