

KU5DSCCHE303: THEORETICAL CHEMISTRY-I

Semester	Course Type	Course Level	Course Code	Credits	Total Hours
V	DSC	300	KU5DSCCHE303	4	60

Learning Approach (Hours/ Week)		Marks Distribution			Duration of ESE (Hours)
Lecture/ Tutorial	Practical/ Internship	CE	ESE	Total	
4	0	30	70	100	2

Course Description: This course discovers the basic concepts of quantum mechanics and group theory. You can learn the history of groundbreaking experiments that led to the development of quantum mechanics. Understand why classical wave equations limitations have to capture the science of microscopic particles and how the Schrödinger equation brings a new perspective. Connect classical and quantum ideas and get comfortable with required mathematical tools for better insight into the concepts of quantum mechanics. Explore the rules governing quantum systems and see how symmetry matters in molecules using point group concepts.

Course Prerequisite: NIL

Course Outcomes:

CO No.	Expected Outcome	Learning Domains
1	To identify the fundamental experiments and theories that led to the development of quantum mechanics, also the limitations of classical models.	U
2	To understand and explain the core postulates of quantum mechanics, including the state function, operator, eigenvalue, and expectation value postulates, and describe their significance and application in solving quantum mechanical problems.	An

3	To apply the Schrödinger equations to various potential problems, such as the particle in a box, and compute quantized energy levels and corresponding wave functions	A
4	To combine knowledge of symmetry elements and operations to systematically identify and classify symmetry point groups of simple molecules, and predict the effects of symmetry on physical properties like dipole moments and optical activity	A

***Remember (R), Understand (U), Apply (A), Analyse (An), Evaluate (E), Create (C)**

Mapping of Course Outcomes to PSOs

	PSO 1	PSO 2	PSO 3	PSO 4	PSO 5	PSO 6	PSO 7
CO 1	3	3	3	2	2	1	0
CO 2	3	3	3	2	2	1	1
CO 3	3	3	3	2	2	1	0
CO 4	3	3	3	3	2	1	1

Course Contents for Classroom Transaction:

M O D U L E	U N I T	DESCRIPTION	HOURS
1	FUNDAMENTAL CONCEPTS IN QUANTUM MECHANICS		12
		Limitations of Bohr atom model –Development of quantum mechanics – Blackbody Radiation and Planck’s Formula	
		Einstein’s Photoelectric effect – Compton effect – de-Broglie hypothesis – Electron diffraction – Davison and Germer Experiment – Young’s double slit experiment – Stern- Gerlach Experiment – Heisenberg’s uncertainty Principle	

2	POSTULATES OF QUANTUM MECHANICS		12
	1	Postulate 1: (State function postulate): – Statement – Physical significance of wave function: Born interpretation of wave function – Ortho-normality of wave function – Well behaved functions – Conditions of well-behaved functions	
	2	Postulate 2 : (Operator postulate): – Statement – Observables and Operators – Examples of different operators: momentum operators, kinetic energy operators, potential energy operators, Hamiltonian operators, Hermitian operators	
	3	Postulate 3: (Eigen value postulate) Statement – Eigen values and eigen functions- Postulate 4 (Expectation value postulate):– Statement – Definition of expectation value – Physical interpretation – Application to operators – Schrödinger's cat paradox	

	4	Postulate 5: (Time-dependent Schrödinger): The classical wave equation – Time-independent Schrödinger wave equation – Deduction of Schrödinger equation from classical wave equation. Stationary waves and steady-state equation	
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	QUANTUM TRANSLATIONAL MOTION		8
3	1	Particle in a one-dimensional box with infinite potential walls – Boundary conditions – Normalized wave functions – Quantization of energies – Plotting energy levels, wave functions and probability densities	
	2	Application of particle in a box to simple conjugated aliphatic hydrocarbons (Free electron model)-Particle in a three-dimensional box – Boundary conditions, wave functions and energies – degeneracy and its connection with symmetry of the box	

	MOLECULAR SYMMETRY		16
4	1	Historical Sketch – Symmetry in everyday life - Symmetry elements and symmetry operations with examples: Identity operation, Symmetry planes and reflections, Proper axes and proper rotations, Improper axes and Improper rotations – Product of symmetry operations – General relation between symmetry operations	
	2	Complete set of symmetry operations of a molecule – Symmetry point groups – Schoenflies notation – GMT of some simple molecules (H ₂ O ₂ , H ₂ O, NH ₃)-Classes of symmetry operations – Systematic identification of point groups (C _n , C _i , C _s , C _{nv} , C _{nh} , D _{nh} only) -Point groups of simple molecules – H ₂ O ₂ , H ₂ O, NH ₃ , N ₂ O ₄ , N ₂ F ₂ , BF ₃	
5	TEACHER SPECIFIC MODULE <i>Directions: Mathematical tools for quantum chemistry & group theory or any other topic relevant to the course</i>		12

1	Complex Numbers – Complex functions – Odd and even functions	
2	Coordinate system: Cartesian and spherical polar coordinates and their relationships. – Basics of differentiation and integration – Solution of a second order ODE – Power series solution of differential equation	
3	Probability: average, variance and standard deviation– Elements of operator algebra: definition – Linear and non-linear operators – Commutator of two operators - Commuting and non-commuting operators – Vector operators – Laplacian operators and their expressions in cartesian and spherical polar coordinates	
4	Matrices and determinants: matrix algebra – character of a square matrix – diagonal matrix, orthogonal and unitary matrices – direct product and direct sum of square matrices – block factored matrices	

Essential Readings:

1. D. A. McQuarrie, “Quantum Chemistry”, University Science Books, 1983 (Viva books, 2003).
2. A.K. Chandra, “Introduction to Quantum Chemistry”, 4th Edition, Tata McGraw-Hill, 1994.
3. I.N. Levine, Quantum Chemistry, 6th Edition, Pearson Education Inc., 2009
4. F.A. Cotton, “Chemical applications of Group Theory”, 3rd Edition, John Wiley & Sons Inc., 2003
5. Arthur M Lesk, “Introduction to Symmetry & Group theory for Chemists”, Kluwer Academic Publishers, 2004
6. Robert L. Carter, ‘Molecular Symmetry and Group Theory’, Wiley India Edition, 2005

Assessment Rubrics:

Evaluation Type		Marks
End Semester Evaluation		70
Continuous Evaluation		30
a)	Test Paper*	12
b)	Assignment	6
c)	Seminar	6
d)	Viva-voce	6
Total		100

***Average mark of the best two written tests may be considered for internal mark.**