K21P 4175

Reg. No. : .....

Name : .....

I Semester M.Sc. Degree (C.B.S.S. – Reg./Supple./Imp.) Examination, October 2021
(2018 Admission 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 : **(8×1=8)**

1. Which of the following functions is acceptable ?
   a) $\psi = x$ b) $\psi = x^2$ c) $\psi = \sin x$ d) $\psi = e^{-x}$
2. What are eigenfunctions ?
3. The energy of a particle in a box is found to be $9\ h^2/8\ ma^2$. Find out the value of principle quantum number.
4. Write the equation for energy of a rigid rotor.
5. Write down the perturbation term for helium atom.
6. What is associate Legendre polynomial ?
7. What are Slater type orbitals ?
8. Define basis set.

SECTION – B

Answer **any eight** questions in **two** or **three** sentences. **Each** question carries **2** marks : **(8×2=16)**

9. Explain Hermitian operator.
10. Evaluate the commutator $[d/dx, d^2/dx^2]$.

P.T.O.

11. State and explain expectation value postulate of quantum mechanics.
12. What is a well behaved wave function ?
13. Write down the wave function corresponding to the energy $6h^2/8ma^2$.
14. Verify that ψ = Asinkx + Bcoskx is a general solution for a particle in a one dimensional box of infinite potential wall.
15. What are Hermite polynomials ? Find out the values of first two Hermite polynomials.
16. Discuss the significance of quantum numbers n, l and m.
17. Using atomic units write the complete Hamiltonian for electronic motion in hydrogen atom in spherical polar coordinates.
18. Mention the problem facing by many electron system. How it can be solved ?
19. What is a spin orbital ?
20. Give the determinantal wave functions of a 3 electron system.

SECTION – C

Answer **any four** questions in short paragraph. **Each** question carries **3** marks : **(4×3=12)**

21. Explain black body radiation.
22. Consider the wave function ψ = A sin kx. Find the eigenvalue of this function for the operator d^2/dx^2.
23. Draw the molecular orbital diagram of CO molecule.
24. How do you apply Huckel theory to allyl system ?
25. What do you mean by self-consistent field method ?
26. Calculate the ground state energy of butadiene molecule using particle in a box model. (C-C single and double bond lengths are 1.54 Å and 1.34 Å respectively)
27. What are Laguerre polynomials ?
28. Draw the radial plot of Px orbital.

SECTION – D

Answer either **a** or **b** of **each** question. **Each** question carries **6** marks : **(4×6=24)**

29. a) Discuss the postulates of quantum mechanics.

OR

b) Explain the method of variation applied to Helium atom.

30. a) What are antisymmetric wave functions ? Construct the slater determinant of a system with four electrons.

OR

b) What is VBT ? Apply VBT to hydrogen molecule.

31. a) Discuss semi empirical and abinitio method used in computational chemistry.

OR

b) What are operators ? Explain different operators used in quantum mechanics.

32. a) Discuss the quantum mechanics of simple harmonic oscillator.

OR

b) Discuss the importance of angular momentum in quantum mechanics. What are ladder operators ?
