22CHP207N

PSG COLLEGE OF ARTS & SCIENCE
(AUTONOMOUS)

MSc DEGREE EXAMINATION DECEMBER 2025
(Second Semester).

Branch – **CHEMISTRY**

QUANTUM MECHANICS AND GROUP THEORY

Time: Three Hours

Maximum: 75 Marks

SECTION-A (10 Marks)
Answer **ALL** questions
ALL questions carry **EQUAL** marks (10 × 1 = 10)

Module No.	Question No.	Question	K Level	CO
1	1	The term ψ^2 represents (a) Electron density (b) Electron momentum (c) Radial function (d) Radial density	K1	CO1
	2	The linear operator, among the following set of operators d / dx; $\sqrt{}$; $\int dx$ (a) d / dx (b) $\int dx$ (c) $\sqrt{}$ (d) Both d / dx and $\int dx$	K2	CO1
2	3	The degeneracy of energy level $14h^2 / 8ml^2$ of a particle in a cubical box is (a) 4 (b) 6 (c) 8 (d) 10	K1	CO2
	4	In a diatomic rigid rotor, the internuclear distance between two atoms is (a) a variable (b) zero (c) infinite (d) a constant	K2	CO2
3	5	A perturbation $H^{\wedge} = V_0 (3\cos^2\Phi - 1)$, where V_0 is a constant, is applied to a rigid rotator undergoing a rotational motion in a plane. The first order energy correction to the ground state is (a) 2 V_0 (b) $V_0 / 4$ (c) $V_0 / 2$ (d) V_0	K1	CO3
	6	The effective nuclear charge of the helium atom using variation theorem is (a) 17/16 (b) 7/16 (c) 17/6 (d) 27/16	K2	CO3
4	7	The number of symmetry elements for a tetrahedral molecule is (a) 13 (b) 15 (c) 20 (d) 24	K1	CO4
	8	Total number of irreducible representation in a group is equal to (a) order (b) class (c) subgroup (d) elements	K2	CO4
5	9	The main constituents of the acid rain are (a) Oxides of nitrogen and hydrogen (b) Oxides of sulphur and phosphorus (c) Oxides of carbon and nitrogen (d) Oxides of sulphur and nitrogen	K1	CO5
	10	Pesticides cause (a) Noise pollution (b) Air pollution (c) Aquatic pollution (d) None of these	K2	CO5

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SECTION - B (35 Marks)

Answer **ALL** questions

ALL questions carry **EQUAL** Marks (5 × 7 = 35)

Module No.	Question No.	Question	K Level	CO
1	11.a.	State and explain the postulates of quantum mechanics.	K3	CO1
		(OR)		
	11.b.	Explain with suitable examples: (i) Eigen functions and Eigen values. (ii) Linear operators.		
2	12.a.	Derive an expression for Eigen function and Eigen value of a simple harmonic oscillator using the Schrodinger wave equation.	K4	CO2
		(OR)		
	12.b.	Write a note on: (i) Zero point energy (ii) Tunnelling.		
3	13.a.	Write a Slater determinant for n – electron atoms.	K3	CO3
		(OR)		
	13.b.	Give an account on Born – Oppenheimer approximation.		
4	14.a.	Describe in detail about symmetry elements and symmetry operations.	K4	CO4
		(OR)		
	14.b.	(i) Construct the character table for C_{3v} point group. (ii) What is meant by isomorphism?		
5	15.a.	Find the symmetry of the vibrational modes of the NH_3 molecule.	K5	CO5
		(OR)		
	15.b.	Describe the symmetry selection rule for IR and Raman spectra.		

SECTION –C (30 Marks)

Answer **ANY THREE** questions

ALL questions carry **EQUAL** Marks (3 × 10 = 30)

Module No.	Question No.	Question	K Level	CO
1	16	Derive the time independent Schrodinger wave equation and mention its application.	K4	CO1
2	17	Solve the Schrodinger wave equation for particle in a three dimensional box.	K4	CO2
3	18	Discuss the application of first order perturbation theory to helium atom.	K5	CO3
4	19	Explain the following: (i) Similarity transformation (ii) Abelian group (iii) Great orthogonality theorem.	K4	CO4
5	20	Determine the hybrid orbitals for H_2O and BF_3 molecules.	K5	CO5

Z-Z-Z END