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(University of Choice)

MASINDE MULIRO UNIVERSITY OF SCIENCE AND TECHNOLOGY (MMUST)

SPECIAL/SUPPLIMENTARY EXAMINATIONS

2021/2022 ACADEMIC YEAR

THIRD AND FORTH YEAR FIRST SEMESTER EXAMINATIONS

FOR THE DEGREE

OF

BACHELOR OF SCIENCE

(CHEMISTRY AND INDIUSTRIAL CHEMISTRY)

COURSE CODE: **SCH 340**

COURSE TITLE: **QUANTUM CHEMISTRY**

DATE: Wednesday, 27th July 2022 **TIME:** 8.00 - 10.00 am

INSTRUCTIONS TO CANDIDATES

- Answer all the Questions

TIME: 2 Hours

Useful Information

$R = 8.314\ JK^{-1}\ mol^{-1}$ or $0.08206\ L\ atm\ K^{-1}\ mol^{-1}$

$1\ atm = 1.01325\ bar = 760\ torr = 1.01325 \times 10^5\ Pa = 760mmHg$

QUESTION ONE (20 MARKS)

a) The energy required for the ionization of a certain atom is $1.224 \times 10^{-18}J$. The absorption of a photon of unknown wavelength ionizes the atom and ejects an electron with velocity $3.09 \times 10^6\ ms^{-1}$. Calculate the wavelength of the incident radiation **[4 marks]**

b) The wavefunction of an electron in the lowest energy state of a hydrogen atom is proportional to $e^{-(r/a0)}$, with $a_0 = 52.9pm$ and r is the distance from the nucleus. Calculate the relative probabilities of finding the electron inside a small volume δV located at:
   i. The nucleus **[2 marks]**
   ii. A distance a_0 from the nucleus **[2 marks]**

c) Discuss any four characteristics of the photoelectric effects **[4 marks]**

d) Explain the meaning and consequences of the of the wave-particle duality **[4 marks]**

e) Briefly discuss any four postulates of quantum mechanics **[4 marks]**

QUESTION TWO (15 MARKS)

a) The following function represents an unnormalized excited state wavefunctions of the hydrogen atom. Normalize it to 1. $\Psi = [3 - r/a_0]e^{-(2r/a_0)}$ **[5 marks]**

b) Is the function in (a) above mutually orthogonal with $\psi = r\sin\Theta\cos\Phi\ e^{-(r/a_0)}$? **[7 marks]**

c) Define, justify, and provide examples of zero-point energy. **[3 marks]**

QUESTION THREE (20 MARKS)

a) Calculate the most probable radius (r) at which an electron will be found when it occupies a 1s orbital of a hydrogenic atom of atomic number Z=2. **[5 marks]**

b) Starting with the classical relation between kinetic energy and linear momentum, construct operator for kinetic energy **[6 marks]**

c) Explain using equations why the ΔE for a particle in a box increases with n^2 **[5 marks]**

d) Identify the levels that may arise from the configurations h^1 and g^1 **[4 marks]**

QUESTION FOUR (15 MARKS)

a) Explain the origin of spin–orbit coupling and how it affects the appearance of a spectrum. **[5 marks]**

b) Normalize the wavefunction $e^{-r/a0}$ used for the hydrogen like atom **[5 marks]**

c) Prove that the Schrodinger equation can be used to imply De Broglie relation **[5 marks]**

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