25P2053

Reg. No……. Name……..

M. Sc DEGREE END SEMESTER EXAMINATION- APRIL 2025

SEMESTER 2: CHEMISTRY / PHARMACEUTICAL CHEMISTRY

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

(For Regular- 2024 Admission)

Time: Three hours Max. Weight: 30

PART A

Answer any 8 questions **Weight: 1**

1. Explain the rule of mutual exclusion with an example (CO1)
2. Is optical activity related to group theory? Explain (CO1)
3. Discuss direct product representation with an example. (CO1)
4. Differentiate between STO and GTO. (CO2)
5. Differentiate coulombs operator and exchange operator (CO2)
6. What is Hellman Feynman Theorem? (CO2)
7. Discuss the MO treatment of Li_2 (CO3)
8. Give the expression for triplet state of H_2 (CO3)
9. Explain how one determines the electron correlation in ammonia molecule (CO4)
10. Write the Z matrix for staggered ethane (CO4)

(1 x 8 = 8)

PART B

Answer any 6 questions **Weights: 2**

11. Derive the hybridization of methane using the concepts of group theory (CO1)
12. Discuss the electronic transition of formaldehyde using symmetry (CO1)
13. Explain the application of perturbation method to an electron in a one-dimensional box with slanted bottom (CO2)
14. Discuss the proof for variation theorem. (CO2)
15. Give a quantum mechanical treatment of sp hybredisation (CO3)
16. Compare VB and MO theories. (CO3)
17. Compare semi empirical and DFT methods (CO4)
18. Write a notes on Molecular Mechanics method (CO4)

(2 x 6 = 12)

PART C

Answer any 2 questions **Weights: 5**

19. Using symmetry criteria, generate the hybridization and SALC for BF3. (CO1)
20. a) Examine the perturbation treatment of Helium atom b) Calculate electron density in butadiene (3 + 2 wt) (CO2)

21. Explain MO treatment of H2+ (CO3)
22. Discuss the various steps involved in the generation of GAMESS input for various calculations. (CO4)

(**5 x 2 =10)**