QP CODE: 24803034

24803034

Reg No : .....

Name : .....

INTEGRATED MSC DEGREE EXAMINATION, MAY 2024

Seventh Semester

INTEGRATED MSC BASIC SCIENCE-CHEMISTRY

CORE - ICH7CR02 - ADVANCED THEORETICAL CHEMISTRY AND COMPUTATIONAL CHEMISTRY

2020 Admission Onwards

ED44B589

Time: 3 Hours | Weightage: 30

Part A (Short Answer Questions)

*Answer any **eight** questions.*

*Weight **1** each.*

1. State and explain Schrodinger equation for Helium atom.
2. Explain the principle of Hartree-Fock method.
3. Write the Hamiltonian operator for He_2^+ molecule-ion.
4. Draw the MO energy level diagram of CO molecule.
5. Give the selection rule in IR spectroscopy.
6. List out the possible electronic transitions in a molecule.
7. Comment on the transformation properties of atomic orbitals.
8. Explain local density approximation.
9. Comment on the geometry optimization in GAMESS.
10. Write a note on CHARMM and its use in molecular mechanics.

(8×1=8 weightage)

Part B (Short Essay/Problems)

*Answer any **six** questions.*

*Weight **2** each.*

11. Explain perturbation treatment on the ground state of the helium atom.
12. Explain Roothan's concept of basis functions.

13. Discuss the quantum mechanical treatment of sp^2 hybridisaton.

14. Discuss the Huckel molecular theory of ethene.

15. Explain the orbital selection rules.

16. Write a note on group theory and optical activity.

17. Explain the notation MP2/6-31G (d,p)//HF/6-31G.

18. Distinguish between ab initio and semiempirical methods.

(6×2=12 weightage)

Part C (Essay Type Questions)

*Answer any **two** questions.*

*Weight **5** each.*

19. State and explain variation method. Illustrate it using the trial function x(a-x) to a particle in a 1 D box.

20. Explain MO and VB theories with suitable examples.

21. Using group theory explain the bonding in the following molecules: (i) BF_3 (ii) CH_4

22. Compare the different Density Functional Theory (DFT) methods.

(2×5=10 weightage)