

UNIVERSITY OF MADRAS
M.Sc. DEGREE PROGRAMME IN CHEMISTRY
 SYLLABUS WITH EFFECT FROM 2023-2024

Title of the Course	PHYSICAL CHEMISTRY-II						
Paper No.	Core XI						
Category	Core	Year	II	Credits	4	Course Code	524C4B
		Semester	IV				
Instructional hours per week	Lecture	Tutorial	Lab Practice		Total		
	4	1	-		5		
Prerequisites	Basic knowledge of physical chemistry						
Objectives of the course	<p>To understand the essential characteristics of wave functions and need for the quantum mechanics.</p> <p>To know the importance of quantum mechanical models of particle in a box, rigid rotor and harmonic oscillator.</p> <p>To apply the quantum mechanics to hydrogen and polyelectronic systems.</p> <p>To familiarize the symmetry in molecules and predict the point groups.</p> <p>To predict the vibrational modes, hybridization using the concepts of group theory.</p>						
Course Outline	<p>UNIT-I: Wave particle duality, Uncertainty principle, Particle wave and Schrodinger wave equation, wave function, properties of wave function. Properties of wave function, Normalized, Orthogonal, orthonormal, Eigen values, Eigen functions, Hermitian properties of operators. Introduction to quantum mechanics-black body radiation, photoelectric effect, hydrogen spectrum. Need for quantum mechanics, Postulates of Quantum Mechanics, Schrodinger wave equation, Time independent and time dependent</p>						
	<p>UNIT-II: Quantum models: Particle in a box-1D, two dimensional and three-dimensional, degeneracy, application to linear conjugated molecular system, free particles, ring systems. Harmonic Oscillator-wave equation and solution, anharmonicity, force constant and its significance. Rigid Rotor-wave equation and solution, calculation of rotational constants and bond length of diatomic molecules.</p>						
	<p>UNIT-III: Applications to Hydrogen and Poly electron atoms: Hydrogen atom and hydrogen like ions, Hamiltonian-wave equation and solutions, radial and angular functions, representation of radial distribution functions. Approximation methods –variation methods: trial wave function, variation integral and application to particle in 1D box. Perturbation method - first order applications. Hartree-Fock self-consistent field method, Hohenberg-Kohn theorem and Kohn-Sham equation, Helium atom-electron spin, Pauli exclusion principle and Slater determination.</p>						
	<p>UNIT-IV: Group theory: Groups, sub groups, symmetry elements, operations, classification-axial and non-axial. Dihedral point groups- C_n, C_{nh}, D_n, D_{nh}, D_{nd}, T_d and O_h. Matrix representation and classes of symmetry operations, reducible irreducible and direct product representation. The Great orthogonality theorem – irreducible representation and reduction formula, construction of character table for C_{2v}, C_{2h}, C_{3v} and D_{2h} point groups.</p>						

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	UNIT-V: Applications of quantum and group theory: Hydrogen Molecule-Molecular orbital theory and Heitler London (VB) treatment, Energy level diagram, Hydrogen molecule ion; Use of linear variation function and LCAO methods. Electronic conjugated system:Huckel method to Ethylene butadiene, cyclopropenyl, cyclo butadiene and Benzene. Applications of group theory to molecular vibrations, electronic spectra of ethylene.
Extended Professional Component (is a part of internal component only, Not to be included in the external examination question paper)	Questions related to the above topics, from various competitive examinations UPSC / TRB / NET/ UGC-CSIR / GATE /TNPSC others to be solved (To be discussed during the Tutorial hours)
Skills acquired from this course	Knowledge, Problem solving, Analytical ability, Professional Competency, Professional Communication and Transferable skills.
Recommended Text	<ol style="list-style-type: none"> 1. R.K. Prasad, Quantum Chemistry, New Age International Publishers, New Delhi, 2010, 4th revised edition. 2. F. A. Cotton, Chemical Applications of Group Theory, John Wiley & Sons, 2003, 2nd edition. 3. A. Vincent, Molecular Symmetry and Group Theory. A Programmed Introduction to Chemical Applications, John and Willy & Sons Ltd., 2013, 2nd Edition. 4. T. Engel & Philip Reid, Quantum Chemistry and Spectroscopy, Pearson, New Delhi, 2018, 4th edition. 5. G. K. Vemulapalli, Physical Chemistry, Prentice Hall of India Pvt. Ltd. 2001. 6. D.A. McQuarrie, Quantum Chemistry, Viva Books PW. Ltd, 2013, 2nd edition.
Reference Books	<ol style="list-style-type: none"> 1. N. Levine, Quantum Chemistry, Allyn& Bacon Inc, 1983, 4th edition. 2. D.A. McQuarrie and J. D. Simon, Physical Chemistry, A Molecular Approach, Viva Books Pvt. Ltd, New Delhi, 2012. 3. R. P. Rastogi & V. K. Srivastava, An Introduction to Quantum Mechanics of Chemical Systems, Oxford & IBH Publishing Co., New Delhi, 1999. 4. R.L. Flurry. Jr, Symmetry Group Theory and Chemical applications, Prentice Hall. Inc, 1980 5. J. M. Hollas, Symmetry in Molecules, Chapman and Hall, London, 2011, Reprint.
Website and e-learning source	<ol style="list-style-type: none"> 1. https://nptel.ac.in/courses/104101124 2. https://ipc.iisc.ac.in/~kls/teaching.html

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Course Learning Outcomes (for Mapping with POs and PSOs)

Students will be able:

CO1: To discuss the characteristics of wave functions and symmetry functions.

CO2: To classify the symmetry operation and wave equations.

CO3: To apply the concept of quantum mechanics and group theory to predict the electronic structure.

CO4: To specify the appropriate irreducible representations for theoretical applications.

CO5: To develop skills in evaluating the energies of molecular spectra.

CO-PO Mapping (Course Articulation Matrix)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO 1	S	S	S	S	M	S	S	S	S	M
CO 2	M	S	S	S	S	M	S	S	S	S
CO 3	S	S	M	S	S	S	S	M	S	S
CO 4	M	S	S	S	S	M	S	S	S	S
CO 5	M	S	M	S	S	M	S	M	S	S

3 – Strong, 2 – Medium, 1 - Low

Level of Correlation between PSO's and CO's

CO /PO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	3	3	3	3	3
CO2	3	3	3	3	3
CO3	3	3	3	3	3
CO4	3	3	3	3	3
CO5	3	3	3	3	3
Weightage	15	15	15	15	15
Weighted percentage of Course Contribution to POs	3.0	3.0	3.0	3.0	3.0

3 – Strong, 2 – Medium, 1 - Low