KIBABII UNIVERSITY

UNIVERSITY EXAMINATIONS
2020/2021 ACADEMIC YEAR
FOURTH YEAR SECOND SEMESTER
MAIN EXAMINATIONS
FOR THE DEGREE OF SCIENCE

COURSE CODE: SCH 411

COURSE TITLE: QUANTUM CHEMISTRY

DURATION: 2 HOURS

DATE: 8/10/2021 **TIME: 8:00-10:00AM**

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

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

1 atm= 1.01325 bar=760 ton=l .01325 x 10^5 Pa= 760mmHg

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

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

$h=6.626xl0^{-34}\ Js$

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

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

a) Define the following terms as used in quantum chemistry **[10** marks]

i. Uncertainty principle

ii. Quanta

iii. Degeneracy

iv. Black body

v. Operator

b) Distinguish between photoelectric effect and Compton effect [3marks]

c) Give the planck's distribution law [2 marks]

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

e) Find the wavelength in Å 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 cm^{-1} [5 marks]

f) 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). 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 $\Psi^2$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 $=1A^0$ [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 $m\frac{d^2X}{d^2} + kX = 0$ 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≠O 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 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^{ax2} is non an *Eigen* function of the same operator. [6marks]

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