

A-Level Chemistry – Organic Synthesis and Analysis

A-Level Chemistry (Edexcel/AQA/OCR, Year 2) · Total marks: 46 · Answers on the last page

This worksheet covers multi-step organic synthesis routes and structure determination using mass spectrometry, infrared (IR) spectroscopy and ^1H NMR spectroscopy. Use A_r values C = 12, H = 1, O = 16, N = 14. Allow about 45 minutes.

Section A – Synthesis routes (skills)

1. State the reagent(s) and condition(s) needed to convert ethanol into ethene. [2]
2. State the reagent(s) and condition(s) needed to convert propene into propan-2-ol, and name the type of reaction taking place. [3]
3. State the reagent(s) and condition(s) needed to convert ethanoic acid into ethyl ethanoate, and name this type of reaction. [3]
4. Bromoethane can be converted into ethanoic acid in two steps.
Give the reagents and conditions for each step, and name the type of reaction occurring in each. [4]

Section B – Spectroscopic analysis (exam-style)

5. A hydrocarbon has molecular formula C_4H_6 .
 - (a) Calculate its degree(s) of unsaturation (index of hydrogen deficiency) using $\text{DoU} = \frac{2C + 2 - H}{2}$.
 - (b) Suggest, giving a reason, one type of structural feature (or combination of features) consistent with this value. [3]
6. In the mass spectrum of butanone ($\text{CH}_3\text{COCH}_2\text{CH}_3$), the molecular ion peak is observed at $m/z = 72$, with fragment peaks at $m/z = 57$ and $m/z = 43$.
 - (a) Confirm that 72 is consistent with the M_r of butanone.
 - (b) Identify the species responsible for the peak at $m/z = 43$, and explain the loss that produces it from the molecular ion.
 - (c) Identify the species responsible for the peak at $m/z = 57$. [5]
7. An unknown compound has $M_r = 60$. Its infrared spectrum shows a very broad, strong absorption across approximately $2500\text{--}3300\text{ cm}^{-1}$ and a strong sharp absorption at 1710 cm^{-1} .
 - (a) Identify the functional group(s) indicated by each absorption.
 - (b) Suggest the identity of the compound, showing that its M_r is consistent with your answer. [4]
8. Propan-1-ol, $\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$, gives a ^1H NMR spectrum with four signals.
Using the $n + 1$ rule, state the splitting pattern (multiplicity) expected for each of the four proton environments, explaining your reasoning for the two CH_2/CH_3 environments with non-adjacent OH. [4]

Section C – Structure elucidation and synthesis (extended)

9. An unknown compound X has the following data:
Mass spectrum: molecular ion peak at $m/z = 88$.
IR spectrum: strong sharp absorption at 1740 cm^{-1} ; no broad absorption in the $2500\text{--}3300\text{ cm}^{-1}$ region.

^1H NMR spectrum: singlet, 3H, $\delta \approx 2.05$; quartet, 2H, $\delta \approx 4.12$; triplet, 3H, $\delta \approx 1.26$.

Deduce the structure of X, explaining how each piece of data supports your answer. [7]

10. Propan-1-ol and propan-2-ol are structural isomers with the same molecular formula, $\text{C}_3\text{H}_8\text{O}$. Explain how ^1H NMR spectroscopy (splitting patterns and/or integration) could be used to distinguish between these two isomers. [3]
11. Design a three-step synthetic route to convert propan-1-ol into propanoic acid via propanenitrile, $\text{CH}_3\text{CH}_2\text{CN}$, given the intermediate step of forming 1-bromopropane. For each step, state the reagent(s), condition(s) and the type of reaction. [6]
12. Explain why the mass spectrum of a compound containing one carbon atom shows a small peak at $M + 1$ (one mass unit above the molecular ion), and state what information the relative height of this peak can, in principle, give about the compound. [2]

Answers

Check your working against these. If an answer does not match, try the question again before looking for the method.

- Concentrated H_2SO_4 (or Al_2O_3 as a solid catalyst), heat – acid-catalysed dehydration (elimination of water).
- Steam ($\text{H}_2\text{O}(g)$) with a phosphoric acid (H_3PO_4) catalyst, high temperature and high pressure. This is an electrophilic addition (hydration) reaction; Markovnikov addition gives the secondary alcohol, propan-2-ol, as the major product.
- Ethanol, with a small amount of concentrated H_2SO_4 catalyst, under reflux. This is esterification (condensation reaction): $\text{CH}_3\text{COOH} + \text{C}_2\text{H}_5\text{OH} \rightleftharpoons \text{CH}_3\text{COOC}_2\text{H}_5 + \text{H}_2\text{O}$
- Step 1: warm with aqueous sodium hydroxide, under reflux – nucleophilic substitution, giving ethanol ($\text{CH}_3\text{CH}_2\text{Br} \rightarrow \text{CH}_3\text{CH}_2\text{OH}$).
Step 2: heat under reflux with excess acidified potassium dichromate(VI) ($\text{K}_2\text{Cr}_2\text{O}_7/\text{H}_2\text{SO}_4$) – oxidation, giving ethanoic acid ($\text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{CH}_3\text{COOH}$).
- (a) $\text{DoU} = \frac{2(4) + 2 - 6}{2} = 2$
(b) Two degrees of unsaturation could be one ring plus one double bond, two double bonds (a diene), or one triple bond (an alkyne) – e.g. but-1-yne or buta-1,3-diene, since each ring or π bond accounts for one degree of unsaturation, and a triple bond counts as two.
- (a) $M_r(\text{C}_4\text{H}_8\text{O}) = 4(12) + 8(1) + 16 = 72$ – consistent.
(b) $m/z = 43$ is the acylium ion CH_3CO^+ , formed by loss of a $\cdot\text{C}_2\text{H}_5$ radical (mass 29) from the molecular ion: $72 - 29 = 43$.
(c) $m/z = 57$ corresponds to loss of a $\cdot\text{CH}_3$ radical (mass 15) from the molecular ion, $72 - 15 = 57$, giving the ion $\text{CH}_3\text{CH}_2\text{CO}^+$.
- (a) The very broad absorption at $2500\text{--}3300\text{ cm}^{-1}$ is the O–H stretch of a carboxylic acid (much broader than an alcohol O–H due to strong hydrogen bonding/dimerisation); the sharp absorption at 1710 cm^{-1} is a C=O stretch.
(b) Ethanoic acid, CH_3COOH : $M_r = 2(12) + 4(1) + 2(16) = 60$ – consistent, and it contains both a C=O and a carboxylic O–H group.
- CH_3 (adjacent to one CH_2 , 2 neighbouring H): triplet.
Middle CH_2 (adjacent to CH_3 and CH_2OH , $3+2 = 5$ neighbouring H): sextet.
 CH_2 next to OH (adjacent to the middle CH_2 , 2 neighbouring H): triplet.
OH proton: singlet, because it exchanges rapidly with traces of water/other OH protons and does not show coupling to neighbouring C–H protons under normal conditions.
- X is ethyl ethanoate, $\text{CH}_3\text{COOC}_2\text{H}_5$.
 $M_r = 4(12) + 8(1) + 2(16) = 88$, matching the molecular ion.
The IR absorption at 1740 cm^{-1} is a C=O stretch (ester carbonyl); the absence of a broad O–H absorption rules out an alcohol or carboxylic acid, consistent with an ester.
In the NMR: the 3H singlet at $\delta \approx 2.05$ is the CH_3 attached to the carbonyl carbon (no adjacent H, so no splitting); the 2H quartet at $\delta \approx 4.12$ is the O- CH_2 group (deshielded by the adjacent O, split into a quartet by the neighbouring CH_3 's 3 protons); the 3H triplet at $\delta \approx 1.26$ is the terminal CH_3 of the ethyl group, split into a triplet by the adjacent CH_2 's 2 protons. The 3:2:3 integration ratio matches $\text{CH}_3\text{COOCH}_2\text{CH}_3$ exactly.
- Propan-2-ol, $(\text{CH}_3)_2\text{CHOH}$, gives a doublet (6H, two equivalent CH_3 groups split by the single adjacent CH proton) and a septet (1H, the CH proton split by 6 equivalent neighbouring protons),

plus an OH singlet – three signals with a 6:1:1 integration ratio. Propan-1-ol, $\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$, gives four signals (triplet, sextet, triplet, OH singlet) with integration ratio 3:2:2:1, and no signal integrating for 6H. The very different number of signals, splitting patterns and integration ratios distinguish the two isomers.

11. Step 1 (propan-1-ol $\rightarrow$ 1-bromopropane): reflux with sodium bromide and concentrated sulfuric acid (generates HBr in situ), or PBr_3 – substitution reaction.
Step 2 (1-bromopropane $\rightarrow$ propanenitrile): heat under reflux with potassium cyanide (KCN) dissolved in ethanol – nucleophilic substitution, extending the carbon chain by one carbon.
Step 3 (propanenitrile $\rightarrow$ propanoic acid): heat under reflux with dilute hydrochloric acid (or dilute NaOH followed by acidification) – hydrolysis of the nitrile to the carboxylic acid.
12. The $M + 1$ peak arises because a small proportion (about 1.1%) of carbon atoms in nature are the ^{13}C isotope rather than ^{12}C ; a molecule containing one ^{13}C atom is one mass unit heavier than the main molecular ion. The relative height of the $M + 1$ peak compared to the M peak increases with the number of carbon atoms in the molecule, so it can be used to estimate how many carbon atoms the molecule contains.

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