Reg. No……. Name……. **26P256**

M.Sc. DEGREE END SEMESTER EXAMINATION : APRIL 2026

SEMESTER 2: CHEMISTRY / PHARMACEUTICAL CHEMISTRY

COURSE: 24P2CHET08/24P2CPHT08 - THEORETICAL AND COMPUTATIONAL CHEMISTRY

(For Regular 2025 Admission and Improvement/Supplementary 2024 Admission)

Time: Three hours Max. Weight: 30

PART A
Answer any 8 questions

Weight : 1

1. Explain the selection rule for electronic transition with an example. (CO1)
2. Discuss the symmetry criterion for optical activity. (CO1)
3. Differentiate between redundant modes and out of plane modes. (CO1)
4. What are the important problems faced in quantum mechanical calculations for many particles compared to a single particle model? (CO2)
5. Discuss Roothan's equations. (CO2)
6. What is Hellman-Feynman Theorem? (CO2)
7. Discuss the MO treatment of F_2 (CO3)
8. Write the term symbol of Be_2 and C_2 (CO3)
9. Explain how one determines the electron correlation in ammonia molecule. (CO4)
10. Differentiate between geometry optimization and single point energy calculation. (CO4)

(1 x 8 = 8)

PART B
Answer any 6 questions

Weights : 2

11. Perform the IR and Raman analysis of water molecule. (CO1)
12. Derive the hybridization of BF_3 using the concepts of group theory. (CO1)
13. Calculate the electron density of butadiene. (CO3)
14. How does slanted bottom affect the energy of an electron in one dimensional box? Discuss. (CO2)
15. Explain the qualitative treatment of Hartree-Fock Self-Consistent Field (HFSCF) method. (CO2)
16. Draw an analogy between Molecular Orbital and Valence Bond theories. (CO3)
17. Explain in brief HF method. (CO4)
18. What are Force Fields? Explain its characteristics and its parametrization. (CO4)

(2 x 6 = 12)

PART C
Answer any 2 questions

Weights : 5

19. a) Predict the hybridization of PCl_5 using the concepts of group theory (3 wt)

    b) Explain the electronic transitions in methanal using concepts of group theory (2 wt). (CO1)

20. a) Explain the proof of variation theorem.

    b) Apply perturbation theorem for the ground state of helium atom (2 +3 wt). (CO2)

21. Explain MO treatment of H_2^+ (CO3)

22. a) Write a short note on DFT method (3 wt).

    b) Explain in detail how Z matrix is generated for various molecules (2 wt). (CO4)

(5 x 2 = 10)