AQA – Nuclear Magnetic resonance spectroscopy – A2 Chemistry P2

1. June/ 2020/Paper_2/No.7

0 7 This question is about NMR spectroscopy.

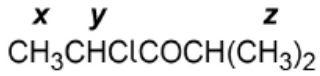
0 7 . 1 A compound is usually mixed with $Si(CH_3)_4$ and either CCl_4 or $CDCl_3$ before recording the compound's ^1H NMR spectrum.

State why $Si(CH_3)_4$, CCl_4 and $CDCl_3$ are used in ^1H NMR spectroscopy.

Explain how their properties make them suitable for use in ^1H NMR spectroscopy.

[6 marks]

0 7 . 2 Deduce the splitting pattern for each of the peaks given by the H atoms labelled ***x***, ***y*** and ***z*** in the ^{1}H NMR spectrum of the compound shown.



[3 marks]

x _____

y _____

z _____

0 7 . 3 Suggest why it is difficult to use **Table B** in the Data Booklet to predict the chemical shift (δ value) for the peak given by the H atom labelled ***y***.

[1 mark]

_____

_____

_____

_____

0 7 . 4 Two isomers of $CH_3CHClCOCH(CH_3)_2$ each have two singlet peaks only in their ^{1}H NMR spectra.
In both spectra the integration ratio for the two peaks is 2:9

Deduce the structures of these two isomers.

[2 marks]

Isomer 1

Isomer 2

2. June/ 2019/Paper_2/No.6 (6.2),(6.)

0 6 . 2 Compounds **A** and **B** both have the molecular formula $C_4H_8Br_2$
A has a singlet, a triplet and a quartet in its ^1H NMR spectrum.
B has only two singlets in its ^1H NMR spectrum.

Draw a structure for each of **A** and **B**.

[2 marks]

A **B**

0 6 . 3 Compounds **C** and **D** both have the molecular formula $C_6H_3Br_3$
C has two peaks in its ^{13}C NMR spectrum.
D has four peaks in its ^{13}C NMR spectrum.

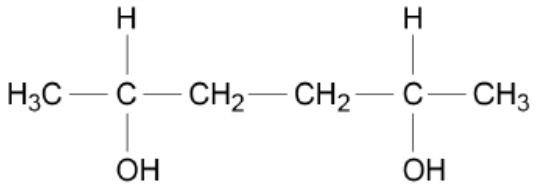
Draw a structure for each of **C** and **D**

[2 marks]

C **D**

3. June/ 2019/Paper_2/No.10 (10.3-10.5)

1 0 . 3 Compounds with molecular formula $C_6H_{14}O_2$ also have a relative molecular mass of 118 to the nearest whole number. These include the diol shown.



Deduce the number of peaks in the ^1H NMR spectrum of this diol.

[1 mark]

1 0 . 4 Draw the structure of a different diol also with molecular formula $C_6H_{14}O_2$ that has a ^1H NMR spectrum that consists of two singlet peaks.

[1 mark]

1 0 . 5 The dicarboxylic acid in question **10.1** and the isomers of $C_6H_{14}O_2$ in Questions **10.3** and **10.4** all have a relative molecular mass of 118

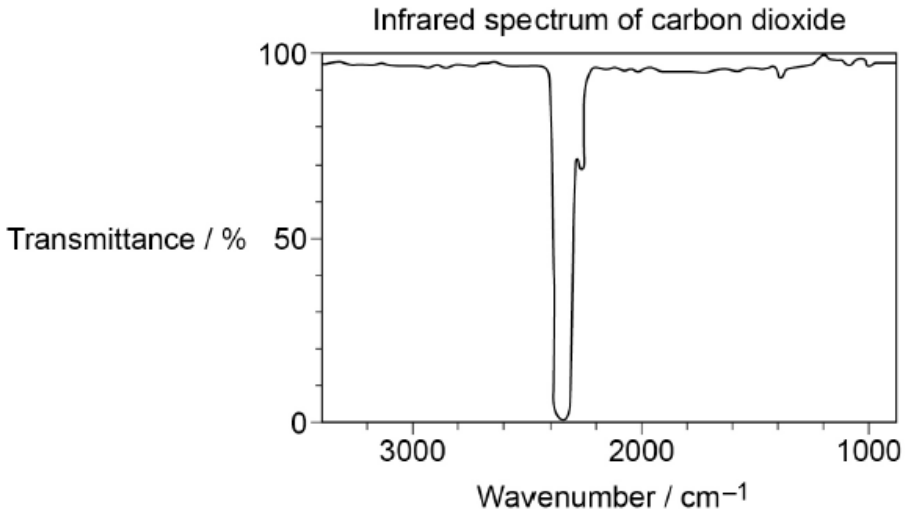
State why the dicarboxylic acid can be distinguished from the two diols by high resolution mass spectrometry using electrospray ionisation.

[1 mark]

4. June/ 2019/Paper_2/No.11 (11.5)

1 1 . 5 Combustion of biodiesel produces greenhouse gases such as carbon dioxide that cause global warming.
Part of the infrared spectrum of carbon dioxide is shown in **Figure 3**.

Figure 3



State how the infrared spectrum of carbon dioxide in **Figure 3** is **not** what you might predict from the data provided in **Table A** in the Data Booklet.

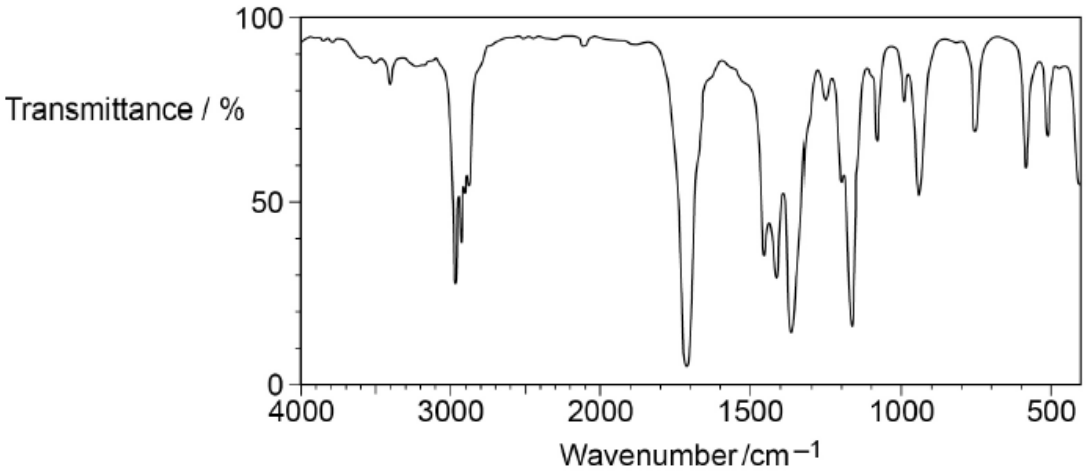
[1 mark]

5. June/2021/Paper_2/No.7

0 7 This question is about spectroscopy.

0 7 . 1 Compound **K** has molecular formula C_4H_8O
Figure 5 shows the infrared spectrum of **K**.

Figure 5



Which functional group does **K** contain?

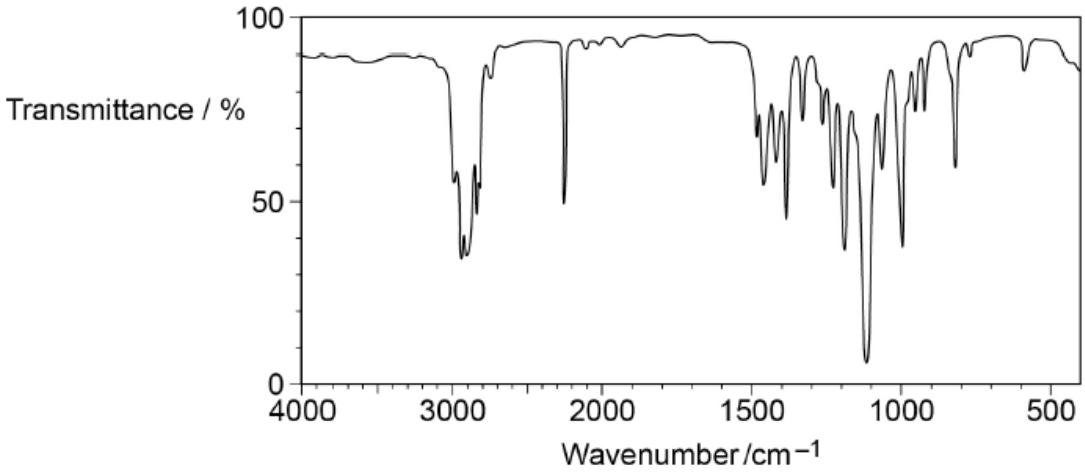
Tick (✓) **one** box.

[1 mark]

Functional Group				
alcohol	alkene	amine	carbonyl	nitrile

0 7 . 2 Compound **L** has molecular formula C_4H_7NO
Figure 6 shows the infrared spectrum of **L**.

Figure 6



L reacts with H_2 in the presence of a nickel catalyst to give compound **M**.

Suggest **three** ways in which the infrared spectrum of **M** is different from the infrared spectrum of **L**.

[3 marks]

1 _____

_____

2 _____

_____

3 _____

_____

0 7 . 3 **Figure 7** shows the ^{1}H NMR spectrum of **Q**, C_3H_7ClO

Figure 7

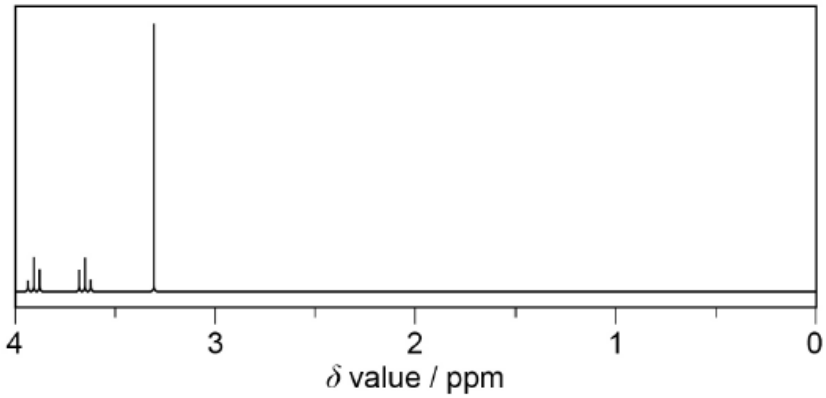


Table 4 shows the chemical shifts (δ values) and integration values for each peak.

Table 4

δ value / ppm	3.95	3.65	3.35
Integration value	0.6	0.6	0.9

Deduce the structure of **Q**.

Explain your answer.

[5 marks]