



24045536

QP CODE: 24045536

Reg No :

Name :

M.Sc DEGREE (CSS) EXAMINATION, DECEMBER 2024**First Semester****CORE - CH500103 - QUANTUM CHEMISTRY AND GROUP THEORY**M.Sc CHEMISTRY, M.Sc ANALYTICAL CHEMISTRY, M.Sc POLYMER CHEMISTRY, M.Sc
APPLIED CHEMISTRY, M.Sc PHARMACEUTICAL CHEMISTRY

2019 ADMISSION ONWARDS

76F830A2

Time: 3 Hours

Weightage: 30

Part A (Short Answer Questions)*Answer any eight questions.**Weight 1 each.*

1. The C_6 axis generates only 2 distinct operations. Justify this statement.
2. Explain why CHCl_3 belongs to C_{3v} point group while CCl_4 belongs to T_d .
3. Write a note on Mulliken symbols.
4. "In an Abelian group all elements must commute with each other" Justify this statement with the help of an example.
- 5.

Reduce the representation.

C_{3v}	E	$2C_3$	$3\sigma_v$
Γ_{RR}	4	1	0

6. How does photoelectric effect show wave particle duality?
7. Identify which of the following functions are eigen functions of the operator d/dx . If so give the eigen value : (a) Ae^{ax} (b) x^2 .
8. Calculate the ground state energy in KJ mol^{-1} for an electron that is confined to a one dimensional infinite potential well with a width of 0.2 nm.
9. Formulate the first three eigen functions of a simple harmonic oscillator.
10. Explain why $1s^3$ configuration is impossible for Li atom by means of Slater determinant concept.

(8×1=8 weightage)



Part B (Short Essay/Problems)

Answer any **six** questions.

Weight **2** each.

11. Distinguish between screw axis and glide plane.
12. (a) What are subgroups? (b) What are classes? Explain each with the help of an example.
13. Formulate the matrix representation for identity, reflection planes, inversion centre and improper axis of rotation.
14. What are reducible and irreducible representations?
15. Discuss the relationships between Cartesian coordinate, spherical polar and cylindrical polar coordinate systems. Convert the cartesian coordinates (1,1,3) to cylindrical polar coordinates.
16. What are Legendre and associated Legendre polynomials? Explain with examples.
17. Evaluate $[L^2 L_x]$ and $[L_x L_z]$.
18. Explain what are spherical harmonics and also determine the first three spherical harmonics.

(6×2=12 weightage)

Part C (Essay Type Questions)

Answer any **two** questions.

Weight **5** each.

19. Construct the Character Table of C_{3v} point group using GOT rules.
20. Construct SALCs for a molecule which belongs to D_{3h} point group.
21. A particle of mass 'm' is confined to move in a three dimensional rectangular box of dimensions a,b, and c. The potential energy is zero inside the box and infinity outside. Derive the expression for eigen function and eigen value.
22. Apply the Schrodinger wave equation to Hydrogen atom and solve the equation by method of separation of variables. Derive the solutions for the radial and angular functions.

(2×5=10 weightage)