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KIBABII UNIVERSITY

UNIVERSITY EXAMINATIONS

2021/2022 ACADEMIC YEAR

FOURTH YEAR SECOND SEMESTER

MAIN EXAM

FOR THE DEGREE OF BACHELOR OF SCIENCE

COURSE CODE: SCH 413

COURSE TITLE: QUANTUM CHEMISTRY

DURATION: 2 HOURS

DATE: 05/09/2022
20/08

TIME: 9:00AM-11:00AM

INSTRUCTIONS TO CANDIDATES

- Answer **QUESTION ONE** (Compulsory) and any other two (2) Questions.
- Indicate **answered questions** on the front cover.
- Start every question on a new page and make sure question's number is written on each page.

This paper consists of 3 printed pages. Please Turn Over



KIBU observes ZERO tolerance to examination cheating

QUESTION ONE (30 Marks)

1a). Define the following terms as used in quantum chemistry. (5marks)

- i. Wavefunction
- ii. Black body
- iii. Photoelectric effect
- iv. Operator
- v. Heisenberg uncertainty principle.

b). A particle of mass 2.00×10^{-26} g is in a one-dimensional box of length 4.00 nm. Find the frequency and wavelength of the photon emitted when this particle goes from the $n = 3$ to the $n = 2$ level. (5marks)

c). State four characteristics of the photoelectric effect (4marks)

d). Give four failures of classical physics (4 marks)

e). State the Significance of ψ and ψ^2 then explain the Born interpretation of the wavefunction, (2 marks)

f). The uncertainty in the position and velocity of a particle are 10^{-10} m and 5.27×10^{-24} m sec⁻¹ respectively. Calculate the mass of the particle. (4marks)

g) Giving examples briefly explain importance of Hermitian operators (3 marks)

h). State the two main origins of zero-point energies for both particle in a box and the harmonic oscillators. Why can't $n \neq 0$ while $v=0$ for a particle in a box and for a harmonic oscillator respectively. (3marks)

QUESTION TWO (20 Marks)

2 a). Find the probability of finding the particle in the first tenth (from $x = 0$ to $x = \frac{L}{10}$) of the box for $n = 1, 2$ and 3 states. (8 marks)

b). Explain the comparison between classical mechanics and quantum mechanics. (8 marks)

c). State characteristics of the Schrödinger's Wave Equation. (4marks)

QUESTION THREE (20 Marks)

- 3 a). Show that $m \frac{d^2X}{dt^2} + kX = 0$ also applies to mass m_1 connected to mass m_2 by a spring exhibiting harmonic motion. (10 marks)
- b). Demonstrate that the ground-state harmonic oscillator wave-function is either
- i. Normalized with the first excited state. (4 marks)
 - ii. Orthogonal with the first excited state. (3 marks)
- c). Calculate the ground-state energy for an electron that is confined to a potential well with a width 0.2 nm. (3 marks)

QUESTION FOUR (20 Marks)

- 4 a). Derive the Schrödinger's wave equation. (10 marks)
- b). Explain the five postulates of quantum mechanics. (10 marks)

QUESTION FIVE (20 Marks)

- 5 a) Calculate the ionization energy E_i for hydrogen like atom of H, He^+ , Li^{2+} and Be^{3+} whose $E_i=13.606 \text{ eV}$. (4 marks)
- b). Determine the term symbol for a hydrogen atom ignoring spin orbit coupling in a) ground-state, b) the 2s orbital, c) the 2p orbital, and d) a 3d orbital. (8 marks)
- c). Determine the trajectory of a projectile fired from a cannon whereby the muzzle is at an angle from the horizontal x-axis and leaves the muzzle with a velocity of Assume that there is no air resistance. (6 marks)
- d). Explain what will happen when the walls of the one-dimensional box are suddenly removed (2marks)

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