

QP CODE: 19002497



Reg No : .....

Name : .....

**M.Sc. DEGREE (C.S.S ) EXAMINATION, NOVEMBER 2019**

**First Semester**

Faculty of Science

**Core - CH500103 - QUANTUM CHEMISTRY AND GROUP THEORY**

(Common to all Branches of Chemistry)

2019 Admission Onwards

9F63094D

Time: 3 Hours

Maximum Weight :30

**Part A (Short Answer Questions)**

Answer any **eight** questions.

Weight **1** each.

1. Prove that  $S_2 = i$  for molecular point groups.
2. Write a note on Hermann Mauguin symbols.
3. " A square of any element is also an element in the same group". Illustrate.
4. Show that inversion operation and rotation operation commute each other.
5. What are block factored matrices?
6. What is meant by black body radiation? Explain.
7. Determine the average value of linear momentum for particle in a one dimensional box.
8. Explain the term degeneracy. What is the maximum degeneracy possible for a particle in a cube ?
9. Write the equations for converting Cartesian co-ordinates to the spherical polar co-ordinates.
10. What are Slater determinants? Write the Slater determinant for Beryllium atom.

(8×1=8 weightage)

**Part B (Short Essay/Problems)**

Answer any **six** questions.

Weight **2** each.

11. Distinguish between  $D_{nh}$  and  $D_{nd}$  point groups





12. Construct GMT for  $C_{2v}$  and  $C_{2h}$  point groups.
13. How does the concept of irreducible representations help in the structure elucidation of molecules?
14. Construct SALCs of  $BF_3$  molecule.
15. Show that the eigenvalues of a Hermitian operator are real.
16. Evaluate  $[L_y, L_x]$ .
17. What are spherical Harmonics? Determine the first three spherical harmonics.
18. What are spin orbitals? How will you construct spin orbitals?

(6×2=12 weightage)

### Part C (Essay Type Questions)

Answer any **two** questions.

Weight 5 each.

19. What do you mean by similarity transformation and classes in group theory? Illustrate using  $C_{3v}$  point group.
20. Construct the character table for  $C_{3v}$  point group.
21. Set up Schrodinger equation and find eigen values and eigen functions for a particle moving on a ring.
22. Write down the Schrodinger equation for the electron in a H atom. Transform the equation into spherical polar co-ordinates and separate into  $\theta$  equation,  $\phi$  equation and R equation. what are the solutions for each ?

(2×5=10 weightage)

