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CHEMISTRY INORGANIC CHEMISTRY II

Level & Board	AQA (A-LEVEL)
TOPIC:	NMR SPECTROSCOPY
PAPER TYPE:	QUESTION PAPER - 2
TOTAL QUESTIONS	10
TOTAL MARKS	24

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NMR Spectroscopy - 2

1. Bromobutane, CH₃CH₂CH₂CH₂Br, can be reacted with hot aqueous sodium hydroxide to prepare butan-1-ol.

The butan-1-ol produced can be analysed by mass spectrometry.

(a) Predict two fragment ions that you would expect to see in the mass spectrum of butan-1-ol and state the m/z value of each ion.

(2)

(b)State a use of mass spectrometry outside of the laboratory.

(1)

- **2.** Which one of the following does not have a singlet peak in its proton n.m.r. spectrum?
 - A. Butyl methanoate
 - **B.** Propyl ethanoate
 - C. Ethyl propanoate
 - D. Methyl butanoate

(1)

- **3.** Compound Q has the molecular formula C₄H₇CIO and does not produce misty fumes when added to water.
 - (a) The infra-red spectrum of Q contains a major absorption at 1724 cm⁻¹.



(1)

(b) The mass spectrum of Q contains two molecular ion peaks at m/z = 106 and m/z = 108. It also has a major peak at m/z = 43.

Suggest why there are two molecular ion peaks.

(1)

(c) A fragment ion produced from Q has m/z = 43 and contains atoms of three different elements.

Identify this fragment ion and write an equation showing its formation from the molecular ion of Q.

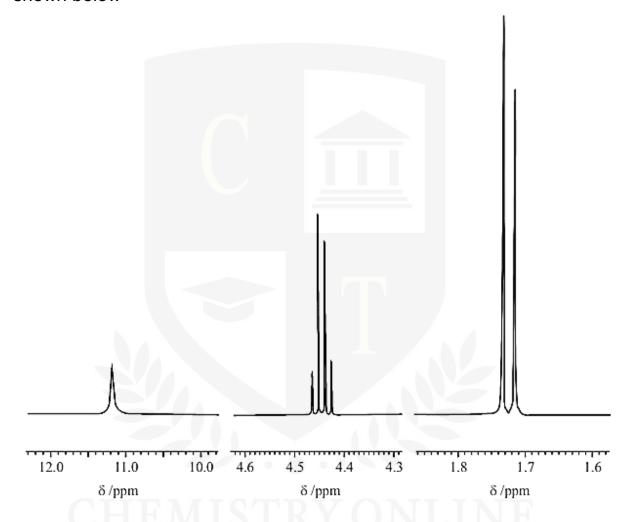
(2)

- **4.** Which one of the following has a singlet peak in its proton n.m.r. spectrum?
 - A. Ethyl propanoate
 - B. propyl methanoate
 - C. hexan-3-one

D. 2-chlorobutane

(1)

5. Three sections of the proton n.m.r. spectrum of CH₃CHClCOOH are shown below



(a) Name the compound CH₃CHClCOOH.

(1)

(b) Explain the splitting patterns in the peaks at δ 1.72 and δ 4.44

(2) (c) Predict the splitting pattern that would be seen in the proton n.m.r. spectrum of the isomeric compound CICH₂CH₂COOH **(1)** 6. Propene reacts with hydrogen bromide to form a mixture of saturated organic products. The proton n.m.r. spectrum of the major organic product has A. 3 peaks with relative intensities 3:2:2 B. 2 peaks with relative intensities 3:4 C. 3 peaks with relative intensities 3:1:3 D. 2 peaks with relative intensities 6:1 **(1)** 7. Proton n.m.r. spectra are recorded using a solution of a substance to which tetramethylsilane (TMS) has been added. (a) Give two reasons why TMS is a suitable standard. **(2)** (b) Give an example of a solvent which is suitable for use in recording an n.m.r. spectrum.

Give a reason for your choice.

(2)

- **8.** How many peaks will be observed in the low-resolution proton n.m.r. spectrum of (CH₃)₂CHCOO(CH₂)₃CH₃?
 - **A**. 4
 - **B.** 5
 - **C.** 6
 - **D.** 7

(1)

9. Butenedioic acid, HOOCCH=CHCOOH, occurs as two stereoisomers.

One of the isomers readily forms the acid anhydride $C_4H_2O_3$ when warmed.

Describe and explain the appearance of the proton n.m.r. spectrum of butenedioic acid.

(3)

10. State the number of peaks in the proton n.m.r. spectra of CH₃CH₂CH₂CH₂OH and of (CH₃)₃COH. (Analysis of peak splitting is not required.)

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