**QP CODE: 21002179**

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**Reg No :** .....

**Name :** .....

## M Sc DEGREE (CSS) EXAMINATION, NOVEMBER 2021

### First Semester

Faculty of Science

### 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

E59F94D4

Time: 3 Hours Weightage: 30

**Part A (Short Answer Questions)**

*Answer any **eight** questions.*

*Weight **1** each.*

1. The $S_5$ axis generates only 4 distinct operations. Which are they and why are they said to be distinct?
2. Identify the point group of pyramidal $AB_3$, $AB_2X$ and $ABX_2$ type molecules. Comment on your observation.
3. What are isomorphic groups? Give two examples.
4. Give the matrix representation of $C_n$ axis when angle of rotation is 360°, 180°, 90°, 60° and 120° respectively.
5. Reduce the representation.

| $C_{2h}$ | E | $C_{2(z)}$ | i | $\sigma_{xy}$ |
|---|---|---|---|---|
| $\Gamma_{RR}$ | 5 | 1 | 1 | 5 |

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. Explain the concept of degeneracy using the wave functions of particle in a cubic box.
9. What are Ladder operators? Explain.
10. What are spin orbitals? Explain.

(8×1=8 weightage)

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

*Answer any **six** questions.*

*Weight **2** each.*

11. Write a note on crystallographic point groups.
12. What do you mean by space groups?
13. Write a short note on Abelian groups. Show that $C_{2v}$ is an Abelian group.
14. Write 4 sub groups each for $O_h$ and $T_d$, point groups.
15. Deduce an expression for total energy of a simple harmonic oscillator using classical mechanics.
16. Explain the relationship between Cartesian and Cylindrical polar coordinates. Convert the Cartesian coordinates (1,1,3) into Cylindrical polar coordinates.
17. Evaluate $[L^2 L_z]$ and $[L_x L_y]$.
18. Explain symmetric and antisymmetric wave functions 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. 'The use of projection operator and reduction formula help in arriving at the SALCs for molecules'. Explain taking $C_{3v}$ point group as an example.
21. Apply Schrodinger equation for a particle in a one dimensional box and discuss the results.
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)