



**University of Kerala**

Discipline	CHEMISTRY				
Course Code	UK5DSCCHE302				
Course Title	PHYSICAL CHEMISTRY II				
Type of Course	DSC				
Semester	5				
Academic Level	300 - 399				
Course Details	Credit	Lecture per week	Tutorial per week	Practical per week	Total Hours/Week
	4	4 hours	-	-	4
Pre-requisites	<p>1. Essential conditions for understanding quantum mechanics, spectroscopy, statistical thermodynamics and group theory include a strong grasp of fundamental principles such as wave-particle duality, electromagnetic radiation interactions, statistical ensembles and symmetry operations.</p> <p>2. Proficiency in mathematical techniques, experimental methodologies, data interpretation, and their applications in various scientific disciplines is crucial for mastering these subjects.</p>				
Course Summary	<p>This course provides a comprehensive understanding of Quantum Mechanics, delving into wave-particle duality, Schrödinger's equation, and energy quantization. Spectroscopy techniques, including rotational spectroscopy, vibrational spectroscopy, electronic spectroscopy, Raman NMR and ESR, are explored for molecular analysis and structural elucidation. Additionally, students study Statistical Thermodynamics and Group Theory for molecular symmetry analysis.</p>				

**Detailed Syllabus:**

Module	Unit	Content	Hrs
I	<b>QUANTUM MECHANICS</b>		<b>12</b>
	1	Failures of Classical mechanics and need for quantum mechanics- Blackbody radiation phenomenon- ultraviolet catastrophe. Formulation of quantum mechanics: The wave nature of sub-atomic particles. de Broglie relation and its experimental proof. The uncertainty principle and its consequences. Time dependent and time independent Schrodinger wave equation for an electron and its significance The postulates of quantum mechanics. Concept of operators: Laplacian, Hamiltonian, linear and Hermitian operators.	5
	2	Eigen function and eigen values. Physical interpretation of wave function. Boundary conditions and well-behaved functions.	4

		Applications of quantum mechanics to simple systems: Solutions of Schrodinger wave equations for a particle in 1D box and particle in 3D box. Harmonic oscillator (No Derivation).	
	3	Atomic Spectra: Space quantization. Spin of electron. Spin orbit coupling. The exclusion principle.	3
<b>II</b>	<b>SPECTROSCOPY I</b>		<b>12</b>
	4	Interaction of electromagnetic radiation with molecules and various types of spectra; Born Oppenheimer approximation. Rotation spectroscopy: Selection rules, intensities of spectral lines, determination of bond lengths of diatomic and linear triatomic molecules, isotopic substitution.	4
	5	Vibrational spectroscopy: Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degrees of freedom for polyatomic molecules, modes of vibration. Vibration-rotation spectroscopy: diatomic vibrating rotator, P, Q, R branches	4
	6	Raman spectroscopy: Quantum theory of Raman effect, Rotational Raman spectrum, Vibrational Raman spectra, Stokes and anti-Stokes lines; their intensity difference, rule of mutual exclusion.	4
<b>III</b>	<b>SPECTROSCOPY II</b>		<b>12</b>
	7	Electronic spectroscopy: Franck-Condon principle, electronic transitions, singlet and triplet states, fluorescence and phosphorescence, dissociation and predissociation.	3
	8	NMR spectroscopy: Principle of NMR, nuclear spin. HNMR, Interaction of nuclear spin with external magnet. Energy level splitting, Precession.	2
	9	Chemical shift. Delta and tau scales. Presentation of NMR spectra, Low and high-resolution spectra of simple molecules like ethanol, 2-chloropropane etc, Spin-spin coupling	2
	10	Electron spin resonance spectroscopy: Principle, Types of substances with unpaired electrons, interaction of electron magnet with external magnet.	2
	11	Energy level splitting. Lande splitting factor, presentation of ESR spectrum, the normal and derivative spectra. Hyperfine splitting. Simple examples of methyl and benzene radicals	3
<b>IV</b>	<b>BINARY LIQUID SYSTEMS &amp; ADSORPTION</b>		<b>12</b>
	12	Liquid-Liquid system: ideal and non-ideal mixtures, Raoult's law, deviations from Raoult's law, vapour pressure - composition, temperature-composition curves, fractional distillation, Azeotropic mixtures.	3
	13	Partially miscible liquid system, critical solution temperature, examples for upper, lower and upper cum lower CST	2

	14	Distribution law, its thermodynamic derivation, Application of distribution law to the study of association and dissociation of molecules	2
	15	Adsorption: Physical and chemical adsorption, Freundlich adsorption isotherm, Derivation of Langmuir adsorption isotherm, Statement and explanation of BET and Gibbs isotherms	3
	16	Determination of surface area of adsorbents by BET equation. Applications of adsorption.	2
<b>V</b>	<b>OPEN ENDED MODULE: Learning through problem solving, seminars, open discussions on real life applications, assignment discussions, Quizzes, Open book exams, etc on the above four modules.</b>		<b>12</b>

**References:**

1. Ira N. Levine, *Quantum Chemistry*, Delhi: PHI Learning, 2014.
2. R L Madan, *Quantum Mechanics and Analytical Techniques*, NEP 2020 Uttar Pradesh Latest Edition 2023 By S. Chand's.
3. *A Text book of Quantum Mechanics*, PM Mathews & K Venkatesan, 2nded, Tata McGraw Hill, (2011).
4. *Introduction to Quantum Mechanics*, David Griffiths, 2<sup>nd</sup>ed., Pearson, (2015).
5. C.N. Banwell, *Fundamentals of Molecular Spectroscopy*, Tata McGraw-Hill Education.
6. Manas Chanda, “*Atomic structure and Chemical bonding in Molecular Spectroscopy*”, Tata McGraw Hill.
7. B. R Puri, L. R Sharma, M. S. Pathania, *Principles of Physical Chemistry*, Vishal Publishing Company.

**Course Outcomes**

No.	Upon completion of the course the graduate will be able to	Cognitive Level	PSO addressed
CO-1	Analyze the fundamental principles and mathematical framework of quantum mechanics to interpret the behavior of subatomic particles, solve simple quantum systems, and explain atomic spectral phenomena and electron properties.	An	PSO-1,2,3
CO-2	Evaluate molecular structure, bonding, and vibrational characteristics by interpreting rotational, vibrational, vibration–rotation, and Raman spectra using the principles of molecular spectroscopy and quantum mechanics.	E	PSO-1,2,3
CO-3	Construct and justify molecular and radical structures	C	PSO-

	by integrating information obtained from electronic, NMR, and ESR spectra and applying the underlying principles of spectroscopic transitions and spin interactions.		1,2,3,5
CO-4	Analyze phase behavior, molecular distribution, and adsorption phenomena by correlating thermodynamic principles, equilibrium laws, and adsorption isotherms with their practical applications.	An	PSO-1,2,3,5
CO-5	Design and communicate innovative solutions to scientific problems by integrating concepts from the course through problem-solving, seminars, discussions, assignments, and reflective evaluation of real-life applications.	C	PSO-1,2,3,4,5

**R-Remember, U-Understand, Ap-Apply, An-Analyse, E-Evaluate, C-Create**

**Name of the Course: PHYSICAL CHEMISTRY II**

**Credits: 4:0:0 (Lecture:Tutorial:Practical)**

CO No.	CO	PO/ PSO	Cognitive Level	Knowledge Category	Lecture (L)/ Tutorial (T)	Practical (P)
1	CO-1	PO-1,6 PSO-1,2,3	An	F, C	L	-
2	CO-2	PO-1,2,3,6 PSO-1,2,3	E	C, P	L	-
3	CO-3	PO-1,2,3,6 PSO-1,2,3,5	C	C, P	L	-
4	CO-4	PO-1,2,3,6 PSO-1,2,3,5	An	C, P	L	-
5	CO-5	PO-1,2,3,4,5,6 PSO-1,2,3,4,5	C	M	L	-

**F-Factual, C- Conceptual, P-Procedural, M-Metacognitive**

**Mapping of COs with PSOs and POs:**

	PSO 1	PSO 2	PSO 3	PSO 4	PSO 5	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO 1	3	3	3	-	-	2	-	-	-	-	3	-	-
CO 2	3	3	3	-	-	3	2	2	-	-	3	-	-
CO 3	3	3	3	-	2	3	2	2	-	-	2	-	-
CO 4	3	3	3	-	2	3	2	2	-	-	2	-	-
CO 5	2	2	3	2	3	3	3	3	2	2	3	-	-

**Correlation Levels:**

Level	Correlation
-	Nil
1	Slightly / Low
2	Moderate / Medium
3	Substantial / High

**Assessment Rubrics:**

- Quiz / Assignment/ Quiz/ Discussion / Seminar
- Midterm Exam
- Programming Assignments
- Final Exam

**Mapping of COs to Assessment Rubrics:**

	Internal Exam	Assignment	Project Evaluation	End Semester Examinations
CO 1	✓	✓		✓
CO 2	✓	✓		✓
CO 3	✓		✓	✓
CO 4	✓		✓	✓
CO 5	✓	✓	✓	