11.1 Spectroscopic Identification

Question Paper

Course	DP IB Chemistry
Section	11. Measurements & Data Processes
Topic	11.1 Spectroscopic Identification
Difficulty	Medium

Time allowed: 70

Score: /53

Percentage: /100

Question 1a

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.

[2 marks]

Question 1b

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.

[2 marks]

Question 1c

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.

[1 mark]

Question 1d

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]

Question 2a

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.

[1 mark]

Question 2b

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.

[2 marks]

Question 2c

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

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

[2 marks]

Question 2d

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**.

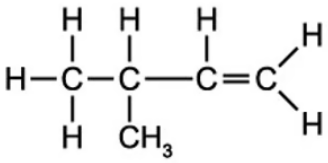
ii) State how an IR spectrum could be used to prove that compound **J** is a carboxylic acid.

[7 marks]

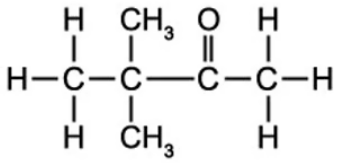
Question 3a

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

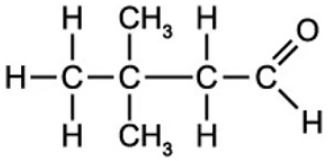
Figure 1



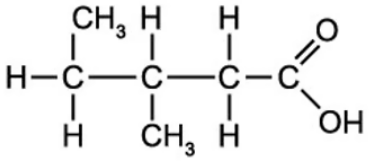
Compound A



Compound B



Compound C



Compound D

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

[2 marks]

Question 3b

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.

[4 marks]

Question 3c

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.

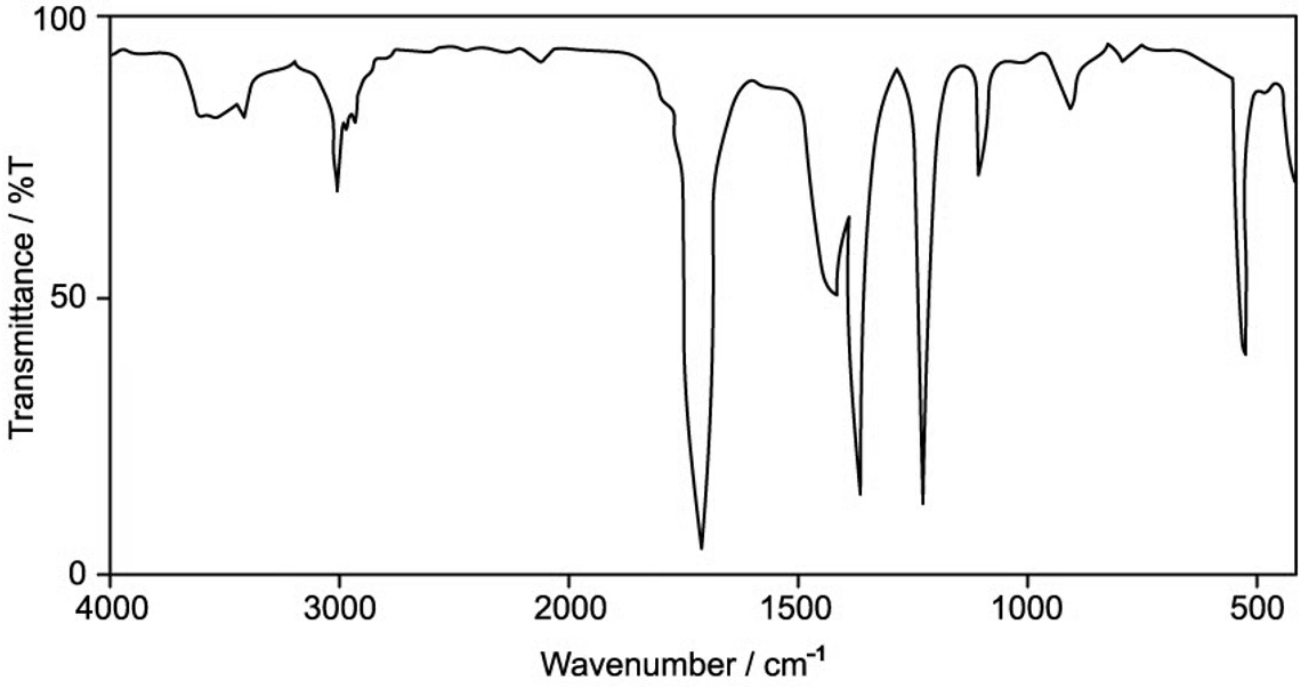
ii) Give the IUPAC name of the alcohol which would need to be used and write an equation using structural formulae for the reaction.

[5 marks]

Question 3d

d) A student claims to have fully oxidised a different primary alcohol than that in part (c). 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.

[3 marks]

Question 4a

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.

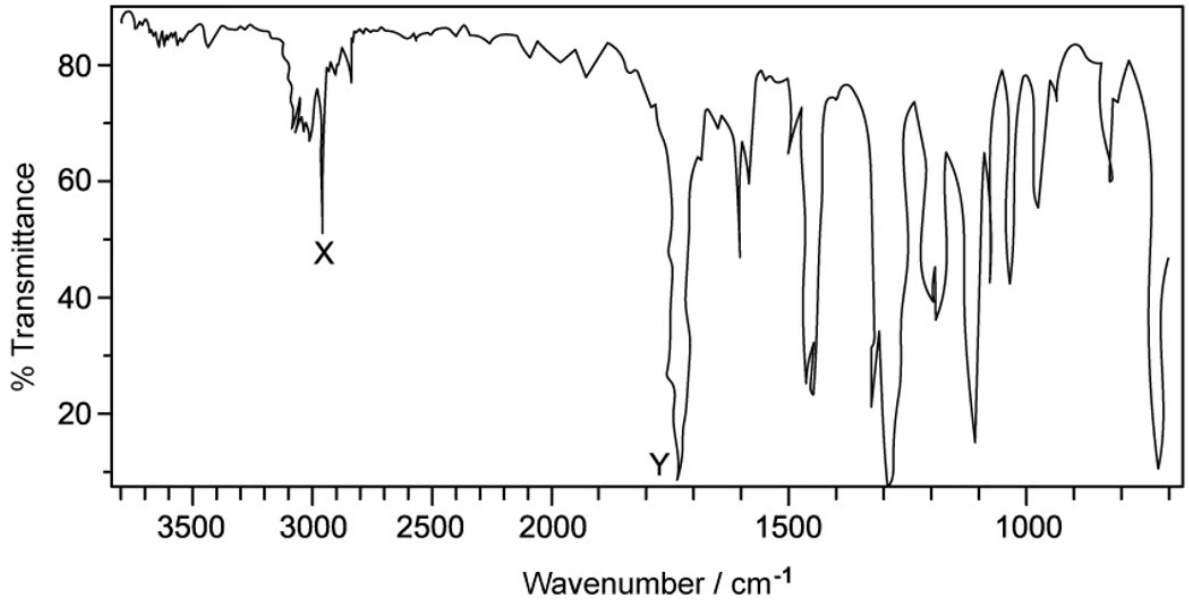
[1 mark]

Question 4b

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



[1 mark]

Question 4c

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

[2 marks]

Question 4d

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.

[4 marks]

Question 5a

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

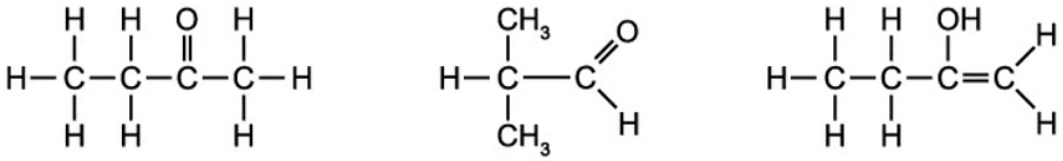
Describe how the group of students could distinguish between the two different alcohols.

[3 marks]

Question 5b

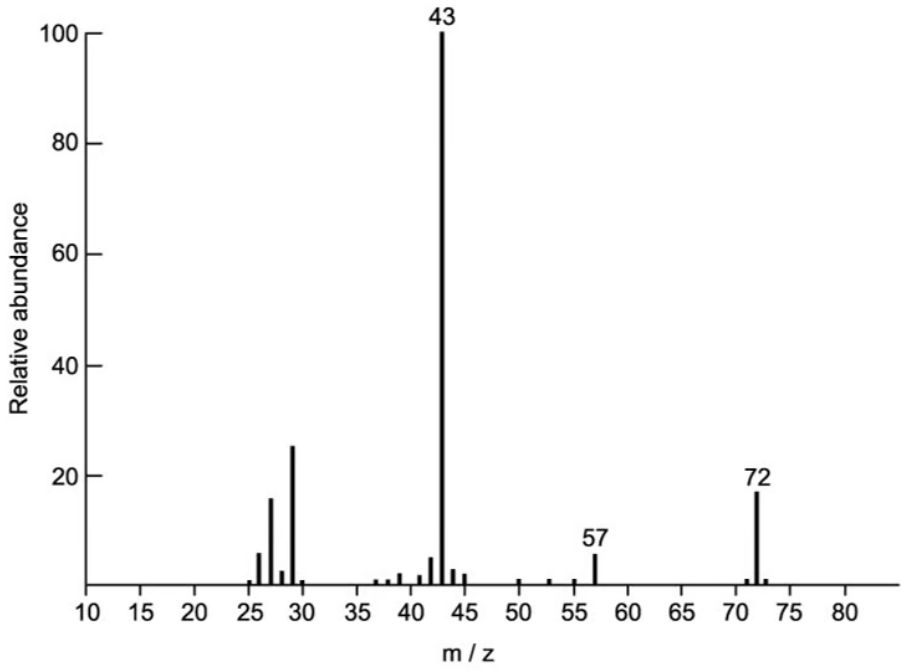
b) One of the students wanted to distinguish between three compounds using mass spectrometry alone. The three compounds are shown below in **Figure 1** and the mass spectrum for one of the compounds is shown in **Figure 2**.

Figure 1



X Y Z

Figure 2



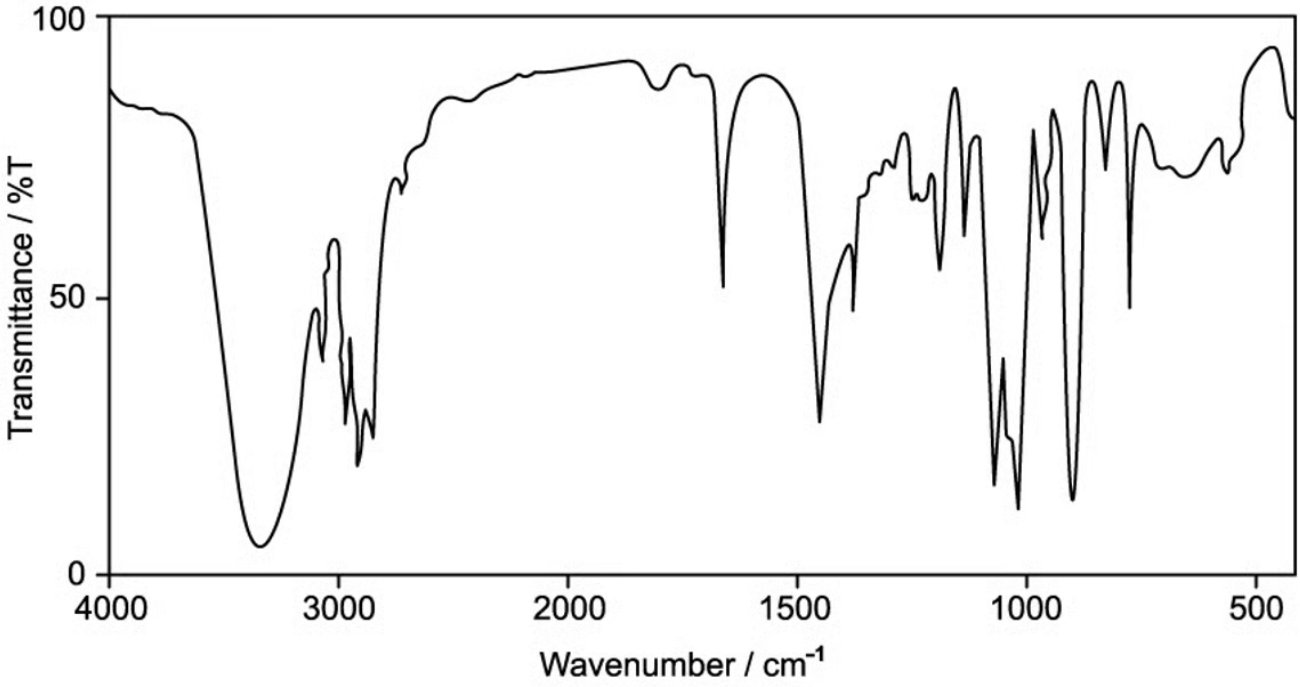
Explain, using **Figure 2**, why determining the exact mass using mass spectrometry alone would not help in distinguishing between the samples of X, Y and Z shown in **Figure 1**.

[3 marks]

Question 5c

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.

[2 marks]

Question 5d

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).

[2 marks]