

QP CODE: 25050649



Reg No :

Name :

MSc DEGREE (CSS) EXAMINATION DECEMBER 2025

First Semester

Core Courses - CH500103 - QUANTUM CHEMISTRY AND GROUP THEORY

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

2019 Admission Onwards

5632ADBD

Time: 3 Hours

Weightage: 30

Part A (Short Answer Questions)

Answer any **eight** questions.

Weight **1** each.

1. "A mirror plane generates only one distinct operation." Verify the statement.
2. Determine the point group of (a) allene (b) tetrafluoro ethylene (c) trifluoromethane (d) benzene (e) naphthalene
3. Write a note on crystallographic point groups.
4. Discuss the essence of Group Multiplication Table.
5. Reduce the representation.

C_{2V}	E	$C_{2(x)}$	σ_{xz}	σ_{yz}
Γ_{RR}	12	-2	2	4

6. The work function for Platinum metal is 8×10^{-19} J. Will a radiation of wavelength 200 nm be able to cause photoelectric effect in it?
7. What are the conditions for acceptable wave functions? Give an example for acceptable wave function.
8. In a cubic box, the energy of the free electron is found to be $E = 12h^2/8ma^2$. Deduce the wave function(s). Is the state a degenerate one?
9. Define the Legendre Polynomial. Obtain the Legendre functions for $l = 0$ and $l = 1$.
10. What are Slater determinants? Write the Slater determinant for Lithium atom.

(8×1=8 weightage)

Part B (Short Essay/Problems)

Answer any **six** questions.

Weight **2** each.

11. What are the mathematical requirements of a point group?





12. Deduce the classes in C_{2v} and C_{3v} point groups.
13. Deduce the matrix representation of C_{2v} point group.
14. State the properties of irreducible representations.
15. Evaluate $[L_z, L_y]$
16. Explain spherical harmonics and discuss how they form the eigen functions for the angular momentum operator L^2 .
17. Explain the radial plot and the radial probability density plot for 1s and 2s electron.
18. Write a note on spin orbitals and discuss on how spin orbitals are constructed.

(6×2=12 weightage)

Part C (Essay Type Questions)

Answer any **two** questions.

Weight **5** each.

19. Construct the Character Table of C_{2h} point group using GOT rules.
20. "Knowledge of group theory simplifies our understanding of bonding in molecules". Justify this statement and explain taking a molecule belonging to C_{2h} point group.
21. Apply Schrodinger equation for a particle in a one dimensional box and discuss the results.
22. Solve the Schrodinger equation for a harmonic oscillator. Give the eigen values and eigen functions for the first three states. Represent the eigen functions graphically.

(2×5=10 weightage)

