QP CODE: 23004970

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Reg No : .....

Name : .....

MSc DEGREE (CSS) EXAMINATION , JULY 2023

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

A0C57D16

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 H_2O molecule .
2. State the selection rules for electronic spectra to occur.
3. Write the Hamiltonian for He .
4. Write one qualitative idea obtained from Hellmann Feynmann theorem.
5. What is core hamiltonian?
6. Draw molecular orbital diagram of Be2..
7. Write the term symbol for the first excited state of Hydrogen molecule.
8. Sketch the plot of an 1s STO function and the STO-1G, STO-2G, STO-3G functions for H atom.
9. What is exchange correlation functional?
10. What is AMBER?

(8×1=8 weightage)

Part B (Short Essay/Problems)

*Answer any **six** questions.*

*Weight **2** each.*

11. Discuss the IR and Raman activity of NH_3 molecule?
12. What are the possible electronic transitions predicted in C_{3v} point group (use direct product rules).

13. How can the time independent perturbation theory be applied to obtain the energy (first correction only) for a non degenerate state?

14. Explain Roothan's concept of basis functions.

15. Construct the wave functions for BeH_2 hybrid orbitals.

16. What are the main assumptions on Huckel Molecular orbital treatment.

17. Explain the scope of computational chemistry.

18. Distinguish between semi empirical and DFT methods.

(6×2=12 weightage)

Part C (Essay Type Questions)

*Answer any **two** questions.*

*Weight **5** each.*

19. Using group theoretical principles, explain the bonding in CH_4 molecule and derive the hybrid orbitals.

20. Discuss the variation treatment for the ground state of helium atom.

21. Explain valence bond (VB) theory and VB theory of H_2 molecule.

22. What is GAMESS/FIRELY format? Give the input file for a) geometry optimization using STO-3G basis set b) optimization + frequency calculation using 6-31G basis set for ammonia molecule?

(2×5=10 weightage)