

PSG COLLEGE OF ARTS & SCIENCE
(AUTONOMOUS)

MSc DEGREE EXAMINATION MAY 2024
(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 commutator of any two quantum mechanical operators that correspond to a wavefunction is a) zero b) non-zero c) infinity d) sometimes zero and sometimes non-zero	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) ∫ dx	K2	CO1
2	3.	The zero-point energy of a particle in a 1D box is a) h ² / 8mL ² b) 9h ² / 8mL ² c) 16h ² / 8mL ² d) 4h ² / 8mL ²	K1	CO2
	4.	The energy gap between the vibrational energy levels of a simple harmonic oscillator is a) hv/2 b) hv c) 5hv/2 d) 3hv/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.	The unit of energy in atomic and molecular calculations is a) Joule b) Hartree c) Dalton d) Calorie	K1	CO3
4	7.	How many numbers of one-dimensional irreducible representations are in the C _{2v} point group? a) Zero b) one c) three d) four	K1	CO4
	8.	Which symmetry element is absent in the ethylene molecule? a) C _∞ (z) b) C ₂ (x) c) C ₂ (y) d) C ₂ (z)	K2	CO4
5	9.	How many Raman signals can be obtained for water molecule? a) One b) Two c) Three d) Four	K2	CO5
	10.	The irreducible representations representing bending vibrations of NH ₃ molecule is a) A ₁ b) E c) A ₁ + E d) 2A ₁	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) What are the conditions for Hermitian operators? (ii) Calculate the de Broglie wavelength of an electron travelling with a momentum of 2.73 × 10 ⁻²⁴ kg. m. s ⁻¹ .	K4	CO1
	11. b	(i) If we locate an electron within 20 pm, then what is the uncertainty in its speed? (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	Obtain the wavefunction and energy equation for a particle in 3D box by solving its Schrodinger wave equation. OR		
	12. b	(i) Draw potential energy level diagram of simple harmonic oscillator. (3.5 Marks) (ii) Write the ground-state normalized wavefunction (ψ_0) and energy equation (E_0) of the simple harmonic oscillator. (3.5 Marks)	K5	CO2
3	13. a	Determine the ground state energy of the He atom using first-order perturbation theory. OR		
	13. b	Discuss the LCAO-MO treatment of H_2^+ ion in detail.	K5	CO3
4	14. a	Answer the following questions from the irreducible character table of the D_{2h} point group given at the end of the question paper: (i) Number of mutually conjugated classes (ii) Order of the group (iii) Number of irreducible representations (iv) Totally symmetric irreducible representation (v) Direct product: $B_{2u} \times B_{3u} =$ (vi) Is D_{2h} an abelian group? (vii) One example for D_{2h} point group OR		
	14. b	(i) Distinguish between an abelian and a cyclic groups. (ii) Direct product of E^2 , in the C_{3v} point group (iii) Explain the improper axis of symmetry in <i>trans</i> -dichloroethylene.	K4	CO4
5	15. a	Obtain the irreducible representations representing vibrational modes of the NH_3 molecule and find out the number of IR bands. OR		
	15. b	Discuss the possible hybridization of water molecule using group theory.	K6	CO5

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	Examine the postulates of quantum mechanics.	K6	CO1										
2	17	Set up the Schrodinger wave equation for the hydrogen atom. From the solutions of $\phi(0)$, $\Theta(0,0)$ and $R(1,0)$ functions, determine the total wavefunction (ψ_{100}) and energy expression (E_{100}) for hydrogen atom.	K5	CO2										
3	18	Show that the delocalization energy of a benzene molecule is 2β using Huckel's approximations method.	K5	CO3										
4	19	(i) Decompose the given reducible representation of C_{2v} point group into its irreducible representations. <table border="1" style="margin-left: auto; margin-right: auto;"> <thead> <tr> <th>C_{2v}</th> <th>E</th> <th>$C_2(z)$</th> <th>σ_{xz}</th> <th>σ_{yz}</th> </tr> </thead> <tbody> <tr> <td>Γ_{red}</td> <td>15</td> <td>-1</td> <td>3</td> <td>3</td> </tr> </tbody> </table> (ii) Construct the irreducible character table for the C_{2v} point group using the Great Orthogonality Theorem.	C_{2v}	E	$C_2(z)$	σ_{xz}	σ_{yz}	Γ_{red}	15	-1	3	3	K5	CO4
C_{2v}	E	$C_2(z)$	σ_{xz}	σ_{yz}										
Γ_{red}	15	-1	3	3										
5	20	How does group theory predict the number of IR and Raman signals for SO_2 molecule? Explain.	K4	CO5										

Given: Irreducible representation character table of D_{2h} point group for answering Question 14.a.6. The D_{2h} Groups

D_{2h}	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	$\sigma(xy)$	$\sigma(xz)$	$\sigma(yz)$	
A_g	1	1	1	1	1	1	1	1	x^2, y^2, z^2
B_{1g}	1	1	-1	-1	1	1	-1	-1	R_x xy
B_{2g}	1	-1	1	-1	1	-1	1	-1	R_y xz
B_{3g}	1	-1	-1	1	1	-1	-1	1	R_z yz
A_u	1	1	1	1	-1	-1	-1	-1	
B_{1u}	1	1	-1	-1	-1	-1	1	1	z
B_{2u}	1	-1	1	-1	-1	1	-1	1	y
B_{3u}	1	-1	-1	1	-1	1	1	-1	x