BENCHMARK

VCE Chemistry Assessments

Chemistry

Solutions

Benchmark Open SAC 4.1: Designing a synthesis pathway

- Writing time is **55 minutes**

Approved materials

- One scientific calculator

Materials supplied

- Data Book

Instructions

- Answer all questions in the spaces provided.
- Write using blue or black pen.

Students are **not** permitted to bring mobile phones or other electronic devices into the room.

Contents pages

Questions (4 questions, 40 marks) 2–9

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Questions

Instructions

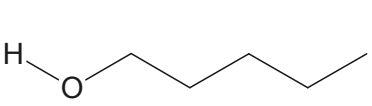
- Answer **all** questions in the spaces provided.
- Write your responses in English.
- Give simplified answers to all numerical questions, with an appropriate number of significant figures; unsimplified answers will not be given full marks.
- Show all working in your answers to numerical questions; no marks will be given for an incorrect answer unless it is accompanied by details of the working.
- Ensure that chemical equations are balanced and that the formulas for individual substances include an indication of state, for example, $H_2(g)$, NaCl(s).
- Unless otherwise indicated, the diagrams in this book are **not** drawn to scale.

Question 1 (8 marks)

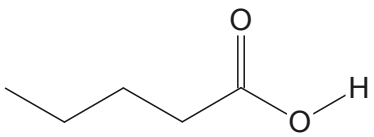
Fuels produced from plant material could replace a proportion of the transport fuels currently produced from crude oil. Esters of pentanoic acid are one family of these renewable fuels, and they can be blended with petrol or diesel. In one road trial, ten vehicles operated on petrol that contained 15% of one of these esters. Together the vehicles travelled 250 000 km, and engineers detected no damage to their engines, tanks or fuel lines.

A researcher plans to make one of these esters, pentyl pentanoate, from pentanoic acid and pentan-1-ol. She first compares the structures and physical properties of the three compounds.

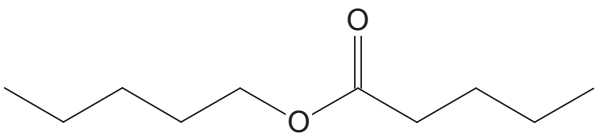
The skeletal formulae of the three compounds are shown below.



pentan-1-ol



pentanoic acid



pentyl pentanoate

The boiling points of the three compounds at normal atmospheric pressure are given in the table below.

Compound	pentan-1-ol	pentanoic acid	pentyl pentanoate
Boiling point (°C)	138	186	204

a. Write the molecular formula of pentyl pentanoate. 1 mark

① $C_{10}H_{20}O_2$

b. Explain why the acid has a higher boiling point than the alcohol. 2 marks

① Both compounds form hydrogen bonds between molecules, as well as dispersion forces.

② The carboxyl group has both a C=O and an O–H, so pentanoic acid forms more hydrogen bonds per molecule (and has larger dispersion forces), so more energy is needed to separate its molecules.

c. The ester cannot form hydrogen bonds between its molecules, but it has a higher boiling point than the acid. Explain this observation. 2 marks

① Pentyl pentanoate molecules are much larger, with more electrons and a greater surface area, so the dispersion forces between them are much stronger.

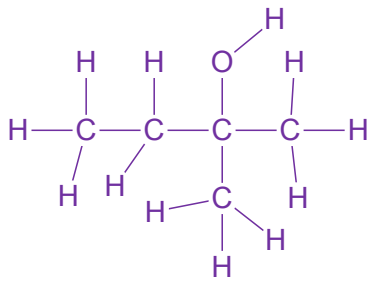
② This increase in dispersion forces outweighs the hydrogen bonding in pentanoic acid, so more energy is needed to separate the ester molecules.

The alcohol used by the researcher has several structural isomers that are also alcohols. Only one of these isomers is a tertiary alcohol.

d. Give the IUPAC name of this tertiary alcohol. 1 mark

① 2-methylbutan-2-ol

e. Draw the structural formula of this tertiary alcohol. Show all atoms and bonds. 2 marks

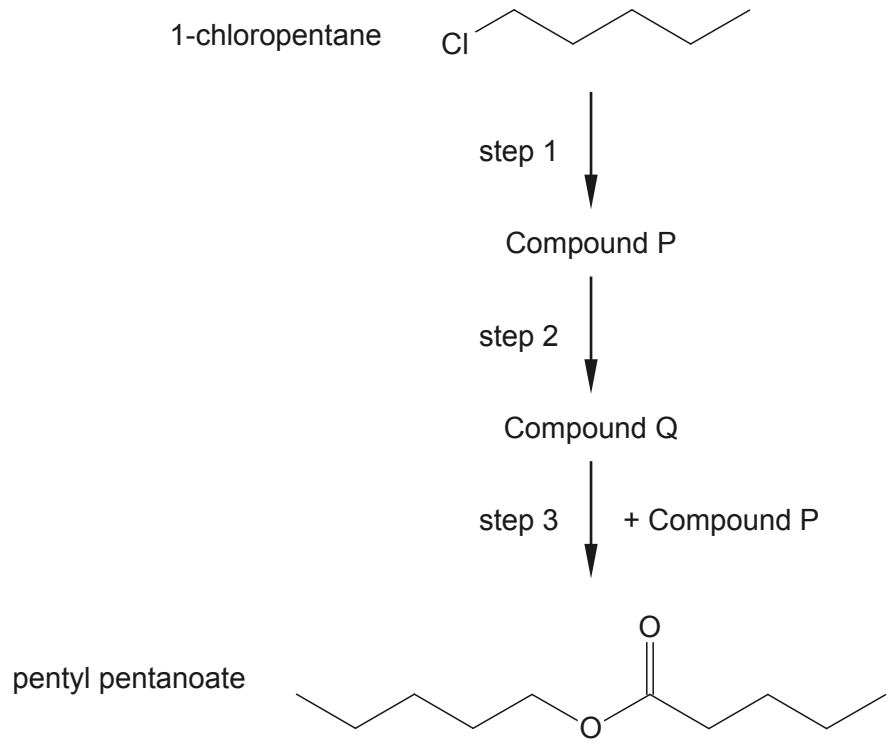


① Hydroxyl group on a carbon atom bonded to three other carbon atoms: a four-carbon chain with a methyl group and the OH on carbon 2.

② Every atom and bond drawn, with the formula $C_5H_{12}O$.

Question 2 (12 marks)

The only organic compound available in the laboratory is 1-chloropentane. The researcher therefore designs a synthesis pathway to produce the ester from this compound, as shown below. Compound P is made in step 1. Half of Compound P is then converted to Compound Q in step 2, and the other half is kept for step 3. Each step requires particular chemicals and reaction conditions.



a. Write the semistructural formulae of Compound P and Compound Q. 2 marks

① P: $CH_3CH_2CH_2CH_2CH_2OH$
② Q: $CH_3CH_2CH_2CH_2COOH$

b. Complete the table by giving the chemicals and conditions needed for each step. 3 marks

Step	Reagents and conditions
1	① NaOH(aq), heat
2	② $Cr_2O_7^{2-}$(aq)/H^+(aq) or MnO_4^-(aq)/H^+(aq), heat under reflux
3	③ Compound P, concentrated H_2SO_4 catalyst, heat

c. Write the balanced equation for step 3, using semistructural formulae. Include states. 2 marks

① $CH_3CH_2CH_2CH_2COOH(l) + CH_3CH_2CH_2CH_2CH_2OH(l) \rightarrow CH_3CH_2CH_2CH_2COOCH_2CH_2CH_2CH_2CH_3(l) + H_2O(l)$

② Equation balanced (1 : 1 : 1 : 1), with every state included.

The researcher starts with 25.0 g of 1-chloropentane. She calculates the theoretical maximum mass of the ester that this quantity could produce.

d. Calculate the maximum mass, in g, of the ester that could be made from this starting material. 2 marks

① $n(C_5H_{11}Cl) = \frac{m}{M} = \frac{25.0}{106.5}$
= 0.23474… mol; two of these are needed for each ester, one through P and one through Q.

② $n(\text{ester}) = \frac{1}{2} \times 0.23474\ldots = 0.11737\ldots$ mol, so m(ester) = n × M = 0.11737… × 172.0
= 20.2 g (to 3 s.f.)

In practice, no reaction step produces the theoretical quantity of product. The researcher follows the pathway above, converting half of Compound P to Compound Q. The percentage yield of each step is shown in the table below.

Step	**1**	**2**	**3**
Percentage yield (%)	88	70	62

e. Calculate the mass, in g, of the ester that the researcher obtains. 3 marks

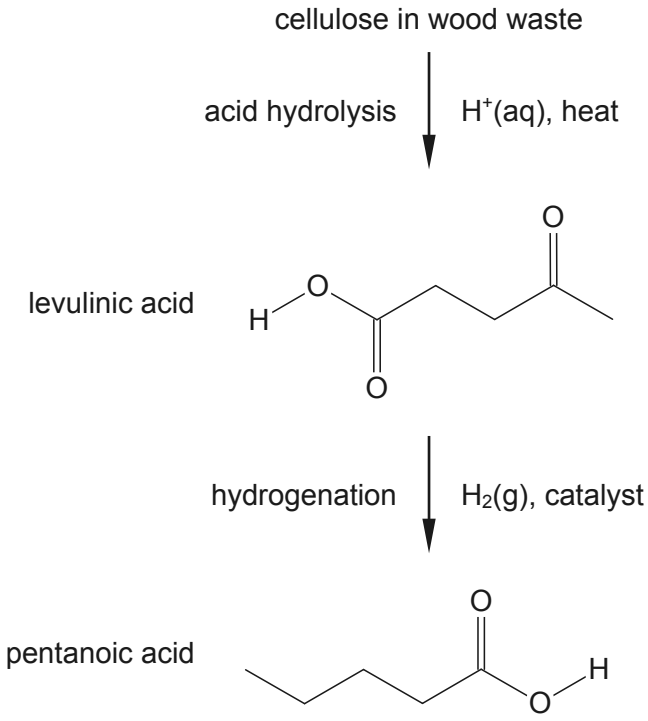
① $n(C_5H_{11}Cl \text{ in each portion}) = \frac{m}{M} = \frac{12.5}{106.5} = 0.11737\ldots$ mol

② n(Q) = 0.11737… × 0.88 × 0.70 = 0.072300… mol, less than n(P) = 0.11737… × 0.88 = 0.10328… mol, so Q is limiting

③ n(ester) = 0.072300… × 0.62 = 0.044826… mol, so m(ester) = n × M = 0.044826… × 172.0 = 7.71 g (to 3 s.f.)

Question 3 (9 marks)

Pentanoic acid can also be produced from wood waste. Compared with food crops, wood waste is inexpensive, widely available and not required for food production. Researchers break down the cellulose in wood by acid hydrolysis to form levulinic acid. This acid then reacts with hydrogen gas over a catalyst, producing the acid used in Question 2. This process is Route B, shown below.



The overall equation for Route B is:

$$CH_3COCH_2CH_2COOH(l) + 2H_2(g) \rightarrow CH_3CH_2CH_2CH_2COOH(l) + H_2O(l)$$

Route A is steps 1 and 2 of Question 2, which convert the starting material, a compound manufactured from crude oil, into the same acid. Route A has a much lower atom economy than Route B.

a. Name the two functional groups present in levulinic acid. 2 marks

① carbonyl group (in a ketone)
② carboxyl group

b. Calculate the atom economy of Route B. 2 marks

① atom economy = $\dfrac{M(C_5H_{10}O_2)}{M(C_5H_8O_3) + 2 \times M(H_2)} \times 100$

② = $\dfrac{102.0}{116.0 + 2 \times 2.0} \times 100 = 85.0\%$

c. Explain how Route B applies two green chemistry principles that Route A does not. 2 marks

① Use of renewable feedstocks: wood waste can be regrown, whereas crude oil is finite.

② Catalysis: the catalyst is not used up, so the hydrogenation needs no oxidant that is consumed and becomes waste. (Accept atom economy or prevention of waste for either mark: Route B has an atom economy of 85.0%, much higher than that of Route A, so less waste forms.)

d. A student claims: “Route B has a higher atom economy than Route A. It will therefore always produce a greater mass of product from the same mass of starting material.” Evaluate this claim. 3 marks

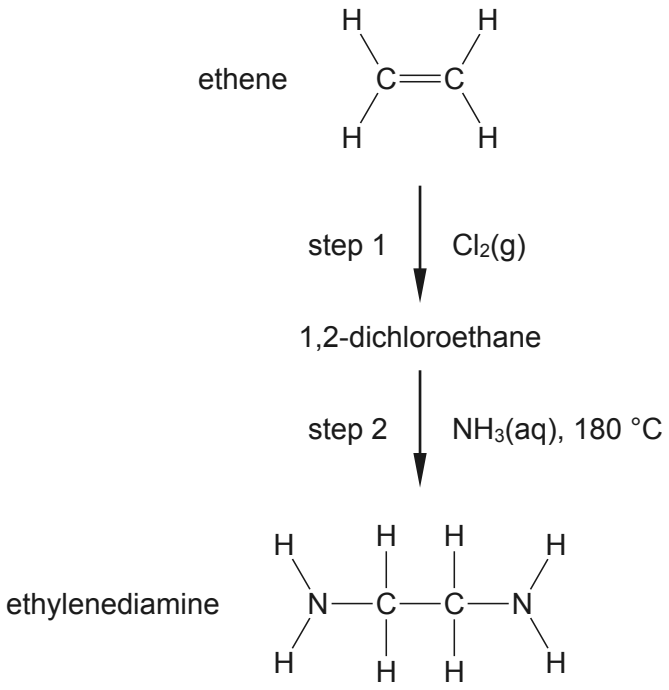
① Atom economy compares the mass of the desired product with the total mass of the reactants in the equation, so a higher value means less waste.

② The mass of product actually obtained depends on the percentage yield of each step, which atom economy does not take into account.

③ The claim is not valid: Route B wastes fewer atoms, but a low yield in any of its steps could still give less pentanoic acid.

Question 4 (11 marks)

Ethylenediamine is an amine that is used in the industrial production of many other chemicals, including some medicines. A company is deciding which of two routes it will use to make this amine. Its decision will consider the environmental effects of each route, the cost of the reactants and the quantity of waste produced. One industrial process starts from ethene and involves two steps, as shown below. In step 2, the product of step 1 reacts with ammonia in water at 180 °C under pressure.



a. Name the type of reaction in step 1. 1 mark

① addition

b. Give the IUPAC name of this amine. 1 mark

① ethane-1,2-diamine

c. In step 2, the products are the amine and ammonium chloride. Write the balanced equation for step 2, using semistructural formulae. Include states. 2 marks

① $ClCH_2CH_2Cl(l) + 4NH_3(aq) \rightarrow H_2NCH_2CH_2NH_2(aq) + 2NH_4Cl(aq)$

② Coefficients 4 and 2 correct, with every state included (accept (aq) for $ClCH_2CH_2Cl$).

d. Calculate the atom economy of step 2. 2 marks

① atom economy = $\frac{M(C_2H_8N_2)}{M(C_2H_4Cl_2) + 4 \times M(NH_3)} \times 100$

② = $\frac{60.0}{99.0 + 4 \times 17.0} \times 100 = 35.9\%$ (to 3 s.f.)

The same amine is also made by passing ethanolamine and ammonia over a nickel catalyst. This route also forms a mixture of other amines. The equation for this reaction is:

$$HOCH_2CH_2NH_2(g) + NH_3(g) \rightarrow H_2NCH_2CH_2NH_2(g) + H_2O(g)$$

The atom economy of this route is 76.9%.

e. In one production run, 2.00×10^3 kg of the organic reactant reacts with an excess of ammonia, producing 1.47×10^3 kg of the amine. Calculate the percentage yield of the amine. 2 marks

① $n(HOCH_2CH_2NH_2) = \frac{m}{M} = \frac{2.00 \times 10^6}{61.0} = 3.2786\ldots \times 10^4$ mol, so the theoretical m(amine) = n × M

$= 3.2786\ldots \times 10^4 \times 60.0 = 1.9672\ldots \times 10^6$ g

② percentage yield = $\frac{\text{actual mass}}{\text{theoretical mass}} \times 100 = \frac{1.47 \times 10^6}{1.9672\ldots \times 10^6} \times 100 = 74.7\%$ (to 3 s.f.)

f. A company must choose one of the two routes to make the amine. Evaluate the two routes with reference to atom economy, catalysis and the products formed. 3 marks

① The ethanolamine route has the much higher atom economy (76.9% compared with 35.9%), so less waste forms for each tonne of product.

② It uses a nickel catalyst that is not used up, while the route from ethene forms ammonium chloride as waste and uses chlorine, a hazardous reactant.

③ However, the ethanolamine route forms a mixture of amines, which lowers the yield and needs separation; on balance it is the better choice where the other amines can be sold.

End of questions

Additional writing space

Additional writing space

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