Master of Science, Chemistry
M. Sc. Chemistry, Semester – II

Course Code	PS02CCHE51	Title of the Course	**Quantum Chemistry**
Total Credits of the Course	4	Hours per Week	4

Course Objectives:	1. The objective of this course is to introduce the students to Quantum Chemistry uses high-level mathematics as a tool to understand atomic and molecular structure and properties, as well as chemical reactivity. 2. This course covers fundamental principles and laws of chemistry. Topics include quantum mechanics, quantum numbers and chemical bonding. 3. This course is aimed to provide the students with a solid understanding of all the fundamental concepts and physical principles in modern inorganic chemistry necessary for the study of the more advanced or specialized courses that follow. The topics discussed include commutation relations, hydrogen like atoms, many electron systems.

Course Content		
Unit	Description	Weightage* (%)
1.	***Commutation relations***: Commutative property; momentum operator; Hamiltonian operator; angular momentum operator; angular momentum operators and their commutation relations; shift operators and their commutation relations; the effect of shift operators on an eigenvalue of the angular momentum; some theorems and problems. ***Translational motion of a particle:*** Free particle; particle in a box with infinite potential barrier; quantization and quantum numbers; symmetry of the wave functions; use of the box model; cubical box and degeneracy; quantum mechanical tunneling and problems	25%
2.	***Rotational motion of a particle:*** Particle on a sphere; normalization of the wave functions; rotation of a diatomic molecule and problems ***Vibrational motion of a particle:*** One dimensional harmonic oscillator; Hermite's differential equation; recursion formula for the Hermite's differential equation; normalization and the characteristic of eigenfunctions of a harmonic oscillator; polynomials of different degree and problems. ***The hydrogen like atoms:*** The r-dependent part of the wave function; Laguerre and associated Laguerre polynomials; radial eigenfunction for various system; total wave functions of hydrogen like atom.	25%
3.	***Approximation methods:*** Dirac notation; time independent perturbation theory for non-degenerate case; n^{th} -order perturbation energy; first order correction	

	to wavefunction; second order correction to energy of the eigenfunction; first order perturbation theory for a degenerate level; the variation theorem. ***Many-electron atoms & angular momenta:*** The wave functions of many electron systems; the He atom; many electron atoms; Hartree-self consistent field methods; angular momenta in many electron atoms; communication with Hamiltonian; spin-orbit Interaction ; energy states of atoms and term symbols; problems.	25%
4.	***Theory of chemical bonding:*** Born Oppenheimer approximation; molecular orbital theory; LCAO approximation; MO theory of bonding in hydrogen molecule ion and hydrogen molecule; Valance bond (VB) theory of bonding in hydrogen molecule ion and hydrogen molecule; LCAOMO treatment of diatomic molecule; VB treatment of diatomic molecule.	25%

Teaching-Learning Methodology	The course with Quantum Chemistry aims to make the students proficient in Inorganic chemistry through the transfer of knowledge in the classroom. This program is designed to encourage the learning strategies that could be incorporated in a comprehensive approach that includes self-directed learning, cooperative learning, and peer education. In the classroom, this will be done through blackboard and chalk lectures, charts, power point presentations, and the use of audiovisual resources that are available on the internet such as virtual lab. The process of effective learning to a great extent will be based on teacher's experiences, identifying the slow learners and individual attention of the teacher towards them. A variety of approaches to teaching learning process, including lectures, seminars, tutorials, peer teaching and learning, practicum and research establishments will be adopted. Problem-solving skills and higher-order skills of reasoning and analysis will be encouraged through teaching strategies. A feedback method with more anonymity will be preferred. An interactive mode of teaching will be used. The students will be encouraged to participate in the discussions and deliver seminars on the course related topics. A problem solving approach will be adopted wherever suitable.	

Evaluation Pattern		
Sr. No.	Details of the Evaluation	Weightage
1.	Internal Written / Practical Examination (As per CBCS R.6.8.3)	15%

2.	Internal Continuous Assessment in the form of Practical, Viva-voce, Quizzes, Seminars, Assignments, Attendance (As per CBCS R.6.8.3)	15%
3.	University Examination	70%

Course Outcomes: Having completed this course, the learner will be able to	
1.	Understand the commutative property and commutation relations of operators
2.	Understand the translational, rotational and vibrational motion of electron.
3.	Calculate the energy levels of electron in translational, rotational and vibrational motion in different dimension.
4	Determine the wave function of electron in translational, rotational and vibrational motion in different dimension.
5	Solve the Schrödinger equation for different model systems.
6	Solve the total wave functions of hydrogen like atom.
7	Understand the Approximation methods such as perturbation method and variation method
8	Determine the energy states of atoms and term symbols.
9	Describe the wave functions of many electron systems.
10	Understand the Born Oppenheimer approximation.
11	Explain the molecular orbital theory and valance bond (VB) theory of bonding in hydrogen molecule ion and hydrogen molecule.
12	Explain the LCAOMO and valance bond treatment of diatomic molecule
13	Determine molecular term symbol

Suggested References:	
Sr. No.	References

1	Introductory Quantum Chemistry, Fourth Edition, **By: A. K. Chandra** : Tata McGraw-Hill Publishing Company Ltd., New Delhi (1994)
2	Quantum Chemistry, **By: R. K. Prasad** : New Age International Publishers (1985)
3	Molecular Quantum Mechanics, **By: P. W. Atkins and R. S. Friedman,** Oxford University Press (1997)
4	An Introduction to Quantum Chemistry, **By: M. Satake, Y. Mido, H. Yasuhisa, S. Taguchi, M. S. Sethi & S. A. Iqbal** Discovery Publishing House New Delhi (1996)
5	Quantum Chemistry, **By: N.Levine**, Prentice Hall of India (p) Ltd. New Delhi (1994)
6	Quantum Chemistry through problem and solutions **By: R. K. Prasad**; New Age International Publishers (1997)

On-line resources to be used if available as reference material
On-line Resources
www.nptel.ac.in
www.swayam.gov.in
www.epgp.inflibnet.ac.in (e-PG pathshala)
www.ndl.iitkgp.ac.in (National Digital Library)

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