WJEC EDUQAS AS CHEMISTRY · COMPONENT 2

CHEMISTRY



EXAM QUESTION PACK

2.8 INSTRUMENTAL ANALYSIS

SCORE	PERCENTAGE
/55	%

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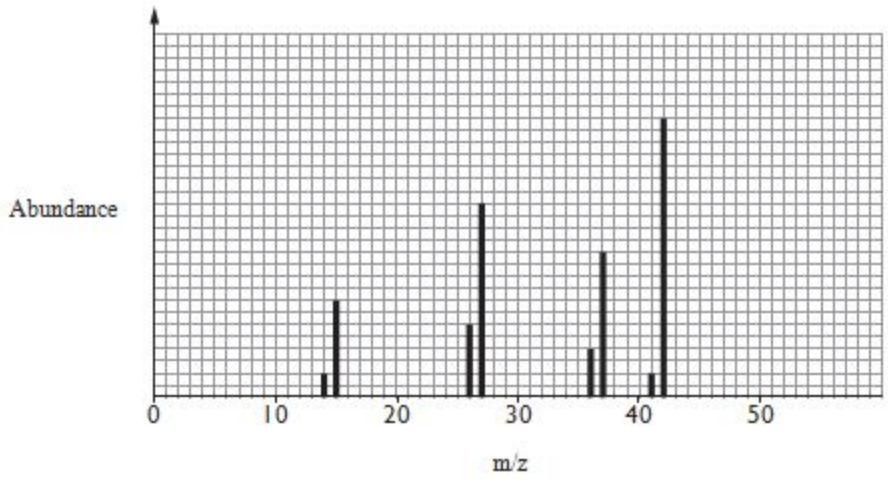
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1. (a) Compound **X** is a straight-chain hydrocarbon that consists of 85.7 % carbon by mass.

(i) Find the **empirical** formula of compound **X**

[3]

(ii) Some peaks from the mass spectrum of **X** are shown below.



Use the empirical formula and the mass spectrum to find the molecular formula of **X**. Show your workings

[2]

(iii) Suggest what information the presence of the peak at m/z 15 gives about the structure of **X**.

[1]

(b) Butene, C_4H_8, is an alkene. Draw **displayed** formulae for three **straight-chain** isomers of C_4H_8. [3]

(Total 9)

2. (a) Propene reacts with hydrogen bromide to give 2-bromopropane.

(i) Draw the mechanism for this reaction.

[3]

(ii) Explain why the product of this reaction is mainly 2-bromopropane rather than 1-bromopropane

[2]

(b) Compound **C** is a compound of carbon, hydrogen and bromine only. Bromine has two isotopes, ^{79}Br and ^{81}Br, in equal abundance. Use all the information below to deduce the structure of compound **C**, giving your reasoning. [6]

QWC [1]

- Compound **C** contains 29.8% carbon, 4.2% hydrogen and 66.0% bromine by mass.
- The mass spectrum of compound **C** contains peaks at m/z of 15, 41 and a pair of peaks at 120 and 122.
- The infrared spectrum of compound **C** has absorptions at 550 cm^{-1}, 1630 cm^{-1} and 3030 cm^{-1}.
- Compound **C** is a Z-isomer.

(Total 12)

3. *(a)* An acid **F** was known to be one of the following.

$CH_3CH_2HC{=}CHCO_2H$	Acid 1	$M_r = 100$
$HO_2CCH_2CH_2CO_2H$	Acid 2	$M_r = 118$

A sample of 1.20 g of acid **F** was burned in excess oxygen. 1.79 g of carbon dioxide was formed.

(i) Calculate the mass of carbon present in the sample of acid **F**. [1]

Mass of carbon = ... g

(ii) The mass of hydrogen in the sample is 0.061 g. Assuming that the rest of the sample is oxygen, calculate the mass of oxygen in the sample.

[1]

Mass of oxygen = ... g

(iii) Use your answers to parts (i) and (ii) to find the empirical formula of acid **F**.

[2]

Empirical formula . . . . . .

(iv) State the identity of acid **F**. Show clearly how you reached this conclusion.

[1]

(v) Describe a chemical test that would distinguish between Acid 1 and Acid 2.You should include the expected results

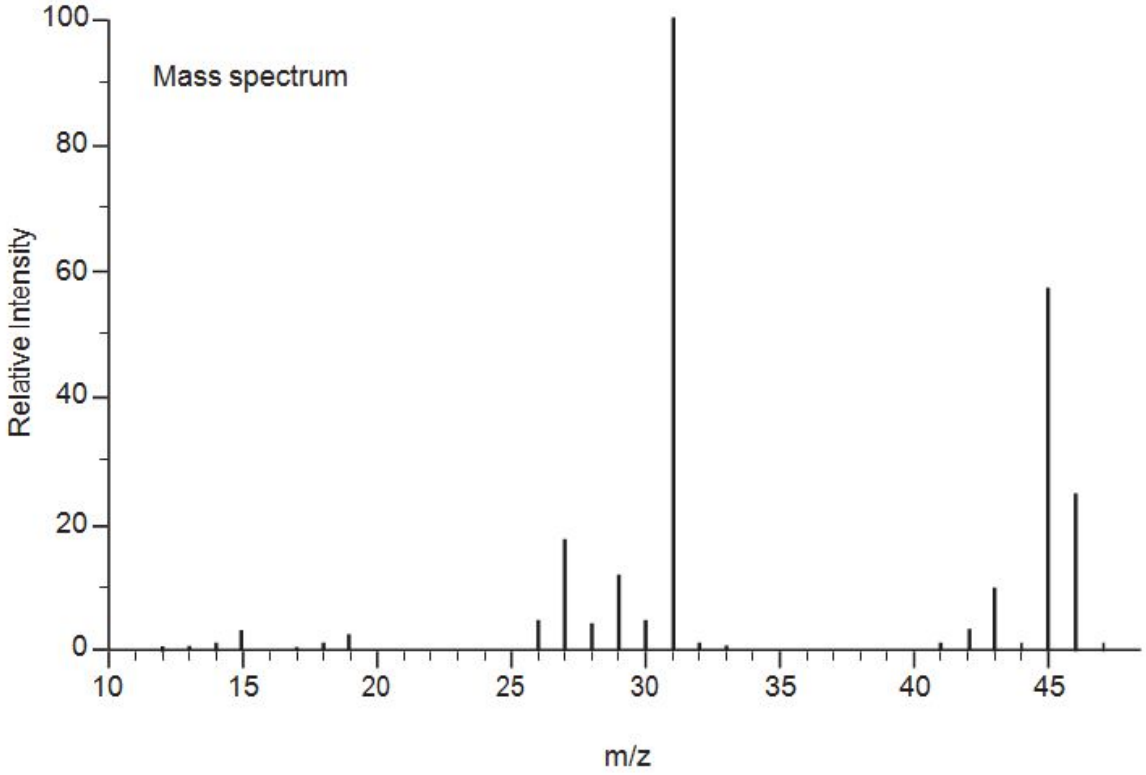
[1]

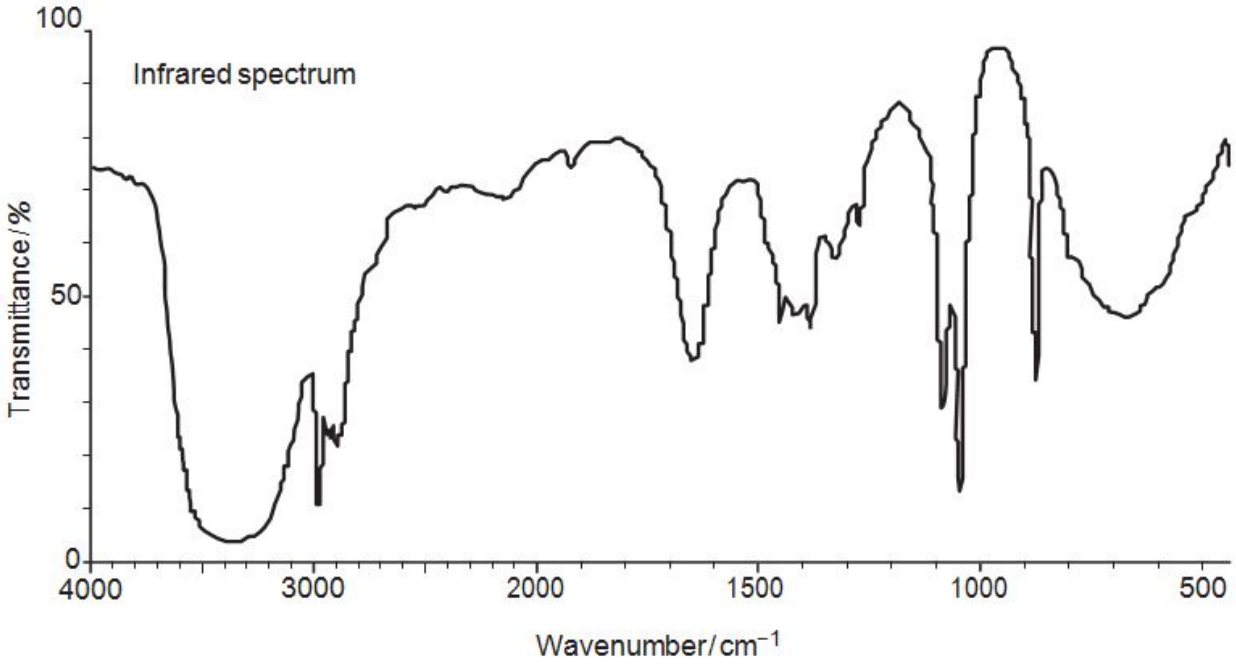
(vi) Draw the structural formula of the alcohol that can be oxidised to form Acid 2.

[1]

(b) Spectra give much information about the structure of organic compounds.

The mass spectrum and infrared spectrum of ethanol, C_2H_5OH, are shown.





(i) What can be deduced by the presence of the peak at m/z 46 in the mass spectrum?

[1]

(ii) What can be deduced by the presence of the peak at m/z 15 in the mass spectrum?

[1]

(iii) What can be deduced by the presence of an absorption peak at 3100 to 3500 cm−1 in the infrared spectrum?

[1]

(c) Ethene can be converted into ethanol and ethanol can be converted into ethene.

For each conversion, state the reagent(s) used and the conditions needed.

[4]

ethene to ethanol

ethanol to ethene

(Total 14)

4. This question concerns isomers with molecular formula $C_5H_{10}O_2$.

(a) Isomers **P**, **Q**, **R** and **S** all react with aqueous sodium carbonate to produce carbon dioxide.

Isomer **P** is a straight-chain compound.

Isomer **Q** contains a chiral carbon centre.

Isomer **R** has only two peaks in its NMR spectrum, both of which are singlets.

Draw the displayed formulae for all **four** isomers. [4]

(b) Isomer **T** is a neutral, sweet-smelling compound and is formed by the reaction between compounds **X** and **Y** in the presence of concentrated sulfuric acid.

Compound **X** has an absorption in its infrared spectrum at 1750 cm^{-1} and a broad absorption around 3000 cm^{-1}.

Compound **Y** can be formed directly from ethanal.

(i)Use **all** the information given to name compounds **X** and **Y**, giving your reasoning. Draw the displayed formula for isomer **T**.

[4] QWC [2]

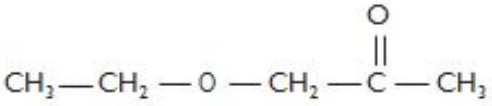
(ii) I. State the reagent needed to form compound **Y** from ethanal

[1]

II. State the role of sulfuric acid in the formation of **T**

[1]

(c) Isomer **U** has the structural formula shown below.



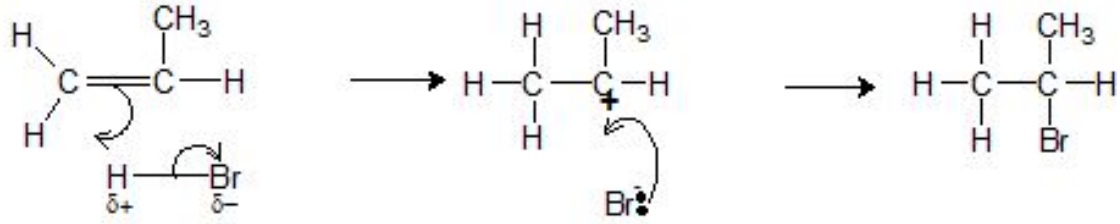
List the peaks which would be found in the NMR spectrum of isomer **U**. Identify which protons are responsible for each peak, giving the approximate chemical shift (ppm) and the splitting of the peak. [4]

(d) Explain which one of isomers **P**, **T** and **U** would have the highest boiling temperature.

[3] QWC [1]

(Total 20)

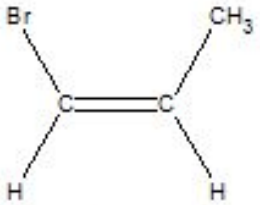
2 (a) (i) 1 mark for arrows in first diagram; 1 mark for arrow in second diagram; 1 mark for all charges



2 max if incorrect isomer given [3]

(ii) 2-bromopropane formed from a secondary carbocation (1)
Secondary carbocations are more stable than primary carbocations (1) [2]

(b) Empirical formula = C_3H_5Br (1)
Molecular formula = C_3H_5Br
(must show use of mass spectrum to gain this mark) (1)
Two molecular ion peaks as there are two isotopes of bromine (1)
Peaks at 15 = CH_3^+ and 41 = $C_3H_5^+$ (1)
550 cm^{-1} = C–Br 1630 cm^{-1} = C=C 3030cm^{-1} = C–H (1)
Molecule is:



(1) [6]

QWC: legibility of text, accuracy of spelling, punctuation and grammar, clarity of meaning [1]

Total [12]

3 (a) (i) Mass C = 1.79 × 12/44 = 0.488 (g) [1]

(ii) Mass O = 0.65 (g) ecf from part (i) [1]

(iii) C : H : O = 0.488/12 : 0.061/1 : 0.65/ 16 = 0.0407 : 0.061 : 0.0406 (1)

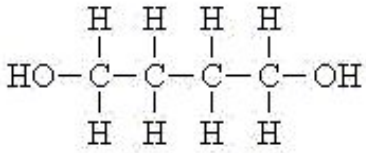
= 2:3:2 empirical formula is $C_2H_3O_2$ (1)

No ecf from incorrect ratios [2]

(iv) *Mr* of empirical formula = 59 so molecular formula is $C_4H_6O_4$ so **F** is acid 2/ molecular formula acid 1 is $C_5H_8O_2$ so empirical formula is not $C_2H_3O_2$ molecular formula acid 2 is $C_4H_6O_4$ so empirical formula is $C_2H_3O_2$ [1]

(v) Bromine turns from brown/red-brown to colourless for Acid 1 [1]

(vi)



[1]

(b) (i) *Mr* / molecular ion (is 46) [1]

(ii) CH_3 (present) [1]

(iii) OH (present) [1]

(c) Ethene to ethanol: steam (1)

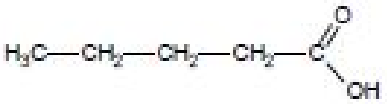
H_3PO_4 (catalyst) (1)

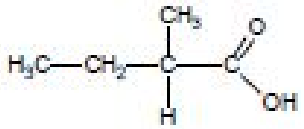
Ethanol to ethene: conc H_2SO_4/ Al_2O_3/ pumice (1)

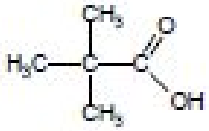
High temperature > 150°C for H_2SO_4
> 300°C for Al_2O_3/ pumice (1) [4]

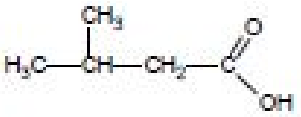
Total [14]

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4 (a) P is  (1)

Q is  (1)

R is  (1)

S is  (1)

[4]

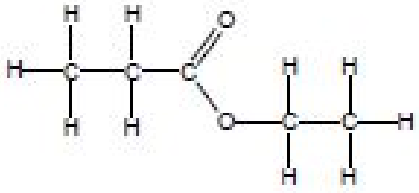
(b) (I) T neutral and sweet-smelling therefore an ester (1)

Infrared spectrum at 1750 cm^{-1} shows C=O and at 3000 cm^{-1} shows O–H therefore X is an acid (1)

Y is an alcohol, formed from ethanal must be ethanol (1)

5 carbons in ester therefore X must be propanoic acid (1)

Structure of T is

 (1)

(Maximum 4 marks) [4]

QWC Legibility of text; accuracy of spelling, punctuation and grammar, clarity of meaning (1)

Selection of a form and style of writing appropriate to purpose and to complexity of subject matter (1) [2]

(II) I Reagent to form Y is $NaBH_4$ / $LiAlH_4$ [1]

II Sulfuric acid acts as a catalyst / removes water so pushes equilibrium to right [1]

(c)

$CH_3(CH_2)$	0.1 to 2.0 ppm triplet (1)
$(CH_3)CH_2O$	3.5 to 4.0 ppm quadruplet (1)
CH_2CO	2.5 to 3.0 ppm singlet (1)
CH_3CO	2.0 to 2.5 ppm singlet (1) [4]

(d) Isomer P (1)

Only P can form hydrogen bonds between molecules (1)

Hydrogen bonds are the strongest intermolecular bonds / need more energy to break hydrogen bonds (1) [3]

QWC The information is organised clearly and coherently, using specialist vocabulary where appropriate [1]

Total [20]