CHEMISTRY ONLINE
TUITION

Phone: +442081445350

www.chemistryonlinetuition.com

Email:asherrana@chemistryonlinetuition.com

CHEMISTRY

ORGANIC CHEMISTRY II

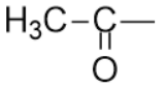
Level & Board	AQA (A-LEVEL)
TOPIC:	NMR SPECTROSCOPY
PAPER TYPE:	SOLUTION - 1
TOTAL QUESTIONS	10
TOTAL MARKS	/28

NMR Spectroscopy - 1

1.

(a)

The singlet peak at $\delta = 2.20$



The three equivalent protons are from the methyl group (CH_3) attached to the carbonyl carbon (C=O).

The presence of the singlet peak at $\delta = 2.20$ ppm, integrating for 3 protons, confirms the presence of an acetyl group in compound Q

(1)

(b)

The singlet peak at $\delta = 3.40$ ppm, integrating for 1 proton, is due to the presence of a hydroxyl (OH) group in compound Q

(1)

(c)

Two triplet peaks show presence of $-CH_2-CH_2-$.

(1)

2. C

(1)

3.

(a)

A is an ester, represented as RCOOR'.

The molecular ion peak in the mass spectrum is at m/z=102, which corresponds to C_4H_{10}.

Subtracting the molecular ion peak of the ester from the molecular ion peak gives 102−44=58, equivalent to C_4H_{10}.

So, $R+R'=C_4H_{10}$

The molecular formula of the ester can be $C_5H_{10}O_2$.

Possible Structure form nmr:
Considering the shifts and integration:

Ethyl Propanoate (Ethyl Propionate):

$CH_3-CH_2-COO-CH_2-CH_3$

The structure is confirmed by the chemical shifts:

- δ 4.13 (2H): $-OCH_2-$ (ethyl group)
- δ 2.32 (2H): $-CH_2-CO-$ (methylene group adjacent to carbonyl)
- δ 1.33 (3H): $-CH_3$ (methyl group adjacent to methylene)
- δ 1.09 (3H): $-CH_3$ (methyl group in ethyl)

So, the molecular formula of the ester can be $C_5H_{10}O_2$.

(3)

(b) What is the ratio of the numbers of each type of proton?

The ratio of the numbers of each type of proton in the ester A is 2:2:3:3.

So, we can interpret this as follows:

- For the peaks at δ 4.13 and δ 2.32: The ratio is 2:2, indicating that these peaks correspond to two different types of protons, each present in equal numbers.

- For the peaks at δ 1.33 and δ 1.09:
- The ratio is 3:3, indicating that these peaks correspond to two other types of protons, each present in equal numbers but in a different ratio compared to the first two types.

(1)

(c)

The splitting patterns in the n.m.r. spectrum shows two CH_2CH_3 groups are present.

(1)

(d)

Following is structure of compound A, labelled with the letters a, b, c and d the four groups of equivalent protons.

$$\overset{a}{C}H_3\ \overset{b}{C}H_2\ COOC\overset{c}{H}_2\ \overset{d}{C}H_3$$

(1)

4. D

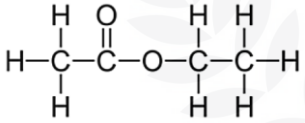
(1)

5.

(a)

Structural formula of the ester.

$CH_3COOCH_2CH_3$



(1)

(b)

There are 3 types of proton which are present in the ester.

(1)

(c) Describe the splitting pattern of the ethyl group in the n.m.r. spectrum of the ester.

CH_3 group:

This will appear as a triplet due to the two adjacent hydrogens on the CH_2 group ($n + 1 = 2 + 1 = 3$).

CH_2 group:
This will appear as a quartet due to the three adjacent hydrogens on the CH_3 group ($n + 1 = 3 + 1 = 4$).

Ethyl group: Triplet for the CH_3 (3 hydrogens) and quartet for the CH_2 (2 hydrogens).

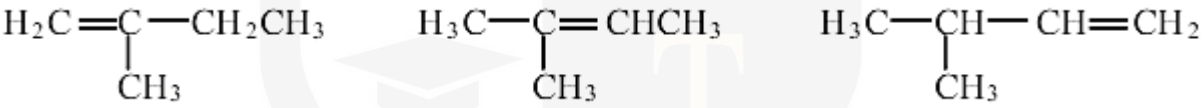
(1)

6. **C**

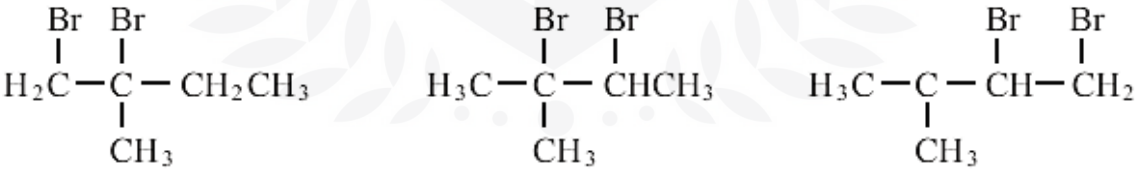
(1)

7.

Structures of the three branched-chain alkenes with molecular formula C_5H_{10}:



Structures of the three dibromoalkanes, $C_5H_{10}Br_2$, formed when these three alkenes react with bromine:



- **Integration Ratio**: 6:3:1
  - **6 hydrogens** from the two methyl (CH_3) groups.
  - **3 hydrogens** from the CH groups adjacent to bromine atoms.
  - **1 hydrogen** on the central carbon.
- **Splitting Patterns**:
  - **6 (CH_3)**: Single (no adjacent hydrogens).

- **3 (CH)**: Doublet (adjacent to the central carbon hydrogen, n + 1 = 1 + 1 = 2).
- **1 (CH)**: Quartet

(4)

8. B

(1)

9.

- **Number of Peaks**: 2 (if 4 peaks are allowed, splitting only)
- **Integration Ratio**: 6:2 or 3:1
- **Splitting of Peaks**:

  - Doublet (6 or 3):
    Each peak representing the hydrogen protons attached to carbon atoms 1 and 4, which are next to one non-equivalent proton on adjacent carbons (2 and 3).

  - Quartet (2 or 1):
    Each peak representing the hydrogen protons attached to carbon atoms 2 and 3, which are next to three non-equivalent protons on adjacent carbons (1 and 4).

(3)

10. D

(1)

DR. ASHAR RANA

CHEMISTRY ONLINE TUITION

Phone: +442081445350
www.chemistryonlinetuition.com
Email: asherrana@chemistryonlinetuition.com

- Founder & CEO of Chemistry Online Tuition Ltd.
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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