



QP CODE: 24018933



24018933

Reg No : .....

Name : .....

**MSc DEGREE (CSS) EXAMINATION , APRIL 2024**

**Second Semester**

**CORE - CH500203 - CHEMICAL BONDING AND COMPUTATIONAL CHEMISTRY**

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

2019 Admission Onwards

C76F2885

Time: 3 Hours

Weightage: 30

**Part A (Short Answer Questions)**

Answer any **eight** questions.

Weight **1** each.

1. Calculate the total character and write down the reducible representation for  $\text{NH}_3$  molecule.
2. Based on orbital selection rule, predict whether  $B_1 - E$  transition is allowed in  $C_{4v}$  point group. Substantiate your prediction.
3. What is the need for approximations in Quantum Mechanics?
4. Highlight the salient features of perturbation theory.
5. Differentiate coulomb operator and exchange operator.
6. Draw molecular orbital diagram of  $\text{F}_2$
7. Draw the Huckel molecular energy levels of Allyl Carbocation.
8. What are Hohenberg Kohn theorems?
9. State three points of differences between ab initio and DFT calculations.
10. What is the meaning of force field and parameterizing a forcefield?

(8×1=8 weightage)

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

Answer any **six** questions.

Weight **2** each.

11. In the IR and Raman spectra of  $\text{H}_2\text{O}$  molecule 3 peaks are observed. Using group theory, justify this observation.





12. What are the possible electronic transitions predicted in  $C_{2v}$  point group? (use direct product rules)
13. How does variation theory help in estimating the energy of the ground state of helium atom?
14. What are Slater type orbitals (STO) and Gaussian type orbitals (GTO), and sketch STO and GTO.
15. Discuss on the major differences between Valence Bond theory and Molecular Orbital theory?
16. Explain the quantum mechanical treatment of  $SP^3$  hybridization.
17. Write short notes on
  - a) conformational search b) global minima c) local minima d) saddle points
18. Write the Z-matrix of a non linear triatomic and a linear triatomic molecule.

(6×2=12 weightage)

### Part C (Essay Type Questions)

Answer any **two** questions.

Weight 5 each.

19. How does group theory help in deducing the hybridisation of  $PCl_5$  molecule? Derive the hybrid orbitals for this molecule.
20. Apply the perturbation theory to evaluate the ground state energy of helium atom.
21. Explain valence bond (VB) theory and VB theory of  $H_2$  molecule.
22. Write short notes on
  - (a) Ab initio methods
  - (b) Electron correlation
  - (c) Configurational Interaction
  - (d) Moller Plesset Perturbation Theory
  - (e) Semi empirical methods

(2×5=10 weightage)

