Reg. No ..... Name **22P1048**

M. Sc. DEGREE END SEMESTER EXAMINATION : OCTOBER 2022

SEMESTER 1 : CHEMISTRY / PHARMACEUTICAL CHEMISTRY

COURSE : **21P1CHET04 / 21P1CPHT04: QUANTUM CHEMISTRY AND GROUP THEORY**

(For Regular - 2022 Admission and Supplementary - 2021 Admission)

Duration : Three Hours Max. Weights: 30

PART A

Answer any 8 questions **Weight: 1**

1.	Show that 120^O rotation and 240^O rotation are conjugate elements of C_{3v} point group.	(An)
2.	Give the reduction formula and explain the terms involved.	(R)
3.	What is an abelian group? Give an example	(U)
4.	How do you fix the principal axis of rotation of molecules in group theory?	(An)
5.	A non-linear molecule possesses four C_3 axis and many vertical planes. What is its point group? What is the maximum number of vertical planes if there is only one C_3 axis	(An)
6.	What is a De-Broglie wave and write the De-Broglie relation?	(A, CO 3)
7.	Explain Photoelectric effect?	(E, CO 3)
8.	What is a normalised wavefunction? Illustrate with an example.	(An, CO 4)
9.	Draw qualitative shapes of the 's' and 'p' atomic orbitals. Indicate with ± the relative signs of the wavefunctions and the position(s) of any nodes.	(A, CO 5)
10.	Define slater determinant.	(U, CO 5)

(1 x 8 = 8)

PART B

Answer any 6 questions **Weights: 2**

11.	Write notes on a) Crystallographic point groups b) Herman Maugin notations c) Schoenflies notation.	(R)
12.	Systematically determine the point group staggered ferrocene. List the elements of the point group	(A)
13.	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)
14.	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)
15.	Stating from [d/dx x]=1, Evaluate the commutator [X, Px] and [X, P_x^2]	(A)
16.	Prove that linear momentum and kinetic energy can be measured simultaneously.	(A, CO 3)

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

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

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

21. What is black body radiation? Explain it with the help of (i) Wein's displacement law (ii) Rayleigh-Jean law and (iii) Plank' law (A, CO 3)

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

(5 x 2 = 10)

OBE: Questions to Course Outcome Mapping

CO	Course Outcome Description	CL	Questions	Total Wt.
CO 2	Apply the principles of group theory in chemical bonding.	A	19, 20	10
CO 3	Understand the foundation and postulates of quantum mechanics.	U	6, 7, 16, 21	9
CO 4	Describe the use of simple models for predictive understanding of different molecular systems and phenomena.	An	8, 22	6
CO 5	Illustrate the concept of atomic orbitals by quantum mechanics.	A	9, 10, 18	4

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