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# CHEMISTRY

## ORGANIC CHEMISTRY II

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

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## NMR Spectroscopy - 2

1.

(a)

Fragment Ion:



Fragment Ion:



Fragment Ion:



(2)

(b)

*One use of mass spectrometry outside of the laboratory is in breathalyzers for detecting alcohol levels in individuals.*

*Additionally, mass spectrometry is used in the monitoring of air pollution, MOT emission testing for vehicles, and various environmental monitoring applications.*

(1)

2. c

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(1)

3.

(a)

*The infra-red spectrum of Q contains a major absorption at  $1724\text{ cm}^{-1}$ .*

*The bond responsible for this absorption is  $\text{C}=\text{O}$  i.e. carbonyl.*

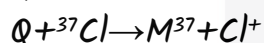
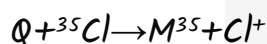
(1)

(b)

The presence of two molecular ion peaks in the mass spectrum of compound Q suggests the occurrence of isotopic substitution.

Chlorine (Cl) has two isotopes, chlorine-35 ( $^{35}\text{Cl}$ ) and chlorine-37 ( $^{37}\text{Cl}$ ), with natural abundances of approximately 75% and 25%, respectively.

So, the presence of these isotopes in the compound can lead to the observation of two molecular ion peaks in the mass spectrum.

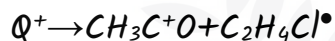


(1)

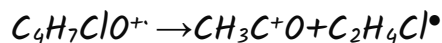
(c)

The fragment ion with  $m/z = 43$  and contains atoms of three different elements corresponds to the formation of a methyl ketone cation ( $\text{CH}_3\text{C}^+=\text{O}$ ) from the molecular ion of Q.

The equation for its formation from the molecular ion of Q can be represented as:



or



$Q^+$  ( $\text{C}_4\text{H}_7\text{ClO}^+$ ) represents the molecular ion of Q,  $\text{CH}_3\text{C}^+=\text{O}$  represents the methyl ketone cation fragment ion, and  $\text{C}_2\text{H}_4\text{Cl}^\bullet$  represents the remainder of the molecular ion after losing the methyl ketone group.

(2)

4. B

(1)

5.

(a)

Name of the compound  $\text{CH}_3\text{CHClCOOH}$ :

2-chloropropanoic acid

Also known as chloroacetic acid.

(1)

(b)

The peak at  $\delta$  1.72 appears as a doublet because it is next to a CH group.

The peak at  $\delta$  4.44 appears as a quartet because it is next to a  $\text{CH}_3$  group. (2)

(c)

In the proton NMR spectrum of the isomeric compound  $\text{ClCH}_2\text{CH}_2\text{COOH}$ , two triplets would be seen in the proton n.m.r. spectrum.

(1)

6. D

(1)

7.

(a)

Reason 1:

TMS is inert, non-toxic, volatile, and easily removed.

Reason 2:

TMS provides a single, intense peak because it has 12 equivalent protons all in the same environment, or its peak is upfield (highly shielded) and away from others, appearing at  $\delta = 0$ .

(2)

(b)

**Solvent:**

$CDCl_3$  or  $CCl_4$

**Reason:**

Proton free or no hydrogens.

(2)

8. C

(1)

9.

For butenedioic acid,  $HOOCCH=CHCOOH$ :

**Two peaks** Maleic acid (cis-isomer) shows two peaks in its proton NMR spectrum.

**No splitting or singlets**

The peaks are singlets because there are no adjacent protons causing splitting.

**(Two) non-equivalent protons:**

The molecule has two distinct proton environments: one for the  $CH=CH$  protons and one for the  $COOH$  protons.

**No adjacent protons**

The  $CH=CH$  protons do not have adjacent protons in the molecule that would cause splitting.

**Same area under the two peaks or same relative intensity**

The area under the two peaks would be the same due to equivalent environments of each type of proton.

(3)

10.

- $CH_3 CH_2 CH_2 CH_2 OH$  (1-butanol): 5 peaks
- $(CH_3)_3 COH$  (tert-butanol): 2 peaks

**Molecule:**  $CH_3 CH_2 CH_2 CH_2 OH$  (1-Butanol)

1-Butanol has the following structure:



**CH<sub>3</sub> group (methyl):**

The hydrogens in the CH<sub>3</sub> group (3 hydrogens) are in one distinct environment.

• **First CH<sub>2</sub> group:**

The hydrogens in the first CH<sub>2</sub> group (2 hydrogens) are in a different environment.

• **Second CH<sub>2</sub> group:**

The hydrogens in the second CH<sub>2</sub> group (2 hydrogens) are in another different environment.

• **Third CH<sub>2</sub> group:**

The hydrogens in the third CH<sub>2</sub> group (2 hydrogens) are in yet another different environment.

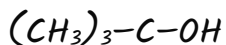
• **OH group (hydroxyl):**

The hydrogen in the OH group (1 hydrogen) is in a unique environment.

So, 1-butanol (CH<sub>3</sub> CH<sub>2</sub> CH<sub>2</sub> CH<sub>2</sub> OH) has 5 distinct hydrogen environments, resulting in 5 peaks in its proton NMR spectrum.

**Molecule: (CH<sub>3</sub>)<sub>3</sub>COH (tert-Butanol)**

tert-Butanol has the following structure:



• **CH<sub>3</sub> groups:**

All three CH<sub>3</sub> groups are equivalent because they are symmetrically attached to the central carbon atom. Thus, all 9 hydrogens in the three CH<sub>3</sub> groups are in one distinct environment.

• **OH group (hydroxyl):**

The hydrogen in the OH group (1 hydrogen) is in a unique environment.

Therefore, tert-butanol ((CH<sub>3</sub>)<sub>3</sub>COH) has 2 distinct hydrogen environments, resulting in 2 peaks in its proton NMR spectrum.



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