Reg. No. :..... **Name** :.....**P228**

M SC DEGREE END SEMESTER EXAMINATION MAY - 2015

SEMESTER -2**M SC CHEMISTRY/ APPLIED CHEMISTRY**

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

Time: 3 Hours MaximumMarks: 75

Section A

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

1. Write the Hamiltonian for He atom in atomic unit by considering independent electron approximation.

2. Calculate the spin multiplicity of an atom in its ground state having outer shell electronic configuration $4s^2 3d^8$.

3. How does RHF method differ from UHF method?
4. What is meant by the Hartree-Fock limit?
5. Write the spectroscopic ground state term symbol for O_2
6. Write down all possible anitsymmetric wave functions for He atom in its first excited state.
7. Why are polarization functions and diffuse functions added in the basis sets? Explain with examples.

8. Why are GTO's more commonly used in quantum mechanical calculations over STO's?
9. How do you explain the direction of the dipole moment in CO?
10. How is configuration interaction different from Møller-Plesset theory?
11. How do you calculate the ionization energy of a molecule?
12. Write an input for calculating transition state using GAMESS program.

13. Explain the Hellman-Feynman theorem.

(2 × 10 =20)

Section B

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

14. Write the Z-matrix representation of eclipsed and staggered 1,2-dichloroethane by keeping a dummy atom at the center of the C=C bond.

15. Sketch the schematic representation of 1s STO function and its approximate wave functions obtained at the STO-1G, STO-2G and STO-3G levels.

16. Show that the angle between the two hybrid orbitals in the *sp*-hybridization in 180º.
17. Explain the term exchange correlation functional using suitable example.
18. Show that the Hartree-Fock ground state wave function is the zeroth-order wave function of Møller-Plesset perturbation theory.

19. How do *Ab inito* methods differ from DFT methods?
20. Justify that the numerical value of the force field energy does not have any physical meaning.
21. How do you construct the hybrid orbitals of boron atom in BF_3 using SALCs?

(5*5= 25)

Section C

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

22. Explain the use of appropriate approximation methods for estimating the effective nuclear charge in He atom.

23. Describe various potential energy terms used in molecular mechanics.
24. Write down the secular determinant for butadiene using HMO theory and estimate the π-bond orders and delocalization energy.

25. Describe the meaning of the notations used in Pople’s basis sets with suitable example.

(15 × 2 = 30)

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