M.Sc DEGREE (CSS) EXAMINATION, MAY 2025

Second Semester

CORE - CH500203 - CHEMICAL BONDING AND COMPUTATIONAL CHEMISTRY

M Sc CHEMISTRY, M Sc POLYMER CHEMISTRY, M Sc ANALYTICAL CHEMISTRY, M Sc APPLIED CHEMISTRY, M Sc PHARMACEUTICAL CHEMISTRY

2019 ADMISSION ONWARDS

C387D898

Time: 3 Hours   Weightage: 30

Part A (Short Answer Questions)

*Answer any **eight** questions.*

*Weight **1** each.*

1. Based on orbital selection rule, predict whether $B_1 - E$ transition is allowed in C_{4v} point group. Substantiate your prediction.

2. How do you relate dissymmetry with optical activity? Explain with an example with relation to group theory.

3. What are trial wave functions?

4. Differentiate coulomb operator and exchange operator.

5. Differentiate Slater type orbitals (STO) and Gaussian type orbitals(GTO).

6. Explain Born-Oppenheimer approximation .

7. Write the spectroscopic term symbol for CO .

8. What is density functional theory used for?

9. Write the z-matrix of methane molecule.

10. What is CHARMM? Explain its use in molecular mechanics?

(8×1=8 weightage)

Part B (Short Essay/Problems)

*Answer any **six** questions.*

*Weight **2** each.*

11. How does internal coordinate system help in analysizing the vibrational modes present in *trans* N_2F_2 molecule?

13. Discuss on the variation treatment for the ground state of helium atom.

14. Apply the time independent perturbation theory to obtain the wave function for a non degenerate state.

15. Construct the wave functions for CH_4 hybrid orbitals

16. Write Hückel determinant of allyl systems, butadiene and benzene. calculate delocalization energy of butadiene .

17. What is double zeta and triple zeta basis sets? Which one is better and why?

18. Distinguish between ab initio and semi empirical methods.

(6×2=12 weightage)

Part C (Essay Type Questions)

*Answer any **two** questions.*

Weight 5 each.

19. Predict the electronic transitions using direct product terms for C_{2v} point group. What are the spin selection rules? Discuss on relaxation in selection rules.

20. Apply perturbation theory to a particle in a 1 dimensional box with slanted bottom.

21. Explain how molecular orbital theory used to explain homonuclear diatomic molecule.

22. Using diagrams explain the following
    a) potential energy surface b)conformational search c) global minima d) local minima e) saddle points

(2×5=10 weightage)