M.Sc. DEGREE END SEMESTER EXAMINATION- NOVEMBER 2025
SEMESTER 1 : CHEMISTRY / PHARMACEUTICAL CHEMISTRY
COURSE : **24P1CHET04 /24P1CPHT04 : QUANTUM CHEMISTRY AND GROUP THEORY**

(For Regular 2025 Admission and Improvement / Supplementary 2024 Admission)

Time : Three Hours   Max. Weights: 30

PART A
Answer any 8 questions   **Weight: 1**

1. How do you fix the principal axis of rotation of molecules in group theory?   (An, CO 1)
2. Define slater determinants with a suitable example.   (U, CO 5)
3. Write complete wave function of Hydrogen like atoms.   (R, CO 4)
4. Prove that *s* orbital is spherically symmetric.   (An, CO 5)
5. What is Linear operator? Write an example .   (R, CO 3)
6. List the symmetry elements and operations of o-dichlorobenzene and para-dichlorobenzene   (U, CO 1)
7. Write the importance of probability density in Quantum mechanics?   (R, CO 4)
8. State GOT and write its expression.   (R, CO 2)
9. Show that the point group of trans-1,2-dichloroethene is abelian.   (An, CO 1)
10. Deduce the matrix representation for reflection about the xy, xz planes and find their product.   (E, CO 2)

(1 x 8 = 8)

PART B
Answer any 6 questions   **Weights: 2**

11. Construct a reducible representation of C_{2v} point group as a set of 3x3 matrices. What are the irreducible representations that can be obtained from these matrices.   (A, CO 2)

12. An electron in a box 0.1nm across, which is the order of magnitude of atomic dimensions. Find the permitted energies in eV?   (A, CO 3)

13. What are space groups ? Distinguish between screw axis and glide planes.   (U, CO 1)

14. What are symmetric and antisymmetric wave functions?   (R, CO 5)

15. Derive the atomic orbital for *l=1, m=0*   (A, CO 5)

16. State the theorem concerning the irreducible representations of a group. Explain the subrules and consequences of GOT in the construction of character table.   (R, CO 2)

17. Generate a reducible representation for C_{2v} point group taking the sigma bond vectors of water molecule as basis vectors. Decompose the resultant reducible representation into linear combination of IR.   (A, CO 2)

18. What are the conditions for accepting a function as a state function?   (A, CO 3)

(2 x 6 = 12)

PART C
Answer any 2 questions   **Weights: 5**

19. Explain the wave mechanical treatment of a particle in a 3D potential box and elaborate the degeneracy of a particle in a cubic box.   (A, CO 3)

20. State the Great Orthogonality theorem. Apply the great orthogonality theorem for C_{3v} point group and derive the character table . (A, CO 2)

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

22. Solve and explain the Schrodinger equation for a particle in a ring. (A, CO 4)

(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, 6, 9, 13	5
CO 2	Apply the principles of group theory in chemical bonding.	A	8, 10, 11, 16, 17, 20, 21	18
CO 3	Understand the foundation and postulates of quantum mechanics.	U	5, 12, 18, 19	10
CO 4	Describe the use of simple models for predictive understanding of different molecular systems and phenomena	U	3, 7, 22	7
CO 5	Illustrate the concept of atomic orbitals by quantum mechanics.	U	2, 4, 14, 15	6

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