M. Sc. DEGREE END SEMESTER EXAMINATION : NOVEMBER 2023
SEMESTER 1 : CHEMISTRY / PHARMACEUTICAL CHEMISTRY
COURSE : **21P1CHET04 / 21P1CPHT04 : QUANTUM CHEMISTRY AND GROUP THEORY**
(For Regular - 2023 Admission and Improvement/Supplementary -2022/2021 Admissions)

Duration : Three Hours   Max. Weights: 30

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

1. Give the reduction formula and explain the terms involved.   (R)

2. What is Ψ in quantum chemistry ? What is the significance of $|\Psi|^2$?   (A, CO 3)

3. What is Linear operator? Write an example .   (R, CO 3)

4. Write the first and second columns of C_{2h} character table   (A, CO 1)

5. Write Hamiltonian operator of Hydrogen-like atoms in spherical polar coordinates.   (U, CO 5)

6. Plot the radial probability distribution curve of the 1s, 2s, and 3s atomic wavefunctions   (A, CO 5)

7. Determine the point group of $B(OH)_3$ assuming that it is a planar molecule.   (E)

8. What is a De-Broglie wave and write the De-Broglie relation?   (A, CO 3)

9. What are subgroups and classes of a group?   (U)

10. 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)

(1 x 8 = 8)

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

11.   Decompose these RR's into linear combination of IRR's .
   a)

C_2v	E	C_2	σ_{xz}	σ_{yz}
T_R	3	1	3	1

   b)

C_3v	E	$2C_3$	$3\sigma_v$
T_R	12	0	2

(A, CO 2)

12.   Solve the Schrödinger wave equation for a particle on a ring.   (A)

13.   Explain Planks law and black body radiation   (U, CO 4)

14.   Construct a reducible representation of C_{2v} point group as a set of 9X9 matrices.   (Cr)

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

16.   An electron in a box 0.10nm across, which is the order of magnitude of atomic dimensions. Find the permitted energies in eV?   (A, CO 3)

17. Generate a reducible representation for D_{3h} point group taking the sigma bond vectors of BF_3 molecule as basis vectors. Decompose the resultant reducible representation into linear combination of IR. (A, CO 2)

18. Construct the group multiplication table of C_{3V} point group (Cr)

(2 x 6 = 12)

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

19. Systematically determine the point groups in SF_4, PCl_3, IF_5, H_3BO_3 and glyoxal molecules. List the elements and classes in each point groups. (An, CO 1)

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

21. Solve the Schrödinger equation for Hydrogen atom by separating the variables; $R(r)$, $\Theta(\theta)$, and $\Phi(\varphi)$ (A, CO 4)

22. State the Great Orthogonality theorem. Write its subrules and consequences. Based on the theorem derive the first and second regions of the character table for C_{2h} point group. (A)

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

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