19001839

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Reg. No.....

Name.....

M.Sc. DEGREE (C.S.S.) EXAMINATION, JUNE 2019

Second Semester

Faculty of Science

Branch : Chemistry

AN 2C 07/AP 2C 07/CH 2C 07/PH 2C 07/POH 2C 07—CHEMICAL BONDING AND COMPUTATIONAL CHEMISTRY

[Common to all Branches of Chemistry]

(2012 Admission onwards)

Time : Three Hours Maximum Weight : 30

Section A

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

1. What is a variational parameter ? How is it used ?
2. What are Slater type orbitals ?
3. What is the importance of Roothen's concept of basis functions ?
4. What are the limitations of Born Oppenheimer approximations ?
5. What are transition moment integrals ?
6. Using HMO method, how will you calculate free valancy ?
7. Discuss the importance of Woodward–Hoffmann rules.
8. What are correlation diagrams ? Why is it required ?
9. Distinguish between double zeta and triple zeta sets.
10. What are the important features of AMBER ?
11. What are Kohn Sham orbitals ? What is its physical meaning ?
12. Construct a firefly programme for the geometry optimization.
13. Identify the steps involved in calculating ionization energies.

(10 × 1 = 10)

Turn over

Section B

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

14. Discuss the qualitative approach of Hellmann - Feynmann theorem.
15. Briefly explain the quantum mechanical treatment of sp^3 hybridization.
16. Distinguish between singlet and triplet state functions.
17. Discuss the molecular orbital treatment of a planar conjugated molecule.
18. Briefly explain the SALC construction of C3v and D3h point groups.
19. With an example, compare the molecular mechanics of computation studies, semiempirical and DFT methods.
20. Discuss the principles of configuration interaction.
21. What is Z- matrix ? Discuss the Z-matrix of a diatomic molecule.

(5 × 2 = 10)

Section C

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

22. Estimate the energy of the ground-state wave function within first-order perturbation theory of a system with particle in a one dimensional box.
23. By taking suitable examples compare the molecular orbital theory and valance band theory.
24. (a) Discuss the qualitative ideas on post Hartree–Fock methods.
    (b) Write an input file for the molecular mechanics methods using computational studies.
25. (a) Distinguish between generalized gradient approximation and local density approximation.
    (b) Explain the applications of quantum mechanics.

(2 × 5 = 10)