OCR A-Level Chemistry A

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

Mark schemes

NMR spectroscopy · 11 questions

Q1 · June 2017 · Paper 2 (Synthesis and analytical techniques) · Q20 · [9 marks]

OCR MARK SCHEME

20(a)

Empirical formula

Mole Ratio C : H : O = 5.88 : 5.92 : 1.47 ✓

Empirical formula = C_4H_4O ✓

Molecular formula

Molecular formula = $C_8H_8O_2$

AND

Evidence of 136 in working or from labelled peak in spectrum ✓

[3 marks]

EXAMINER GUIDANCE

ALLOW $\frac{70.58}{12.0} : \frac{5.92}{1.0} : \frac{23.50}{16.0}$

ALLOW *4:4:1 if linked to C:H:O*

Alternative method for 3 marks:

C: $\frac{136 \times 70.58/100}{12.0} = 8$

H: $\frac{136 \times 5.92/100}{1.0} = 8$

O: $\frac{136 \times 23.50/100}{16.0} = 2$

20(b)

Functional groups

Phenol **AND** ketone ✓

Explanation

Links phenol to (weak) acidity

AND

no reaction with Na_2CO_3 (so not carboxylic acid) ✓

Links 2,4-DNP(H) or Brady’s reagent observation to carbonyl

AND

Tollens’ reagent observation (so not an aldehyde) ✓

[3 marks]

DO NOT ALLOW *any other functional groups for first marking point.*

ALLOW *identity of functional groups in the explanation if not stated on functional group prompt line.*

ALLOW *“aldehyde or ketone” in place of carbonyl*

20(c)

Carbon NMR analysis

Peaks between 110–160 ppm are the (four) aromatic (carbon environments) ✓

Compound contains a C=O between 190 - 200 ppm

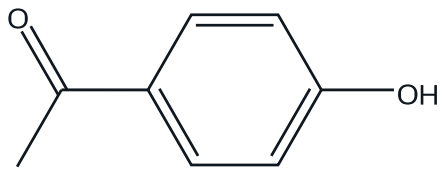
AND

ALLOW *peaks to be identified by:*

- Peaks labelled on spectrum
- Peaks indicated on a chemical structure
- Peaks indicated from within text

Compound contains a C-C at 20-30 ppm ✓

Structure



✓

Note: If identifying aromatic peaks from the spectrum all four peaks should be indicated.

***ALLOW** any combination of skeletal **OR** structural **OR** displayed formula as long as unambiguous*

[3 marks]

Q2 · June 2022 · Paper 2 (Synthesis and analytical techniques) · Q12 · [1 mark]

Answer: **A**

$CH_3CH_2COOCH_2CH_3$

Q3 · June 2022 · Paper 2 (Synthesis and analytical techniques) · Q15 · [1 mark]

Answer: **B**

Only 1 and 2

Q4 · June 2023 · Paper 2 (Synthesis and analytical techniques) · Q1 · [1 mark]

Answer: **C**

D_2O

Q5 · June 2023 · Paper 2 (Synthesis and analytical techniques) · Q23 · [6 marks]

OCR MARK SCHEME

23

Level 3 (5–6 marks)

Structure is either $CH_3CH_2COOCH_2C(CH_3)_3$ **OR** $(CH_3)_3CCH_2COOCH_2CH_3$

AND

Most of the data analysed.

There is a well-developed line of reasoning which is clear and logically structured. The information presented is relevant and substantiated.

Level 2 (3–4 marks)

Structure is an ester of $C_8H_{16}O_2$ with some key features present

AND

EXAMINER GUIDANCE

Indicative scientific points:

1. Empirical Formulae

- $C : H : O = \frac{66.63}{12.0} : \frac{11.18}{1.0} : \frac{22.19}{16.0} = 5.55 : 11.18 : 1.39 = 4 : 8 : 1$
- Empirical formula = C_4H_8O

2. Molecular Formulae

- uses $m/z = 144.0$ to determine molecular formula as $C_8H_{16}O_2$

3. Functional group

From IR,

- → C=O from ~1740 cm^{-1}

Analyses some of the data from at least 3 of the scientific points.

There is a line of reasoning presented with some structure. The information presented is relevant and supported by some evidence.

Level 1 (1–2 marks)

Attempts analysis from at least 2 of the scientific points.

There is an attempt at a logical structure with a line of reasoning. The information is in the most part relevant.

0 marks

No response or no response worthy of credit.

[6 marks]

***IGNORE** references to C–O peaks*

No reaction with 2,4-DNP

- → no carbonyl/no ketone and aldehyde
- Likely to be an ester

4. ^{1}H NMR analysis

- δ = 0.9 ppm, singlet, 9H $-C(CH_3)_3$
- δ = 1.2 ppm, triplet, 3H CH_3CH_2-
- δ = 2.2 ppm, quartet, 2H CH_3CH_2CO
- δ = 4.1 ppm, singlet, 2H $-OCH_2-$

***ALLOW** approximate values for chemical shifts.*

Structure

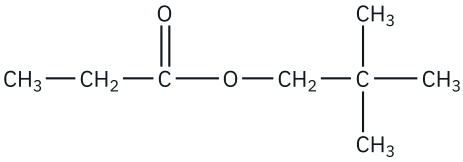
***ALLOW** any combination of skeletal **OR** structural **OR** displayed formula as long as unambiguous*

Key features consistent with chemical shift data and relative peak areas

- O-CH_2
- $C(CH_3)_3$
- $CH_3CH_2C{=}O$

Correct Structure

- $CH_3CH_2COOCH_2C(CH_3)_3$



Q6 · June 2023 · Paper 2 (Synthesis and analytical techniques) · Q9 · [1 mark]

Answer: **C**

Q7 · June 2024 · Paper 2 (Synthesis and analytical techniques) · Q14 · [1 mark]

Answer: **B**

Only 1 and 2

Q8 · June 2024 · Paper 2 (Synthesis and analytical techniques) · Q24 · [6 marks]

OCR MARK SCHEME

24

Level 3 (5–6 marks)

Structure is $C_6H_5CHCH_3CHO$

AND

Analyses data from all 3 scientific points

There is a well-developed line of reasoning which is clear and logically structured. The information presented is relevant and substantiated.

Level 2 (3–4 marks)

Structure with most key features including O atom(s)

AND

Analyses data from at least 2 of the scientific points

There is a line of reasoning presented with some structure. The information presented is relevant and supported by some evidence.

Level 1 (1–2 marks)

Attempts analysis from at least 2 of the scientific points

There is an attempt at a logical structure with a line of reasoning. The information is in the most part relevant.

0 marks

No response or no response worthy of credit.

[6 marks]

EXAMINER GUIDANCE

Indicative scientific points:

1. Empirical (and Molecular) Formulae

- $C : H : O = \frac{80.60}{12.0} : \frac{7.46}{1.0} : \frac{11.94}{16.0} = 6.72 : 7.46 : 0.746 = 9 : 10 : 1$
- Empirical formula = $C_9H_{10}O$

2. Mass spectrum and IR

Mass spectrum

- uses $m/z = 134$ to give molecular formula: $C_9H_{10}O$
- Any possible fragments:

- m/z = 105 $C_6H_5CHCH_3^+$

- m/z = 77 $C_6H_5^+$

- m/z = 29 CHO^+

IR

- C=O from ~1700 cm^{-1}
- Likely to be aldehyde or ketone
- C=C (arenes) ~1500 cm^{-1}

ALLOW *Data Sheet ranges*

3. ^1H NMR

- δ = 1.4 ppm, doublet, 3H CH_3CH-
- δ = 3.8 ppm, quintet, 1H next to 4 adjacent H
- δ = 7.3 ppm, singlet, 5H C_6H_5-

- δ = 9.0 ppm, doublet, 1H - CHCHO

ALLOW *approximate values for chemical shifts*

Structure

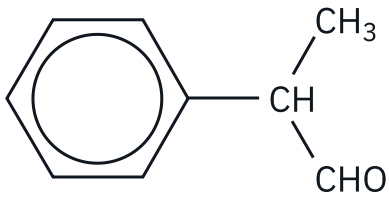
ALLOW *any combination of skeletal* ***OR*** *structural* ***OR*** *displayed formula as long as unambiguous*

ALLOW *correct Kekulé representation of benzene*

Key features

- Benzene ring
- C=O
- CH_3

Correct structure



- $(C_6H_5CHCH_3CHO)$

Aspects of the communication statement being met might typically include:

- Structures given are feasible and unambiguous
- Easy to follow layout on empirical formula calculation
- Empirical formula is shown to be same as molecular
- IR peaks linked clearly to bond it refers to not just functional groups
- Positive charge given on MS fragments
- MS fragments plausible for the molecular formula determined

- Clear information for each NMR peak
- No additional irrelevant/incorrect information given

Q9 · June 2025 · Paper 2 (Synthesis and analytical techniques) · Q15 · [1 mark]

Answer: **D**

Only 1

Q10 · November 2020 · Paper 2 (Synthesis and analytical techniques) · Q22 · [8 marks]

OCR MARK SCHEME

22(a)

$CDCl_3$ used as a solvent ✓

D_2O used to identify OH **OR** NH protons ✓

[2 marks]

EXAMINER GUIDANCE

Example and use required for each mark

ALLOW *for 1 mark, D_2O as a solvent*

22(b)

Level 3 (5–6 marks)

Structure I has a viable chemical structure of $C_6H_9NO_2$ which has the key features consistent with spectral data

AND

Most of the data analysed

There is a well-developed line of reasoning which is clear and logically structured. The information presented is relevant and substantiated.

Level 2 (3–4 marks)

Compound I has a viable chemical structure of $C_6H_9NO_2$ with most of the key features consistent with spectral data

AND

Some of the spectral data analysed.

There is a line of reasoning presented with some structure. The information presented is relevant and supported by some evidence.

Level 1 (1–2 marks)

Correct determination of empirical formula and/or molecular formula.

OR

Indicative scientific points:

Empirical and Molecular Formulae

C : H : N : O

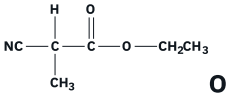
$= \frac{56.69}{12.0} : \frac{7.09}{1.0} : \frac{11.02}{14.0} : \frac{25.20}{16.0}$

OR 4.72 : 7.09 : 0.787 : 1.575

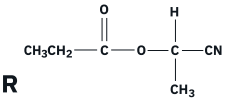
= 6 : 9 : 1 : 2

- Empirical formula = $C_6H_9NO_2$
- m/z = 127.0 and empirical formula mass (127) used to determine molecular formula as $C_6H_9NO_2$

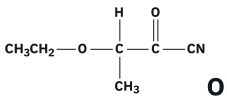
Structures of compound I



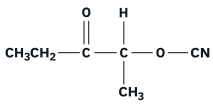
OR



OR



OR



Analyses some of the IR and NMR data.

OR

Analyses most of the NMR data.

There is an attempt at a logical structure with a line of reasoning. The information is in the most part relevant.

0 marks

No response or no response worthy of credit.

[6 marks]

ALLOW *any combination of skeletal* ***OR*** *structural* ***OR*** *displayed formula as long as unambiguous*

Key features

- C ≡N
- C=O in aldehyde, ketone, ester, amide, acid anhydride
- CH_3 group that would give a doublet
- CH_3 group that would give a triplet
- CH_2 group that would give a quartet

^{1}H NMR and IR analysis

^{1}H NMR spectrum

- δ = 4.2 ppm, quartet, 2H CH_3–CH_2–O
- δ = 2.9 ppm, quartet, 1H CO–CH–CH_3
- δ = 1.7 ppm, doublet, 3H CO–CH–CH_3
- δ = 1.3 ppm, triplet, 3H CH_3–CH_2

IR spectrum

- peak at 1750 (cm^{-1}) is C=O
- peak at 2280 (cm^{-1}) is C ≡N

ALLOW *ranges from Data Sheet*

IGNORE *references to C–O peaks*

Q11 · November 2021 · Paper 2 (Synthesis and analytical techniques) · Q21 · [6 marks]

OCR MARK SCHEME

21

Level 3 (5–6 marks)

Compounds **D, E AND F** correctly identified

AND

EXAMINER GUIDANCE

Indicative scientific points may include:

Observations from Test-tube tests

Most of the observations and NMR data analysed.

There is a well-developed line of reasoning which is clear and logically structured. The information presented is relevant and substantiated.

Level 2 (3–4 marks)

Most of compounds D, E **AND** F correctly identified

AND

Some of the observations and NMR data analysed.

There is a line of reasoning presented with some structure. The information presented is relevant and supported by some evidence.

Level 1 (1–2 marks)

Most of compounds D, E **AND** F correctly identified

OR

Some of compounds **D, E AND F** correctly identified

AND

Analyses some of the observations or NMR data

OR

Analyses most of the observations from the test-tube tests.

OR

Analyses most of the NMR data.

OR

Analyses some of the observations and NMR data

There is an attempt at a logical structure with a line of reasoning. The information is in the most part relevant.

0 marks

No response or no response worthy of credit.

[6 marks]

2,4 DNP	**D** has no C=O
	E and **F** have C=O present
$H^+/Cr_2O_7^{2-}$	**D** is primary **OR** secondary alcohol
	E and **F** are ketones
	(negative test shows not aldehydes)
Br_2	**D**, **E** and **F** have no C=C/are saturated

^{13}C NMR analysis

D:

- 3 carbon environments/types of C
- δ = 24, 36 ppm C–C
- δ = 73 ppm, C–O

^{1}H NMR analysis

E:

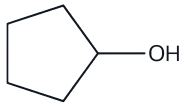
- δ = 2.4 ppm, quartet $CH_3–CH_2–C=O$
- δ = 1.1 ppm, triplet $CH_3–CH_2–$

F:

- δ = 2.6 ppm, heptet/multiplet $(CH_3)_2–CH–C=O$
- δ = 2.1 ppm, singlet, $CH_3–C=O$
- δ = 1.1 ppm, doublet $CH_3–CH–$

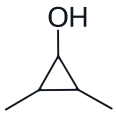
Structures

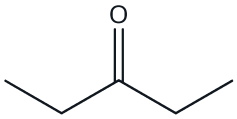
ALLOW *any combination of skeletal* ***OR*** *structural* ***OR*** *displayed formula as long as unambiguous*



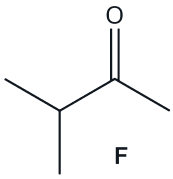
D

OR





E



F

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