M Sc DEGREE (CSS) EXAMINATION, DECEMBER 2023

First Semester

CORE - CH500103 - QUANTUM CHEMISTRY AND GROUP THEORY

M Sc CHEMISTRY, M Sc ANALYTICAL CHEMISTRY, M Sc APPLIED CHEMISTRY , M Sc PHARMACEUTICAL CHEMISTRY, M Sc POLYMER CHEMISTRY

2019 ADMISSION ONWARDS

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Time: 3 Hours   Weightage: 30

Part A (Short Answer Questions)

*Answer any **eight** questions.*

*Weight **1** each.*

1. The S_3 axis generates only 2 distinct operations. Which are they and why are they said to be distinct?

2. What is a screw axis? Explain using an example.

3. Depict the GMT of C_{2v} point group.

4. Give the matrix representation of translational vectors in C_{2v} point group.

5. State the properties of irreducible representations.

6. Prove that the wave functions $Y_1 = A_1cos(npx/a)$ and $Y_2 = A_2sin(npx/a)$ are orthogonal with the range 0 < x < a.

7. Explain the concept of degeneracy using the wave functions of particle in a cubic box.

8. Write the recursion formula. Explain its significance.

9. Find the commutator of angular momentum operator $[L_x, L^2]$.

10. How can the shape of s and p orbitals be obtained from polar plots?

(8×1=8 weightage)

Part B (Short Essay/Problems)

*Answer any **six** questions.*

*Weight **2** each.*

11. Duscuss briefly about the point groups associated with molecules of high symmetry?

12. Assign Mulliken symbols and substantiate your answer.

	E	$2C_4$	C_2	$2\sigma_v$	σ_v'
Γ_1	1	1	1	1	1
Γ_2	1	1	1	-1	-1
Γ_3	1	-1	1	1	-1
Γ_4	1	-1	1	-1	1
Γ_5	2	0	-2	0	0

13. What are the features of an abelian group?

14. Reduce the representations.

C_{3v}	E	$2C_3$	$3\sigma_v$
$\Gamma_{RR}(1)$	21	0	3
$\Gamma_{RR}(2)$	15	0	3

15. Discuss the failures of classical mechanics and the success of quantum theory in the explanation of black body radiation.

16. Explain the relationship between Cartesian and Cylindrical polar coordinates. Convert the Cartesian coordinates (1,1,3) into Cylindrical polar coordinates.

17. What is the relevance of spin orbitals? Discuss on how spin orbitals are constructed.

18. Discuss on symmetric and antisymmetric wave functions. Explain with suitable examples.

(6×2=12 weightage)

Part C (Essay Type Questions)

*Answer any **two** questions.*

Weight 5 each.

19. What are character tables? Applying GOT to C_{2v} point group, derive the character table.

20. "Knowledge of group theory simplifies our understanding of bonding in molecules". Justify this statement and explain taking a molecule belonging to C_{2v} point group.

21. Apply the Schrodinger wave equation to a particle in a one dimension box and hence arrive at the wave function and possible energy values.

22. Solve the Schrodinger equation for a non planar rigid rotator. Discuss the results.

(2×5=10 weightage)