Bachelors with Chemistry as Major
7th Semester
Title of the course: Quantum Mechanics and Spectroscopy

Course Code: CHM722J2 **Credits:** Theory-4, Tutorials-2

Theory (4 credits: 60 Hours) **Max. Marks**: 100, **Min Marks:** 36

Course Objectives:

- To understand theorigin of quantum mechanics and strangeness in quantum mechanical formulation.
- To understand Schrodinger equation and apply the quantum mechanical formulation for evaluating someatomic and molecular properties.
- Understand basics of spectroscopy and its power to understand structure and reactivity of molecules.

Learning outcomes:

On completion of the course, the student should be able to:

- Appreciate the importance of transition from classical to quantum mechanics for understanding atomic/molecular world.
- Apply quantum mechanical formulations to simple systems so as to distinguish between the quantum results from the expected classical ones.
- Understand and interpret the rotational, vibrational and electronic spectra of simple molecules under the realm of quantum mechanics.

Unit I:Understanding genesis of quantum mechanics (15 hours)

Limitation of Classical mechanics: Wave-particle duality of radiation:Black-body radiation, Planck's radiation law, photoelectriceffect, heat capacity of solids and atomic spectra.
Quantum strangeness:Wave-particle duality of matter: outcomes of doublet slit experiment, Heisenberg's uncertainty principle and Copenhagen interpretation, Quantum mechanical paradoxes (Schrodinger's cat and Einstein's bubble thought experiments).
Time independentSchrodinger wave equationsand itsimportance, physicalinterpretation of the wave function, Postulates of quantum mechanics.

Unit II:Formalism and Applications of Quantum mechanics (15 hours)

Introduction to operators. Algebra & commutation ofoperators with numerical problems. Linear and Hermitian operators, Hamiltonian operator.Eigen functions & eigen values. Orthogonality & normalization of wave functions.
Particle in a one/three-dimensional box and rigid rotator; Harmonic oscillator and H-like atoms, radial and angular wave functions of H-like atom.

Unit- III:Molecular spectroscopy-I (15 hours)

***Spectroscopy*:**Introduction, electromagnetic radiation, regions of the spectrum, line width of the peaks and peak broadening,Statement of Born-Oppenheimer approximation.

***Rotational spectroscopy*:**Moment of inertia, classification of molecules on the basis of moment ofinertia. Energy of a rigid diatomic rotor, selection rules for rotational transition and associated

spectrum, relative population of rotational levels and spectral intensity, determination of bond length.

Vibrational Spectroscopy:Classical and quantum mechanical (qualitative) treatment of simpleharmonic oscillator, selection rules for vibrational transition, pure vibrational spectrum of a diatomic molecule, determination of force constant, relation of force constant with bond length and bond energy, vibrational degrees of freedom.Vibration-rotation spectroscopy: diatomic vibrating rotator, P, Q, R branches.

Unit-IV: Molecular spectroscopy-II (15 hours)

Raman spectroscopy: Classical and Quantum theories of Raman scattering, Molecular polarizability, rotational, vibrational Raman spectra. Selectionrules; rule of mutual exclusion. Applications.

Electronic Spectroscopy: Vibronic transitions. Intensity of spectra—the Franck-Condon principle. Different types of electronic transitions; nomenclature and labels of electronic states.

Books Recommended:

1. Physical Chemistry- A Molecular Approach - D. A. McQuarie& J. D. Simon, University Science Books, 1997.
2. Quantum Chemistry - Ira. N. Levine, 7th Edition, Pearson, 2009.
3. Principles of Physical Chemistry; B.R. Puri, L.R. Sharma and L.S. Pathania; 47th Edn.,Vishal Pubs & Co, 2017.
4. Quantum Chemistry, R. K. Prasad, 2nd Edition, New Age Publishers, 2001.
5. Fundamentals of Molecular Spectrsocopy; C.N.Banwell, E.M.Mc Cash; 4th edn; Tata McGrawHill; 1994.
6. Quantum Chemistry and Spectroscopy, 2018, by Thomas Engel, Philip Reid, Pearson Publications.
7. Physical Chemistry, 2017, by David W. Ball, Cengage India Private Limited, second Edition.

Tutorials (2 credits: 60 Hours) Max. Marks: 50, Min Marks: 18

1. Understanding genesis of quantum mechanics through online videos demonstrating the early development of quantum mechanics, outcomes of doublet slit experiment and the quantum paradoxes.
2. See the videos related to particle in a 1D and 3D boxes and solve some basis problems related to degeneracy, energy calculation, energy difference calculations and plot wave function in Microsoft excel for interpretation.
3. Problems related to calculation of Bond length and intensity of microwave transitions of diatomic molecules assuming them to be rigid rotators.
4. Problems related to calculation of bond strength and bond energy of the using the IR transitions for simple diatomic molecules.