K23P 3260

Reg. No. : .....

Name : .....

First Semester M.Sc. Degree (CBSS – Supple. (One Time Mercy Chance)/Imp.) Examination, October 2023
(2014 to 2022 Admissions)
CHEMISTRY
CHE1C.01 : Theoretical Chemistry – 1

Time : 3 Hours Max. Marks : 60

SECTION – A

(Answer **all** questions in **one** word or **one** sentence. **Each** question carries **one** mark)

1. Find the normalization of ψ = ASinx, where x = 0 to π.
2. Prove Hamiltonian operator is a Hermitian operator.
3. A particle is confined in 3-D box having energy $9h^2/8ma^2$. Write down the possible energy states.
4. Write down the quantum mechanical postulate for operator and justify Hamiltonian operator satisfy the postulate.
5. Write two differences between variation treatment and perturbation treatment.
6. What is meant by Kronecker delta ? Find the Kronecker delta for $\sqrt{2}$ /aSinπx and $\sqrt{2}$ /aSin2πx, limit 0 to a.
7. What is meant by quantum mechanical tunnelling ?
8. Explain the term split valence basis set. **(8×1=8)**

SECTION – B

(Answer **any eight** questions. **Each** question carries **2** marks)

9. Discuss Planck's hypothesis of black body radiation.
10. Find the expectation value of momentum of particle in 1-D box.

P.T.O.

11. Write down the Slater determinant for He atom.
12. Discuss the advantages of *Ab initio* method.
13. Prove that the Sinkx is an eigen function of a Hamiltonian operator.
14. Briefly explain the postulates for an ideal wavefunction.
15. Compare the energy equations for a harmonic oscillator, derived classically and quantum mechanically.
16. What are the assumptions of Huckel MO theory ?
17. Differentiate linear operator and non-linear operator with suitable examples.
18. Show that x and Px do not commute.
19. Justify the conversion of polar coordinates to spherical polar coordinates while solving the H atom.
20. Justify the need for approximation methods to solve energy of a multi-electron atom. **(8×2=16)**

SECTION – C

(Answer **any four** questions. **Each** question carries **3** marks)

21. State and explain the perturbation theory and derive the energy of a particle in slanted bottom.
22. Show that $[L^2, L_z] = 0$.
23. Write a brief account of classification of basis sets.
24. Discuss semi-empirical methods in computational chemistry.
25. Explain the following (a) linear operator (b) symmetry breaking.
26. Derive the principle quantum number of hydrogen atom.
27. Explain L-S coupling with an appropriate example.
28. What is meant by recursion formula in harmonic oscillator ? Show that the recursion formula provides odd gives odd values and even gives even values. **(4×3=12)**

SECTION – D

(Answer **any four** questions. **Each** question carries **6** marks)

29. A) Derive quantum mechanically the energy of a Simple Harmonic Oscillator and its wave function.

OR

B) Derive and discuss the variation treatment of Helium atom and compare the energy to experimental value.

30. A) Discuss and solve the rigid rotor by quantum mechanical treatment. How it is useful to solve the energy of hydrogen atom ?

OR

B) Give an account of MO theory of conjugated systems and explain the aromaticity of benzene.

31. A) Briefly discuss Self Consistent Field theory with suitable illustrations.

OR

B) Elaborate the spin of an electron and comment about its coupling with angular momentum.

32. A) Compare the MO treatment and VB treatment of H_2 molecule.

OR

B) Briefly discuss the hybridization and geometry of the following molecules :
   a) Methane
   b) Water
   c) Acetylene. **(4×6=24)**
