

QP CODE: 23003255



Reg No : .....

Name : .....

**M Sc DEGREE (CSS) EXAMINATION, APRIL 2023**

**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

07EAB500

Time: 3 Hours

Weightage: 30

**Part A (Short Answer Questions)**

*Answer any **eight** questions.*

*Weight **1** each.*

1. "A molecule may have  $S_n$  axis even if  $C_n$  and  $\sigma_h$  does not exist independently" Do you agree with the statement? Why?
2. State the standard reduction formula.
3. What do you mean by space groups?
4. What are cyclic groups? Explain using an example.
5. What is meant by the term "class" in group theory? Explain using an example.
6. Highlight the significance of recursion relation.
7. Find the commutator of angular momentum operator  $[L_y, L^2]$ .
8. What are Ladder operators? Explain.
9. What are radial and angular plots? Explain.
10. What are spin orbitals? Explain.

(8×1=8 weightage)

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

*Answer any **six** questions.*

*Weight **2** each.*

11. Explain the different point groups present in linear molecules.



12. Deduce the matrix representation for  $C_n$  and  $S_n$ .
13. What is block diagonalisation? How is it helpful?
14. Write a note on transformation properties of atomic orbitals.
15. Light of wavelength  $4360 \text{ \AA}$  caused photoelectric emission of electrons whose kinetic energy is measured as  $0.45 \text{ eV}$ . Calculate the threshold frequency needed for photo-electric emission of electrons.
16. Which of the following functions are eigenfunctions of  $d^2/dx^2$  (a)  $e^{x^2}$ , (b)  $x^2$ , (c)  $\sin x$ , (d)  $3\cos x$ , (e)  $\sin x + \cos x$ . Give the eigenvalue for each eigenfunction.
17. Discuss the significance of spherical harmonics. Give an example of the real form of spherical harmonics.
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. Construct the Character Table of  $C_{2v}$  point group using GOT rules.
20. Construct SALCs for trans  $N_2F_2$  molecule.
21. A particle of mass 'm' is confined to move in one dimension between  $x=0$  and  $x=a$ . The potential energy is zero between  $x=0$  and  $x=a$  and infinity when  $x < 0$  and when  $x > a$ . Write the time independent schrodinger wave equation and obtain the eigen function and eigen value.
22. Derive the expression for normalized wave function for a particle in a 3D box with sides of length a, b and c and discuss the degeneracies of the first three energy levels.

(2×5=10 weightage)

