QP Code: U25C049

Reg. No : .....
Name : .....

ST MARY'S COLLEGE (AUTONOMOUS), THRISSUR-20

III SEMESTER (FYUGP) DEGREE EXAMINATIONS, OCTOBER 2025
B. Sc. Chemistry
CHE3CJ201 : THEORETICAL CHEMISTRY I : BASIC QUANTUM CHEMISTRY
2024 Admission Onwards
(Credits: 4)

Time: 2 Hours **Maximum Marks: 70**

Section A

*Answer **all**. Each question carries **3** Marks.* ***(Ceiling: 24 Marks)***

1. What are the characteristics of blackbody radiation? Give an example of a blackbody.
2. The threshold wavelength of a metal is 6800 A^o. Calculate the threshold frequency and work function. [h = 6.625×10^{-34} Js]
3. Explain the term quantum tunnelling and its significance.
4. Discuss the terms Laplacian and Hamiltonian Operators.
5. Give the angular distribution plots for the *p*-orbitals.
6. What is meant by 'degeneracy'?
7. Describe the bonding in the O_2 molecule through orbital overlap within the framework of Valence Bond Theory.
8. What are the basic principles of Molecular Orbital Theory?
9. What are the coefficients of *s*, p_x, and p_y orbitals in the wave function of the sp^2 hybrid orbital constructed by LCAO?
10. Define Hybridization. What is the need of hybridization?

Section B

*Answer **all**. Each question carries **6** Marks* ***(Ceiling: 36 Marks)***

11. Derive the de Broglie relation and explain its significance.
12. Discuss the line spectrum of the Hydrogen atom.
13. Illustrate the concept of the spin quantum number through the Stern-Gerlach experiment.

Turn Over

14. Write down the Hamiltonian for Hydrogen-like systems and also give the corresponding time-independent Schrodinger equation.

15. Discuss the postulates of Quantum mechanics.

16. Compare the bond length of NO, NO^+, and NO^- using bond order derived from the MO configuration.

17. What is a molecular orbital (MO) diagram? Explain why the energy order of the molecular orbitals of N_2 differs from that of the O_2 molecule.

18. Compare the theoretical and experimental potential energy profiles of the H_2 molecule. What causes any discrepancies?

Section C

*Answer **any one**. Each question carries **10** Marks* ***(1x10=10marks)***

19. Explain the structure and geometry of PCl_5, CH_4, BH_3, and BeF_2 molecules with the help of the concept of hybridization.

20. Solve the wave function and energy of the particle in a 1D box using the Schrödinger wave equation and plot the wave and probability densities as well.

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