20001119

20001119

Reg. No.....

Name.....

M.Sc. DEGREE (C.S.S.) EXAMINATION, NOVEMBER 2020

Second Semester

Faculty of Science

Branch : Chemistry

AN2C07/AP2C07/CH2C07/PH2C07/POH2C07—CHEMICAL BONDING AND COMPUTATIONAL CHEMISTRY

(2012—2018 Admissions)

[Common to all Branches of Chemistry]

Time : Three Hours Maximum Weight : 30

Section A

Answer any **ten** *questions.*
Each question carries weight 1.

1. What is a trial function ? What if any restrictions are there on the choice of trial function ?
2. Why approximation theorems are needed in quantum mechanics ?
3. Discuss the Pauli's exclusion principle based on quantum mechanical treatment.
4. What is meant by non - crossing rule ?
5. What is free valancy ? What is its significance ?
6. What are transition moment integrals ?
7. What is Jahn—Teller effect ?
8. How will you study the non-bonded interactions using computational method ?
9. Discuss the basic principles of configuration interactions.
10. Discuss the use of CHARMM in molecular mechanics.
11. Discuss the scope and future of computational chemistry.
12. What is meant by geometry optimization ?
13. What is Koopmans' theorem ?

(10 × 1 = 10)

Turn over

Section B

Answer any **five** *questions.*
Each question carries weight 2.

14. Distinguish between symmetric and antisymmetric wave functions.
15. Given any Hamiltonian, and given a trial function, write down the integrals that need to be solved to get the variational energy.
16. Discuss the valance bond theory of hydrogen molecule.
17. Explain the postulates of Born - Oppenheimer approximations.
18. Discuss the SALC construction of C2v and C2h point groups.
19. With an example, compare the molecular mechanics of computation studies, *ab initio* and semiempirical methods.
20. Describe the basic principle of hybrid functionals.
21. Briefly explain the classification of basic sets.

(5 × 2 = 10)

Section C

Answer any **two** *questions.*
Each question carries weight 5.

22. a) Illustrate the variation theorem for hydrogen atom.
    b) Explain the Hellmann – Feynman theorem.
23. a) Explain the molecular orbital treatment of the diatomic molecule CO.
    b) Explain the Hückel molecular orbital theory of ethane.
24. a) Construct a hybrid orbital with CH_4.
    b) Using suitable graphic packages, identify HOMO visualization of molecular orbitals.
25. a) What are force fields ? What are the important features of force fields ?
    b) Explain the DFT method.

(2 × 5 = 10)