I Semester M.Sc. Degree (CBSS-Reg./Suppl./Imp.)
Examination, October - 2019
(2014 Admn. Onwards)
CHEMISTRY
CHE1C.01: THEORETICAL CHEMISTRY - I

Time : 3 Hours

Max. Marks : 60

SECTION-A

Answer **All** questions in one word or sentence. Each question carries **1** mark. **(8x1=8)**

1. Write down Hamiltonian operator for an N-particle system.
2. What are stationary states?
3. What are the conditions to be satisfied for the particle to be in a box?
4. Classify the following into even and odd functions: $\tan x$; $(3+x)(3-x)$
5. E_1 and E_2 correspond to the energies of proposed trial functions, φ_1 and φ_2 for a system with latter being the most realistic guess. If E_0 is the real energy, write down these energies in ascending order.
6. What is Pauli's antisymmetry principle?
7. State Born-Oppenheimer approximation.
8. Calculate the number of basis functions for carbon atom using 6-31 1G basis set.

SECTION - B

Answer **Eight** questions. Answer may be **two** or **three** sentences. Each question carries **2** marks. **(8 x 2= 16)**

9. Normalize the function, $\sin(2\pi x)$ with x varies between 0 and 1.
10. Express (x+iy) in terms of spherical polar coordinates.
11. Explain orthonormalized functions.

P.T.O.

K19P 1477

12. Write down the del squared operator in spherical polar coordinates.
13. What is Rodrigues formula?
14. Give the potential energy diagrams of SHO and hydrogen molecule. Why do these differ?
15. Write down possible spin function and orbital functions for the electronic configuration, $1s^1\ 2s^1$.
16. State two limitations of perturbation methods.
17. Write down the Slater determinant for the ground state of Li atom and show that all three electrons cannot occupy the 1s orbital.
18. What are split-valence basis sets? Give an example.
19. How will you calculate the π- charge density of conjugated molecule?
20. Write down the ground state term symbol of i) C_2; ii) CO

SECTION – C

Answer **Four** questions in short paragraph for each. Each question carries **3** marks.   (4x3=12)

21. Explain Davisson-Germer experiment. What it demonstrates?
22. What is zero point energy? What are their values for a planar rigid rotor and SHO? Justify that these values are in agreement with Heisenberg's uncertainty principle.
23. Write down the Schrodinger equation of Hydrogen atom in spherical polar coordinates and separate the variables.
24. Write down the explicit form of complete wave function and energy of nonplanar rigid rotor explaining each term.
25. Explain self consistent field method.
26. State and prove variational theorem.
27. Differentiate between STO and GTO.
28. Give the MO and VB approximation for the ground state of H_2 molecule and highlight the basic difference between the two.
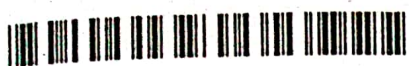
SECTION - D

Answer either **a** or **b** of each question. Each question carries **6 marks**.

(4x6=24)

29. a) Deduce time dependent Schrodinger equation from classical wave equation.

(OR)

b) Explain the postulates of Quantum mechanics.

30. a) Arrive at the energy and wave function of planar rigid rotor.

(OR)

b) Explain radial distribution functions. Plot these for 1s, 2s, 2p, 3p and 4d.

31. a) Derive first order perturbation correction to energy for a nondegenerate system.

(OR)

b) Derive the various atomic term symbols for carbon atom and arrange them in the order of energy.

32. a) Explain Hartree-Fock theory for molecules.

(OR)

b) Calculate the C-C π-bond order in benzene using Huckel molecular orbital treatment.

_____