

G 2797

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Reg. No.....

Name.....

M.Sc. DEGREE (C.S.S.) EXAMINATION, AUGUST 2016

Second Semester

Faculty of Science

Branch : Chemistry

**AN2 C07/AP2 C07/CH2 C07/PH2 C07/POH2 C07—CHEMICAL BONDING AND
COMPUTATIONAL CHEMISTRY**

(Common to all branches of Chemistry)

[2012 Admissions]

Time : Three Hours

Maximum Weight : 30

Section A

Answer any ten questions.

Each question carries a weight of 1.

1. Calculate the average potential and kinetic energies of a harmonic oscillator in the ground state. Compare the results obtained with the classical results.
2. Distinguish between symmetric and antisymmetric wave functions.
3. Discuss the singlet and triplet state functions of H_2 .
4. What are the steps involved for the calculations of free valency ?
5. Draw the MO diagram of water.
6. What are the basic principles of configuration interaction ?
7. Deduce the steps involved in ionization energy calculation using computational methods.
8. What is meant by free valance ?
9. By taking a simple example, discuss briefly the spin orbitals for many electron atoms.
10. What is meant by non-crossing rule ?
11. What is meant by Z-matrix ?
12. What are the rules for constructing the wave functions for the hybrid orbitals ?
13. What are *four* useful chemical properties (quantities) that DFT calculates ?

(10 × 1 = 10)

Turn over

Section B

Answer any five questions.

Each question carries a weight of 2.

14. Explain the Density Functional Theorem.
15. What are Slater type orbitals ? How they are different from Gaussian type orbitals ?
16. Taking a simple example, compare the MO and VB theories.
17. What are molecular mechanics methods in computation chemistry ? Discuss.
18. Discuss the variation treatment for ground state of helium atom.
19. What are the steps involved in identifying HOMO visualizations of molecular orbitals ?
20. What is meant by semiempirical MO treatment ?
21. Pick out the important features of force fields for MM3 and MMFF.

(5 × 2 = 10)

Section C

Answer any two questions.

Each question carries a weight of 5.

22. What are the applications of Computation chemistry ?
23. Discuss the Hartree Self-Consistent Field method. Explain its qualitative treatment.
24. Explain the MO treatments of homonuclear diatomic molecules, Be₂ and N₂.
25. What are symmetry adapted linear combinations ? Discuss it for C_{2v}, C_{3v} and D_{3h} point groups.

(2 × 5 = 10)