15P2033

Reg. No..... Name.....

M.Sc. DEGREE END SEMESTER EXAMINATION APRIL 2017

SEMESTER **– 2: CHEMISTRY**

COURSE**: 15P2CHET07-15P2CPHT07: CHEMICAL BONDING AND COMPUTATIONAL CHEMISTRY**

(For Supplementary - 2015 Admission)

Time: Three Hours Max. Marks: 75

Section A

*(Answer any **ten** questions, Each question carries **2 marks)***

1. What is a trial function? Give an example.
2. State Hellmann-Feynman theorem and explain the terms.
3. What do you mean by Hartree-Fock limit?
4. State and explain Pauli's exclusion principle.
5. Explain Born-Oppenheimer approximation.
6. How will you generate a multi reference configuration interaction wave function?
7. What is correlation energy?
8. Obtain the spectroscopic term symbols for the ground state of B_2 molecule.
9. Differentiate between Slater and Gaussian functions?
10. What are saddle points? What do they imply?
11. What are the important features of MMFF?
12. Explain the term free-valency.
13. Explain the significance of Hohenberg-Kohn theorems.

(2 x 10 = 20)

Section B

*(Answer any **five** questions, Each question carries **5 marks)***

14. Write a note on first order perturbation theory.
15. (a) Construct the spin-orbitals for the ground state of He atom.
    (b) Draw the MO energy level diagram for CO molecule.
16. Using group theory construct the hybrid orbitals in CH_4 molecule.
17. Discuss Møller Plesset Perturbation Theory.
18. What are basis sets? Discuss (a) double zeta and (b) split valence basis sets

19. Write short note on semiempirical methods highlighting basic principles and terminology.
20. What is Z-matrix? Obtain the Z-matrix for ammonia molecule.
21. (a) Write down the slater determinant for the ground state of Be atom.
    (b) Construct spin orbitals for a multi electron system.

(5 × 5 = 25)

Section C

(*Answer any* ***two*** *questions, Each question carries* ***15 marks)***

22. Compare and contrast MO theory and VB theory with suitable example
23. What do you mean by electon correlation? Suggest a method to find it in the case of HF molecule using GAMESS. Show the relevant input files.
24. Obtain the SALCs for the pi orbitals of cyclopropenyl group.
25. Write the structure for Gaussian input file for water molecule.

(15 × 2 = 30)

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