



22001594

QP CODE: 22001594

Reg No : .....

Name : .....

**M Sc DEGREE (CSS) EXAMINATION, JULY 2022****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

053E6CA3

Time: 3 Hours

Weightage: 30

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

1. What is meant by pitch and fold of screw axis?
2. What are the features of an abelian group?
3. What are subgroups? Explain using an example.
4. Formulate the matrix representation for  $S_n$ .
5. What is meant by trace of a matrix? Explain with the help of an example.
6. How does photoelectric effect account for the particle nature of radiation?
7. Prove that operator multiplication can be non commutative.
8. Explain the significance of spherical harmonics?
9. Explain the term 'Ladder operator'.
10. What are symmetric and antisymmetric wave functions?

(8×1=8 weightage)

**Part B (Short Essay/Problems)***Answer any six questions.**Weight 2 each.*

11. List out the symmetry operations generated by the following:  $S_3$  &  $S_6$ . Also identify the distinct operations.





12. Identify the symmetry elements present and hence the point group of benzene.
13. Assign Mulliken symbols and substantiate your answer.

$D_{3h}$	E	$2C_3$	$3C_2$	$\sigma_h$	$2S_3$	$3\sigma_v$
$\Gamma_1$	1	1	1	1	1	1
$\Gamma_2$	1	1	-1	1	1	-1
$\Gamma_3$	2	-1	0	2	-1	0
$\Gamma_4$	1	1	1	-1	-1	-1
$\Gamma_5$	1	1	-1	-1	-1	1
$\Gamma_6$	2	-1	0	-2	1	0

14. What are isomorphic groups. Illustrate using  $C_{2v}$  and  $C_{2h}$  point group.
15. Discuss the case of the particle in a one dimensional box with one finite potential barrier.
16. Deduce an expression for total energy of a simple harmonic oscillator using classical mechanics.
17. Describe the Eigen values and eigen functions of a particle in a ring.
18. Evaluate  $[L_x L_z]$

(6×2=12 weightage)

### Part C (Essay Type Questions)

Answer any **two** questions.

Weight 5 each.

19. Applying Great Orthogonality theorem, construct the character table for  $C_{3v}$  point group.
20. Discuss the concept of SALCs and construct the SALCs for  $NH_3$  molecule.
21. Solve the Schrodinger equation for a particle in 3 dimensional box.
22. Set up the Schrodinger equation for hydrogen atom, in spherical polar coordinates and separate it into three ordinary differential equations by the method of separation of variables.

(2×5=10 weightage)

