KIBABII UNIVERSITY

UNIVERSITY EXAMINATIONS
2017/2018 ACADEMIC YEAR

FOURTH YEAR SECOND SEMESTER
SUPPLEMENTARY EXAMINATIONS

FOR THE DEGREE OF SCIENCE

COURSE CODE: SCH 411

COURSE TITLE: QUANTUM CHEMISTRY

DURATION: 2 HOURS

DATE: 01/10/2018 **TIME: 11:30-1:30PM**

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.
- You are provided with graph papers where necessary.

This paper consists of 4 printed pages. Please Turn Over

Useful Information

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

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

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

$IJ = CV = lKgm^2s^{-2}$

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

$N_A = 6.022\ X10^{23}$ /molecules

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

a) Define the following terms as used in quantum chemistry **[4 marks]**

i. Ritzs combination
ii. The harmonic oscillator
iii. Uncertainty principle
iv. Orbital

b) State the properties of black body **[3 marks]**

c) Calculate the wavelength of a photon needed to excite a transition between neighbouring energy levels of a harmonic oscillator of effective mass equal to that of a proton (1.0078 u) and force constant 855 N m^{-1} **[5 marks]**

d) Calculate the value of **[x]** and **[x^2]** for a particle in a one dimensional box **[4 marks]**

e) What are the electron configuration for H^-, Li^+ O^{2-},F^-,Na^+ and Mg^{2+} **[4 marks]**

f) The work faction for metallic caesium is 2.14eV. Calculate kinetic energy and the speed of electron ejected by light of wave length 250nm. **[4 marks]**

g) A photodetector produces 0.68μW when exposed to radiation of wavelength 245 nm. How many photons does it detect per second? **[3 marks]**

State two basic principle of classical mechanic

h) Calculate the minimum uncertainity in the speed of a ball of a mass 500g that is known to be within 5.0μm of certain point on a bat **[3 marks]**

QUESTION TWO (20MARKS)

a) Arrange the species O_2^+, O_2, O_2^- in order of increasing bond length and comment on the stability of these species **[6 marks]**

b) Normalize the molecular orbital Ψ =N(A-B) state the meaning of the overlap integral S in this probability of this wavefunction. **[8 marks]**

c) Starting from the general formula for kinetic energy, prove that the energy of separation of a particle confined into some box of length L increases with the value n and decreases with the increase in the length of the box. **[6 marks]**

QUESTION THREE (20MARKS)

a) Identify which of the following functions are eigenfunctions of the operator d/dx: (i) e^{ikx} (ii) cos kx, (iv) kx, (v) e^{-ax^2}. Give the corresponding eigenvalue where appropriate. **[6 marks]**

b) Explain why Einstein's introduction of quantization accounted for the properties of heat capacities at low temperatures. **[6 marks]**

c) Starting from the operator $I_z = xp_y - yp_x$, prove that in spherical polar coordinates $1_z = -i\hbar\partial/\partial\varphi$ **[6 marks]**

d) State the four postulates of quantum mechanics **[2 marks]**

QUESTION FOUR (20M A R KS)

a) Normalize the wave function, sin(a+x) **[10 marks]**

b) Discuss the two main origins of zero-point energies for both particle in a box and the harmonic oscillators. Why can't $n\neq0$ while $v=0$ for a particle in a box and for a harmonic oscillator respectively. **[5 marks]**

c) Give the possible term symbols for Sc [Ar] $3d^14s^2$ and Br [Ar] $3d^{10}4s^24p^5$. **[5 marks]**

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