



MACHAKOS UNIVERSITY

University Examinations for 2021/2022 Academic Year

SCHOOL OF PURE AND APPLIED SCIENCES

DEPARTMENT OF PHYSICAL SCIENCES

SECOND YEARSEMESTER EXAMINATION FOR

**BACHELOR OF SCIENCE IN TELECOMMUNICATION AND INFORMATION
TECHNOLOGY**

BACHELOR OF SCIENCE APPLIED PHYSICS AND TECHNOLOGY

BACHELOR OF SCIENCE IN ANALYTICAL CHEMISTRY

BACHELOR OF EDUCATION (SPECIAL NEEDS)

BACHELOR OF SCIENCE IN MATHEMATICS

BACHELOR OF SCIENCE IN BIOLOGY

BACHELOR OF EDUCATION SCIENCE

SCH 200: ATOMIC STRUCTURE AND CHEMICAL BONDING

DATE:

TIME:

INSTRUCTIONS

- The paper consists of **two** sections.
- Section **A** is **compulsory** (30 marks)
- Answer any **two** questions from section **B** (each 20 marks)

SECTION A (COMPULSORY)

QUESTION ONE (30 MARKS)

- (a) (i) State Heisenberg uncertainty principle (2 marks)
- (ii) Calculate the uncertainty in the velocity of a cricket ball of mass 150 g if the uncertainty in its position is of order of $1\text{\AA}$ (3 marks)
- (b) State the stringent six conditions a wave-function must satisfy to be acceptable. (6 marks)
- (c) (i) Define zero point energy (2 marks)
- (ii) The force constant for H^{18}F molecule is 966 Nm^{-1} . Calculate the zero-point vibrational energy for this molecule for a harmonic potential. (4 marks)
- (d) Write down the time independent Schrödinger (TISE) for a 1-dimensional quantum problem. Clearly State the meaning of constants in your equation. (3 marks)
- (e) A wave function has the value $\Psi(x) = A\sin x$ between $x = 0$ and $x = \pi$ but zero elsewhere
- (i) Normalize the wave function (2 marks)
- (ii) Find the probability that the particle is between $x = 0$ and $x = \frac{\pi}{4}$ (2 marks)
- (iii) The probability that the particle is between $x = 0$ and $x = \frac{\pi}{2}$ (2 marks)
- (f) A particle limited to the x axis has the wave function $\Psi(x) = ax^2 + ibx$ between $x = 0$ and $x = 1$; $\Psi(x) = 0$ elsewhere. Find the expectation value $\langle x \rangle$ of the particle's position. (4 marks)

SECTION B: ANSWER ANY TWO QUESTIONS

QUESTION TWO (20 MARKS)

- (a) Calculate the wavelength of electrons that have been accelerated from rest through a potential difference of 45 kV. (4 marks)
- (b) H^{80}Br molecule was placed in a harmonic oscillator with a difference of $3.20 \times 10^{-21}\text{ J}$ in adjacent energy levels. Calculate the force constant for the oscillator (3 marks)
- (c) A particle in a one dimensional infinite potential well is in the $n = 1$ state. Calculate the probability that the particle will be located in the range $0.5a \leq x \leq 0.75a$ where a is the

width of the well. Recall the particle in a box wave function is $\Psi_n = \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{n\pi x}{a}\right)$

[Hint use: $b = \frac{\pi}{a}$] (5 marks)

- (d) Calculate the energy emitted when electrons of 1.0 g atom of hydrogen undergo transition giving the spectral lines of lowest energy in the visible region of its atomic spectra. (3 marks)

- (e) A particle is constrained to move in a one-dimensional box between $x = a$ and $x = b$. The potential energy is such that the particle cannot be outside these limits and the wave function is given by $\Psi = \frac{A}{x^2}$ where A is a real normalization constant. Determine the value of the normalization constant A . (5 marks)

QUESTION THREE (20 MARKS)

- (a) (i) Define lattice energy (2 marks)
- (ii) Using Born Haber cycle calculate the lattice enthalpy of magnesium chloride from the following data.

Enthalpy of atomization of $\text{Mg}_{(s)} = 148 \text{ kJmol}^{-1}$

First ionization energy of $\text{Mg}_{(g)} = 738 \text{ kJmol}^{-1}$

Second ionization energy of $\text{Mg}_{(g)} = 1451 \text{ kJmol}^{-1}$

Enthalpy of atomization of $\text{Cl}_{2(g)} = 122 \text{ kJmol}^{-1}$

Electron affinity of $\text{Cl}_{(g)} = -349 \text{ kJmol}^{-1}$ (7 marks)

Enthalpy of formation of $\text{MgCl}_{2(s)} = -641 \text{ kJmol}^{-1}$

- (b) Define the following: (3 marks)

- (i) Molecular orbital
- (ii) Bonding molecular orbital (BMO)
- (iii) Anti-bonding molecular orbital (ABMO)

- (c) Explain why the first ionization energy of molecular oxygen O_2 (1175 kJ mol^{-1}), is lesser than the first ionization energy of O (1314 kJmol^{-1}) (4 marks)

- (d) Determine the bond order and magnetic property of the following molecules

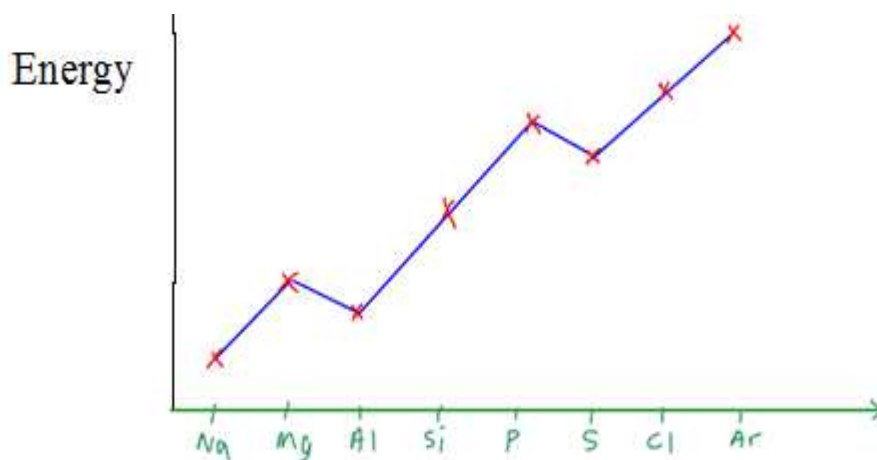
- (i) O_2 (2 marks)
- (ii) N_2 (2 marks)

QUESTION FOUR (20 MARKS)

- (a) Using a relevant example define orbital degeneracy (2 marks)
- (b) A particle travelling in the negative x direction has a wave-function given by $\psi(x) = e^{-ikx}$
- (i) Show that this wave function is an Eigen-function of the momentum operator and thus that the momentum is known exactly. (3 marks)
- (ii) What is the uncertainty in the momentum of the particle? (2 marks)
- (c) List the four quantum numbers and state their designations/functions in quantum chemistry (8 marks)
- (d) Calculate the de Broglie wavelength of an electron in the first Bohr orbit in the hydrogen atom (5 marks)

QUESTION FIVE (20 MARKS)

- (a) Using the VSEPR model draw and predict the molecular geometry of the following molecules
- (i) SnCl_2 (4 marks)
- (ii) AsCl_5
- (b) Explain the trend in the first ionization energy in the third period of the periodic table



- (c) A diatomic molecule HX (X is an unknown atom) has a harmonic vibrational force constant $k = 9.680 \times 10^5 \text{ g/s}^2$. The harmonic vibrational frequency in wavenumbers is 4143.3 cm^{-1} .
- (i) Calculate the reduced mass of the molecule HX (2 marks)

- (ii) Identify atom X (2 marks)
- (d) Assume that you prepare a more general state that is a superposition of the first and the third stationary state so that $\psi(x,0) = A[u_1(x) - iu_3(x)]$. Assuming that the stationary states are normalized already, calculate the normalization constant A. (5 marks)
- (e) Sketch the radial distribution functions of 1s, 2s and 3s orbitals of hydrogen atom on the same axis. (3 marks)

Useful Information

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

$$c = 2.998 \times 10^8 \text{ m/s} ;$$

$$R_H = 1.097 \times 10^7 \text{ m}^{-1}$$

$$1 \text{ eV} = 1.602 \times 10^{-19} \text{ J}$$

$$m_e = 9.10 \times 10^{-31} \text{ kg} ;$$

$$\epsilon_0 = 8.85418 \times 10^{-12} \text{ Fm}^{-1} ;$$

$$E_n = -\frac{me^4}{8\epsilon_0^2 n^2 h^2}$$

$$r_n = \frac{\epsilon_0 n^2 h^2}{\pi m_e e^2}$$

$$1 \text{ amu} = 1.66054 \times 10^{-27} \text{ kg} ;$$

$$\int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx = \frac{a}{2},$$

$$\int_0^a x \sin^2\left(\frac{n\pi x}{a}\right) dx = \frac{a^2}{4},$$

$$\int \sin^2 bx \, dx = \left[\frac{x}{2} - \frac{\sin(2bx)}{4b} \right] ;$$

$$\int_0^\infty e^{-\beta x^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{\beta}} ;$$

$$\text{Momentum operator, } P_x = i\hbar \frac{d}{dx} ;$$

$$\int_0^a \sin\left(\frac{n\pi x}{a}\right) \sin\left(\frac{m\pi x}{a}\right) dx = \int_0^a \cos\left(\frac{n\pi x}{a}\right) \cos\left(\frac{m\pi x}{a}\right) dx = \frac{a}{2} \delta_{mn} \text{ (m and n are integers)}$$

$$\sin \alpha \sin \beta = \frac{1}{2} \cos(\alpha - \beta) - \frac{1}{2} \cos(\alpha + \beta) ;$$

$$\int \cos(bx) dx = \frac{1}{b} \sin(bx)$$

$$\int_0^a x^2 \sin^2\left(\frac{n\pi x}{a}\right) dx = \frac{a^3}{6} - \frac{a^3}{4n\pi^2}$$

