K22P 1567

Reg. No. : .....

Name : .....

I Semester M.Sc. Degree (CBSS – Reg./Sup./Imp.) Examination, October 2022
(2019 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. Write down the expression for Fock operator.
2. Define free valence.
3. Express the energy equation of a Harmonic oscillator.
4. Define minimal basis set.
5. What are Lagendre polynomial ?
6. Write down the Hamiltonian for He atom in atomic unit.
7. Write down the perturbation term for H_2 molecule.
8. Draw the angular distribution diagram of 2pz orbital.

SECTION – B

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

9. State variation theorem.
10. Define STO and GTO.
11. Discuss the hybridization of water molecule.
12. What are commutators ?

P.T.O.

13. State Pauli's antisymmetry principle.

14. What are Coulomb integrals ?

15. Write down the molecular term symbol for O_2 molecule.

16. Give any two assumptions of Huckel's theory.

17. What is meant by semi empirical methods ?

18. Explain Born-Oppenheimer approximation.

19. Write down the minimum energy at which degeneracy exist for particle in one dimensional box.

20. How dual character of electron is confirmed ?

SECTION – C

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

21. What is an eigen function ? Explain with example.

22. Define spherical harmonics.

23. Draw the molecular orbital diagram of LiH molecule.

24. Briefly give the assumptions of VBT.

25. Find the commutators of d/dx and d^2/dx^2 for the function e^{-ikx}.

26. What is meant by complex conjugate ?

27. What is a Laplacian operator ?

28. Find the first order correction in energy of a particle in a box model.

SECTION – D

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

29. a) Explain Huckel's theory of molecular orbital using suitable example.

OR

b) Discuss the complete quantum mechanical treatment of a rigid rotator.

30. a) Compare and contrast VBT and MOT.

OR

b) Explain Hartree-Fock-self-consistent field method.

31. a) Give a brief account of approximation method used in quantum mechanics.

OR

b) Discuss the operator postulates in quantum mechanics.

32. a) How MOT is successful in explaining the bonding in H_2^+ ion ?

OR

b) Discuss valence bond theory applied to H_2 molecule.