Lecture Plan

Name of the college: Government College of Arts, Science and Commerce, Sanquelim- Goa

Name of Faculty: Dr. Amarja Prashant Naik	**Subject: Chemistry**	
Paper code: CHC-105 Physical Chemistry	**Program: TY BSc**	**Division: NA**
Academic year: 2024- 2025	**Semester: V**	**Total Lectures: 30**

Course Objectives:

- To study the mathematical concepts (integration, derivation, exponential trigonometric function.)
- To study optical activity, polarization, dipole moment and methods of determination of dipole moments and structure of molecules.
- To define the principles, hypothesis, postulates of quantum mechanics in Quantum chemistry.
- To apply the basic mathematical concepts in quantum chemistry.
- To draw the wave functions, orbital diagrams and the graphs involved.
- To solve the numerical, explain and interpret the wave functions.
- To study the electromagnetic spectrum, terms, principles involved.
- To study Rotational spectra of diatomic molecules, determination of bond lengths and qualitative description

Expected Course Outcome:

At the end of the course students will be able to

- Define the terms involved in Quantum chemistry, electrochemistry, and molecular structure.
- State the laws, principles of quantum chemistry, molecular structure and nuclear chemistry. postulates of quantum mechanics

Student Learning Outcome:

- Able to apply the knowledge of quantum chemistry in solving problems.
- Able to determine bond length, moment of inertia.
- Distinguish between rotational, vibrational spectroscopy.

Month	Lecture From	Lecture To	No. of lectures allotted	Topic, Subtopic to be covered	Exercise/ Assignment	ICT Tools	Reference books
June	28/06/2024	29/06/2024	02	Mathematical Concepts: Derivatives and integrations, trigonometric functions, exponential functions	Exercise	Google Classroom	1. Gurdeep Raj, Advanced Physical Chemistry Goel Publication 2. Barnwell, C. N. & McCash, E.M., Fundamentals of Molecular Spectroscopy, 4th Ed. 3. Puri Sharma and Pathania Principles of Chemistry Vishal Publication
				Second derivatives of the functions	Exercise	Google Classroom	
July	01/07/2024	06/07/2024	02	De-Broglie hypothesis,	Exercise	Google Classroom	
				Heisenberg Uncertainty principle	Exercise	Google Classroom	
	08/07/2024	13/07/2024	02	Sinusoidal wave function	Exercise	Google Classroom	
				Terms involved in Quantum mechanics: Normalisation, orthogonality, observables, operators, stationary states, and variables.	Exercise	Google Classroom	

		15/07/2024	20/07/2024	02	Schrodinger equation and its application to free particle and particle in a box	Exercise	Google Classroom
					Quantisation of energy levels,	Exercise	Google Classroom
		22/07/2024	31/07/2024	02	Zero – point energy	Exercise	Google Classroom
					Schrodinger equation in Cartesian and spherical polar	Exercise	Google Classroom
						Exercise	Google Classroom
	August	1/08/2024	3/02/2024	02	Extension to two- and three-dimensional boxes, separation of variables	Exercise	Google Classroom
					Degeneracy. Operators (Hermitian, non-Hermitian), eigen value and eigen functions,	Exercise	Google Classroom
		5/08/2024	10/08/2024	02	Physical significance of wave function, examples of operators, Hamiltonian operators	Exercise	Google Classroom
					Quantum mechanical operators and commutation rules	Exercise	Google Classroom
		12/08/2024	17/08/2024	02	Postulates of quantum mechanics, wave functions	Exercise	Google Classroom
					Probability distribution functions, nodal properties.	Exercise	Google Classroom

4. H. Kaur spectroscopy Pragati edition

	19/08/2024	24/08/2024	02	Interaction of electromagnetic radiation with molecules and various types of spectra, Born Oppenheimer approximation.	Exercise	Google Classroom
				Rotational Spectroscopy: selection rules, intensities of spectral lines	Exercise	Google Classroom
	26/08/2024	31/08/2024	02	Determination of bond lengths of diatomic and linear triatomic molecules	Exercise	Google Classroom
				Isotopic substitution and introduction to Vibrational spectroscopy:	Exercise	Google Classroom
				Classical equation of vibration, computation of force constant,	Exercise	Google Classroom
September	2/09/2024	7/09/2024	02	Amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies	Exercise	Google Classroom
				Fundamental frequencies, overtones, hot bands, degree of freedom for polyatomic molecules	Exercise	Google Classroom
	16/09/2024	21/09/2024	02	Modes of vibration, concept of group frequencies.	Exercise	Google Classroom

					Vibration –rotation spectroscopy: Diatomic vibrating rotator	Exercise	Google Classroom	
		16/09/2024	21/09/2024	02	P, Q, R branches Raman spectroscopy	Exercise	Google Classroom	
					Qualitative treatment of Rotational Raman effect	Exercise	Google Classroom	
		23/09/2024	30/09/2024	02	Vibrational Raman spectra	Exercise	Google Classroom	
					Introduction to Raman effect	Exercise	Google Classroom	
	October	1/10/2024	5/10/2024	02	Stokes and Anti-stokes lines	Exercise	Google Classroom	
					Intensity difference of Raman effect, stokes and antistokes lines	Exercise	Google Classroom	
		7/10/2024	12/10/2024	02	Quantum theory of Raman effect	Exercise	Google Classroom	
					Classical theory of Raman effect			
		14/10/2024	22/10/2024	02	Rule of mutual Exclusion principle.	Exercise	Google Classroom	
					Examples of Rule of mutual Exclusion principle.	Exercise	Google Classroom	

***Assessment Rubrics**

Component	Max Marks
ISA 1	10
ISA 2	10
Practical	50
Project	---
Semester End Exam	80