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(University of Choice)

MASINDE MULIRO UNIVERSITY OF SCIENCE AND TECHNOLOGY (MMUST)

UNIVERSITY EXAMINATIONS 2021/2022 ACADEMIC YEAR THIRD YEAR MAINEXAMINATIONS FOR THE DEGREE OF BACHELOR OF SCIENCE IN CHEMISTRY

COURSE CODE: SCI 465

COURSE TITLE: MATERIAL SCIENCE

DATE: 29TH APRIL 2022 **TIME:** 12.00PM - 2.00PM

INSTRUCTIONS TO CANDIDATES

TIME: 2 Hours

Answer question ONE and any THREE of the remaining

Symbols used bear the usual meaning.

QUESTION ONE (COMPULSORY) (30 MARKS)

(a). A uniform steel wire of length 4 m and area of cross section $3.0 \times 10^{-6} m^2$ is extended by 1 mm. Calculate the energy stored in the wire if the elastic limit is not exceeded. (Youngs modulus = $2.0 \times 10^{11} Pa$) (5 marks)

(b). Consider a unit cell carrying a plane whose intercepts are;

$x' = 1.5r \; y' = 0.5r \; z' = 0.25r$, where r is the atomic radius. Obtain the miller indices describing this plane. (8 marks)

(c). Obtain the Packing Fraction of a face centered structure. (5 marks)

(d). Show that the cation: anion ratio is equal to 0.732 for a material with body centered cubic structure. (8marks)

(e). Wood contains a natural polymer based on cellulose molecule. Describe the structure of wood that make it strong and stiff. State the circumstances under which it is weak. (4 marks)

QUESTION TWO (20 MARKS)

(a). The lattice constants for KBr and NaCl are respectively 0.66nm and 0.56 nm. Given that $r_0 = 0.33\text{Å}$ for KBr and $r_0 = 0.56\text{Å}$ for NaCl , calculate the

i. F-center absorption energies (5 marks)

ii. F- absorption wavelength (5 marks)

(b). The energy contribution between two ions in a material is given by $E_c = \frac{-e^2}{4\pi\varepsilon_0 r}.\alpha$, show that the total potential energy at $r = r_0$ is given by;

$E = \frac{-e^2}{4\pi\varepsilon_0 r_0}.\alpha\left[1 - \frac{1}{m}\right]$, where α is Madelung constant and m is Born exponent. (10marks)

QUESTION THREE(20 MARKS)

(a). The bulk modulus of a material at absolute zero is; $K = -v\left(\frac{dP}{dv}\right)$ and the compressibility is $\beta = \frac{1}{K} = -\frac{1}{v}\left(\frac{dv}{dP}\right)$. Using the first law of thermodynamics, show that the repulsive component n of the material is $n = 1 + \frac{72\pi\varepsilon_0 r_0^4}{Ae^2\beta}$ (10 marks).

(b). An example of a solution-hardened material is steel. Using well labeled diagrams, describe how steel is made pointing out the types of solid solution. (10 marks)

QUESTION FOUR (20 MARKS)

(a). The total energy per Kmol of a crystal is $(r) = N_A\left[\frac{B}{r^n} - \frac{Ae^2}{4\pi\varepsilon_0 r}\right]$. By minimizing this energy, show that;

i. $B = \frac{Ae^2 r_0^{n-1}}{4\pi\varepsilon_0 n}$ (5marks)

ii. The equilibrium energy per kMol of the crystal is

$$U_0 = -\left[\frac{Ae^2 N_A}{4\pi\varepsilon_0 r_0}\right]\left[\frac{n-1}{n}\right] \text{ (5 marks)}$$

(a). Using the Born-Lande equation equation, Calculate the lattice energy for sodium chloride for which $r_0 = 2.81\text{Å}$ and Obtain the molar lattice energy for the same crystal (10marks)

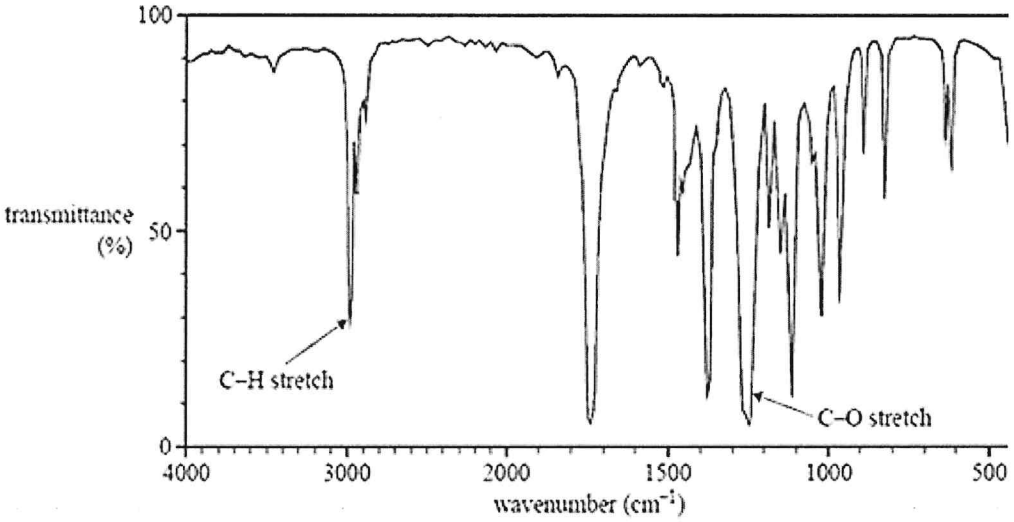
(c) Name four types of ionization methods commonly used in Mass-Spectrometry and classify each as either a "hard" or "soft" ionization method. **(4 marks)**

(d) A small sample of a purified ester mixture was passed through a gas chromatograph (GC) attached to a mass spectrometer. The chromatogram showed two peaks, indicating that the ester mixture contained two different fatty acid methyl esters, A and B. The peak area of each compound and the mass-to-charge ratio of the molecular ion of each compound are shown in the following table. Assume that the charge on each molecular ion is +1.

Methyl ester	Peak area	Mass-to-charge ratio of the molecular ion
A	1000	270
B	2000	298

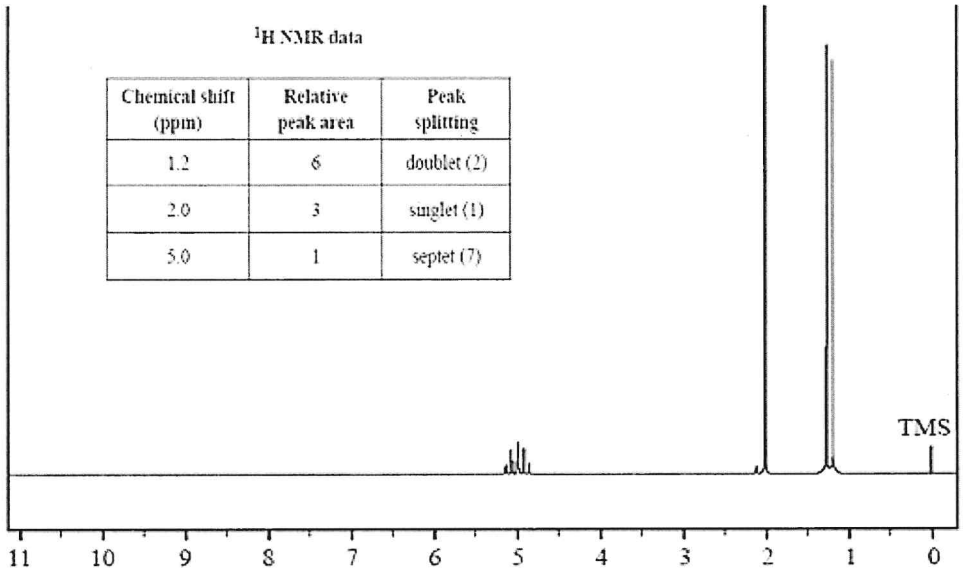
i. The mass spectrum of methyl ester A corresponds to that of methyl palmitate, $CH_3(CH_2)_{14}COOCH_3$. What are the name and semi-structural formula of methyl ester B? **(2 marks)**

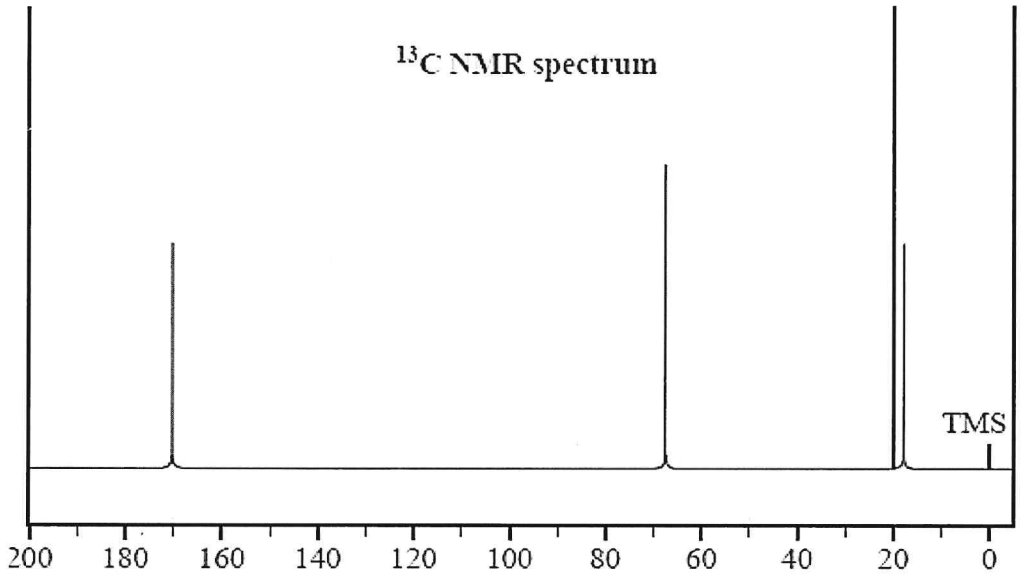
ii. While cleaning out a laboratory shelf labelled 'Carboxylic acids and esters', a chemist discovers a bottle simply labelled '$C_5H_{10}O_2$'. To identify the molecular structure of the contents of the bottle, a sample is submitted for analysis using infrared spectroscopy, and ^1H and ^{13}C NMR spectroscopy. The spectra are shown below.



^{1}H NMR data

Chemical shift (ppm)	Relative peak area	Peak splitting
1.2	6	doublet (2)
2.0	3	singlet (1)
5.0	1	septet (7)





(e) Use the IR spectrum to determine:

i. determine the various functional groups present in the compound **(2 marks)**

ii. whether the molecule is a carboxylic acid or an ester **(1 marks)**

Provide reasons for your answer.

(f) Using the information provided in the ^{1}H and ^{13}C NMR spectra, identify the number of different chemical environments for hydrogen and carbon in this molecule **(2 marks)**

(g) Draw a structure for this molecule **(1 mark)**

Question 4 — 17 marks

(a) What are ion selective electrodes? Explain its working principle **(4 marks)**

(b) Explain the measurement of PH by potentiometry and discuss the advantages **(5 marks)**

(c) Briefly outline the steps involved in an Anodic Stripping Voltammetry (ASV) analysis **(5 marks)**

(d) Explain why ASV has the best detection limits of any voltammetric methods available today **(3 marks)**