Reg. No ..... Name **24P1053**

M.Sc. DEGREE END SEMESTER EXAMINATION - NOVEMBER 2024

SEMESTER 1 : CHEMISTRY / PHARMACEUTICAL CHEMISTRY

COURSE : **24P1CHET04 /24P1CPHT04 : QUANTUM CHEMISTRY AND GROUP THEORY**

(For Regular - 2024 Admission)

Duration : Three Hours Max. Weights: 30

PART A

Answer any 8 questions **Weight: 1**

1. Explain inversion operation with the help of an illustrative example. (U, CO 1)
2. Write the Schrodinger equation for a particle on a sphere in spherical polar co-ordinates. (R, CO 4)
3. An Eigen function of the operator d^2/dx^2 is $\Psi = e^2x$. Find the corresponding eigen value. (An)
4. Plot the radial probability distribution curve of the 1s, 2s, and 3s atomic wave functions. (A, CO 5)
5. Define S_5 axis of symmetry. Find the distinct operations generated by S_5 axis. (An, CO 1)
6. Determine a representation of C_{2v} point group by taking p_x,p_y and p_z orbitals as basis vectors. Is the representation reducible or irreducible in each case. (A, CO 2)
7. The set of symmetry operations of a molecule is {E, C, C_3^2, C_2, C_2', C_2'', i, S_6, S_6^5, σ_d, σ_d', σ_d''}. What is the point group of the molecule? (E, CO 1)
8. Explain Photoelectric effect. (E, CO 3)
9. Suggest an example for a molecule having C_5 axis, horizontal plane and determine the point group if the molecule has C_2 axes perpendicular to C_5 axis. (E, CO 1)
10. Express the Laplacian operator, $(Del)^2$, in spherical coordinates. (R)

(1 x 8 = 8)

PART B

Answer any 6 questions **Weights: 2**

11. Systematically determine the point group of staggered ferrocene. List the elements of the point group. (A, CO 1)
12. Write the determinantal wave functions of He and write the properties of determinants. (U, CO 4)
13. What is the superposition rule in operator postulate? Write down the operators of (1) Position (2) Linear momentum (3) Kinetic energy (4) Total energy. (E)
14. Derive the relation between cartesian coordinates and spherical polar coordinates. (A, CO 4)
15. Explain all types of symmetry elements and symmetry operations that are possible in a molecule with higher order symmetry. (R, CO 1)

16. Determine whether the following functions are acceptable or not as state functions over the indicated intervals (a) e^{-x} (0, ∞) (b) e^{-x} (-∞, +∞) (c) $Sin^{-1}x$(-1, +1) (d) Sinx/x (0, ∞) (A, CO 4)

17. Write the Mullicken rules to designate the irreducible representations in a character table. Explain how the Mullicken notations are assigned to different IR's of C_{2h} point group. (An)

18. The operations of a point group are {E, $2C_4(z)$, C2, $2C_2'$, $2C_2''$, i, $2S_4$, $2\sigma_v$, $2\sigma_d$}. Identify the point group, order of the group. How many irreducible representations does it have? (A, CO 1)

(2 x 6 = 12)

PART C

Answer any 2 questions **Weights: 5**

19. State the Great Orthogonality theorem. Based on the theorem derive the complete character table for C_{2v} point group. (A, CO 2)

20. Evaluate the commutator a) $[L_x,L_y]$ b) $[L_y,L_z]$ and c) $[L_z,L_x]$ (A)

21. Derive Time dependent and independent Schrodinger wave equations? (A, CO 4)

22. Define SALC. Generate the SALC orbitals of boron trifluoride molecule with sigma bond vectors as basis. (A, CO 2)

(5 x 2 = 10)

OBE: Questions to Course Outcome Mapping

CO	Course Outcome Description	CL	Questions	Total Wt.
CO 1	Explain the fundamentals of group theory.	R	1, 5, 7, 9, 11, 15, 18	10
CO 2	Apply the principles of group theory in chemical bonding.	A	6, 19, 22	11
CO 3	Understand the foundation and postulates of quantum mechanics.	U	8	1
CO 4	Describe the use of simple models for predictive understanding of different molecular systems and phenomena	U	2, 12, 14, 16, 21	12
CO 5	Illustrate the concept of atomic orbitals by quantum mechanics.	U	4	1

Cognitive Level (CL): Cr - CREATE; E - EVALUATE; An - ANALYZE; A - APPLY; U - UNDERSTAND; R - REMEMBER;