



CHEMISTRY ONLINE
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Phone: +442081445350

www.chemistryonlinetuition.com

Email: asherrana@chemistryonlinetuition.com

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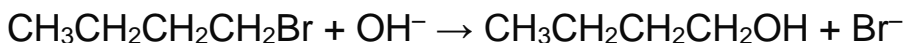
ORGANIC CHEMISTRY II

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, $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{Br}$, 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)

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3. Compound Q has the molecular formula C_4H_7ClO 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} .

Identify the bond responsible for this absorption.

(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)

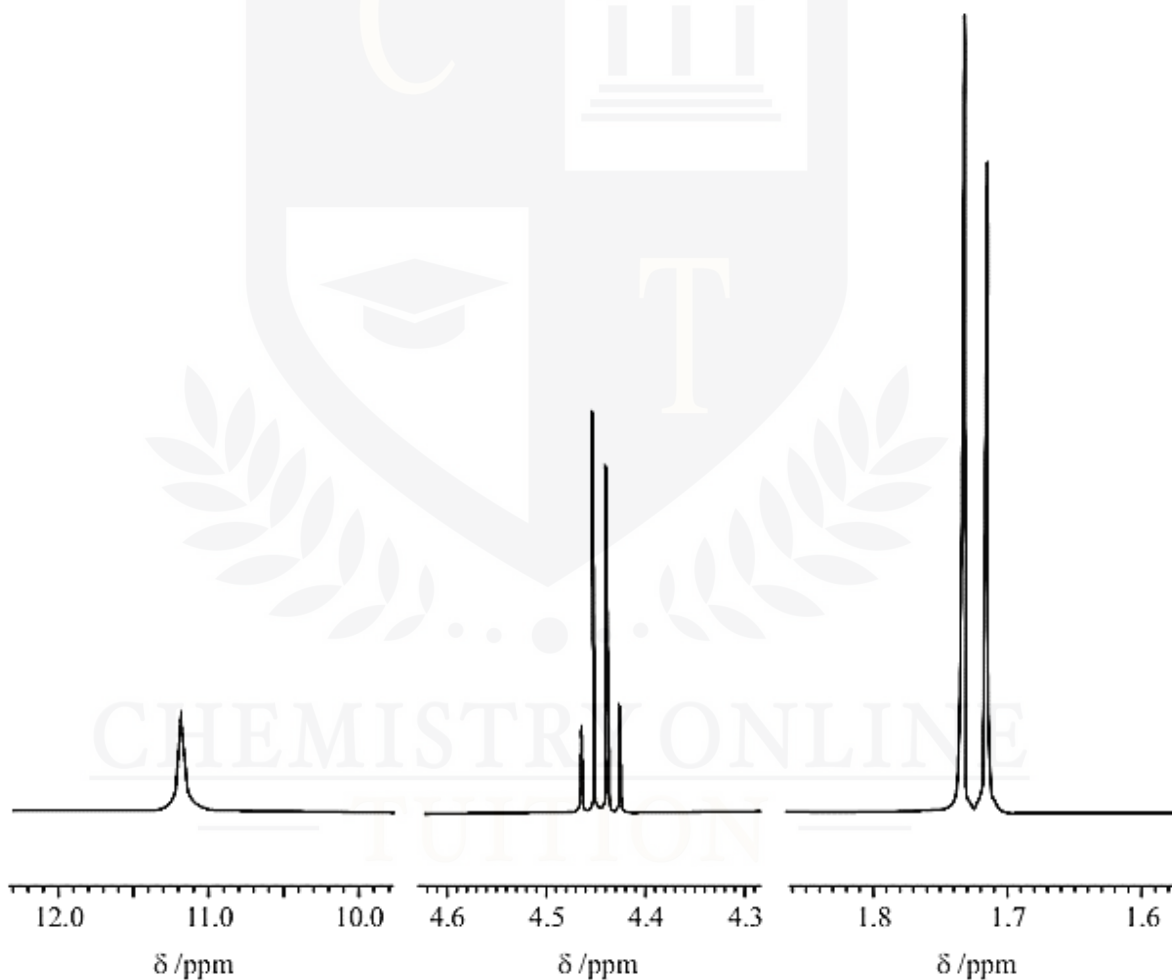
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4. Which one of the following has a singlet peak in its proton n.m.r. spectrum?

- 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 $\text{CH}_3\text{CHClCOOH}$ are shown below.



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(a) Name the compound $\text{CH}_3\text{CHClCOOH}$.

(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 $\text{ClCH}_2\text{CH}_2\text{COOH}$.

(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)

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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 $(\text{CH}_3)_2\text{CHCOO}(\text{CH}_2)_3\text{CH}_3$?

- A. 4
B. 5
C. 6
D. 7

(1)

9. Butenedioic acid, $\text{HOOCCH}=\text{CHCOOH}$, occurs as two stereoisomers.

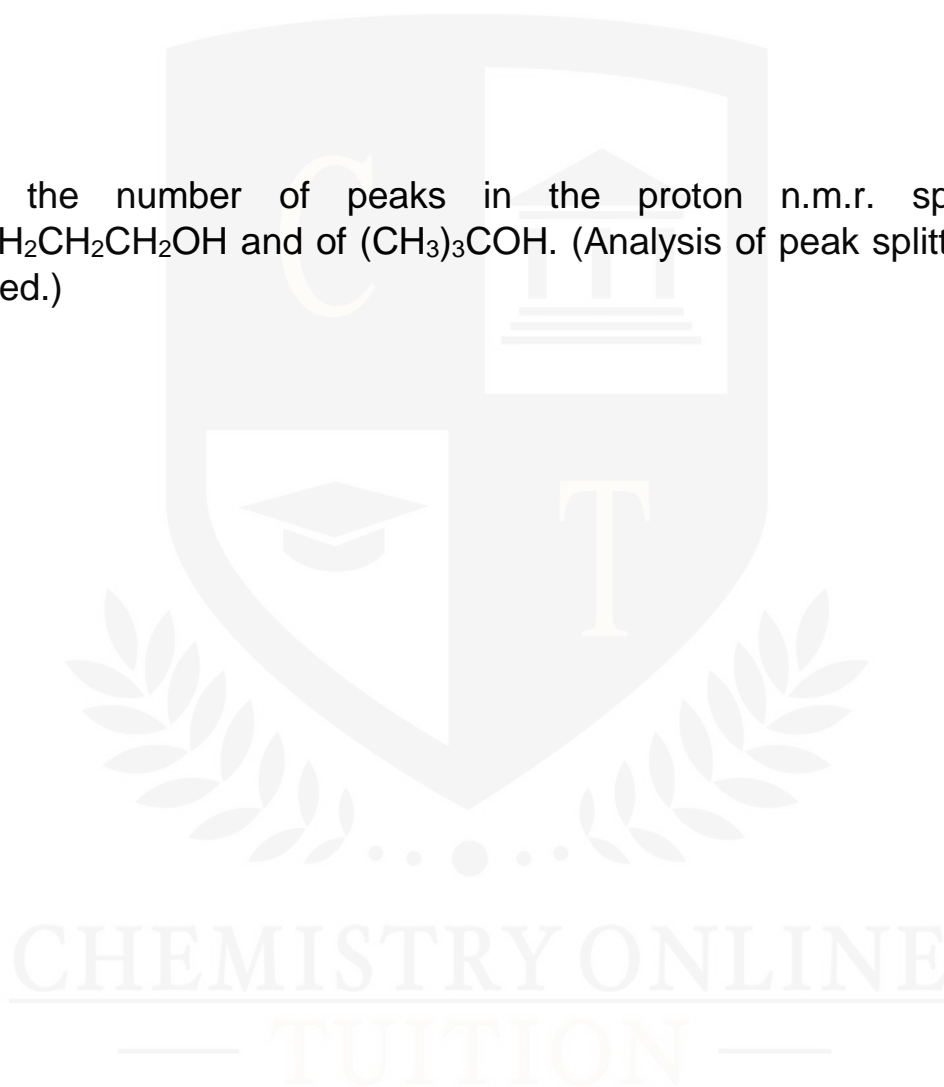
One of the isomers readily forms the acid anhydride $\text{C}_4\text{H}_2\text{O}_3$ when warmed.

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 $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{OH}$ and of $(\text{CH}_3)_3\text{COH}$. (Analysis of peak splitting is not required.)

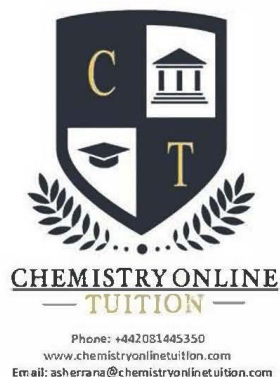
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DR. ASHAR RANA



- Founder & CEO of Chemistry Online Tuition Ltd.
- Tutoring students in UK and worldwide since 2008
- Chemistry, Physics, and Math's Tutor

CONTACT INFORMATION FOR CHEMISTRY ONLINE TUITION

- UK Contact: 02081445350
- International Phone/WhatsApp: 00442081445350
- Website: www.chemistryonlinetuition.com
- Email: asherrana@chemistryonlinetuition.com
- Address: 210-Old Brompton Road, London SW5 OBS, UK