KIBABII UNIVERSITY

UNIVERSITY EXAMINATIONS
2019/2020 ACADEMIC YEAR

SECOND YEAR SECOND SEMESTER
MAIN EXAMINATIONS

FOR THE DEGREE OF BED (SCIENCE)

COURSE CODE: SCH 411

COURSE TITLE: QUANTUM CHEMISTRY

DURATION: 3 HOURS

DATE: 10TH NOVEMBER, 2020 **TIME: 2:00PM-5:00PM**

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 **4** printed pages. Please Turn Over

Useful Information

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

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

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

$1J = CV = 1Kgm^2s^{-2}$

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

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

QUESTION O N E (30 M A R K S)

a) Define the following terms as used in quantum chemistry [**8** marks]

i. Wave-function

ii. Photo electric effect

iii. Wave-particle duality

iv. Black body

b) Calculate the minimum uncertainty in the velocity of an electron if the uncertainty in its position is 100pm [5 marks]

c) Calculate the wavelength of the line with n=5 in the Balmer series of the spectrum of atomic hydrogen. [5 marks]

d) What is the ground state energy for an election that is confined to a potential well with a width of 0.2 nm? [5 marks]

e).What is the de-Broglie wavelength of an electron that has been accelerated through a potential difference of 100v. [5 marks]

f) State two basic principle of classical mechanic [2 marks]

QUESTION TWO (20 MARKS)

a).Derive the Schrödinger's Wave Equation as used in quantum chemistry [10marks]

b). State significance of the Schrödinger's Wave Equation [6marks]

c). Explain the meaning of Ψ^2 and Ψ [4marks]

QUESTION THREE (20 MARKS)

a) Show that $m\frac{d^2X}{d^2} + kX = 0$ also applies to mass m_1 connected to mass m_2 by a spring exhibiting harmonic motion [6 marks]

b) Normalize the molecular orbital $\Psi = N(A-B)$ state the meaning of the overlap integral S in thisprobability of this wave function. [6 marks]

c) What is the Ritzs combination principle [4marks]

d) Calculate the ionization energy Ei for hydrogen like atom of H, He^{+}, Li^{2+} And Be^{3+} whose Ei=13.606 ev [4marks]

QUESTION FOUR (20 MARKS)

a). Explain the five postulates of quantum mechanics [10 marks]

b).What are the reduced mass and moment of inertia of HCl?. The equilibrium internuclear distance Re is 127.5pm. What are the values of L, L_Z and E for the state with j=1? Atomic masses of some of H=1.007825 $.10^{-3}kgmol^{-1}$and Cl^{35}= $34.96885.10^{-3}kgmol^{-1}$ and

h=$1.054.10^{-34}$ [10marks]

QUESTION FIVE (20 MARKS)

5a). State three modes of motion [3 marks]

b). Discuss the two main origins of zero-point energies for both particle in a box and the harmonic oscillators. Why can't n≠O while v=0 for a particle in a box and for a harmonic oscillator respectively. [3marks]

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 1 e^{-} species from Hydrogen to Neon [6marks]

d) Show that e^{ax} is an *Eigen* function of the operator d/dx and find corresponding *Eigen* value. Also show that e^{ax2} is non an *Eigen* function of the same operator. [5marks]

e). Draw the schematic diagram for the lowest energy molecular or orbital of Homo-nuclear diatomic molecules [3marks]

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