National Qualifications 2026

X813/77/02

Chemistry
Section 1 — Questions

TUESDAY, 12 MAY

9:00 AM – 12:00 NOON

Instructions for the completion of Section 1 are given on *page 02* of your question and answer booklet X813/77/01.

Record your answers on the answer grid on *page 03* of your question and answer booklet.

You may refer to the Chemistry Data Booklet for Higher and Advanced Higher.

You must leave your answer booklet on your desk; if you do not, you could lose all the marks for this paper.

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A/PB

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SECTION 1 — 25 marks

Attempt ALL questions

1. Which of the following elements is found in the d-block of the periodic table?

A Calcium

B Carbon

C Chromium

D Curium

2. Which of the following statements is true for a Co^{2+} ion in its ground state?

A It has 5 unpaired electrons.

B It has 8 electrons in s orbitals.

C It has 13 electrons in the third main energy level.

D Its electrons with the highest energy are in the third main energy level.

3. What is the coordination number of the transition metal in $[Pt(NH_3)_2(OH_2)_2]Cl_2$?

A 2

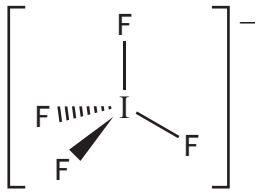
B 3

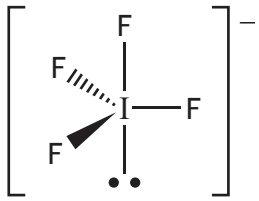
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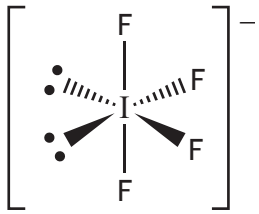
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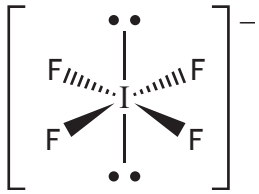
4. Which diagram best represents the arrangement of atoms in the IF_4^- ion?

A non-bonding pair of electrons is represented by • •

A 

B 

C 

D 

5. What is the pH of a 0.25 mol l^{-1} solution of calcium hydroxide, $Ca(OH)_2$?

A 13.7

B 13.4

C 0.6

D 0.3

[Turn over

6. $NH_3 + NH_3 \rightleftharpoons NH_4^+ + NH_2^-$

Which line in the table shows the correct conjugate acid and conjugate base in this equilibrium?

	Conjugate acid	Conjugate base
A	NH_3	NH_4^+
B	NH_4^+	NH_3
C	NH_2^-	NH_4^+
D	NH_4^+	NH_2^-

7. Which of the following indicators is the most suitable for the titration of sodium hydroxide with ethanoic acid?

A *p*-Nitrophenol

B Thymolphthalein

C Bromophenol blue

D Bromothymol blue

Questions **8** and **9** refer to the equilibrium mixture below.

$$2SO_2(g) + O_2(g) \rightleftharpoons 2SO_3(g) \qquad \Delta H° = -197 \text{ kJ mol}^{-1}$$

8. The equilibrium mixture was found to contain 0.2 moles of SO_2, 0.2 moles of O_2 and 16 moles of SO_3.

Which of the following is correct?

A $K > 1$ and $\Delta G° > 0$

B $K > 1$ and $\Delta G° < 0$

C $K < 1$ and $\Delta G° > 0$

D $K < 1$ and $\Delta G° < 0$

9. Which of the following changes in reaction conditions will decrease the equilibrium constant for this reaction?

A Increasing the temperature

B Decreasing the temperature

C Increasing the pressure

D Decreasing the pressure

10.

Substance	K_a
X	1.85×10^{-11}
Y	1.57×10^{-10}
Z	1.61×10^{-5}

Using the information in the table, identify the statement that must be correct.

A X is a stronger acid than Y.

B X is a weaker base than Z.

C Y is a weaker acid than Z.

D Y is a stronger base than X.

11. Which of the following is likely to have the lowest standard entropy at 50 °C?

A Caesium

B Calcium

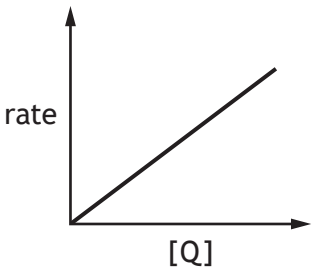
C Mercury

D Rubidium

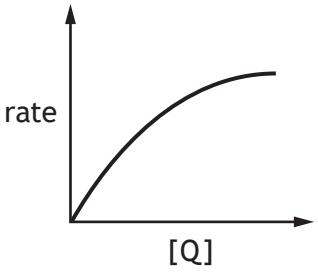
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12. Which of the following graphs would be obtained for a reaction that is first order with respect to reactant Q?

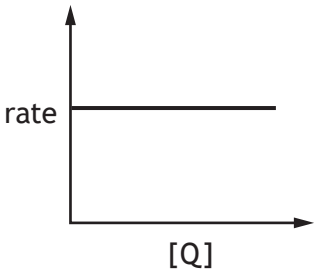
A



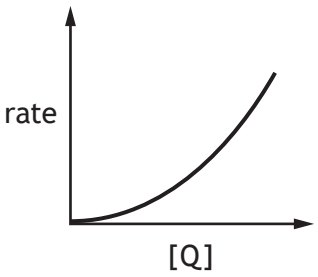
B



C



D



13. For the reaction

$$2A + 2B \longrightarrow C$$

the mechanism is

$$A + 2B \longrightarrow X \quad \text{(slow)}$$

$$X + A \longrightarrow C \quad \text{(fast)}$$

Which of the following would be second order?

A Overall order of the reaction
B Order of the reaction with respect to A
C Order of the reaction with respect to B
D Order of the reaction with respect to X

14. Which of the following has the fewest sigma bonds?

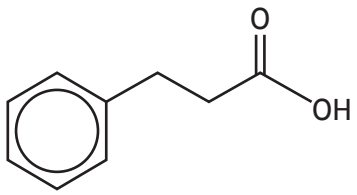
A Pentane
B Pent-1-ene
C Pent-1-yne
D Cyclopentane

15. Lycopene and vitamin A are coloured organic compounds.
Lycopene is red and vitamin A is yellow.
Which line in the table is correct for lycopene when compared to vitamin A?

	Size of energy gap between HOMO and LUMO	**Wavelength of light absorbed**
A	larger	longer
B	smaller	longer
C	larger	shorter
D	smaller	shorter

[Turn over

16. Hydrocinnamic acid has the structure shown.



Hydrocinnamic acid will not react with

A ethanol

B bromine solution

C sodium hydroxide

D concentrated sulfuric acid.

17. Alcohol **X** does not react with hot copper(II) oxide but produces alkene **Y** when dehydrated with hot concentrated sulfuric acid.

Alkene **Y** reacts with bromine solution to form 1,2-dibromo-2-methylpropane.

Which of the following is alcohol **X**?

A $(CH_3)_3COH$

B $CH_3CH_2CH(OH)CH_3$

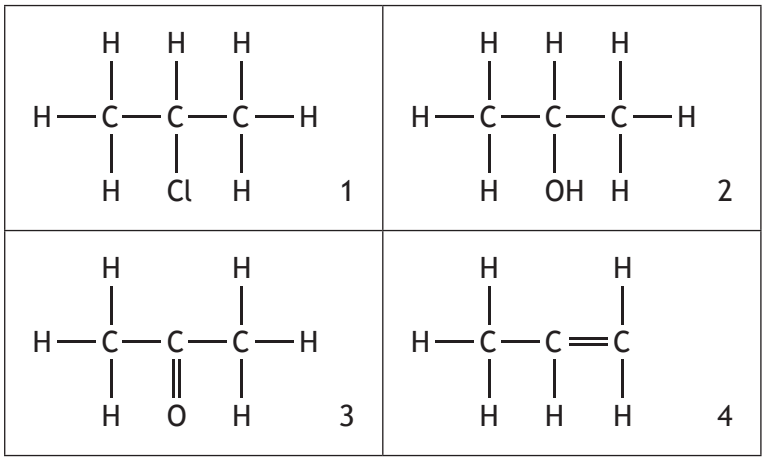
C $CH_3CH_2C(CH_3)_2OH$

D $CH_3CH(CH_3)CH_2OH$

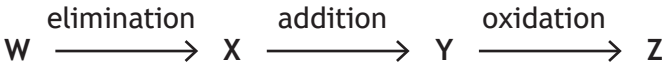
18. Which line in the table is correct for primary amines as the chain length increases?

	Boiling point	**Solubility in water**
A	increases	increases
B	decreases	decreases
C	increases	decreases
D	decreases	increases

19.



Which line in the table correctly identifies **W**, **X**, **Y** and **Z** in the reaction sequence?



	W	X	Y	Z
A	1	4	2	3
B	2	4	3	1
C	1	4	3	2
D	2	4	1	3

20. The major product in the reaction of HCl with $CH_3CH_2C(CH_3)CH_2$ is

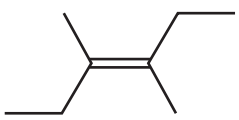
A 1-chloro-2-methylbutane

B 2-chloro-2-methylbutane

C 3-chloro-3-methylbutane

D 4-chloro-3-methylbutane.

21.



The systematic name of the molecule shown above is

A *cis*-2,3-diethylbut-2-ene

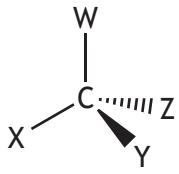
B *trans*-2,3-diethylbut-2-ene

C *cis*-3,4-dimethylhex-3-ene

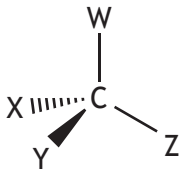
D *trans*-3,4-dimethylhex-3-ene.

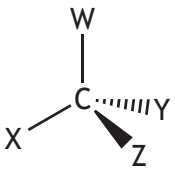
[Turn over

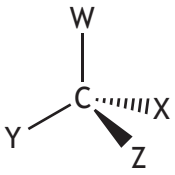
22. The diagram represents one enantiomer of an optically active compound where **W**, **X**, **Y** and **Z** are four different groups.

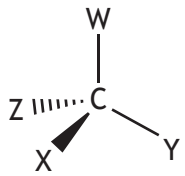


Which of the following represents the other enantiomer of this compound?

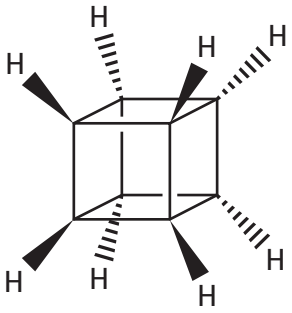
A 

B 

C 

D 

23. The structure of cubane, C_8H_8, is shown.



cubane

How many peaks would be seen in the low resolution ^1H NMR spectrum of cubane?

A 1
B 2
C 4
D 8

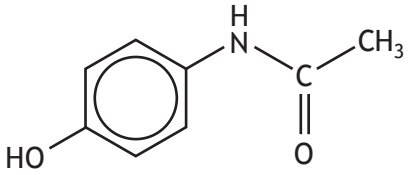
24. 200 cm^3 of water is added to 50 cm^3 of 2 mol l^{-1} sodium hydroxide solution.

The approximate concentration of the diluted sodium hydroxide solution in mol l^{-1}, is

A 0.1
B 0.2
C 0.4
D 0.5

[Turn over

25. A structural formula for paracetamol is shown.



If one tablet contains 500 mg of paracetamol, how many tablets would be needed to obtain one mole of paracetamol?

A 294

B 302

C 0.294

D 0.302

[END OF SECTION 1. NOW ATTEMPT THE QUESTIONS IN SECTION 2 OF YOUR QUESTION AND ANSWER BOOKLET.]

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National Qualifications 2026

Mark

X813/77/01

Chemistry
Section 1 — Answer grid and Section 2

TUESDAY, 12 MAY
9:00 AM – 12:00 NOON

X8137701

Fill in these boxes and read what is printed below.

Full name of centre

Town

Forename(s)

Surname

Number of seat

Date of birth
Day Month Year

Scottish candidate number

You may refer to the Chemistry Data Booklet for Higher and Advanced Higher.

Total marks — 110

SECTION 1 — 25 marks

Attempt ALL questions.

Instructions for the completion of Section 1 are given on *page 02*.

SECTION 2 — 85 marks

Attempt ALL questions.

Write your answers clearly in the spaces provided in this booklet. Additional space for answers and rough work is provided at the end of this booklet. If you use this space you must clearly identify the question number you are attempting. Any rough work must be written in this booklet. You should score through your rough work when you have written your final copy.

Use **blue** or **black** ink.

Do not remove any exam materials. You must leave this booklet on your desk; if you do not, you could lose all the marks for this paper.

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SECTION 2 — 85 marks

Attempt ALL questions

1. Potassium can be detected by spectroscopy.

(a) Using orbital box notation, write the electronic configuration for a potassium atom in its ground state. **1**

(b) Complete the table below showing the quantum numbers and values for the outer electron in a potassium atom in its ground state. **1**

Quantum number	n	l		m_s
Value	4		0	$+\frac{1}{2}$

[Turn over

1. (continued)

(c) When a sample containing potassium is heated, an emission spectrum consisting of a series of lines at discrete wavelengths is produced.

(i) State the effect on the electrons when potassium is heated. **1**

(ii) Explain why a series of lines is produced. **1**

(iii) The shortest wavelength of light in an emission spectrum corresponds to the first ionisation energy of an element.

(A) Calculate the wavelength of light, in nm, corresponding to the first ionisation energy of potassium. **2**

(B) Predict how the shortest wavelength of light in the emission spectrum of caesium would compare to that of potassium. **1**

2. Mercury forms different compounds.

(a) The decomposition of mercury(II) oxide led to the discovery of oxygen gas.

$$HgO(s) \rightarrow Hg(\ell) + \tfrac{1}{2}O_2(g)$$

Substance	ΔH_f° (kJ mol^{-1})	S° (J K^{-1} mol^{-1})
Hg(ℓ)	0	76.0
$O_2(g)$	0	205
HgO(s)	−90.7	70.7

Using information from the table, calculate

(i) ΔS° in J K^{-1} mol^{-1} **1**

(ii) the temperature, in K, at which the reaction becomes feasible. **2**

[Turn over

2. (continued)

(b) Mercury vapour is toxic if inhaled.

A person inhales 6 litres of air per minute. The air contains 2.5×10^{-5} ppm of mercury vapour.

Calculate the mass of mercury vapour, in mg, inhaled in 8 hours. **1**

(c) Over time, inhaled mercury can accumulate in hair.

The concentration of mercury in hair can be measured using atomic absorption spectroscopy.

Explain how atomic absorption spectroscopy can be used to determine the concentration of mercury. **2**

3. Silver metal and silver compounds have many different uses.

(a) Silver metal can be used to make jewellery.

(i) Over time, a black coating of silver(I) sulfide appears on the surface of silver jewellery.

Two possible reactions have been suggested for the formation of silver(I) sulfide.

Reaction 1 $2Ag(s) + H_2S(g) \rightarrow Ag_2S(s) + H_2(g)$

Reaction 2 $2Ag(s) + \frac{1}{2}O_2(g) + H_2S(g) \rightarrow Ag_2S(s) + H_2O(\ell)$

The table shows the ΔG_f° values for the substances involved in these reactions.

Substance	ΔG_f° (kJ mol^{-1})
Ag(s)	0
$H_2S(g)$	–33.0
$Ag_2S(s)$	–40.3
$H_2(g)$	0
$O_2(g)$	0
$H_2O(\ell)$	–237

(A) Using the data in the table, explain if reaction **1** or **2** is more likely to be responsible for the black coating of silver(I) sulfide. **1**

(B) ΔG can be determined by experiment.

Explain why ΔG is likely to be different to ΔG° for each reaction. **1**

3. (a) (continued)

MARKS DO NOT WRITE IN THIS MARGIN

(ii) Coloured enamel is often used to decorate silver jewellery.

A yellow pigment, which is used to produce coloured enamel, contains the complex ion $[Fe(CN)_6]^{4-}$.

(A) Name the complex ion $[Fe(CN)_6]^{4-}$. **1**

(B) Explain fully why the complex ion $[Fe(CN)_6]^{4-}$ is yellow. **2**

(b) Silver(I) nitrate solution can be used in a back titration to determine the sodium chloride content of cheese.

50.0 cm^3 of 0.100 mol l^{-1} silver(I) nitrate solution was reacted with the chloride ions in a 5.27 g sample of cheese.

$$Ag^+(aq) + Cl^-(aq) \rightarrow AgCl(s)$$

The resulting mixture was filtered and the filtrate containing the excess $Ag^+(aq)$ ions was made up to 500 cm^3 in a standard flask.

The number of moles of excess $Ag^+(aq)$ ions was determined by titrating a 100 cm^3 sample of this solution with 0.0503 mol l^{-1} of $SCN^-(aq)$ ions.

The average titre was found to be 13.7 cm^3.

$$Ag^+(aq) + SCN^-(aq) \rightarrow AgSCN(s)$$

(i) Calculate the number of moles of excess $Ag^+(aq)$ ions in the 500 cm^3 standard flask. **1**

3. (b) (continued)

(ii) Calculate the percentage by mass of sodium chloride in this cheese. **2**

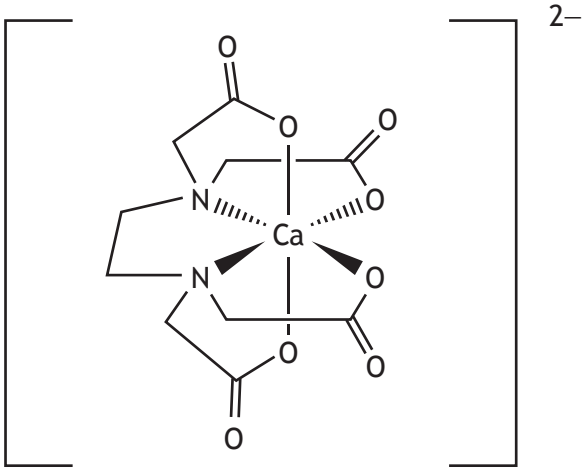
[Turn over

4. Copper can form different coloured compounds. A common copper compound is $CuSO_4 \cdot 5H_2O$, which is found as bright blue crystals.

Using your knowledge of chemistry, describe how an unknown sample of bright blue crystals could be determined to be $CuSO_4 \cdot 5H_2O$. **3**

5. Water hardness is a measure of the concentration of Ca^{2+} and Mg^{2+} ions present in water.

(a) The concentration of Ca^{2+} ions in water can be determined by titration with EDTA to form the ion shown.



Ca^{2+}– EDTA ion

(i) (A) Name this type of titration. **1**

(B) State the term used to classify the EDTA ligand in this titration. **1**

(C) State how EDTA bonds to the calcium ion. **1**

(ii) Zinc(II) sulfate is a primary standard and can be used to standardise the EDTA solution.

(A) State one characteristic of a primary standard. **1**

(B) State the purpose of standardising the EDTA solution. **1**

5. (a) (continued)

MARKS DO NOT WRITE IN THIS MARGIN

(iii) A 50.0 cm^3 sample of water was titrated with 0.00941 mol l^{-1} standardised EDTA solution.

The titre volume was 14.3 cm^3.

$$Ca^{2+} + EDTA^{4-} \rightarrow [CaEDTA]^{2-}$$

Calculate the concentration of calcium ions, in mol l^{-1}, in the water sample. **1**

(b) A second water sample had a calcium ion concentration of 0.00247 mol l^{-1}.

Water hardness is usually expressed in mg l^{-1} of calcium carbonate, $CaCO_3$.

Water hardness	Concentration of calcium carbonate (mg l^{-1})
Soft	below 50
Moderately soft	50 to 99
Slightly hard	100 to 149
Moderately hard	150 to 199
Hard	200 to 300
Very hard	over 300

Calculate the concentration of calcium carbonate, in mg l^{-1}, and determine the water hardness. **1**

6. The Williamson synthesis can be used to make ethers by nucleophilic substitution.

(a) The steps in the synthesis of the ether $CH_3CH_2OCH_3$ are

Step 1 $2CH_3CH_2OH + 2Na \rightarrow 2CH_3CH_2ONa + \mathbf{X}$

Step 2 $CH_3CH_2ONa + CH_3Cl \rightarrow CH_3CH_2OCH_3 + NaCl$

(i) Write the formula for substance **X**. **1**

(ii) The nucleophile in step **2** is $CH_3CH_2O^-$.

Name this nucleophile. **1**

(iii) Step **2** proceeds via an S_N2 mechanism.

Using structural formulae and curly arrow notation, outline the mechanism for step **2**. **2**

(iv) Write the systematic name of $CH_3CH_2OCH_3$. **1**

[Turn over

6. (continued)

(b) The rate equation for the formation of another ether is

$$\text{rate} = k[CH_3O^-][CH_3Cl]$$

Reaction	$[CH_3O^-]$ (mol l^{-1})	$[CH_3Cl]$ (mol l^{-1})	Initial reaction rate (mol l^{-1} s^{-1})
1	0.04	0.04	
2	0.12	0.04	3.15×10^{-6}

(i) Calculate the initial reaction rate, in mol l^{-1} s^{-1}, for reaction **1**. **1**

(ii) Using the data from reaction **2**, calculate the value for the rate constant, k, including the appropriate units. **2**

6. (b) (continued)

(iii) The activation energy, E_a, in kJ mol^{-1}, can be calculated for a reaction using a variation of the Arrhenius equation

$$E_a = 2.303\ RT \log\left(\frac{A}{k}\right)$$

where: R is 8.314 J K^{-1} mol^{-1}

T is the temperature in K

A is the pre-exponential factor

k is the rate constant

Calculate the activation energy, E_a, in kJ mol^{-1}, for this reaction at 500 K if the value for the pre-exponential factor is 718 l mol^{-1} s^{-1} and the rate constant is 6.04×10^{-4} l mol^{-1} s^{-1}. **1**

[Turn over

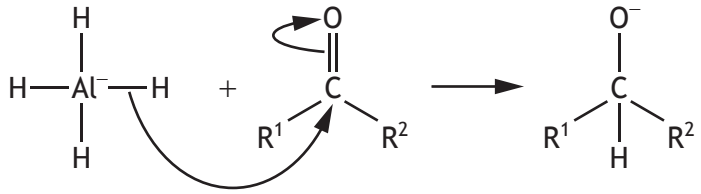
7. Lithium aluminium hydride, $LiAlH_4$, is a reagent used in organic synthesis.

(a) Aldehydes and ketones react with lithium aluminium hydride to produce the corresponding alcohol.

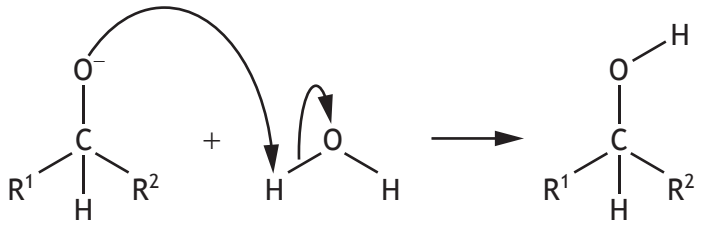
(i) Name this type of reaction. **1**

(ii) The general mechanism for the reaction is shown.

Step 1



Step 2



(A) Step **1** involves nucleophilic attack on the carbonyl group and the breaking of the pi bond between carbon and oxygen.

(I) Explain why the carbon atom of the carbonyl group can be attacked by a nucleophile. **1**

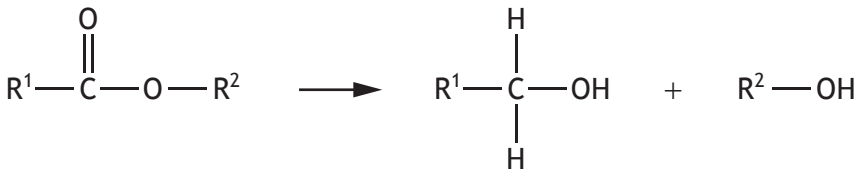
(II) Suggest a reason why the pi bond between carbon and oxygen is broken rather than the sigma bond. **1**

(B) State why the water can be described as an acid in step **2**. **1**

MARKS

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(b) Esters can react with lithium aluminium hydride to produce two alcohols.

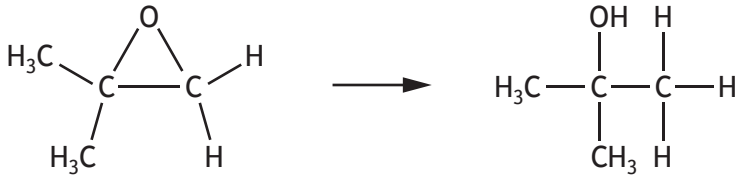


When ester **X** reacts with lithium aluminium hydride, 3-methylbutan-1-ol and propan-2-ol are produced.

Draw a structural formula for ester **X**. **1**

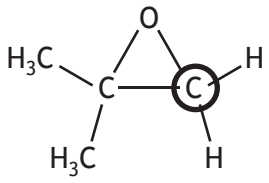
(c) Lithium aluminium hydride can be used to produce alcohols from cyclic ethers. In this reaction a C–O bond in the ring is broken.

2-Methylpropan-2-ol can be produced from a cyclic ether as shown.



(i) Name the other alcohol that could be produced from this cyclic ether. **1**

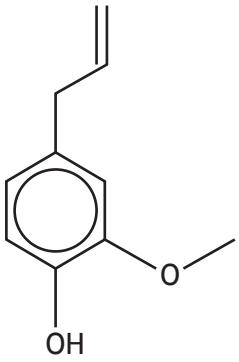
(ii) The reaction to produce 2-methylpropan-2-ol proceeds via an S_N2 mechanism with nucleophilic attack on the circled carbon atom.



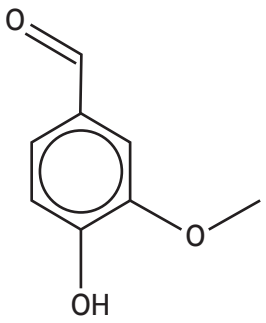
Suggest why the circled carbon atom is the more likely carbon atom in the ring to be attacked by a nucleophile. **1**

8. Vanillin is the main component of vanilla essence, used as a flavouring in foods.

(a) Vanillin can be synthesised from eugenol.

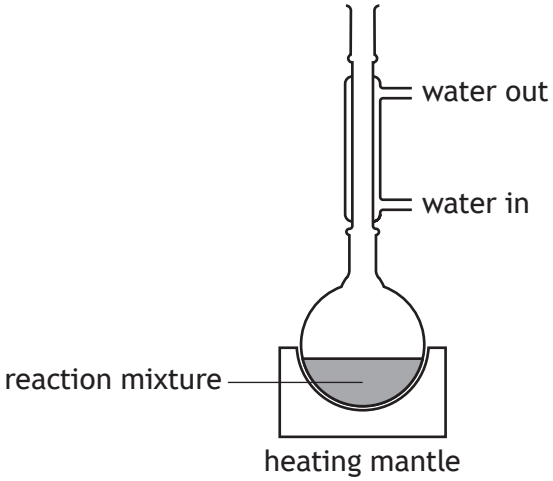


eugenol



vanillin

(i) The diagram shows the apparatus used to heat the reaction mixture.



(A) Name the technique shown in the diagram. **1**

(B) State what else should be added to the round-bottomed flask to ensure safe heating of the reaction mixture. **1**

8. (a) (continued)

(ii) Once the reaction is complete, vanillin is extracted from the reaction mixture and purified by recrystallisation.

Outline the steps that should be carried out to recrystallise vanillin. **2**

(iii) One mole of eugenol theoretically produces one mole of vanillin.

The percentage yield was found to be 16%.

Calculate the mass of vanillin ($GFM = 152$ g), in g, produced from 3.16 g of eugenol ($GFM = 164$ g). **2**

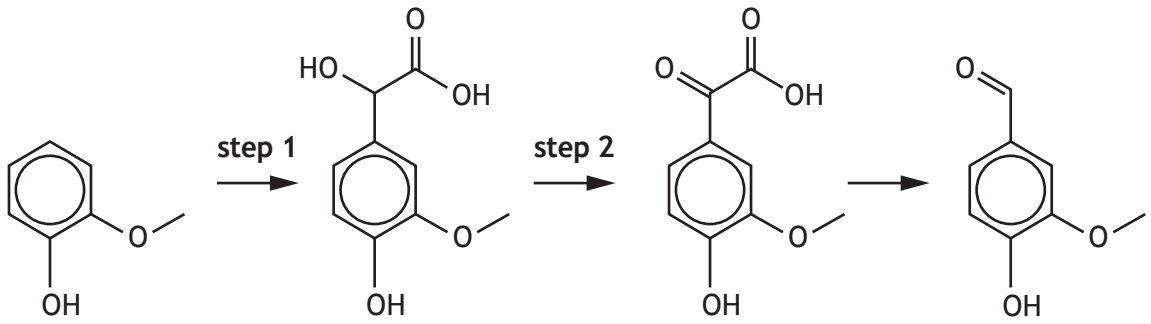
(iv) The literature melting point range of pure vanillin is 80 – 81 °C.

Explain fully the effect impurities have on the melting point range compared to a pure sample. **2**

[Turn over

8. (continued)

(b) Vanillin can also be synthesised from guaiacol as shown.



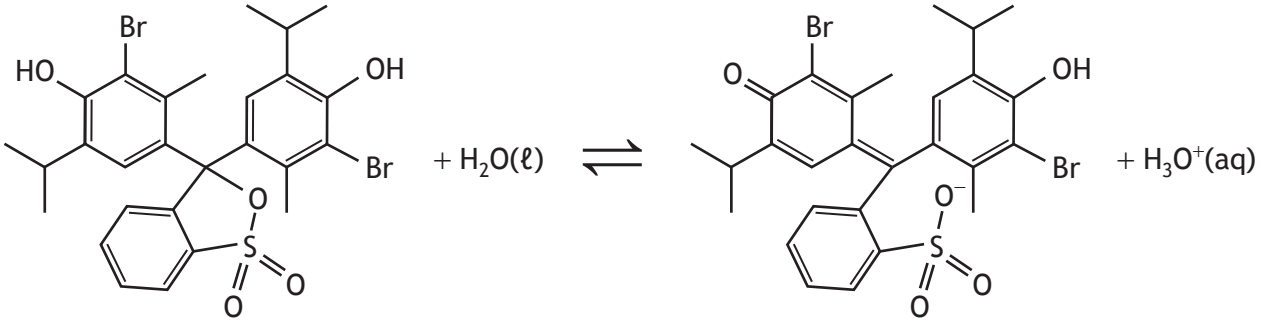
(i) Suggest the type of reaction taking place in step **1**. **1**

(ii) Suggest a reagent that could be used for step **2**. **1**

9. Many chemical reactions require the measurement and control of pH.

Equilibria exist in aqueous solutions of acid-base indicators and buffers.

Bromothymol blue is an example of an acid-base indicator.



yellow blue

An acid buffer consists of a solution of a weak acid and one of its salts made from a strong base.

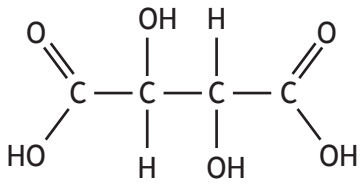
Ethanoic acid is an example of a weak acid used to make an acidic buffer.

$$CH_3COOH(aq) + H_2O(\ell) \rightleftharpoons CH_3COO^-(aq) + H_3O^+(aq)$$

Using your knowledge of chemistry, discuss how equilibria are involved in the action of acid-base indicators and buffers to measure and control pH. **3**

[Turn over

10. Tartaric acid is a weak acid found in grapes.



tartaric acid

(a) Tartaric acid dissociates in two stages. The equation for the first stage dissociation of tartaric acid is

$HOOCCH(OH)CH(OH)COOH(aq) + H_2O(\ell) \rightleftharpoons HOOCCH(OH)CH(OH)COO^-(aq) + H_3O^+(aq)$

(i) Complete the equation to show the second stage dissociation of tartaric acid. **1**

$HOOCCH(OH)CH(OH)COO^-(aq) + H_2O(\ell) \rightleftharpoons$

(ii) The pH of a tartaric acid solution is determined by its first stage dissociation ($pK_a = 2.98$).

Calculate the concentration of a tartaric acid solution, in mol l^{-1}, with a pH of 2.75. **2**

(b) Tartaric acid is a waste product in the winemaking industry. It can be removed by solvent extraction using the solvent MIBK.

(i) The systematic name for MIBK is 4-methylpentan-2-one.

Draw the skeletal structural formula of 4-methylpentan-2-one. **1**

10. (b) (continued)

(ii) In an extraction, 50 cm^3 of aqueous tartaric acid solution and 50 cm^3 of MIBK were shaken together and left to settle into two layers.

(A) Name the piece of apparatus that should be used for this extraction. **1**

(B) After equilibrium was established, the concentration of tartaric acid in the MIBK layer was found to be 0.0477 mol l^{-1}.

tartaric acid(aq) $\rightleftharpoons$ tartaric acid(MIBK) $K = 0.649$

(I) Write the expression for this equilibrium constant, K. **1**

(II) Calculate the number of moles of tartaric acid remaining in the aqueous layer. **1**

(C) Suggest an improvement to the procedure that would maximise the number of moles of tartaric acid extracted from 50 cm^3 of aqueous tartaric acid solution using 50 cm^3 of MIBK. **1**

[Turn over

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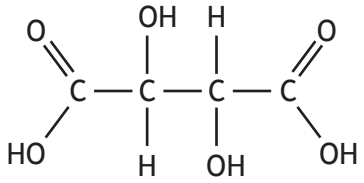
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(c) Tartaric acid has optical isomers.

(i) Optical isomers occur in compounds that have chiral centres.

Circle all the chiral centres in the structure of tartaric acid shown. **1**

(An additional structure, if required, can be found on *page 32*.)

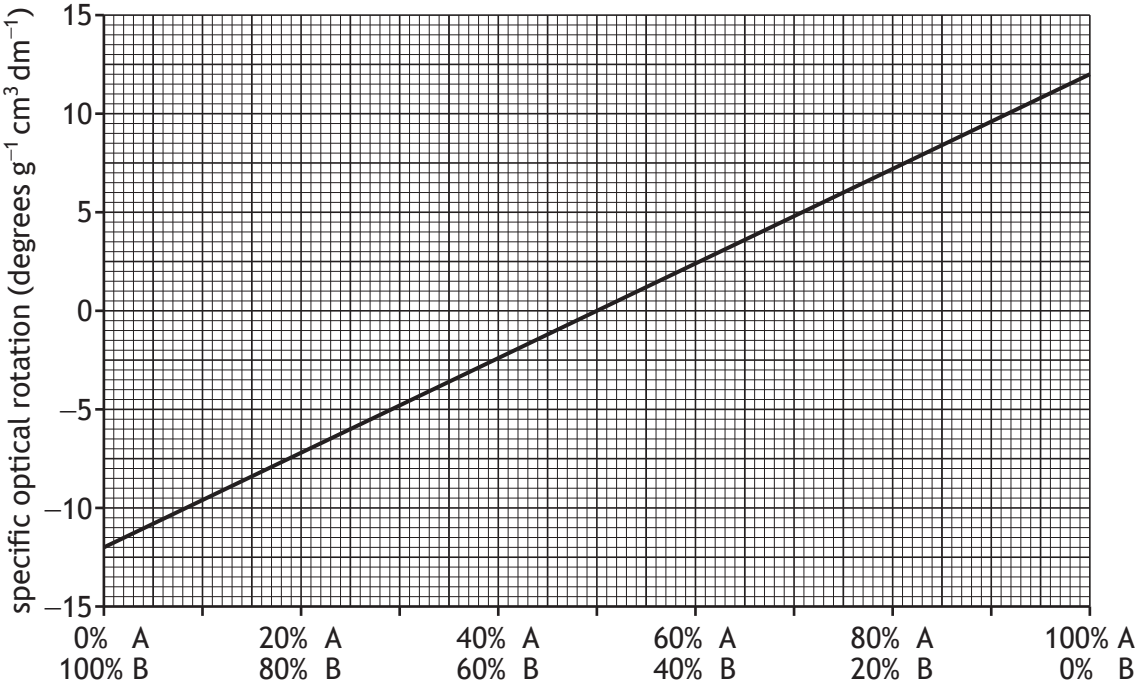


tartaric acid

(ii) Optical isomers rotate plane polarised light.

A polarimeter is used to measure the angle of rotation of plane polarised light.

The optical rotation of solutions containing different percentages of two optical isomers of tartaric acid, A and B, was measured.



composition of isomer mixture

(A) Draw an **X** on the line on the graph above to show the point that corresponds to a racemic mixture. **1**

(An additional graph, if required, can be found on *page 32*.)

10. (c) (ii) (continued)

(B) The observed optical rotation of a sample depends on the concentration of the sample and the path length.

This is shown in the equation

$$[\alpha] = \frac{\alpha_{observed}}{c \times l}$$

where: $[\alpha]$ is the specific optical rotation, in degrees $g^{-1}\,cm^3\,dm^{-1}$

$\alpha_{observed}$ is the observed optical rotation, in degrees

c is the concentration, in $g\,cm^{-3}$

l is the path length, in dm (1 dm = 10 cm)

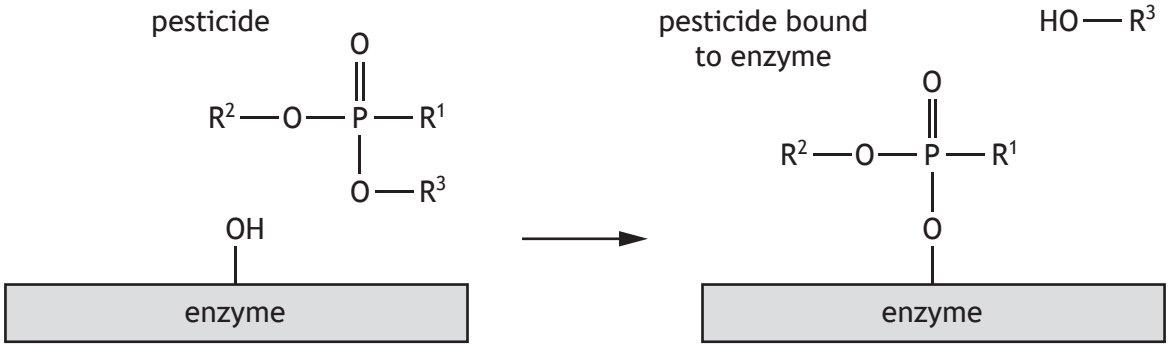
Calculate the observed optical rotation, in degrees, for a mixture of optical isomers containing 67% of isomer A, if the concentration of the solution is 1.35 $g\,cm^{-3}$ and the path length is 20 cm. **2**

[Turn over

11. Acetylcholine is a natural compound which stimulates nerves and muscles in the body.

(a) The breakdown of acetylcholine is catalysed by an enzyme.

Some pesticides can inhibit the activity of this enzyme by binding to an area of the enzyme and blocking the reaction normally catalysed there.



(i) State the area of the enzyme that the pesticide binds to. **1**

(ii) The inhibiting effects of the pesticide on the enzyme can be long lasting.

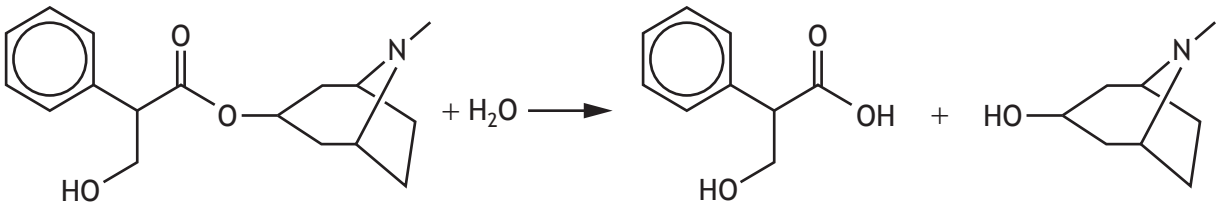
Suggest, by considering how the pesticide binds to the enzyme, why the effects can be long lasting. **1**

11. (continued)

(b) The drug atropine can be used to relax muscles in the eye by preventing acetylcholine from binding to receptors.

(i) State the classification of drug used to describe atropine. **1**

(ii) Atropine is broken down in the body to form tropic acid and tropine.



atropine tropic acid tropine

(A) State the type of reaction taking place. **1**

(B) Write the molecular formula for tropic acid. **1**

[Turn over

12. Creatine is a molecule that is found in some dietary supplements.
A sample of pure creatine was analysed to determine its structure.

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(a) Elemental microanalysis gave the following results.

Element	Percentage (%)
Carbon	36.6
Nitrogen	32.1
Oxygen	24.4
Hydrogen	6.9

Calculate the empirical formula of creatine. **2**
(*Clearly show your working for the calculation.*)

(b) A sample of creatine was analysed by mass spectrometry.

(i) The molecular formula for creatine was determined to be $C_4H_9N_3O_2$.
Predict the m/z value of the molecular ion peak. **1**

(ii) The mass spectrum of creatine has a peak at m/z 15.
Suggest a possible ion fragment that may be responsible for this peak. **1**

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(c) Creatine contains a carboxyl, an amine, an alkyl and an alkyl amine group.

The bonds in these groups can be identified using infrared spectroscopy.

(i) State the effect that infrared radiation has on the bonds within a molecule. **1**

(ii) Complete the table to show the bonds that are responsible for the peaks found in the infrared spectrum of creatine. **1**

(An additional table, if required, can be found on *page 33*.)

Bond responsible for peak	Wavenumber (cm^{-1})
O–H	2798
	1700
	1449
	1242

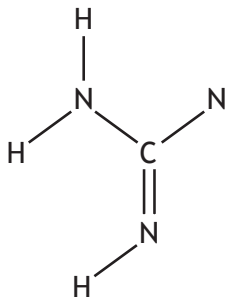
(d) The creatine molecule has no neighbouring hydrogen environments.

Predict the effect this would have on the splitting of the peaks in the high-resolution ^{1}H NMR spectrum. **1**

(e) Part of the structural formula for creatine is shown.

By considering all the evidence, complete the structural formula for creatine. **1**

(An additional structure, if required, can be found on *page 33*.)



[END OF QUESTION PAPER]