



KIBABII UNIVERSITY

UNIVERSITY EXAMINATIONS
2020/2021 ACADEMIC YEAR
FOUR YEAR SECOND SEMESTER
SPECIAL/SUPP' EXAMINATIONS
FOR THE DEGREE OF SCIENCE

COURSE CODE: SCH 411

COURSE TITLE: QUANTUM CHEMISTRY

DURATION: 2 HOURS

DATE: 20/1/2022

TIME: 2-4PM

INSTRUCTIONS TO CANDIDATES

- Answer **QUESTION ONE** (Compulsory) and any other two (2) Questions
- Indicate answered questions on front cover.
- Start every question on a new page and make sure question's number is written on each page.
- You are provided with graph papers where necessary.

This paper consists of 4 printed pages. Please Turn Over 

KIBU Observes ZERO tolerance to examination cheating

Useful Information

$$R = 8.314 \text{ JK}^{-1} \text{ mol}^{-1} \text{ or } 0.08206 \text{ L atmK}^{-1} \text{ mol}^{-1}$$

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

$$e = 1.60217662 \times 10^{-19} \text{ C}$$

$$IJ = CV = 1 \text{ Kgm}^2 \text{ s}^{-2}$$

$$h = 6.626 \times 10^{-34} \text{ Js}$$

$$N_A = 6.022 \times 10^{23} / \text{molecules}$$

QUESTION ONE (30 MARKS)

- a) Define the following terms as used in quantum chemistry [10 marks]
- Uncertainty principle
 - Quanta
 - Degeneracy
 - Black body
 - Operator
- b) Distinguish between photoelectric effect and Compton effect [3marks]
- c) Give the planck's distribution law [2 marks]
- d) Calculate the ionization energy E_i for hydrogen like atom of H, He^+ , Li^{2+} and Be^{3+} whose $E_i = 13.606 \text{ eV}$ [3 marks]
- e) Find the wavelength in \AA of the line in Balmer series that is associated with drop of the electron from the fourth orbit. The value of Rydberg constant is $109,676 \text{ cm}^{-1}$ [5 marks]
- f) What is the ground state energy for an electron that is confined to a potential well with a width of 0.2 nm ? [5 marks]
- e). State four characteristics of the photoelectric effect [4 marks]

QUESTION TWO (20 MARKS)

- a). Explain the five postulates of quantum mechanics [10 marks]
- b). Explain the comparison of classical mechanics with quantum mechanics [8marks]
- c) State the shortcomings of Bohr' model of the atom [2 marks]

QUESTION THREE (20 MARKS)

- a). Derive the Schrödinger's Wave Equation as used in quantum chemistry [10marks]
- b). State characteristics of the Schrödinger's Wave Equation [6marks]
- c). Explain the meaning of Ψ^2 and Ψ [4marks]

QUESTION THREE (20 MARKS)

- a) Calculate the minimum uncertainty in the velocity of an electron if the uncertainty in its position is 100pm [3 marks]
- b) Calculate the energy required for a transition from $n_x = n_y = n_z = 1$ to $n_x = n_y = n_z = 2$ for an electron in a cubic hole of a crystal having edge length = 1Å^0 [3marks]
- c) Explain what is meant by harmonic oscillator as used in quantum theory [2 marks]
- d) Explain what happens if the walls of the one dimensional box are suddenly removed [3marks]
- e) 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 [6 marks]
- f) Explain quantum mechanical principles that are involved in the formation of hybrid orbitals from atomic orbitals [6 marks]

QUESTION FIVE (20 MARKS)

- 5a). State three modes of motion [3 marks]
- b). Calculate the expected ground state energy of a hydrogen atom electron assumed to be present in a three-dimensional cubical box of 0.1nm length if the ground-state energy of the electron in one-dimensional box of 0.3nm length is 4eV [4 marks]
- c). 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. [2marks]
- c). Calculate the most probable radius r at which an electron will be found when it occupies a 1s orbital of a hydrogen atom of atomic number Z and tabulate values for $1 e^-$ species from H to Ne [5marks]
- d) Show that e^{ax} is an *Eigen* function of the operator d/dx and find corresponding *Eigen* value. Also show that e^{ax^2} is non an *Eigen* function of the same operator. [6marks]

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