Chemistry

QP CODE: 20000782

17

Reg No : .....

Name : .....

MSc DEGREE (CSS) EXAMINATION , NOVEMBER 2020

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

54E7C630

Time: 3 Hours Weightage: 30

Part A (Short Answer Questions)

Answer any **eight** questions.

Weight **1** each.

1. How many vibrational modes are present in NH_3 and trans N_2F_2 molecules.
2. How does the departure from cubic symmetry result in a forbidden transition becoming allowed? Explain
3. Write down the Hamiltonian for H_2 molecule
4. What is Hellmann-Feynman theorem.
5. What is Fock operator
6. Write Schrödinger equation for molecules and explain
7. Compare the bond energy, bond length and magnetic behavior of CN and CN^-
8. What is generalized gradient approximation?
9. Write the z-matrix of ammonia 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. Discuss the IR and Raman activity of trans N_2F_2 molecule
12. What are the orbital selection rules? Explain.
13. What are the important problems faced in quantum mechanical calculations for many particles compared

to a single particle model

14. What are Slater type orbitals (STO) and Gaussian type orbitals (GTO), and sketch STO and GTO
15. Construct the wave functions for CH_4 hybrid orbitals
16. Explain Hückel Molecular Orbital (HMO) theory of allyl system
17. What is meant by SCF procedure? Explain.
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. How does group theory help in deducing the hybridisation of BF_3 molecule? Derive the hybrid orbitals for this molecule.
20. Illustrate variation theorem using suitable trial wave function for particle in a one dimensional box
21. Compare and construct MO and VB theories
22. What are the applications of Computational Chemistry?

(2×5=10 weightage)