24U320 (Pages: 2) Name : .....

Reg. No : .....

THIRD SEMESTER UG DEGREE EXAMINATION, NOVEMBER 2025

(FYUGP)

CC24UCHE3CJ201 - THEORETICAL CHEMISTRY-I: BASIC QUANTUM CHEMISTRY

(B.Sc. Chemistry - Major Course)

(2024 Admission - Regular)

Time: 2.0 Hours Maximum: 70 Marks

Credit: 4

Part A (Short answer questions)

Answer ***all*** questions. Each question carries 3 marks.

1. What is Bohrs frequency rule? [Level:2] [CO1]
2. Differentiate between a spin orbital and a spatial orbital, with an example. [Level:2] [CO2]
3. How did Einstein extend Plank's quantum theory? [Level:2] [CO1]
4. Find the eigen value for wave function $\Psi=3e3x$; for the operator d/dx. [Level:2] [CO2]
5. Explain how the Stern–Gerlach experiment demonstrated the quantization of electron spin. Why was this result unexpected from a purely classical point of view? [Level:1] [CO2]
6. State variation theorem. [Level:2] [CO3]
7. Write MO configuration of CO molecule and calculate bond order. [Level:3] [CO3]
8. Calculate the uncertainty in the momentum of a particle whose uncertainty in position is of the order 1A. [Level:3] [CO2]
9. For a particle in a 3D cubic box, determine the degeneracy of the energy level corresponding to quantum numbers (nx,ny,nz)=(2,2,1). [Level:3] [CO2]
10. State the Born–Oppenheimer approximation. Why is it valid to treat nuclei as fixed while solving the electronic Schrödinger equation? [Level:1] [CO3]

(Ceiling: 24 Marks)

Part B (Paragraph questions/Problem)

Answer ***all*** questions. Each question carries 6 marks.

11. Describe how quantum tunnelling explains the working principle of the Scanning Tunnelling Microscope (STM). [Level:2] [CO2]

12. An electron at rest is accelerated through 10 kV potential. The de Broglie wavelength (in Å) of the electron is _____. (round off to three decimal places) [Given: Mass of an electron, me = 9.11×10^{-31} kg; Planck's constant (h) = 6.63×10^{-34} J s; 1 eV = 1.6×10^{-19} J] [Level:3] [CO1]

13. Write the time-independent Schrödinger equation for a free particle in one dimension and write the general form of the wave function. [Level:2] [CO2]

14. Calculate the ground state energy of an electron confined in a one dimensional box of length 0.3 nm. Also calculate its energy when it is in n=3 level. [Level:3] [CO2]

15. Make comparison of of VB and MO theories. [Level:2] [CO3]

16. Give three differences between bonding and antibonding molecular orbitals. [Level:2] [CO3]

17. Explain penetration and shielding effects. [Level:2] [CO2]

18. Discuss shape of PCl_5 molecule on the basis of hybridization. [Level:2] [CO4]

(Ceiling: 36 Marks)

Part C (Essay questions)

Answer any ***one*** question. The question carries 10 marks.

19. Evaluate the coefficients of sp^2 hybrid orbitals using LCAO and draw the schematic plot. [Level:2] [CO4]

20. (a) What are quantum numbers? [Level:2] [CO2]
    (b) Discuss the significance of each quantum number.

(1 × 10 = 10 Marks)

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