



22002453

QP CODE: 22002453

Reg No :

Name :

MSc DEGREE (CSS) EXAMINATION , NOVEMBER 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

B6BAA014

Time: 3 Hours

Weightage: 30

Part A (Short Answer Questions)

Answer any *eight* questions.

Weight *1* each.

1. Differentiate between redundant modes and out of plane bending modes using an example.
2. What is meant by d-p mixing?
3. What is the principle of variation method?
4. Give the mathematical approach of Perturbation method.
5. State and Explain Hartree-Fock equations.
6. Draw the MO energy level diagram of N_2 molecule.
7. What are the important aspect in drawing a correlation diagram?
8. What is a Potential Energy Surface?
9. What is local density approximation?
10. The numerical value of the force field has no physical meaning. Comment on this statement.

(8×1=8 weightage)



Part B (Short Essay/Problems)

Answer any **six** questions.

Weight **2** each.

11. Discuss how internal coordinate system helps in analyzing the vibrational modes present in NH_3 molecule?
12. What are the orbital selection rules? Explain.
13. Explain the application of perturbation theory to an electron in a one dimensional box with slanted bottom.
14. Explain the Qualitative treatment of Hartree-Fock Self-Consistent Field (HFSCF) method.
15. Write and Explain Born-Oppenheimer approximation.
16. Explain the quantum mechanical treatment of SP hybridization.
17. Write a note on semi-empirical methods used in computational chemistry.
18. Explain how to build a Z-matrix.

(6×2=12 weightage)

Part C (Essay Type Questions)

Answer any **two** questions.

Weight **5** each.

19. Derive the hybrid orbitals for PCl_5 molecule using group theory.
20. Apply the variation method to hydrogen atom using the trial function $e^{-\alpha r}$
21. Using HMO theory set up and solve the Huckel secular determinantal equation for the allyl system which consist of allyl radical, cation and anion. calculate the delocalization energy for the three species and construct molecular diagrams.
22. Compare the basic principles of the different computational methods in chemistry?

(2×5=10 weightage)

