Reg. No ..... Name **19P2045**

MSc DEGREE END SEMESTER EXAMINATION - MARCH/APRIL 2019

SEMESTER 2 : CHEMISTRY / PHARMACEUTICAL CHEMISTRY

COURSE : **16P2CHET08 / 16P2CPHT08 : THEORETICAL AND COMPUTATIONAL CHEMISTRY**

(For Regular – 2018 Admission and Supplementary – 2017/2016 Admissions)

Time : Three Hours Max. Marks: 75

Section A
Answer any 10 (2 marks each)

1. Given the following space part of an approximate wavefunction for Li^+ ion: $1/\sqrt{2}$ [1s(1)2p$_1$(2) + 2p$_1$(1)1s(2)], write a physically possible spin part for this wavefunction.
2. State the variation theorem. Mention its significance.
3. Explain how the Roothaan equations arise in the Hartree–Fock method. What additional approximations do they represent?
4. Construct the molecular orbital energy level diagram of LiH molecule.
5. Determine the term symbols for He_2 and He_2^+.
6. Calculate the π-bond order of ethylene in the first excited state.
7. What are the allowable spin functions for a two-electron system?
8. How does the software realize that the job of optimization of molecule is complete?
9. What is exchange correlation functional?
10. What is a saddle point? Explain its significance.
11. What is a protein structure file format?
12. Describe the torsional terms in a molecule.
13. Explain the notation MP2/6-311G(d,p)//HF/STO-3G

(2 x 10 = 20)

Section B
Answer any 5 (5 marks each)

14. Explain the independent electron model.
15. Explain the variation treatment for the ground state of helium atom.
16. Write a note on HFSCF theory.
17. Using HMO theory, determine the energies and wave functions of the pi electron system in allyl group.
18. Show that $c_1 = c_2$ in the ground state valence bond wave function of hydrogen molecule, given by
$\psi_{VB} = c_1\psi_1 + c_2\psi_2$.

19. Prove that the three sp^2 hybrid orbitals are directed at angles of 120° with respect to one another.
20. Distinguish between ab initio methods and semiempirical methods
21. What is double zeta and triple zeta basis sets? Which one is better and why?

(5 x 5 = 25)

Section C
Answer any 2 (15 marks each)

22. Explain perturbation method. How is perturbation method applied to evaluate the ground state energy of He atom.
23. Apply HMO theory to determine the wavefunctions and corresponding energies of π MOs of benzene. Sketch the MOs.
24. Explain the basic principles of computational chemistry based on Density Functional Theory (DFT)
25. Explain MM-MD simulation protocol. Write a flow chart for the molecular dynamics simulation of glycine in water. Analyse the results of the simulation.

(15 x 2 = 30)