AQA A-Level Chemistry

NMR mark scheme · goes with “NMR” · whiteboardchemistry.com/revision/aqa-a-level-chemistry/exam-questions

Mark schemes

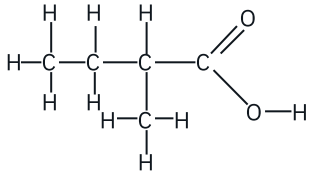
NMR · 7 questions

Q1 · June 2024 · Paper 2 · Q6 · [12 marks]

(a) $C_4H_9COOH + NaHCO_3 \rightarrow C_4H_9COONa + CO_2 + H_2O$

[1 mark]

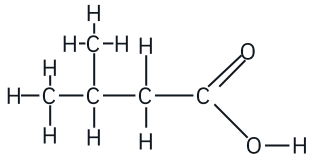
(b)



$CH_3CH_2CH(CH_3)COOH$

[1 mark]

(c) M1



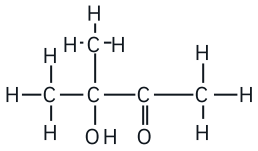
M1 $(CH_3)_2CHCH_2COOH$

M2 6:1:2:1 (Any order)

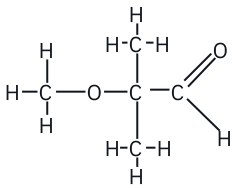
M2 Allow ECF for a 5 carbon carboxylic acid

[2 marks]

(d) M1



Or

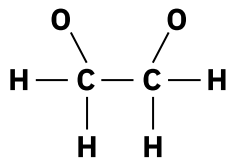
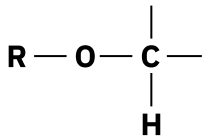
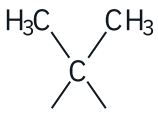
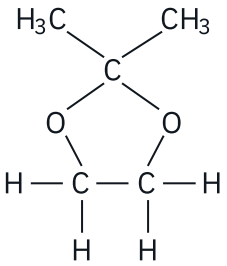
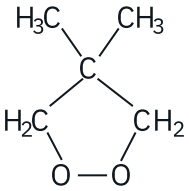


Adjacent C has no (non-equivalent) H attached (so no splitting/spin-spin coupling takes place)

M1 $(CH_3)_2C(OH)COCH_3$ or $CH_3OC(CH_3)_2CHO$

[2 marks]

(e)

	**Scores M1 and M2**	**Allow M1 for**	
	Scores M3 and M4	Allow M3 for	RCH_3
	Scores M5		This structure also scores M5 
^{13}C peaks	= 3	M6	Allow ECF from their M5 of $C_5H_{10}O_2$

[6 marks]

Q2 · June 2017 · Paper 3 · Q29 · [1 mark]

Answer: **D**

Q3 · June 2018 · Paper 3 · Q16 · [1 mark]

Answer: **C**

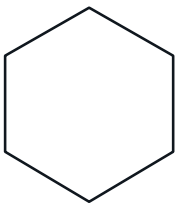
Q4 · June 2025 · Paper 2 · Q7 · [12 marks]

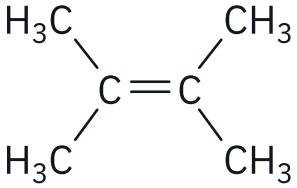
07.1

M1 84.09396 = (6 × 12.00000) + (12 × 1.00783)

Hence C_6H_{12}

M2 and M3 Structures e.g.





M4 Look for a peak at 1620–1680 cm^{-1}

M5 Alkene has this peak for C=C or cycloalkane doesn't

[5 marks]

07.2

This question is marked using Levels of Response.

Level 3 5–6 marks

All stages are covered and the explanation of each stage is correct and virtually complete

(i.e. two from stages 1, 2 and 3)

Answer communicates the whole explanation, including equations, coherently and shows a logical progression through all three stages

Level 2 3–4 marks

All stages are covered (NB 'covered' means min one from each stage) but the explanation of each stage may be incomplete or may contain inaccuracies

OR two stages covered and the explanations are generally correct and virtually complete

(i.e. two from 2 stages either 1, 2 or 3)

Answer is coherent and shows some progression through all three stages. Some steps in each stage may be incomplete

Level 1 1–2 marks

Two stages are covered (NB 'covered' means min one from a stage) but the explanation of each stage may be incomplete or may contain inaccuracies

OR only one stage is covered but the explanation is generally correct and virtually complete

(i.e. two from stages 1, 2 or 3)

Answer shows some progression between two stages

Level 0

Insufficient correct chemistry to gain a mark.

Stage 1 ^{13}C NMR

1a (5 peaks so) there are 5 (different) C environments

1b (2) peaks with chemical shift 190–220 ppm so there are (2 different C=O) aldehyde / ketone groups

1c (3) peaks with chemical shift 5–50 ppm so could be C–C alone or C–C and R–CO–C

Stage 2 ^{1}H NMR chemical shift data

2a peak at chemical shift 0.7 – 1.4 R–CH_3 or R_2CH_2

2b peak at chemical shift 2.1 – 2.6 R–CO–CH

2c peak at chemical shift 2.6 – 2.8 R–CO–CH

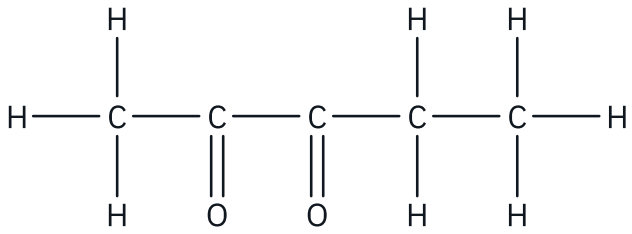
Stage 3 ^{1}H splitting

3a Triplet (0.7 – 1.4 CH) next to CH_2

3b Singlet (2.1 – 2.6 CH) no H on adjacent C

3c Quartet (2.6 – 2.8 CH) next to CH_3

M7 $CH_3CH_2COCOCH_3$ or



[7 marks]

Q5 · November 2021 · Paper 3 · Q11 · [1 mark]

Answer: **B**

Its ^{13}C NMR spectrum has 3 peaks.

Q6 · June 2022 · Paper 2 · Q6 · [6 marks]

This question is marked using Levels of Response.

Level 3 5-6 marks	**All stages are covered and each stage is generally correct and virtually complete. Answer is communicated coherently and shows a logical progression from Stage 1 to Stages 2 and 3 Covers at least 1 point for stage 1, 3 for stage 2 and 3 for stage 3.**
Level 2 3-4 marks	All stages are covered but stage(s) may be incomplete or may contain inaccuracies Covers at least 1 point for stage 1 stage 2 and stage 3. OR two stages are covered and are generally correct and virtually complete. Covers at least 1 point for stage 1, and 3 for stage 2 or stage 3 OR 3 for stage 2 and 3 for stage 3 Answer is communicated mainly coherently and shows a logical progression from Stage 1 to Stages 2 and 3.
Level 1 1-2 marks	Two stages are covered but stage(s) may be incomplete or may contain inaccuracies OR only one stage is covered but is generally correct and virtually complete. Answer includes isolated statements but these are not presented in a logical order.
0 marks	Insufficient correct chemistry to gain a mark.

Indicative Chemistry content

Stage 1: infrared

1a) (broad peak) at 3400 cm^{-1} (any value from 3230-3550) indicates OH in alcohols

1b) peak at 1720 cm^{-1} (any value from 1680-1750) indicates C=O

Stage 2: ^{1}H nmr

2a) peak at 3.9 ppm integration 1 so 1 H-C-O AND quartet so adjacent to CH_3 (stated or shown)

2b) peak at 3.7 ppm integration 1 so HO-C-(stated or shown)

2c) peak at 2.1 ppm integration 3 so H_3C-C=O AND singlet so no adjacent H (stated or shown)

2d) peak at 1.2 ppm integration 3 so H_3C- AND doublet so adjacent to CH (stated or shown)

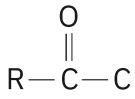
2e) sum of integration values = 8 Hence $C_4H_8O_2$

Stage 3: ^{13}C nmr

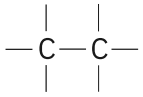
3a) peak at 210 ppm C=O aldehydes or ketones

3b) peak at 75 ppm C–O (alcohols, ethers or esters)

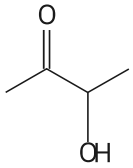
3c) peak at 25 ppm



3d) peak at 20 ppm



3e) structure



Q7 · June 2023 · Paper 2 · Q5 · [11 marks]

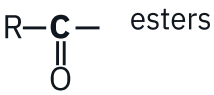
(a) C=O

[1 mark]

(b) Tick in the box for 7 ONLY

[1 mark]

(c)

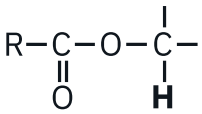


Ignore acids

[1 mark]

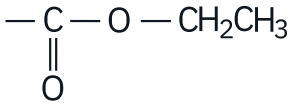
(d) M1 (Quartet) because neighbouring C has 3H

M2 (At δ = 4.1 ppm) because connected to single bonded O of ester or



M3 (Triplet) because neighbouring C has 2H

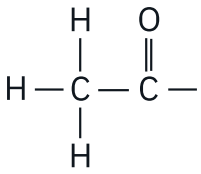
M4 (At δ = 1.26 ppm) because R_2CH_2 or RCH_3



Ignore use of integration

[5 marks]

(e)



[1 mark]

(f) Cannot deduce splitting patterns of peaks (at about δ = 2.60)

Or

No integration values

Allow

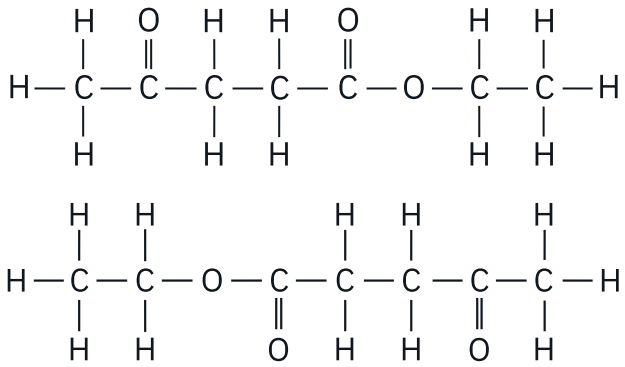
Peaks at δ = 2.60 and δ = 2.56 ppm overlap

OR

spectrum at δ = 2.60 is second order

[1 mark]

(g)



[1 mark]

Source: AQA A-Level Chemistry past papers. Reproduced for revision at whiteboardchemistry.com.

Stuck on any of these? One-to-one online A-Level chemistry tuition with Joe White, an experienced examiner: whiteboardchemistry.com/tuition