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

M. Sc DEGREE END SEMESTER EXAMINATION - MARCH 2020

SEMESTER 2 : CHEMISTRY / PHARMACEUTICAL CHEMISTRY

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

(For Regular - 2019 Admission & Supplementary 2018/2017/2016 Admissions)

Time : Three Hours Max. Marks: 75

Section A

Answer any 10 (2 marks each)

1. Show that the Slater determinant formalism automatically incorporates the Pauli's exclusion principle by evaluating the He ground-state wave function, giving both the electrons the same quantum numbers.
2. How can you tell if one basis set is better than another in calculating the total energy of an atom?
3. Explain how the Roothaan equations arise in the Hartree–Fock method. What additional approximations do they represent?
4. Electrons in bonding molecular orbitals render stability to the bond. Why?
5. Show that $\psi_{sp} = \frac{1}{\sqrt{2}}(2s \pm 2p_z)$ is normalized.
6. Estimate the free valence index of carbon atoms in butadiene.
7. What is the concept of correlation diagrams in chemical bonding?
8. Explain the term Pople style basis sets with one example.
9. How does the software realize that the job of optimization of molecule is complete?
10. What is exchange correlation functional?
11. Describe non bonded interactions and electrostatic interactions in a molecule.
12. What is a protein structure file format?
13. What are the two basic approaches for parameterizing a forcefield?

(2 x 10 = 20)

Section B

Answer any 5 (5 marks each)

14. Explain the independent electron model.
15. What is the consequence of electron correlation in solving Schrodinger equation?
16. Show using an example that the following two formulations of the Pauli's exclusion principle are equivalent:
    a) Wave functions describing a many-electron system must change sign under the exchange of any two electrons.
    b) No two electrons may have the same values for all four quantum numbers.
17. Give an account of the Valence Bond theory of H_2 molecule.
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. A hybrid orbital has 25% *s*- and 75% *p*-character. Construct the wave functions for this set of hybrid orbitals.
20. State and explain Hohenberg-Kohn theorems. How are they implemented?.
21. Explain the relation between variation principle and SCF procedure.

(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. Discuss the Molecular Orbital treatment of H_2^+ ion. Sketch the molecular orbitals formed and explain the bonding.

24. a) Distinguish between potential energy diagram and potential energy surface.
    b) Compare and contrast the potential energy diagrams of ethane and butane.
    c) Explain how the potential energy diagram of butane can be generated using Gaussian software.

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)