MACHAKOS UNIVERSITY

University Examinations 2022/2023

SCHOOL OF PURE AND APPLIED SCIENCES

DEPARTMENT OF PHYSICAL SCIENCES

SECOND YEAR FIRST SEMESTER EXAMINATION FOR

BACHELOR OF SCIENCE (TELECOMMUNICATIONS AND INFORMATION TECHNOLOGY)

BACHELOR OF SCIENCE (ANALYTICAL CHEMISTRY)

BACHELOR OF EDUCATION (SCIENCE)

BACHELOR OF EDUCATION (SPECIAL NEEDS)

BACHELOR OF SCIENCE (MATHEMATICS)

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

QUESTION ONE (COMPULSORY) (30 MARKS)

(a) (i) State **four** limitations of valence bond theory (VBT) (4 marks)

(ii) Using the molecular bond theory (MO) explain the existence or non-existence of He_2 molecule (He = 2) (2 marks)

(b) State the stringent **five** conditions a wave-function must satisfy to be acceptable. (5 marks)

(c) (i) Calculate the shortest wavelength in Layman series and determine its corresponding frequency. (4 marks)

(ii) Calculate de Broglie wavelength associated with an electron moving with a speed of $5.4 \times 10^6\ m/s$ (2 marks)

(d) Write down the time dependent Schrödinger (TDSE) for a 1-dimensional quantum problem. Clearly State the meaning of constants in your equation. (3 marks)

(e) The state of a free particle of mass m in a one dimension is described by the following quantum wave function:

$$\psi(x) = \begin{cases} 0 & x < -a \\ A(a - |x|) & -a \leq x \leq a \\ 0 & x > a. \end{cases}$$

(i) Determine A using normalization condition (3 marks)

(ii) What is the probability that a measurement of the particle's position will reveal it to be in the range [0, a/2]? (2 marks)

(f) (i) State Heinsenberg Uncertainty principle (2 marks)

(ii) For a particle moving freely along the x-axis, show that the Heisenberg uncertainty principle can be written in the alternative form: $\Delta\lambda\Delta x = \frac{\lambda}{4\pi}^2$

(3 marks)

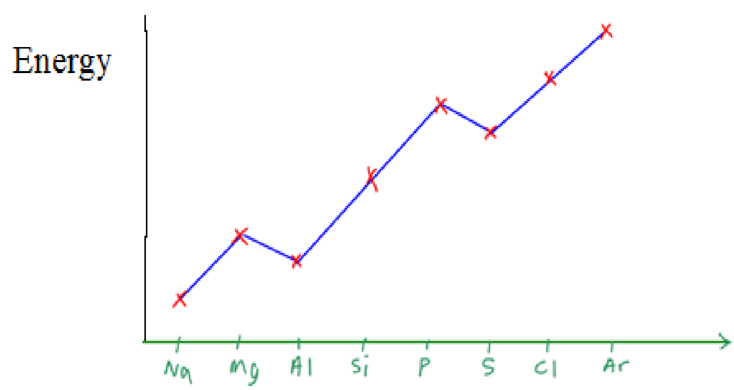
SECTION B

QUESTION TWO (20 MARKS)

(a) State the electronic configuration of the following:

(i) Co^{3+} (ii) Y (iii) Ru (3 marks)

(b) Explain the trend and anomalies in the first ionization energies in the following period



(4 marks)

(c) Draw the molecular orbital energy level diagram for NO and calculate the bond order of the molecule (5 marks)

(d) $H^{80}Br$ molecule was placed in a harmonic oscillator with a difference of $3.20 \times 10^{-21}\, J$ in adjacent energy levels. Calculate the force constant for the oscillator (3 marks)

(e) A particle in a one dimensional infinite potential well is in the n = 1 state. Calculate the probability when the particle is located in the range $0.5a \le x \le 0.75a$ where the width of the well is "a" Recall the particle in a box wave function is $\Psi_n = \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{n\pi x}{a}\right)$

use: $b = \frac{\pi}{a}$] (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 $Mg_{(s)}$ = 148 $kJmol^{-1}$

First ionization energy of $Mg_{(g)}$ = 738 $kJmol^{-1}$

Second ionization energy of $Mg_{(g)}$ = 1451 $kJmol^{-1}$

Enthalpy of atomization of $Cl_{2(g)}$ = 122 $kJmol^{-1}$

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

Enthalpy of formation of $MgCl_2(s)$ = -641 $kJmol^{-1}$

(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)

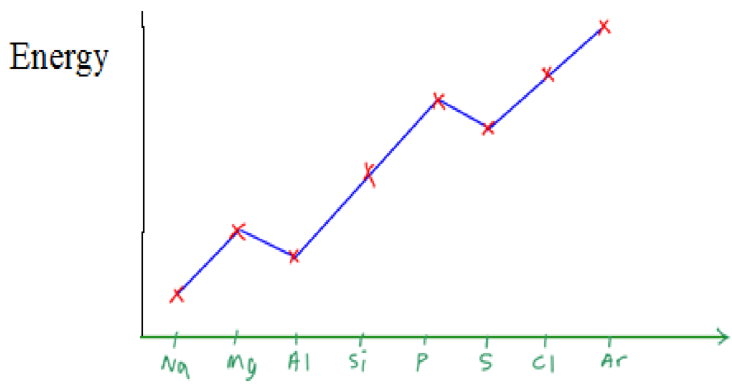
QUESTION FIVE (20 MARKS)

(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



(4 marks)

(c) A diatomic molecule HX (X is an unknown atom) has a harmonic vibrational force constant $k = 9.680 \times 10^5$ 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

$h = 6.626\times10^{-34}\ Js$; $c = 2.998\times10^{8}\, m/s$; $R_H = 1.097\times10^{7}\, m^{-1}$

$1\ eV = 1.602\times10^{-19}$ J $\quad m_e = 9.10\times10^{-31}\, kg$; $\quad \varepsilon_0 = 8.85418\times10^{-12}\ Fm^{-1}$;

$$E_n = -\frac{me^4}{8\varepsilon^2{}_0 n^2 h^2} \qquad r_n = \frac{\varepsilon_0 n_n^2 h^2}{\pi m_e e^2}$$

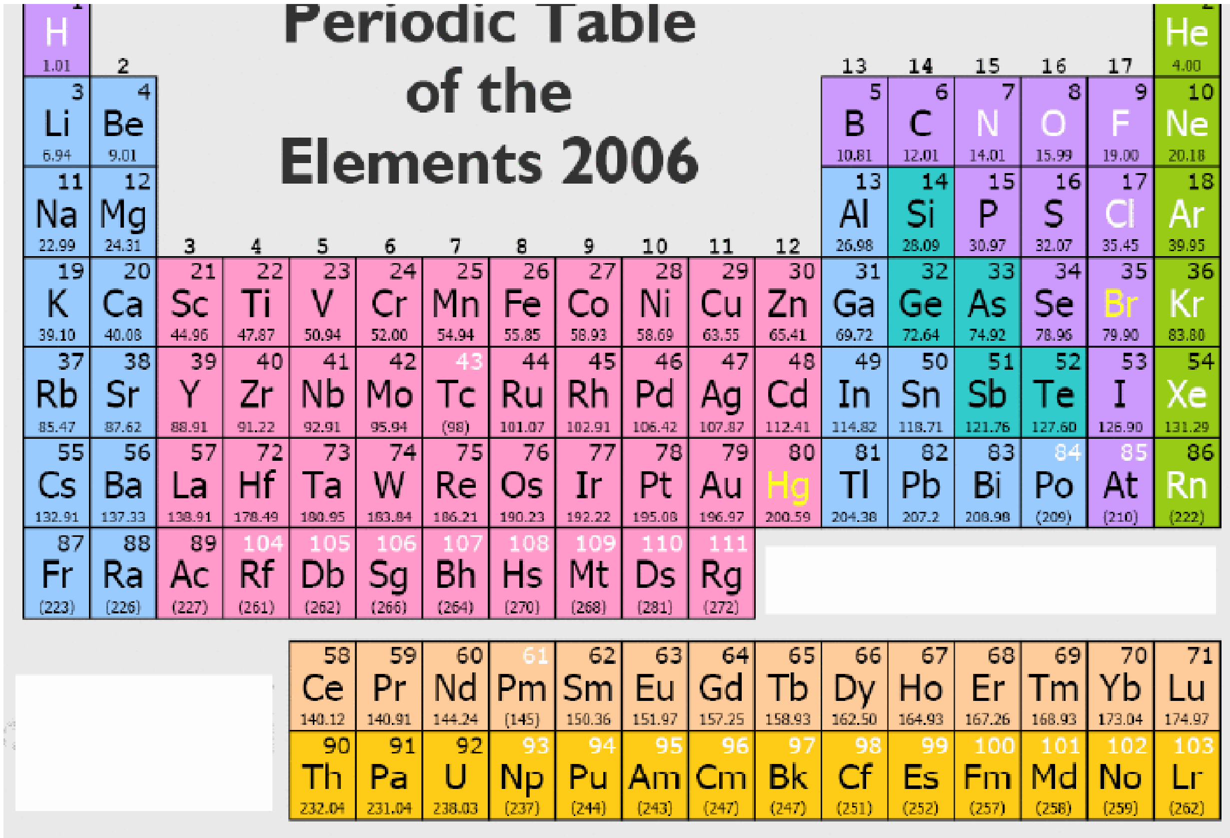
$1\, amu = 1.66054\times10^{-27} kg$; $\quad \int_o^a \sin^2\left(\frac{n\pi x}{a}\right)dx = \frac{a}{2}$, $\quad \int_0^a x\sin^2\left(\frac{n\pi x}{a}\right)dx = \frac{a^2}{4}$,

$\int \sin^2 bx\, dx = \left[\frac{x}{2} - \frac{\sin(2bx)}{4b}\right]$; $\quad \int_0^\infty e^{-\beta x^2} dx = \frac{1}{2}\sqrt{\frac{\pi}{\beta}}$; $\quad$ Momentum operator, $P_x = i\hbar\frac{d}{dx}$;

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

$\sin\alpha\sin\beta = \frac{1}{2}\cos(\alpha-\beta) - \frac{1}{2}\cos(\alpha+\beta)$; $\quad \int \cos(bx)dx = \frac{1}{b}\sin(bx)$

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



Periodic Table of the Elements 2006

	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	
1 H 1.01																	2 He 4.00
3 Li 6.94	4 Be 9.01											5 B 10.81	6 C 12.01	7 N 14.01	8 O 15.99	9 F 19.00	10 Ne 20.18
11 Na 22.99	12 Mg 24.31											13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.07	17 Cl 35.45	18 Ar 39.95
19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.87	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.69	29 Cu 63.55	30 Zn 65.41	31 Ga 69.72	32 Ge 72.64	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (98)	44 Ru 101.07	45 Rh 102.91	46 Pd 106.42	47 Ag 107.87	48 Cd 112.41	49 In 114.82	50 Sn 118.71	51 Sb 121.76	52 Te 127.60	53 I 126.90	54 Xe 131.29
55 Cs 132.91	56 Ba 137.33	57 La 138.91	72 Hf 178.49	73 Ta 180.95	74 W 183.84	75 Re 186.21	76 Os 190.23	77 Ir 192.22	78 Pt 195.08	79 Au 196.97	80 Hg 200.59	81 Tl 204.38	82 Pb 207.2	83 Bi 208.98	84 Po (209)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra (226)	89 Ac (227)	104 Rf (261)	105 Db (262)	106 Sg (266)	107 Bh (264)	108 Hs (270)	109 Mt (268)	110 Ds (281)	111 Rg (272)							
				58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm (145)	62 Sm 150.36	63 Eu 151.97	64 Gd 157.25	65 Tb 158.93	66 Dy 162.50	67 Ho 164.93	68 Er 167.26	69 Tm 168.93	70 Yb 173.04	71 Lu 174.97
				90 Th 232.04	91 Pa 231.04	92 U 238.03	93 Np (237)	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (262)