



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 Legendre 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 ?

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K22P 1567

-2-



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.



-3-

K22P 1567

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.