IB · DP · Chemistry

2 hours 14 questions

Structured Questions: Paper 2

11.1 Spectroscopic Identification

11.1.1 Index of Hydrogen Deficiency / 11.1.2 Mass Spectrometry / 11.1.3 Nuclear Magnetic Resonance Spectroscopy / 11.1.4 Infrared Spectroscopy

Easy (5 questions)	/33
Medium (5 questions)	/53
Hard (4 questions)	/28
Total Marks	**/114**

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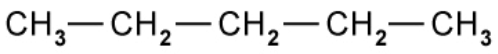
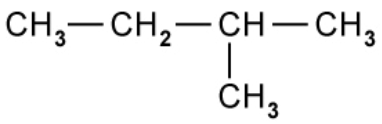
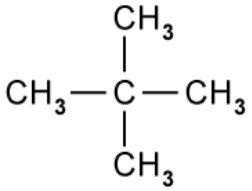
Easy Questions

1 (a) Three isomers of pentane are shown below.

A 

B 

C 

Give the IUPAC names of isomers **B** and **C.**

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(2 marks)

(b) Predict the number of different hydrogen environments in each of the isomers from part (a).

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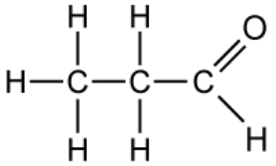
(3 marks)

(c) The displayed formula of propanal is shown.



State the number of ^{1}H NMR signals that would appear in the ^{1}H NMR of propanal and state the ratio of the area under the peaks in which they would appear.

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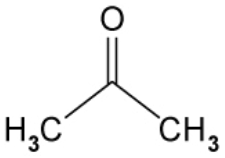
(2 marks)

(d) Propanal and propanone, shown below, both have the same molecular formula C_3H_6O.



Explain how propanone gives a different 1H NMR spectrum compared to propanal.

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(2 marks)

Using section 27 of the data booklet, state the chemical shift for the ^{1}H NMR of propanone.

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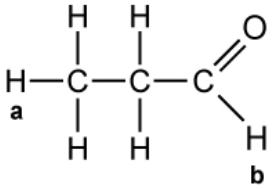
(e) **(1 mark)**

2 (a) Using section 27 of the data booklet, state the chemical shift for hydrogens **a** and **b** in the ^{1}H NMR of propanal.



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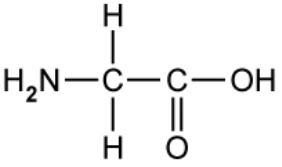
(2 marks)

(b) The structure of the amino acid glycine is shown below.



State the number of peaks found in the ^{1}H NMR spectrum of glycine.

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(1 mark)

(c) State the ratio of the areas under the hydrogen peaks for glycine.

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(1 mark)

(d) The chemical shift for the protons in the NH_2 protons in glycine is 1.0 - 4.5 ppm.

Using section 27 of the data booklet, predict the other ^{1}H NMR chemical shifts for glycine.

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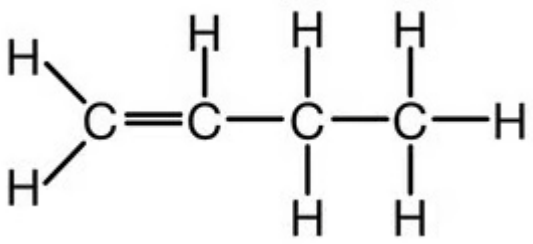
(1 mark)

3 (a) Deduce the hydrogen deficiency of but-1-ene.



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(1 mark)

(b) Phenol acid has the molecular formula C_6H_6O.

Deduce the index of hydrogen deficiency of phenol.

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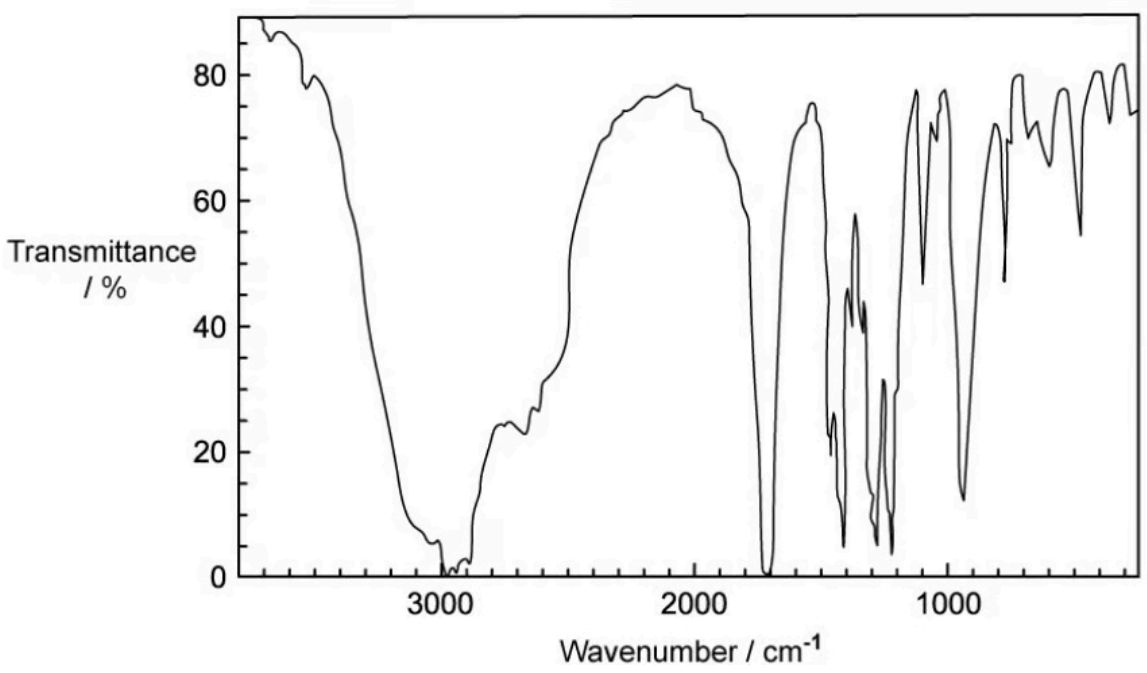
(1 mark)

(c) Under certain conditions, butan-1-ol can be oxidized to the compound with the infrared spectrum shown below.



Using section 26 of the data booklet, state the name of the compound that has produced the spectrum shown.

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(1 mark)

(d) State what the molecular (parent) ion, M^+ peak, in the mass spectrum of a hydrocarbon containing ^{12}C and ^{1}H represents.

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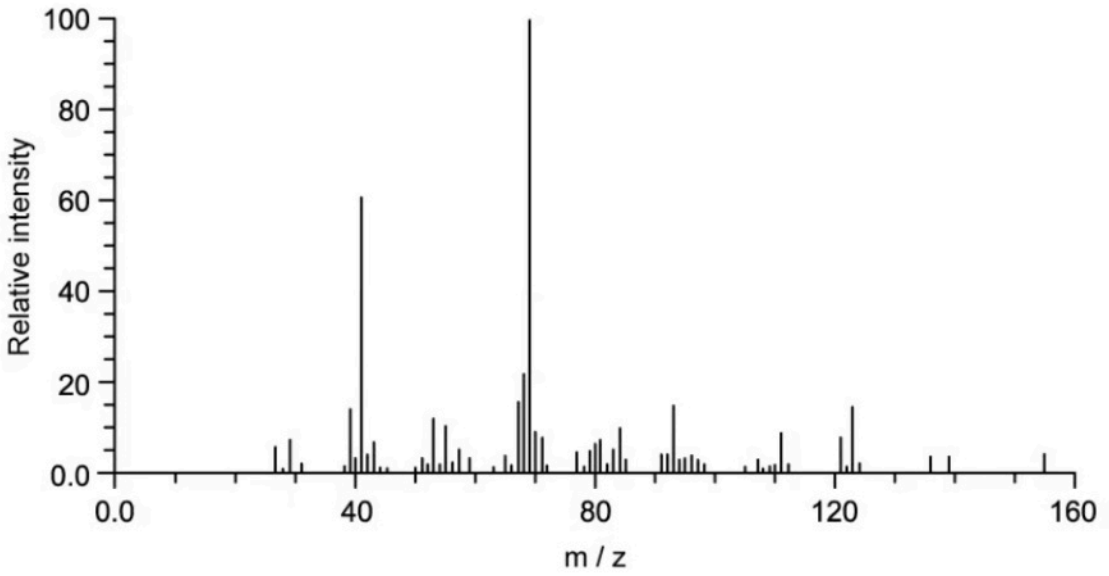
(1 mark)

4 (a) Geraniol is an organic molecule that contains alkene and alcohol functional groups.

The mass spectrum of geraniol is shown below.



i) State how this mass spectrum can be used to confirm the molar mass of geraniol. [1]

ii) Give the formula of an ion that could be responsible for the peak at *m/ z* = 69. [1]

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(2 marks)

(b) A sample of propan-2-ol was heated under reflux with potassium dichromate(VI) acidified with sulfuric acid, and then the mixture was distilled.

Apart from the peaks due to the C—C and C—H bonds, what peak(s) would be present in the infrared spectrum of the distillate.

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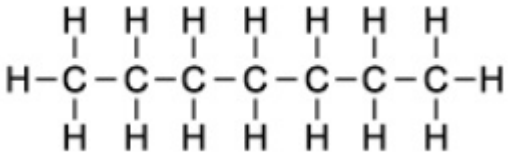
(1 mark)

(c) The compound shown below can be analysed to obtain infrared and mass spectra.



Using section 28 of the data booklet, suggest the molecular formulae of the ions responsible for peaks in the mass spectrum with the following m/e values.

i) 15 [1]

ii) 100 [1]

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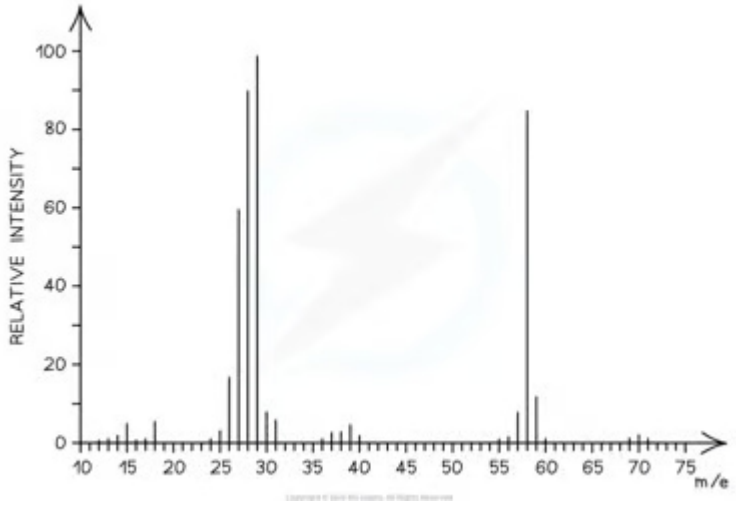
(2 marks)

(d) The mass spectrum shown below was obtained for propanal, CH_3CH_2CHO.



i) Use the mass spectrum to show that the empirical and the molecular formulae of the compound mentioned are the same. [1]

ii) Using section 28 of the data booklet, suggest the species responsible for the peak at *m/z* = 29. [1]

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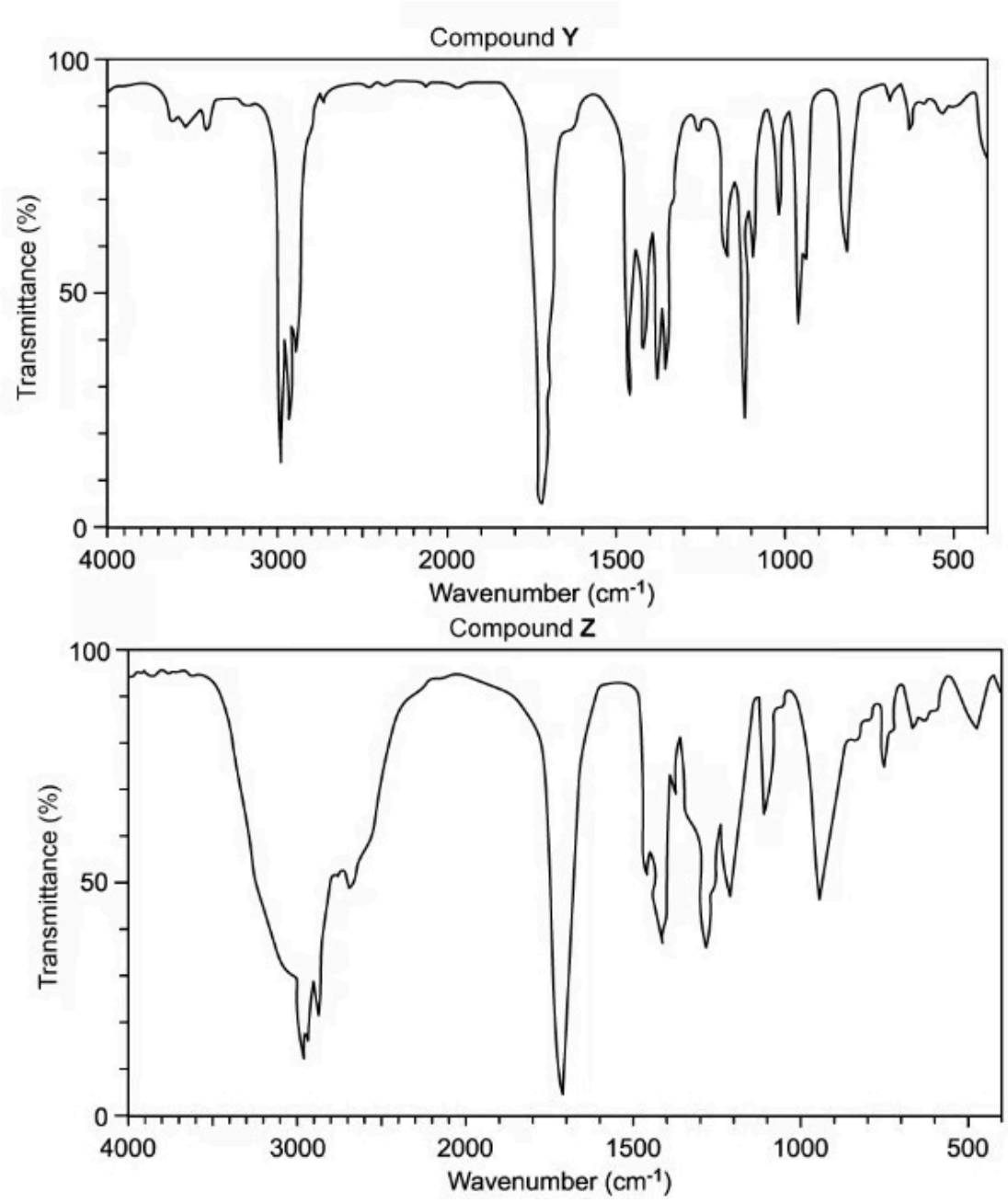
(2 marks)

5 (a) This question is about some isomeric alcohols with the molecular formula $C_5H_{12}O$.

Some alcohols were heated with potassium dichromate(VI) and sulfuric acid. The organic compounds were separated from the reaction mixtures and purified.

The infrared spectra of two of these organic compounds are shown below.



Using section 26 of the data booklet, deduce the type of compound responsible for each spectrum.

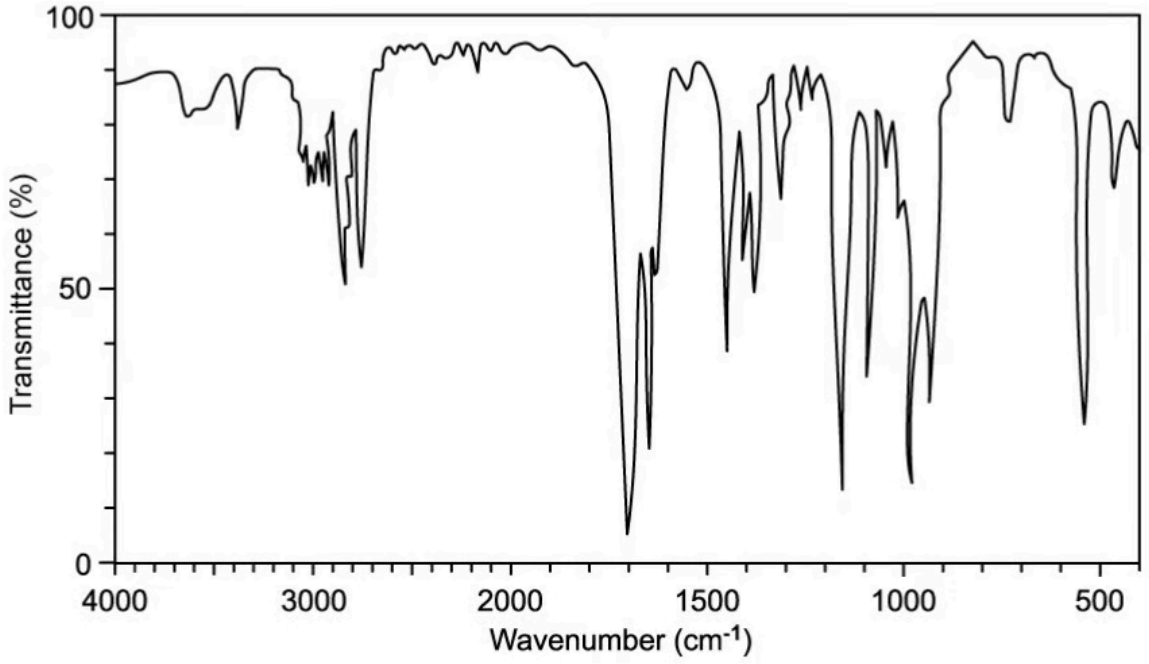
Include in your answer references to wavenumbers and their corresponding bonds.

(2 marks)

(b) State what is meant by the term '*fingerprint region*' on infrared spectra and explain how this can be used to identify primary, secondary and tertiary halogenoalkanes.

(2 marks)

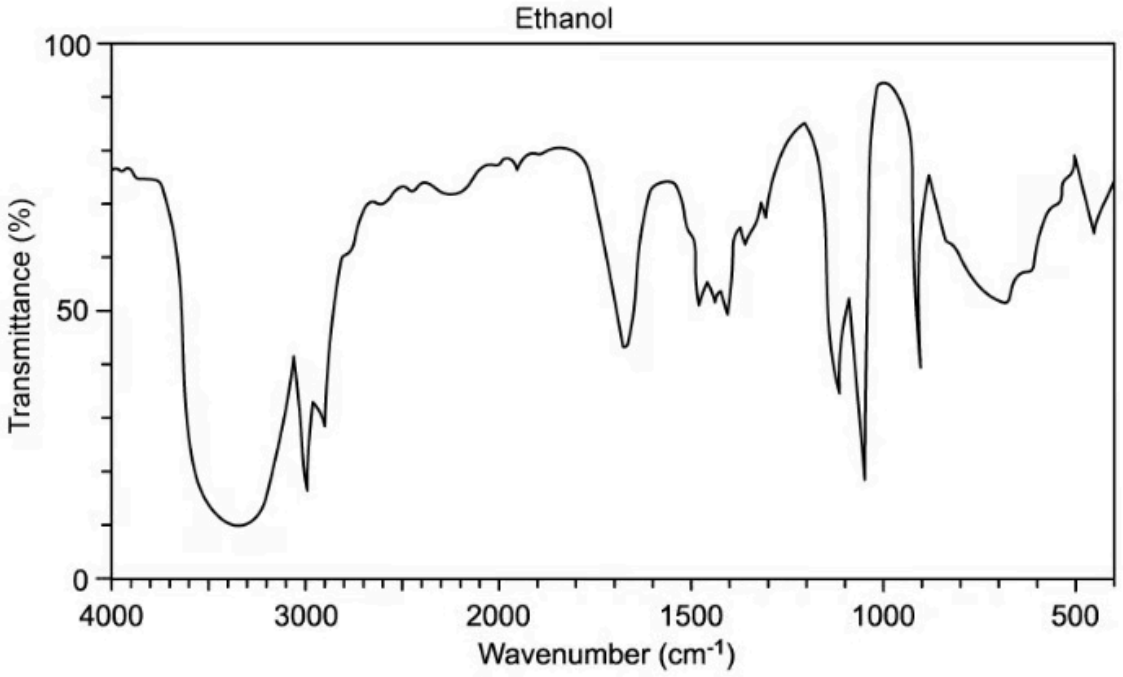
(c) The infrared spectrum a student obtained of an organic molecule which contains carbon, hydrogen and oxygen atoms is shown below.

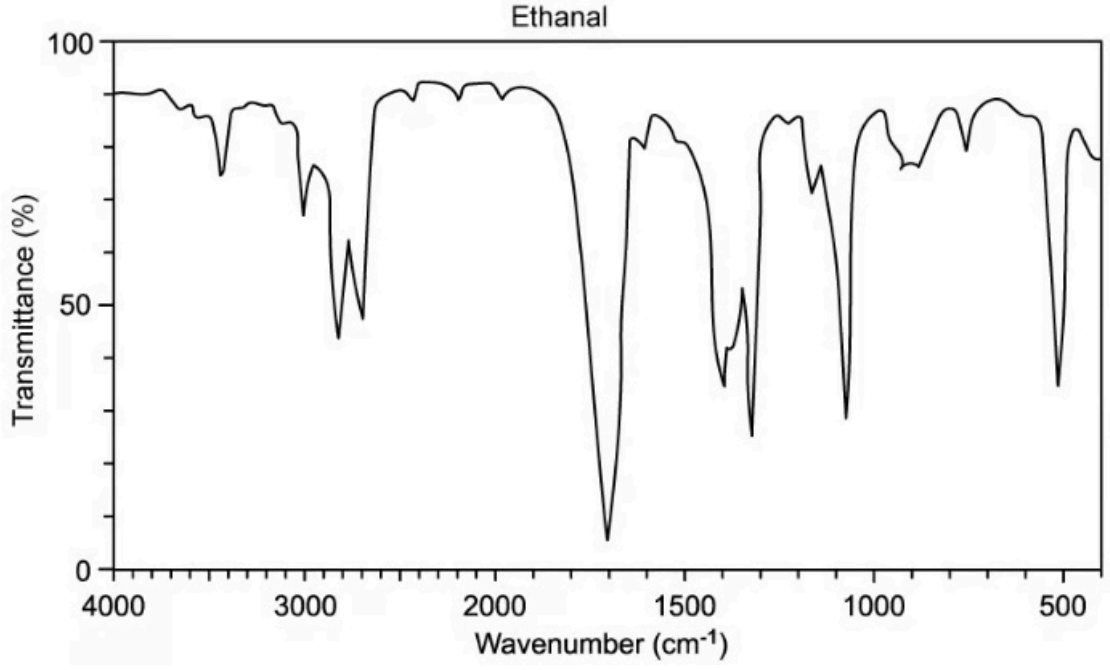


Use section 26 of the data booklet and information from the infrared spectrum to explain how the student deduced that the spectrum shows the presence of a carbonyl group.

(1 mark)

(d) In an experiment to prepare a sample of ethanal, CH_3CHO, ethanol, C_2H_5OH, is reacted with acidified potassium dichromate (VI) and the reaction mixture is distilled. The infrared spectra for ethanol and ethanal are shown below.





i) State the bonds that give rise to the absorption in the ethanol spectrum at 3400 cm^{-1} and the absorption in the ethanal spectrum at 1720 cm^{-1}. [1]

ii) Explain why the absorption at 3400 cm^{-1} in the ethanol spectrum does not appear in the spectrum for ethanal. [1]

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(2 marks)

Medium Questions

1 (a) Often, scientists will use analytical techniques such as infrared spectroscopy to determine if a desired reaction has taken place. Outline how infrared spectroscopy generates useful information about an organic molecule.

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(2 marks)

(b) A chemist uses infrared spectroscopy to distinguish between two organic molecules, a primary alcohol, and an aldehyde.

Use section 26 of the data booklet to state, with a reason, how the chemist could use the IR spectra produced to distinguish between these two molecules.

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(2 marks)

(c) The chemist fully oxidized the alcohol from part (b) and used IR spectroscopy to prove that the reaction had taken place.

State how the chemist could use infrared spectroscopy to determine that the reaction had taken place. Use section 26 of the data booklet to support your answer.

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(1 mark)

(d) The chemist then heated 1-chloro-3-methylbutane under reflux with a solution of sodium hydroxide to produce a different primary alcohol.

i) Name the product of the reaction following the IUPAC rules and draw the condensed structural formula of the product.

ii) State the index of hydrogen deficiency, IHD, of the product you have drawn in part (i) and state what this tells you about the molecule.

(4 marks)

2 (a) Toluene is a common organic chemical with many industrial and commercial applications. Toluene is also known as methylbenzene.

Draw the displayed structure of toluene.

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(1 mark)

(b) State the number of ^{1}H NMR signals that would be seen on the NMR spectrum of toluene and state the ratio of the area under the peaks in which they would appear.

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(2 marks)

(c) Another derivative of benzene has the molecular formula C_8H_{10}.

Draw the structures of the four possible isomers of this derivative.

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(2 marks)

(d) Infrared spectroscopy is a common analytical tool used in chemistry, to identify or distinguish between different organic compounds. These could be compounds such as toluene which contain a benzene ring, or any other organic compound. IR is often used alongside other analytical tools, such as mass spectrometry, to help identify the unknown.

An organic molecule, **J**, has the following composition by mass.

62.1% carbon

10.3% hydrogen

27.6% oxygen

In the mass spectrum of **J**, the molecular ion peak has a value of *m/z* = 116.

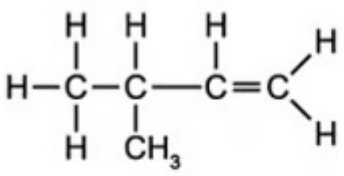
i) Use this information to determine the molecular formula of **J**.

ii) State how an IR spectrum could be used to prove that compound **J** is a carboxylic acid.

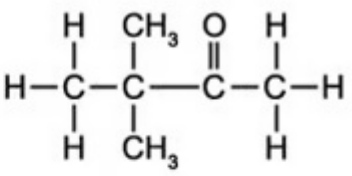
(7 marks)

3 (a) You are provided with the following selection of organic compounds, to investigate using test-tube reactions and spectroscopy.

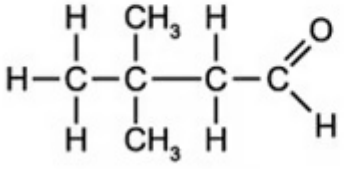
Figure 1



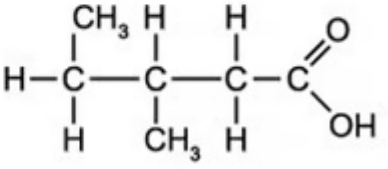
Compound A



Compound B



Compound C



Compound D

State the index of hydrogen deficiency, IHD, of compound B and what this tells you about the molecule.

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(2 marks)

(b) State the simple test-tube reactions that could be done to distinguish between Compound A and Compound D from part (a), including the observations that could be made.

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(4 marks)

(c) Compound D in part (a) can be formed from an alcohol if the correct reagents and conditions are used for the reaction.

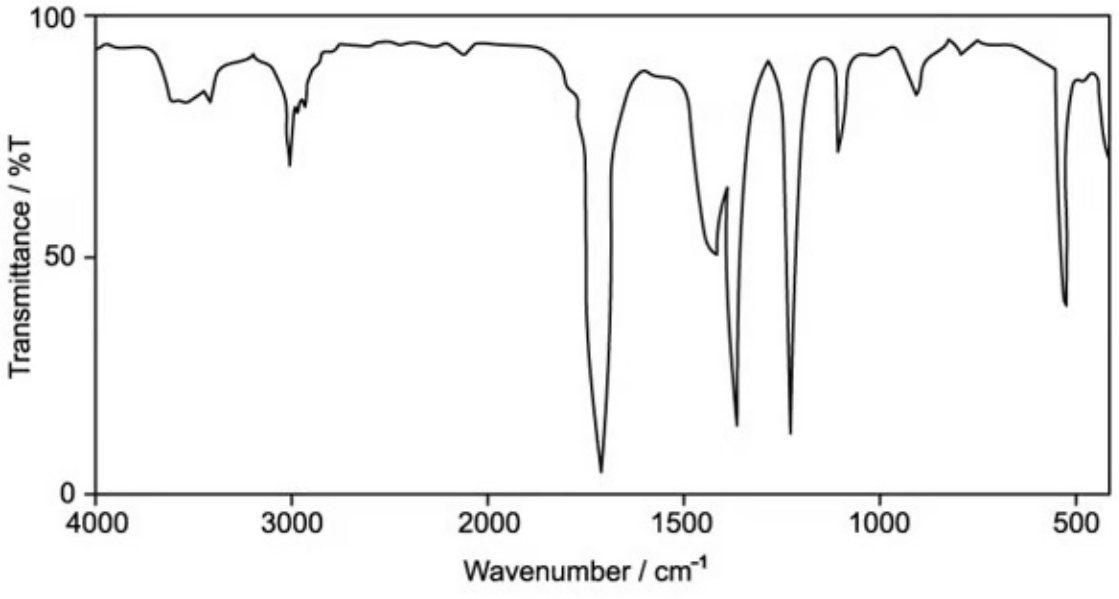
i) State the reagents, conditions and any observations that would be made during the above reaction.

ii) Give the IUPAC name of the alcohol which would need to be used and write an equation using structural formulae for the reaction.

(5 marks)

(d) A student claims to have fully oxidised a different primary alcohol than that in part The student analysed their product and obtained the following IR spectrum.

Figure 2



Use the spectrum in **Figure 2** and section 26 of the data booklet to suggest whether full oxidation has taken place.

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(3 marks)

4 (a) The analytical instruments used for identification of organic compounds are constantly being improved.

Mass spectroscopy is one such analytical tool which provides key information used to identify an unknown compound.

An unknown compound has the empirical formula C_2H_4O, and its mass spectrum has a molecular ion peak at *m/z* 84.

Deduce the molecular formula of the compound.

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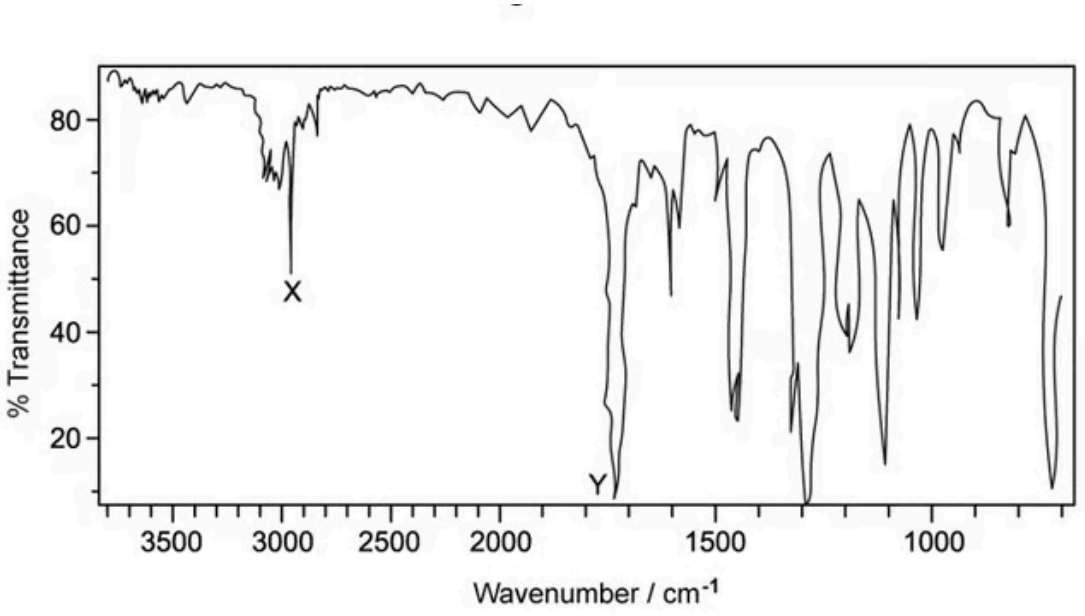
(1 mark)

(b) **Figure 1** below shows the IR spectrum of the unknown compound in part (a).

Identify the bonds which are causing peak X and peak Y on the spectrum, using section 26 of the data booklet.

Figure 1



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(1 mark)

(c) The unknown compound is a carboxylic acid. Deduce the two possible carboxylic acid structural isomers.

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(2 marks)

(d) For each of the isomers drawn in part (c), state the number of signals which would be seen in an ^{1}H NMR spectrum and the ratio of the areas under the peaks.

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(4 marks)

5 (a) A group of students are asked to distinguish between four samples of different organic compounds.

The four samples are as follows:

- A primary alcohol
- A tertiary alcohol
- An aldehyde
- A carboxylic acid

Describe how the group of students could distinguish between the two different alcohols.

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(3 marks)

(b) One of the students wanted to distinguish between three compounds using mass spectrometry alone. The three compounds are shown below in **Figure 1** and the mass spectrum for one of the compounds is shown in **Figure 2**.

Figure 1

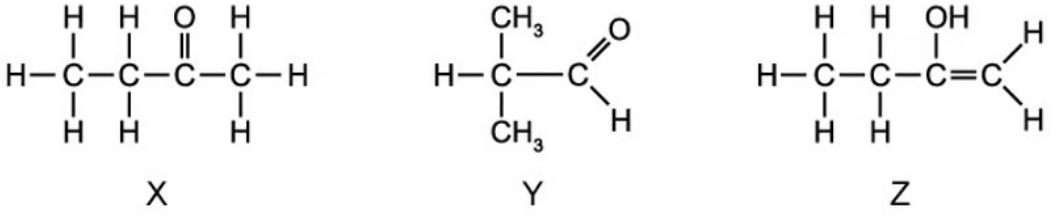
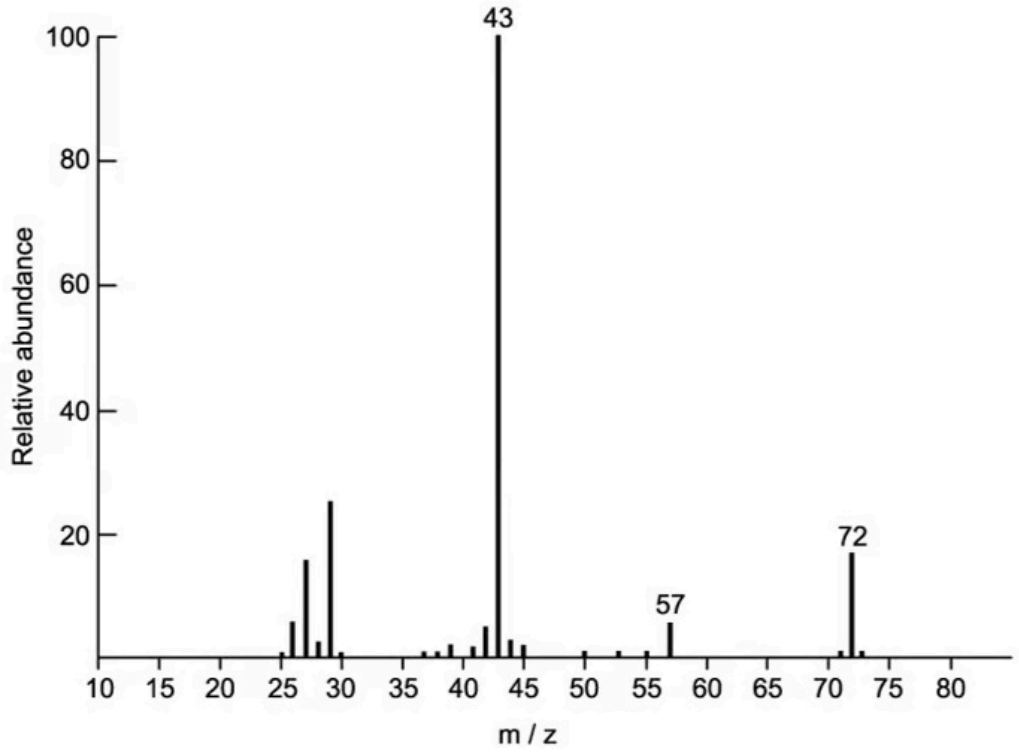


Figure 2



Explain, using **Figure 2**, why determining the exact mass using mass spectrometry alone would not help in distinguishing between the samples of X, Y and Z shown in **Figure 1**.

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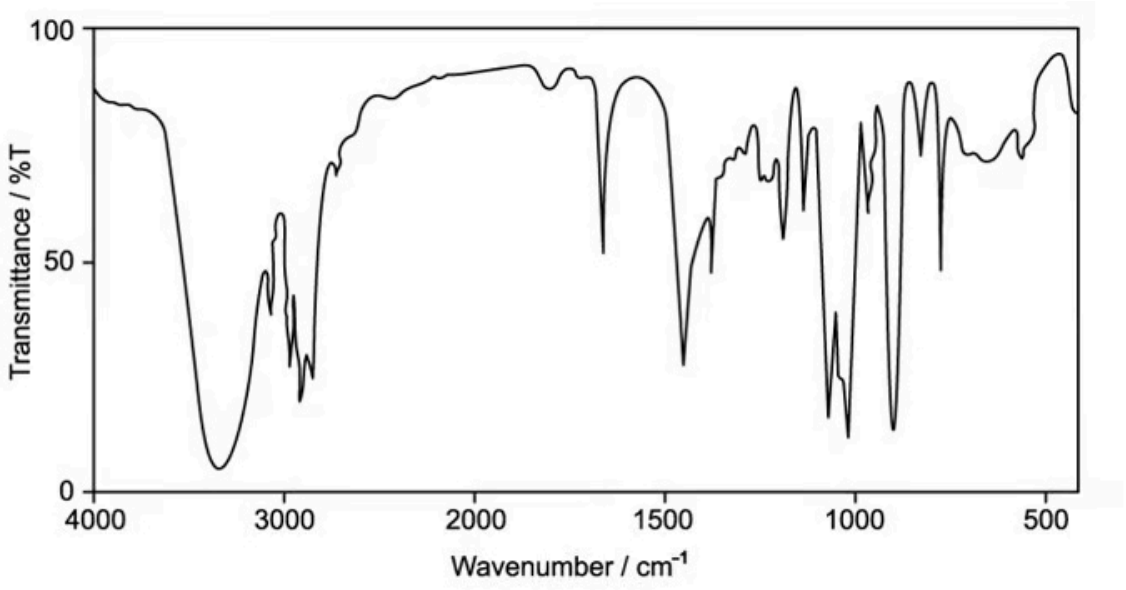
(3 marks)

(c) The three compounds from **Figure 1** in part (b) were analysed using IR spectroscopy. The spectrum of one of the compounds is shown below:

Figure 3



Identify which of the three compounds X, Y or Z this spectrum belongs to. Justify your choice.

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(2 marks)

(d) State, with a reason, how infrared spectroscopy would be used to distinguish between the compounds X and Y from **Figure 1** in part (b).

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(2 marks)

Hard Questions

1 (a) Zanamivir is an inhibitor used to treat infections caused by the influenza A and B viruses.

Using section 37 of the data booklet, deduce the hydrogen deficiency of Zanamivir.

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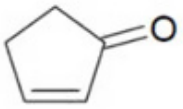
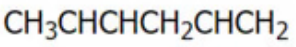
(1 mark)

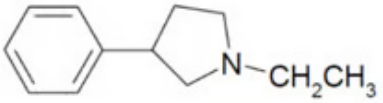
(b) Determine which of the following molecules has the same IHD and state the IHD value.



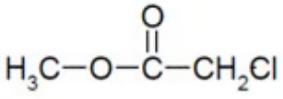
I



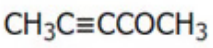
II



III



IV



V

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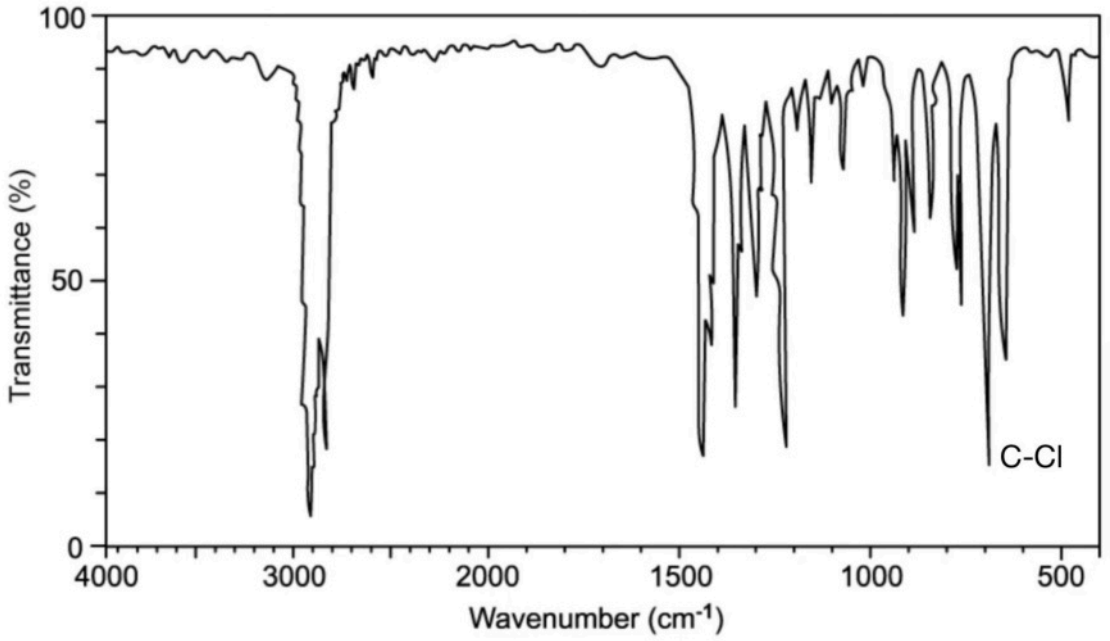
(1 mark)

2 (a) An alcohol can be prepared by hydrolysing the halogenoalkane $C_2H_5CHBClCH_3$ with aqueous sodium hydroxide. The infrared spectrum for $C_2H_5CHClCH_3$ is shown below with the C–Cl bond absorption labelled.



Using section 26 of the data booklet deduce how IR spectroscopy will change as a result of the above reaction.

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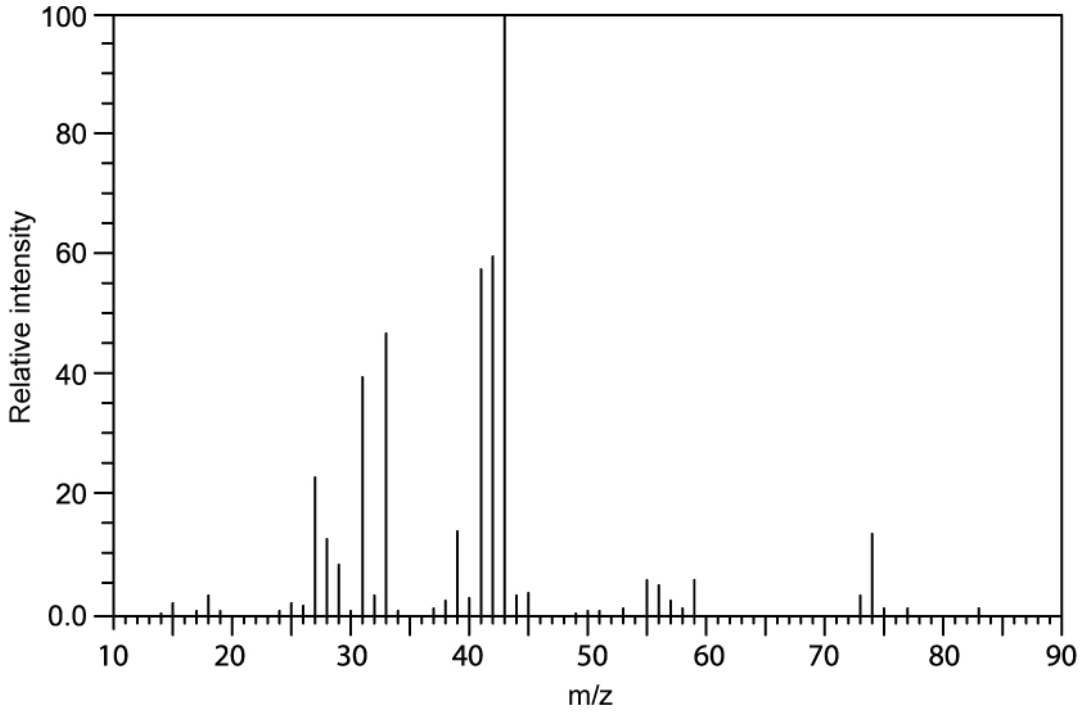
(2 marks)

(b) The mass spectrum of $(CH_3)_2CHCH_2OH$ is shown below.



Deduce which ion is responsible for the peak with the greatest relative intensity.

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(1 mark)

(c) Alcohol **X** has the following percentage composition by mass. Carbon = 68.2%, hydrogen = 13.6%, oxygen = 18.2%. The molecular ion peak in the mass spectrum for alcohol **X** occurs at *m/z* = 88.

i) Use this information and section 6 of the data booklet to show that the molecular formula for alcohol **X** is $C_5H_{12}O$. Include your working.

[2]

ii) When alcohol **X** is oxidised, a carboxylic acid can be formed. State what information this gives about alcohol **X**.

[1]

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.....

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(3 marks)

(d) The mass spectrum of alcohol **X** has a major peak at *m/z* = 45.

i) Draw the structure of the species that could give this peak.

[1]

ii) Alcohol **X** has a branched chain. Deduce the structural formula and IUPAC name of alcohol **X**. Justify your answer.

[2]

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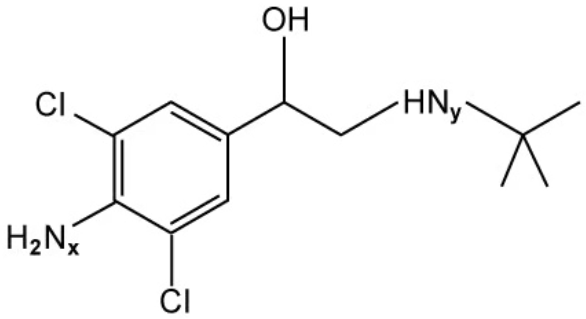
(3 marks)

3 (a) Clenbuterol, shown below, is considered a performance enhancing drug and is believed to increase short term work rate and cardiovascular output.



Deduce the functional groups marked *x* and *y* and state to which class they belong to.

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(2 marks)

(b) Determine the m/z value of the molecular ion, M^+, of clenbuterol. Justify your answer.

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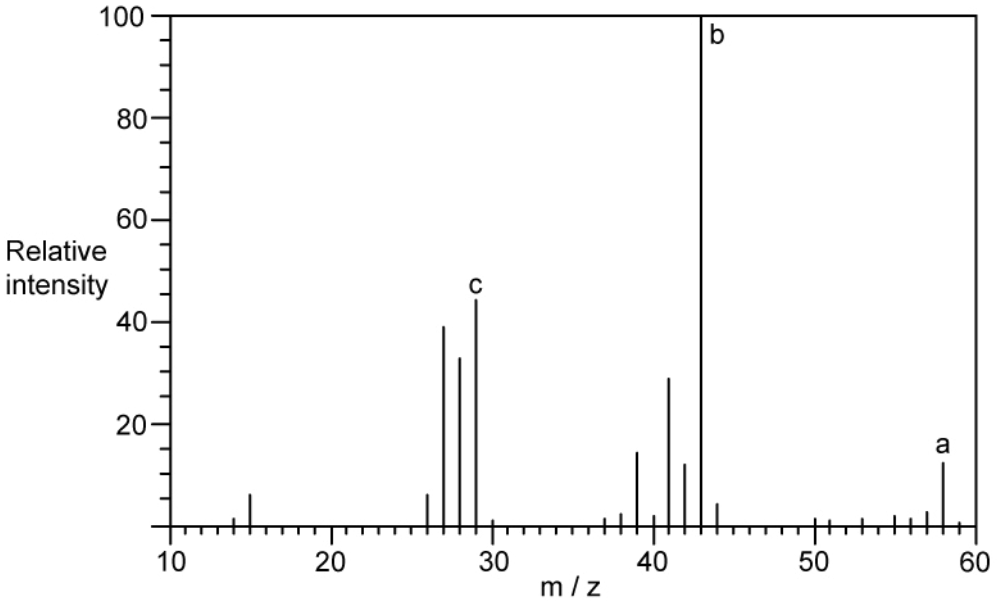
(2 marks)

(c) Two students, **P** and **Q**, were provided with the mass spectrum of an alkane, shown in below. Student **P** analysed peaks **a** and **b** and concluded that the alkane was one of two structures. Student **Q** analysed peaks **a**, **b** and **c** and was able to identify one possible alkane structure.



i) Deduce which fragments of the alkane correspond to peaks **a**, **b** and **c**.

[3]

ii) Suggest why the two students obtained different conclusions.

[2]

(5 marks)

4 (a) Four samples containing isomeric alcohols with molecular formula $C_4H_{10}O$, were studied using ^1H NMR spectroscopy

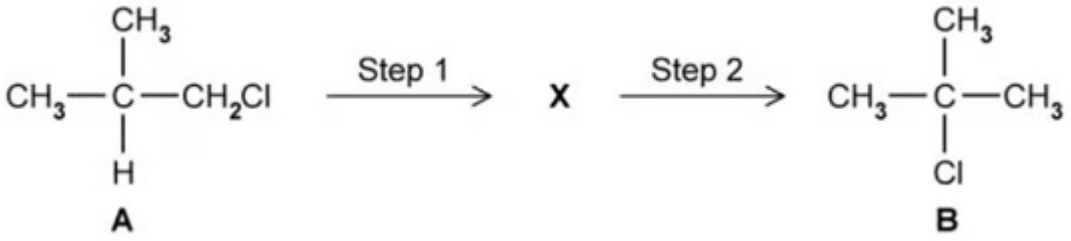
Draw structural formulas of the alcohols and deduce the number of peaks in the NMR spectrum of each alcohol

(4 marks)

(b) Two of the alcohols produce the same number of peaks in an ^1H NMR spectrum. Suggest how they may be distinguished, by further spectroscopy analysis.

(2 marks)

(c) Compound A can be converted into compound B via an intermediate species.



Suggest how you would be able to determine the difference between Compounds **A** and **B** by analysis of their ^1H NMR spectra.

(2 marks)