MSc DEGREE EXAMINATION MAY 2026

(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	What is the fundamental concept of wave-particle dualism? i) Particles can only be waves ii) Waves can only be particles iii) Particles can exhibit both wave-like and particle-like behavior iv) Waves can only exhibit particle-like behavior	K1	CO1
	2	Explain the significance of orthonormal wave functions. i) They are not orthogonal ii) They are not normalized iii) They are both orthogonal and normalized iv) They are only orthogonal	K2	CO1
2	3	What is the ground state energy of a hydrogen atom? i) -13.6 eV ii) -3.4 eV iii) 0 eV iv) 13.6 eV	K1	CO2
	4	Which is not a characteristics of a rigid rorator? i) diatomic ii) fixed bond length iii) centrifugal distortion iv) equally spaced energy levels	K2	CO2
3	5	Name the approximation method used for calculating energy levels in a helium atom using a trial wave function. i) Perturbation theory ii) Variation method iii) LCAO-MO method iv) Born-Oppenheimer approximation	K1	CO3
	6	Explain the concept of electron spin and its relation to the Pauli exclusion principle. i) Electron spin leads to symmetric wave functions ii) Electron spin leads to antisymmetric wave functions iii) Electron spin has no relation to Pauli principle iv) Electron spin determines energy levels directly	K2	CO3
4	7	Find the number of symmetry operations in C_{2v} point group. i) 2 ii) 4 iii) 6 iv) 8	K1	CO4
	8	Summarize the main difference between reducible and irreducible representations. i) Dimensionality ii) Symmetry elements iii) Basis functions iv) Orthogonality	K2	CO4
5	9	Choose the point group of BF_3 molecule. i) C2v ii) C3v iii) D3h iv) Td	K1	CO5
	10	Summarize the symmetry elements present in C_{2v} point group. i) E, C2, σv ii) E, C3, σv iii) E, C2, σh iv) E, σv, σh	K2	CO5

Cont...

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.	Derive the time-independent Schrödinger equation using the separation of variables procedure.	K2	CO1
		(OR)		
	11.b.	Extend the concept of orthonormal wave functions to a set of three wave functions, and show that they satisfy the orthonormality condition.		
2	12.a.	Apply the particle-in-a-box model to explain the energy levels of a conjugated polyene.	K3	CO2
		(OR)		
	12.b.	Apply the correspondence principle to show how the energy levels of a harmonic oscillator approach classical behavior at high quantum numbers.		
3	13.a.	Create a diagram showing molecular orbitals for ethylene using Huckel's theory.	K4	CO3
		(OR)		
	13.b.	Differentiate between the anharmonic oscillator and harmonic oscillator energy levels.		
4	14.a.	Assess the symmetry elements present in the C_2v point group.	K5	CO4
		(OR)		
	14.b.	Determine the point group of a molecule with C_3 axis and $3\sigma v$ planes.		
5	15.a.	Compose the vibrational modes of NH_3 molecule using group theory.	K6	CO5
		(OR)		
	15.b.	Adapt the concept of hybrid orbitals to explain the shape of H_2O molecule.		

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	Determine the eigen values of the Hamiltonian operator for a particle in a one-dimensional box, and discuss the physical significance of the results.	K2	CO1
2	17	Build a 3D box model to explain degeneracy in a cubical box.	K3	CO2
3	18	Examine the Born-Oppenheimer approximation's impact on molecular calculations.	K4	CO3
4	19	Assess the significance of Great Orthogonality theorem in group theory.	K5	CO4
5	20	Discuss the classification of vibrational modes in SO_2 and $POCl_3$.	K6	CO5

Z-Z-Z END