OCR A-Level Chemistry A

Organic synthesis, IR and mass spectra mark scheme · goes with “Organic synthesis, IR and mass spectra” · whiteboardchemistry.com/revision/exam-questions/ocr-a-level-chemistry/

Mark schemes

Organic synthesis, IR and mass spectra · 11 questions

Q1 · June 2023 · Paper 2 (Synthesis and analytical techniques) · Q19 · [6 marks]

OCR MARK SCHEME

19

Level 3 (5–6 marks)

A three stage synthesis in the correct order

AND

Equations for each stage are mostly correct

AND

Most reagents correct

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)

Synthesis includes at least two stages in any order **OR** uses NH_3 and HBr in the correct order (without chain extension)

AND

some of the reagents and some equations correct

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)

Planned synthesis includes reagents for any two stages

OR

Describes one stage with reagents and equation mostly correct

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

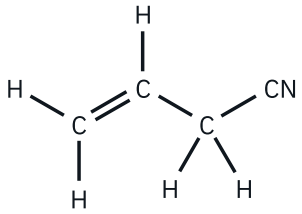
Indicative scientific points may include:

***IGNORE** conditions*

Stage 1: Reaction with CN^-

- Reagents: CN^- (in ethanol)
- Equation: $H_2C{=}CHCH_2Br + CN^- \rightarrow H_2C{=}CHCH_2CN + Br^-$

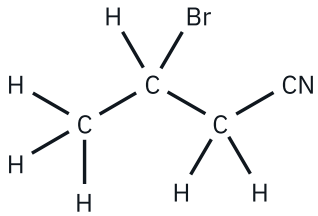
Intermediate 1



Stage 2: Addition of HBr to C=C

- Reagents: HBr
- Equation: $H_2C{=}CHCH_2CN + HBr \rightarrow CH_3CHBrCH_2CN$

Intermediate 2



Stage 3: Reduction of CN

- Reagents: H_2 (with Ni)
- Equation: $H_3CCHBrCH_2CN + 2H_2 \rightarrow CH_3CHBrCH_2CH_2NH_2$

Needs CN^- before HBr

– CN^- would react with both Br atoms

Needs HBr before H_2

– H_2 would react with C=C

Alternative three stage syntheses:

Alternative using $LiAlH_4$

Caution - Can be done as stage 2 or 3

- Reagents: $LiAlH_4$
- Equation: $H_2C{=}CHCH_2CN + 4[H] \rightarrow H_2C{=}CHCH_2CH_2NH_2$

OR

$H_3CCHBrCH_2CN + 4[H] \rightarrow CH_3CHBrCH_2CH_2NH_2$

Needs CN^- before HBr and $LiAlH_4$

Can have HBr and $LiAlH_4$ in any order

Alternative using radical substitution:

Stage 1: Reaction with CN^-

- Reagents: CN^- (in ethanol)
- Equation: $H_2C{=}CHCH_2Br + CN^- \rightarrow H_2C{=}CHCH_2CN + Br^-$

Stage 2: Reduction of CN and C=C

- Reagents: H_2 (with Ni)
- Equation: $H_2C{=}CHCH_2CN + 3H_2 \rightarrow CH_3CH_2CH_2CH_2NH_2$

Stage 3: Reaction with Br_2

- Reagents: Br_2 (with UV)
- Equation: $CH_3CH_2CH_2CH_2NH_2 + Br_2 \rightarrow CH_3CHBrCH_2CH_2NH_2 + HBr$

Needs CN^- before H_2

Needs H_2 before Br_2

Two stage synthesis using NH_3 and HBr forming product with no lengthening of carbon chain

Stage 1: Reaction of NH_3

- Reagents: NH_3 (in ethanol)
- Equation: $H_2C{=}CHCH_2Br + NH_3 \rightarrow H_2C{=}CHCH_2NH_2 + HBr$

OR $2NH_3 \rightarrow NH_4Br$

Stage 2: Addition of HBr to C=C

- Reagents: HBr
- Equation: $H_2C{=}CHCH_2NH_2 + HBr \rightarrow CH_3CHBrCH_2NH_2$

Needs NH_3 before HBr

– HBr would react with C=C

Q2 · June 2024 · AS Paper 1 (Breadth in chemistry) · Q18 · [1 mark]

Answer: **D**

Carboxylic acid and ketone.

Q3 · June 2024 · AS Paper 2 (Depth in chemistry) · Q6 · [6 marks]

OCR MARK SCHEME

6

Level 3 (5–6 marks)

A comprehensive description including most of the evidence to justify the correct structure of X.

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)

Explains two scientific points with few omissions **OR** some aspects from all three

AND

an attempt at a feasible structure with either a C=O **OR** COOH

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)

Determines the correct empirical/molecular formula

OR

Some aspects from two scientific points are given

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 worthy of credit.

[6 marks]

EXAMINER GUIDANCE

LOOK ON THE SPECTRA for labelled peaks.

Indicative scientific points may include:

1. Empirical formula

Element	%mass	Ar	moles	
C	40.91	12	3.41	
H	4.54	1	4.54	
O	54.55	16	3.41	

Empirical formula = $C_3H_4O_3$

ALLOW *Alternative method using M_r of 88 i.e.*

$$C = \frac{88 \times (40.91/100)}{12} = 3 \text{ etc.}$$

2. Spectra and Molecular formula

Mass spectrum

- molecular ion peak m/z or $M_r = 88$
- molecular formula = $C_3H_4O_3$

IR

- peak at 2500 to 3500 cm^{-1} is O–H
- peak at 1630 to1820 cm^{-1} is C=O

3. Functional groups and structure of X

- X contains a carboxylic acid

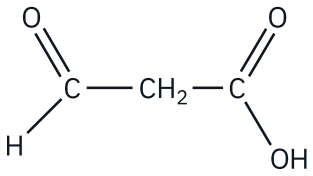
- X doesn't decolourise Br_2 so no C=C bond
- Mass spectrum fragment peak(s) identified e.g.

- m/z = 43 for CH_3CO^+

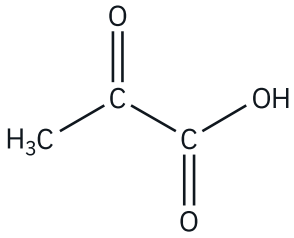
- m/z = 29 CHO^+

- m/z =15 due to CH_3^+

- Structure of X



OR



Aspects of the communication statement might typically have been met when evidence is presented in a logical and clear order making good use of all the evidence given.

Some points which may be seen where communication is good include:

- Easy to follow layout on empirical formula calculation
- Empirical formula is same as molecular formula i.e. not given as $CH_{1.33}O$
- 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.
- No additional irrelevant/incorrect information given

Q4 · June 2024 · Paper 2 (Synthesis and analytical techniques) · Q11 · [1 mark]

Answer: **D**

$(CH_3)_2C(OH)COOH$

Q5 · June 2024 · Paper 2 (Synthesis and analytical techniques) · Q7 · [1 mark]

Answer: **A**

Infrared radiation causes bonds in CH_4 molecules to vibrate more.

Q6 · June 2025 · AS Paper 1 (Breadth in chemistry) · Q19 · [1 mark]

Answer: **D**

$H_3CCH{=}CHCH_2CH_3$

Q7 · June 2025 · AS Paper 1 (Breadth in chemistry) · Q20 · [1 mark]

Answer: **B**

CH_3CH_2CHO

Q8 · June 2025 · AS Paper 2 (Depth in chemistry) · Q6 · [6 marks]

OCR MARK SCHEME

6(a)(i)

P : CH_3CO^+ ✓

Q : $CH_3COCH_2CH_3^+$ ✓

[2 marks]

EXAMINER GUIDANCE

ALLOW *correct structural* ***OR*** *skeletal* ***OR*** *displayed formula* ***OR*** *mixture of the above for both structures*

+ charge (anywhere on structure) required for each response

ALLOW *one mark if both formulae are correct but with no charge/incorrect charge*

ALLOW *one mark if both formulae are correct but incorrectly labelled P/Q*

6(a)(ii)

(M+1 peak due to small proportion of) Carbon-13 / C-13

[1 mark]

6(b)(i)

(causes bonds to) vibrate more (and absorb energy) ✓

[1 mark]

DO NOT ALLOW *Bond breaking*

6(b)(ii)

Functional Group

Alcohol

OR

Alkene ✓

Name of functional group required not just bond

Explanation

Marks can be awarded from anywhere in response – does not need to be on the correct line.

IGNORE *Alkane*

DO NOT ALLOW *any other functional group*

IGNORE *'hydroxyl' for 'alcohol'*

O–H **AND** broad peak at 3200 - 3600 cm^{-1}

OR

C=C **AND** sharp peak at 1620 -1680 cm^{-1} ✓

Explanation must contain bond and either an appropriate range or value given within range stated.

[2 marks]

If no or incomplete explanation, check spectrum for annotations – credit can be given from correctly labelled peaks.

ALLOW *'OH' or 'hydroxyl' for 'O-H'*

IGNORE *all other bonds, except O-H and C=C, even if incorrect*

Q9 · June 2025 · Paper 2 (Synthesis and analytical techniques) · Q12 · [1 mark]

Answer: **A**

Catalytic ozone depletion

Q10 · June 2025 · Paper 2 (Synthesis and analytical techniques) · Q17 · [6 marks]

OCR MARK SCHEME

17

Level 3 (5–6 marks)

Correct calculation of mass of D required

AND

Gives correct reagents for both stages of the synthesis in the correct order with both equations mostly correct

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)

Correct calculation of mass of D required

AND

Gives correct reagents for one stage of the synthesis with equation mostly correct

OR

Calculation of mass of D is partly correct

AND

Gives correct reagents for both stages of the synthesis

OR

Gives correct reagents for both stages of the synthesis, in the correct order, with equations mostly correct

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)

Calculation of mass of D is partly correct

OR

Gives correct reagents for both stages of the synthesis

OR

EXAMINER GUIDANCE

Indicative scientific points may include:

Calculation of mass of D

Using moles:

- $n(F) = \frac{2.50}{102} = 0.0245...$ (mol)
- $n(D) = \frac{0.0245... \times 100}{31.5} = 0.0778...$ (mol)
- $m(D) = 0.0778... \times 122.5 = 9.53$ (g)

Using mass:

- Theoretical $m(F) = \frac{2.50 \times 100}{31.5} = 7.94$ (g)
- Theoretical $n(D) = \frac{7.94}{102} = 0.0778...$ (mol)
- $m(D) = 0.0778... \times 122.5 = 9.53$ (g)

ALLOW *small slip/rounding errors such as errors in M_r e.g. use of M_r of 101 instead of 102 for F*

Note: allow use of calculator value, or values rounded to min. 3SF

Examples of partly correct calculations:

Mass = 0.946 (g) from $\frac{0.0245... \times 31.5}{100} \times 122.5$ (inverted % yield)

Mass = 3.00 (g) from $0.0245... \times 122.5$ (omission of % yield)

Describes one stage of the synthesis with reagents and equation mostly correct

OR

Attempts to calculate the mass of D but makes little progress

AND

Correct reagent for one stage of the synthesis

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]

Mass = 6.61 (g) from M_r values wrong way round

Synthesis

In equations, **ALLOW** any unambiguous formulae

IGNORE *conditions or solvents*

Stage 1 (oxidation of 2° alcohol)

Reagents: $H^+/Cr_2O_7^{2-}$

ALLOW $K_2Cr_2O_7$ ***OR*** $Na_2Cr_2O_7$ ***AND*** H_2SO_4

ALLOW *names for reagents e.g. acidified dichromate, if no formulae given*

IGNORE *Roman numerals e.g. (VI), unless incorrect*

Equation:



Stage 2 (substitution of Cl)

Reagents: NaOH **OR** KOH **OR** OH^-

ALLOW H_2O

Equation:



ALLOW *correct ionic equation/mechanism showing* OH^- *and* Cl^-



IF *stage 2 (substitution of Cl) attempted first*

Equation:



Then oxidation step follows

Equation:



Aspects of the communication statement might typically have been met when:

- All information given is correct and relevant using appropriate scientific language, for example:

○ no additional incorrect reagents e.g. NaOH and H_2SO_4 for substitution

○ use of an inappropriate acid e.g. HCl for oxidation

- Equations are correctly balanced
- Calculations are set out in a clear and logical way
- No small slips/rounding errors
- Final value for mass given to an appropriate number of significant figures/decimal places.

Q11 · June 2025 · Paper 2 (Synthesis and analytical techniques) · Q23 · [10 marks]

OCR MARK SCHEME EXAMINER GUIDANCE

23(a)

Functional group and reasoning for compound K

alcohol

AND

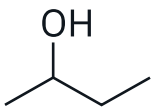
OH

AND

peak at 3200 – 3600 (cm^{-1}) ✓

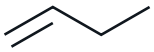
Possible structures of K, L and M

K =



✓

L =



✓

M =



✓

[4 marks]

DO NOT ALLOW *any other functional group e.g. phenol, carboxylic acid*

IGNORE *'hydroxyl' for 'alcohol'* ***BUT ALLOW*** *for O-H*

ALLOW *any stated value in range 3100 to 3600 (cm^{-1}) (consistent with spectrum provided)*

IGNORE *reference to C-O*

If no or incomplete answer, check spectrum for annotations – credit can be given from a correctly labelled peak (values are not needed)

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

ALLOW *one mark if L and M both correct but in the wrong boxes*

23(b)

Level 3 (5–6 marks)

Structure is either $CH_3CH_2COOCH(CH_3)_2$ **OR** $(CH_3)_2CHCOOCH_2CH_3$

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 has a molecular formula of $C_6H_{12}O_2$ with at least two key features present

AND

Analyses some of the data from the NMR

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)

Indicative scientific points:

1. Empirical Formula

- C : H : O = $\frac{62.07}{12.0} : \frac{10.34}{1.0} : \frac{27.59}{16.0}$ = 5.17 : 10.34 : 1.72 = 3 : 6 : 1
- Empirical formula = C_3H_6O
- **ALLOW** Alternative method using M_r of 116 e.g $\frac{(0.6270 \times 116)}{12}$ = 6

2. Molecular Formula and Mass Spectrum

- uses m/z = 116.0 to determine molecular formula as $C_6H_{12}O_2$
- Any possible fragments, for example:

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]

- m/z = 43 $(CH_3)_2CH^+$

- m/z = 29 $CH_3CH_2^+$

3. ^{1}H NMR analysis

- δ = 1.1 ppm, triplet, 3H CH_3CH_2–
- δ = 1.4 ppm, doublet, 6 H $–CH(CH_3)_2$
- δ = 2.4 ppm, quartet, 2H CH_3CH_2CO
- δ = 4.4 ppm, heptet, 1H $–OCH(CH_3)_2$

ALLOW *approximate values for chemical shifts.*

ALLOW *multiplet for heptet*

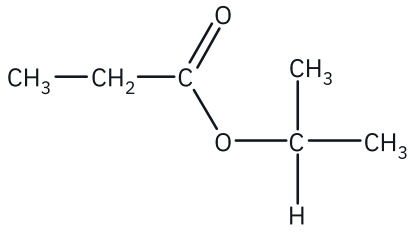
4. Structure

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

Key Features

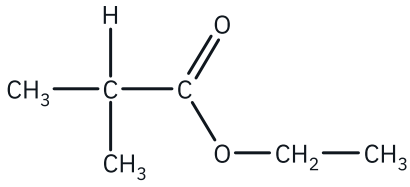
- Carbonyl -C=O
- C-O bond
- Ethyl group $-CH_2CH_3$
- Dimethyl group $-C(CH_3)_2$

Correct structure



Justified from NMR chemical shift analysis

OR



Justified from MS fragment as $(CH_3)_2CHCO^+$ at 71

Aspects of the communication statement being met might typically includes;

- Structures given are feasible and unambiguous
- Justifying the correct structure from the evidence
- Easy to follow layout on empirical formula calculation
- Plausible MS fragments (ideally with a positive charge shown)
- Clear information for each NMR peak, including use of correct terminology for splitting patterns
- No additional irrelevant/incorrect information given

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