VICTORIAN CERTIFICATE OF EDUCATION

CHEMISTRY – SAC 4

Analysis of Secondary data

Reading time: 5 minutes

Writing time: 60 minutes

Student's Name: Solutions

Teacher: _____

Structure of booklet

Section	Number of Questions	Number of questions to be answered	Marks
Short Answer	5	5	49
		Total:	**49**

Directions to students

Materials

- Students **are permitted** to bring into the examination room: pens/pencils, highlighters, erasers, sharpeners, rulers, and an approved scientific calculator.
- Students are **NOT permitted** to bring into the examination room: white out liquid/tape, phones or electronic devices, including smart watches.
- Students are provided with the following: Question and answer book of **8** pages and VCAA Data booklet.

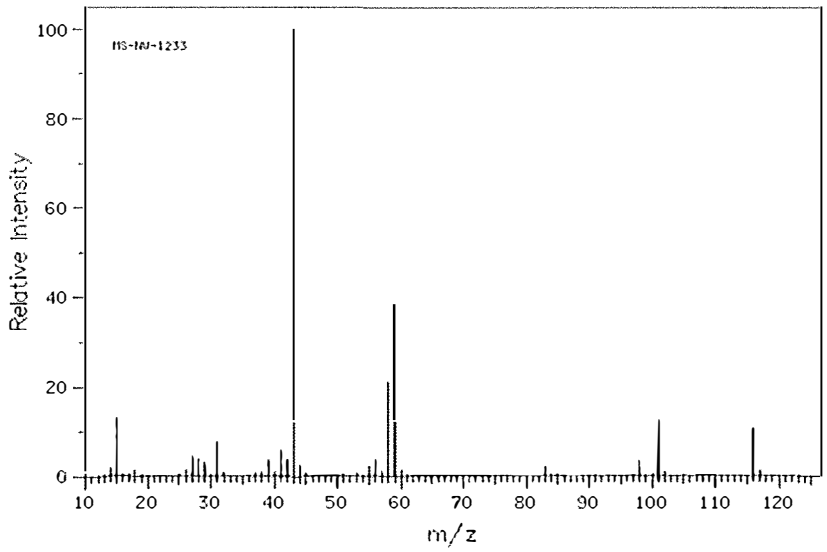
The task

- Please ensure that you write your name and teacher's name on this booklet. This paper consists of short answer questions.
- There are a total of **49** marks available.
- Be sure to include states with all chemical equations.
- All numerical answers need to be quoted to the correct number of significant figures.
- All working out must be shown in the space provided.

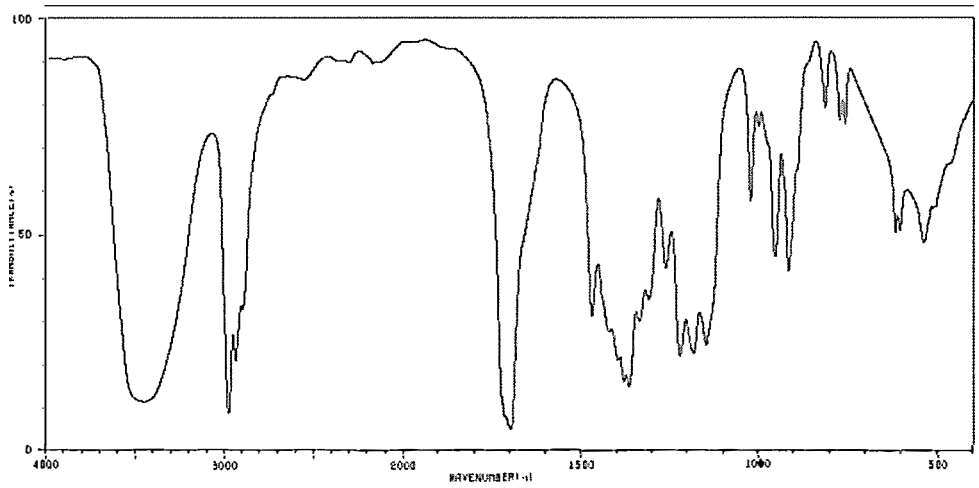
Question 1 (12 marks):

Five bottles of organic compounds are found in a cupboard where the label only contained the empirical formula of the compound which was C_3H_6O. It was decided to try and identify the structure of the substance using mass spectroscopy, IR spectroscopy and NMR spectroscopy. The spectra are given below. It was also tested whether the substance would react with NaOH and there was **no** evidence of a reaction.

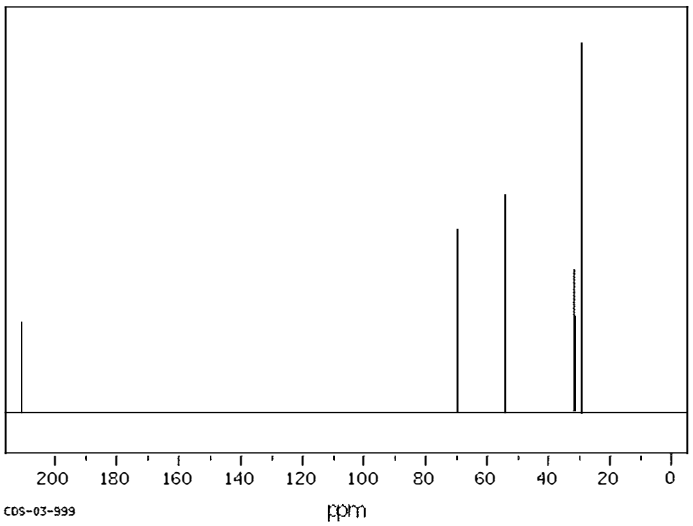
Mass Spectra



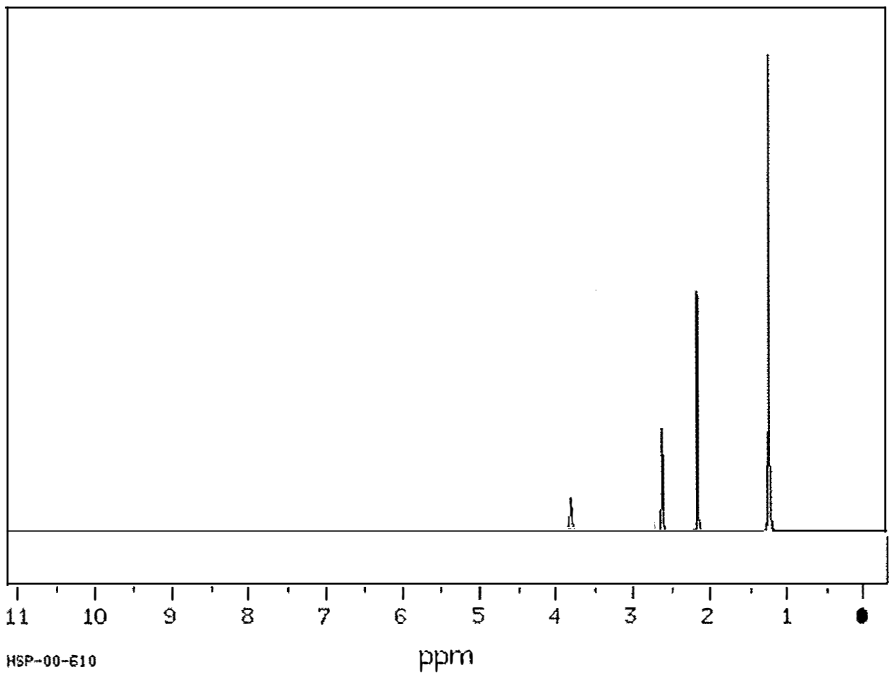
IR spectra



^{13}C NMR



^{1}H NMR



a. Determine the molecular formula of the unknown compound. Show all working. (2 marks)

$C_6H_{12}O_2$

$72 + 12 + 32 = 106 = m/z$.

b. The mass spectra identified a peak at 15m/z. State the species responsible for this peak.(1 mark)

CH_3^+

c. Identify 2 characteristic peaks from the IR spectra. (2 marks)

C=O - 1700 cm^{-1} & 3500 - OH (alcohol)

d. Why are **different** frequencies of infrared radiation (IR) absorbed by this molecule as shown in the IR spectrum. (2 marks)

Different covalent bonds present - (1)

Either => Different masses of atoms - (1)

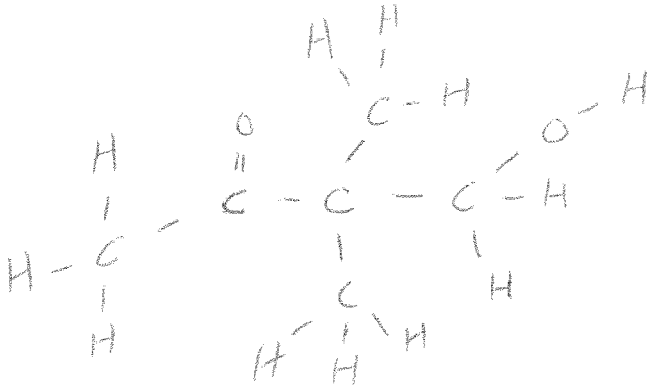
Different bond strengths - (1)

e. State the number of hydrogen and carbon environments present in the molecule. (2 marks)

Number of hydrogen environments: 4

Number of carbon environments: 5

f. Draw the structural formula of the molecule (note there is no splitting in the H NMR). (2 marks)



g. Explain why the peak at 1.2ppm on the ^{1}H NMR spectra contains no splitting. (1 mark)

The adjacent C atom has no Hydrogens attached to it
↓
non equivalent

Question 2 (8 marks):

5 unlabelled bottles of organic substances were found in the chemical storeroom. Also found were 5 labels that was assumed are meant to be used, these labels (in alphabetical order) are, chlorobutane, butanoic acid, butanol, but-2-ene and 2-hydroxybutanoic acid.

To determine the identity of the unknown chemicals Dr Lewis conducted a series of laboratory tests. Her results are summarised in the table below.

	A	B	C	D	E
Addition of bromine (Br_2)	No reaction	No reaction	No reaction	Solution turned colourless	No reaction
Addition of potassium permanganate ($KMnO_4$)	No reaction	No reaction	Solution changes colour from purple to colourless	No reaction	Solution changes colour from purple to colourless
Addition of sodium hydrogen carbonate ($NaHCO_3$)	No reaction	Bubbles produced	Bubbles produced	No reaction	No reaction

a. Using the results above, identify each of the unknown compounds: (5 marks)

A: chlorobutane

B: butanoic acid

C: 2-hydroxybutanoic acid

D: but-2-ene

E: butanol

b. Butanol has two potential isomers, butan-1-ol and butan-2-ol. Briefly explain a simple experiment that could be conducted in a chemistry classroom to determine which isomer is present in the bottle. Be sure to explain the **potential results** and what it would indicate. (3 marks)

Any reasonable lab experiment. Not IR or HPLC

1) React with acidified permanganate & gently heat. Butan-1-ol & Butan-2-ol will both turn the permanganate clear.

2) Then test with blue litmus paper & the sample that turns it red must be butanoic acid. Hence, it was originally butan-1-ol.

Question 3 (12 marks):

Detective Razos was suspicious over the stated alcohol content of ethanol is his favourite beer. The states alcohol content was 4.5%(m/v) of ethanol. He decided to investigate his suspicions using a titration with acidified potassium dichromate. The overall reaction is given below:

$$3CH_3CH_2OH_{(l)} + 2Cr_2O_7^{2-}{}_{(aq)} + 16H^+_{(aq)} \rightarrow 3CH_3COOH_{(aq)} + 4Cr^{3+}_{(aq)} + 11H_2O_{(l)}$$

A simplified method of the process Detective Razos followed is given below:

1. Take a 25.00mL sample of beer and add to a 100.0mL volumetric flask and make up to the calibration mark with distilled water.
2. Use a 20.00mL aliquot of the diluted beer sample and titrate with 0.1290M potassium dichromate.

The titre results obtained in this experiment were 16.75mL, 17.49mL, 17.97mL, 17.55mL and 17.52mL.

a. Write the half equation for ethanol → ethanoic acid (including states) (2 marks)

$CH_3CH_2OH \longrightarrow CH_3COOH$

$C_2H_6O_{(aq)} + H_2O_{(l)} \longrightarrow C_2H_4O_{2(aq)} + 4H^+_{(aq)} + 4e^-$

b. Calculate the average titre for Detective Razos' results. (1 mark)

$\frac{17.49 + 17.55 + 17.52}{3} = 17.52\ ml$

c. Calculate the concentration (in molarity) of ethanol in the diluted beer sample. (3 marks)

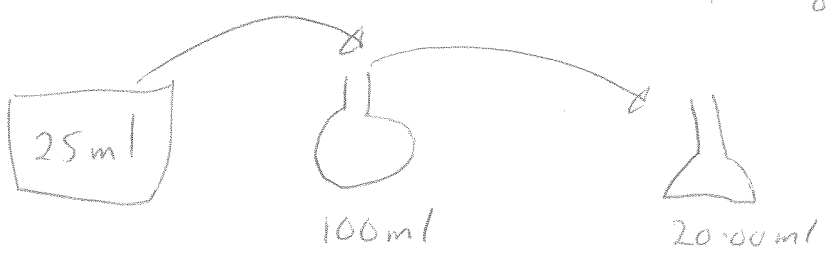
$n(Cr_2O_7)^{2-} = 0.01752 \times 0.1290 = 2.26 \times 10^{-3}\ mol$ — (1)

$n(CH_3CH_2OH) = 3/2 \times 2.26 \times 10^{-3} = 3.39 \times 10^{-3}\ mol$ — (1)

$\Rightarrow [CH_3CH_2OH] = \frac{3.39E^{-3}}{0.02}$

$= 0.170M$

$Cr_2O_7^{2-}$
20.00 ml
0.1290 M



d. Calculate the concentration (in molarity) of ethanol in the beer (give your answer to the correct number of significant figures). 4 fold dilution (2 marks)

$\Rightarrow 0.170 \times {}^{100}/_{25} = 0.6780\,M.$ (4 s.f) ~ 1 mark

e. Convert the 4.5%(m/v) stated on the beer bottle to a molar concentration. (2 marks)

$4.5\,\% = 45\,g/L$

$\Rightarrow [ethanol] = \frac{45}{46} = 0.978\,M$

f. Compare your answers to part d. and e. above to compare the manufacturers claim to Detective Razos' results. Give **one** potential error that could have caused this discrepancy. (2 marks)

0.678 M < 0.978 M ; => significantly less ethanol than manufacturer's claim.

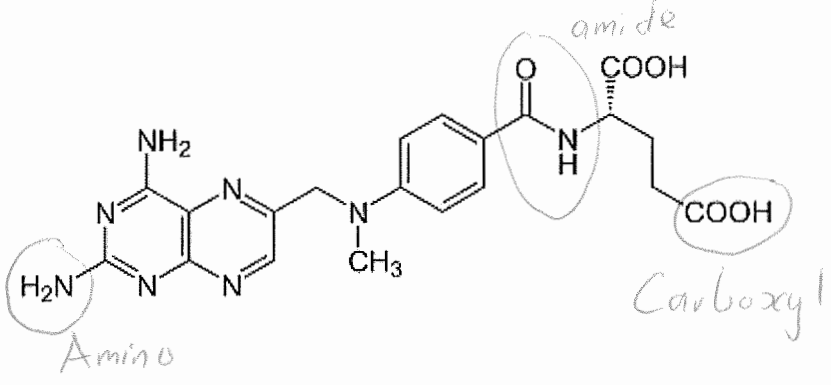
=> reason ethanol has oxidised to ethanal & ethanoic acid

=> Beer was diluted by company prior.

Question 4 (13 marks):

Research Fellow Jacqui is part of a team of medical researchers investigating the use of methotrexate (MXT) in the treatment of breast cancer patients. MXT is a medication that acts as a competitive inhibitor for the enzyme dihydrofolate reductase (DHFR), which is an enzyme responsible for the synthesis of tetrahydrofolate. Tetrahydrofolate is responsible for the formation of proteins and DNA synthesis.

DHFR is 1000 times more likely to bind to MXT than it is to its usual substrate, dihydrofolate. The structure of MXT is given below.



a. On the diagram of MXT above, circle and name two different functional groups. (2 marks)

b. MXT is a competitive inhibitor. Define the term competitive inhibitor. (1 mark)

A chemical that competes with a substrate for the active site of an enzyme. (Thus blocking the ability of the substrate to be broken down)

with dihydrofolate (1) mark

c. Explain how the formation of tetrahydrofolate would change when a patient is administered a drug containing MXT. (3 marks)

The drug MXT would compete for the active site of the enzyme DHFR. This interferes with the ability of the substrate to be broken down & produce tetrahydrofolate. (1) mark

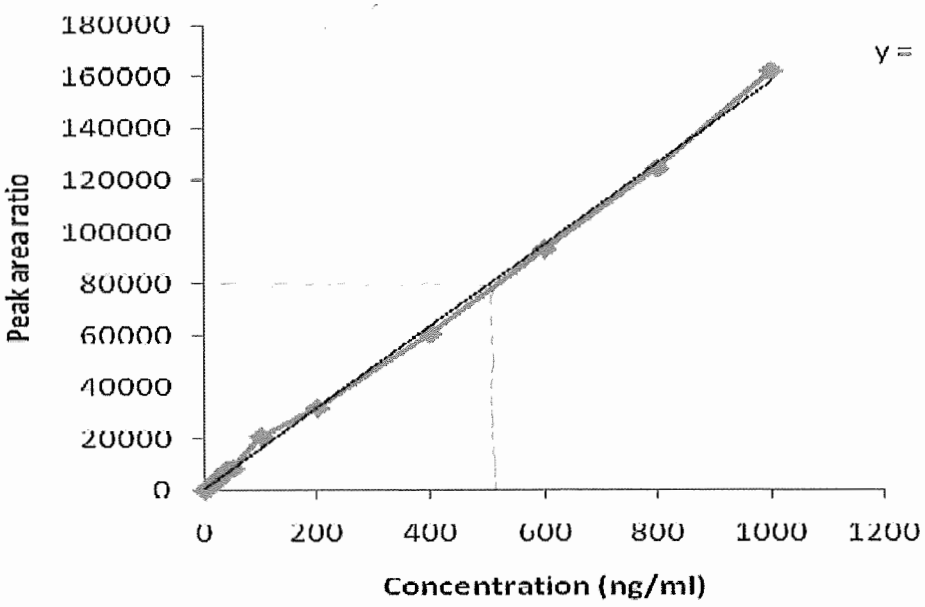
Hence with a lower production of tetrahydrofolate => & protein & DNA synthesis & risk of breast cancer. – (1) mark

d. To extract the MXT molecule from a solid tablet in order to be tested, should Jacqui use propan-1-ol or water to allow more effective separation? Explain your reasoning. (2 marks)

Water => (1) mark

As water is more polar than propan-1-ol it will form more hydrogen bonds with the many polar functional groups on MXT – (1) mark.
=> better separation.

Following extraction of MXT from the tablet, the research team used high performance liquid chromatography (HPLC) to create a standard curve demonstrating the relationship between the concentration of MXT versus the peak area from a retention time of 6.5 minutes. The medication produced a peak area ratio for MXT of 80,000.

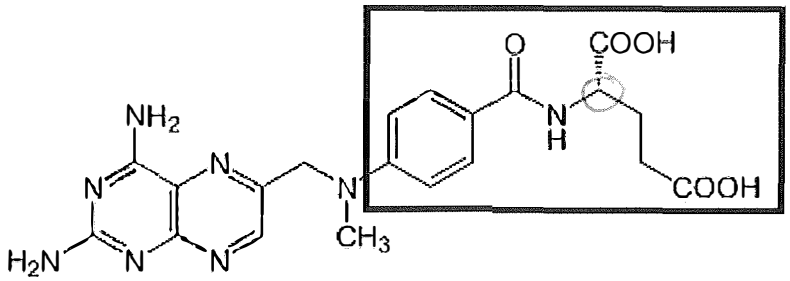


e. Determine the concentration of MXT in the tablet in g/L. (2 marks)

range 500 – 550 ng/ml – (1)

=> 0.500 mg/ml = 0.500 g/L. – (1)

f. MXT is known to have **1 chiral centre**. This chiral centre is inside the box on the diagram below.



i. Circle the chiral centre inside the box on the diagram above. (1 mark)

ii. State the number of optical isomers MXT has. (1 mark)

2

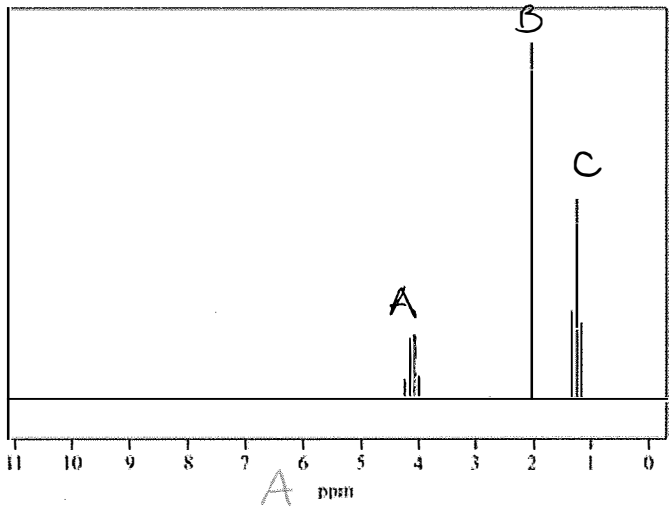
g. Another medication was tested and has a peak area for MXT of 400,000. What could be done to accurately calculate the concentration of MXT in this sample. (1 mark)

Dilute the sample medication to within the range of the calibration curve. -①

(Dilute sample = not enough for 1 mark)

Question 5 (4 marks):

The ^{1}H NMR for a compound with the molecular formula $C_4H_8O_2$ is given below.

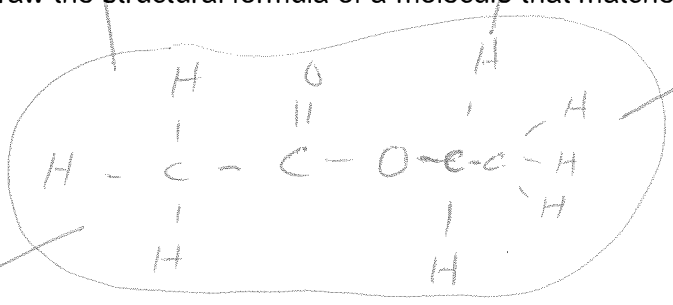


B

A

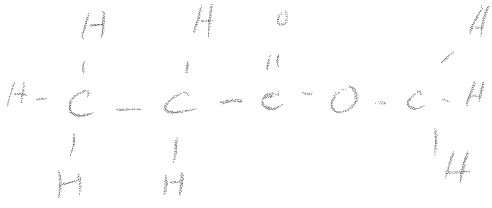
a. Draw the structural formula of a molecule that matches the NMR spectral data above. (2 marks)

2 marks



C

or



chemical shift = 2.0

b. On your structural formula, label each hydrogen with the letter A, B or C to indicate which environment in the NMR spectra above it belongs to. (2 marks)

END OF SAC