QP CODE: 22000491

22000491

Reg No : .....

Name : .....

MSc DEGREE (CSS) EXAMINATION , JANUARY 2022

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

66AFFBBD

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 $A_1 – A_2$ transition is allowed in C_{3v} point group. Substantiate your prediction.
2. What are the conditions for a molecule to be optically active?
3. Write the Hamiltonion for Li atom.
4. Differentiate coulomb operator and exchange operator.
5. Explain Gaussian type orbitals.
6. Write the spectroscopic term symbol for HF molecule .
7. Draw the Huckel molecular energy levels of Allyl Carbanion.
8. List any 5 scopes of computational chemistry.
9. What is basis function?
10. What is meant by GAMESS / FIREFLY keywords?

(8×1=8 weightage)

Part B (Short Essay/Problems)

*Answer any **six** questions.*

*Weight **2** each.*

11. Explain redundant and out of plane modes using an example.
12. What are the possible electronic transitions predicted in C_{3v} point group? (use direct product rules).

13. Write and explain variation treatment for the ground state of helium atom.

14. Explain the Qualitative idea of Hellmann-Feynman theorem.

15. Explain spin orbitals of Hydrogen molecule.

16. Explain the Semiempirical MO treatment of planar conjugated molecules.

17. What are local density approximation and generalized gradient approximation? Explain.

18. Distinguish between ab initio and DFT methods.

(6×2=12 weightage)

Part C (Essay Type Questions)

*Answer any **two** questions.*

*Weight **5** each.*

19. Using cartesian coordinate method and internal coordinate method, give the number and symmetry of vibrational modes for NH_3 and H_2O molecules.

20. What is Perturbation method? Discuss on time-independent perturbation method and the first order correction to energy and finally arrive at the wave function.

21. Explain Molecular Orbital (MO) theory, MO theory of H_2 molecule,

22. "Molecular Mechanics as a computational tool". Discuss the features of this method for large systems and the programmes developed

(2×5=10 weightage)