PSG COLLEGE OF ARTS & SCIENCE
(AUTONOMOUS)

MSc DEGREE EXAMINATION MAY 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.	Questions	K level	CO
1	1.	The product of two wave functions of a particle in 1D-box, say $\psi(n=1)$ and $\psi(n=2)$, is a) one b) zero c) infinity d) always a fraction	K1	CO1
	2.	One of the following is not a linear operator. a) Taking square root b) d/dx c) d^2/dx^2 d) $\int dx$	K2	CO1
2	3.	The energy expression for the rigid rotator is given by a) $E_J = (\hbar^2/2I)\ J(J+1)$ b) $E_J = (2I/\hbar^2)\ J(J+1)$ c) $E_J = J(J+1)/2I\ \hbar^2$ d) $E_J = (2I\hbar^2)\ /\ J(J+1)$	K1	CO2
	4.	The energy difference (ΔE) between any two consecutive energy levels of a particle in a 1-D box is a) $2h^2/8mL^2$ b) $(2n+1)h^2/8mL$ c) $h^2/8mL^2$ d) $(3n+1)h^2/8mL^2$	K2	CO2
3	5.	In the perturbation method, which of the following terms is neglected in the Hamiltonian operator? a) total kinetic energy b) The nuclear–electronic attraction c) electronic – electronic repulsion d) electronic – nuclear repulsion	K2	CO3
	6.	According to the Born-Oppenheimer approximation, the nuclear wave function ψ_n is given by a) $E_e\psi_n = E\psi_n$ b) $\hat{H}_n\ \psi_n = E\psi_n$ c) $(\hat{H}_n + E_e)\ \psi_n = E\psi_n$ d) $\Psi = \psi_e\psi_n$	K1	CO3
4	7.	The character of (3×3) matrix representation of $C_2(z)$ rotational operation is a) 3 b) 1 c) -1 d) zero	K1	CO4
	8.	The point group of the Cl_2 molecule is a) $C_{\infty}v$ b) $C_{2}v$ c) $D_{\infty h}$ d) C_i	K2	CO4
5	9.	How many infrared (IR) signals can be obtained for an ammonias molecule? a) One b) Two c) Three d) Four	K2	CO5
	10.	The irreducible representations representing out-of-plane deformation vibration modes of $[PtCl_4]^{2-}$ is a) $A_{2u} + B_{2u}$ b) $2\ B_{2u}$ c) $E_g + B_{2u}$ d) $2\ A_{2u}$	K2	CO5

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.	(i) Distinguish between ψ and ψ^2 (ii) What is the probability of finding the particle in a region of volume 3 pm^3 having a probability density of 0.2 pm^{-3}?	K4	CO1
		(OR)		
	11.b.	(i) Distinguish between matter waves and electromagnetic waves. (ii) Show that operators, AB≠BA for a function f(x), If operator A= d/dx and operator B=x^2.		

Cont...

2	12.a.	Solve the Schrodinger wave equation of particle in a 1D box to obtain the normalized wavefunction and energy equation.	K5	CO2
		(OR)		
	12.b.	Obtain the solutions for the Schrodinger wave equation of a rigid rotator.		
3	13.a.	Determine the ground state energy of the He atom using first-order perturbation theory.	K5	CO3
		(OR)		
	13.b.	Explain Pauli's antisymmetric principle by taking H_2 as an example.		
4	14.a.	Answer the following questions from the irreducible character table of the D_{3h} point group D_{3h} | E | $2C_3$ | $2C_2$ | σ_h | $2S_3$ | $3\sigma_v$ | | A_1' | 1 | 1 | 1 | 1 | 1 | 1 | | x^2+y^2, z^2 A_2' | 1 | 1 | −1 | 1 | 1 | −1 | R_z | E' | 2 | −1 | 0 | 2 | −1 | 0 | (x,y) | (x^2-y^2, xy) A_1'' | 1 | 1 | 1 | −1 | −1 | −1 | | A_2'' | 1 | 1 | −1 | −1 | −1 | 1 | z | E'' | 2 | −1 | 0 | −2 | 1 | 0 | (R_x, R_y) | (xz, yz) (i) Number of mutually conjugated classes (ii) Order of the group (iii) Number of irreducible representations (iv) S_3^3 =? (v) $A_2' \times A_1''$ = (vi) Is D_{3h} an abelian group?	K4	CO4
		(OR)		
	14.b.	(i)Distinguish between an abelian and a non-abelian group (ii)Direct product of E^2, in the C_{3v} point group Show that "$S_2 = i$" in the C_{2h} point group.		
5	15.a.	Obtain the irreducible representations representing vibrational modes of the water molecule.	K6	CO5
		(OR)		
	15.b.	Discuss how group theory predicts sp^2 hybridization is present in BF_3 molecule. D_{3h} | E | $2C_3$ | $2C_2$ | σ_h | $2S_3$ | $3\sigma_v$ | | A_1' | 1 | 1 | 1 | 1 | 1 | 1 | | x^2+y^2, z^2 A_2' | 1 | 1 | −1 | 1 | 1 | −1 | R_z | E' | 2 | −1 | 0 | 2 | −1 | 0 | (x,y) | (x^2-y^2, xy) A_1'' | 1 | 1 | 1 | −1 | −1 | −1 | | A_2'' | 1 | 1 | −1 | −1 | −1 | 1 | z | E'' | 2 | −1 | 0 | −2 | 1 | 0 | (R_x, R_y) | (xz, yz)		

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	Discuss the postulates of quantum mechanics.	K6	CO1
2	17	Set up the Schrodinger wave equation for the hydrogen atom. Determine solution for the ground-state wavefunction and Energy expression of hydrogen atom.	K5	CO2
3	18	Obtain the delocalization energy of a butadiene molecule using Huckel's Molecular Orbital Theory.	K5	CO3
4	19	(i)Decompose the given reducible representation of C_{3v} point group into its irreducible representations. C_{3v} | E | $C_3(z)$ | $3\sigma_v$ Γ_{red} | 15 | 0 | 3 (ii)Construct the irreducible character table for the C_{3v} point group using the Great Orthogonality Theorem.	K5	CO4
5	20	How does group theory predict the number of IR and Raman signals for $POCl_3$ molecule? Explain.	K4	CO5

Z-Z-Z END