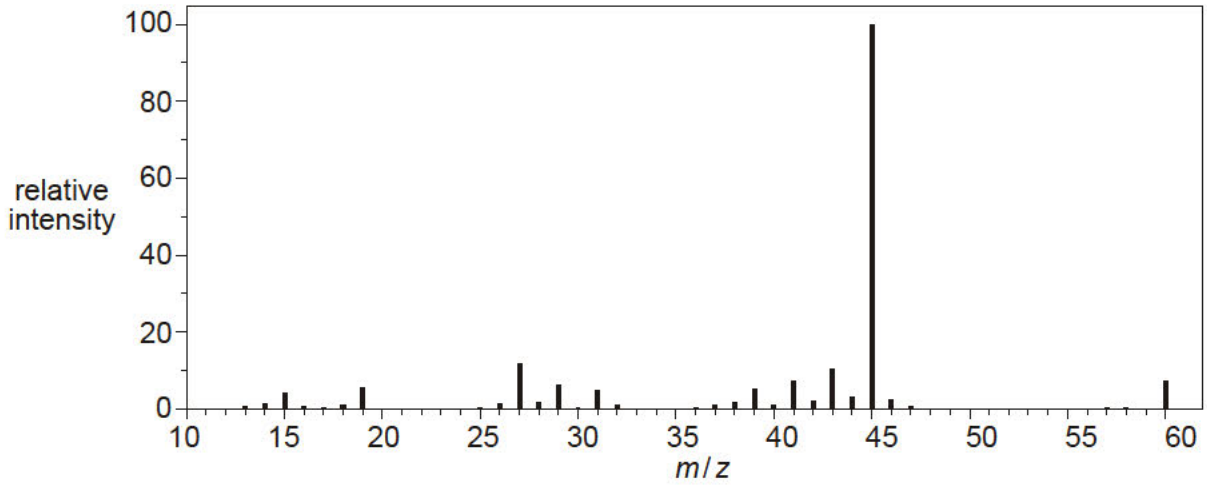
F322: Chains, Energy and Resources
2.2.3 Modern Analytical Techniques

1. Alcohol **E** is one of the following alcohols.

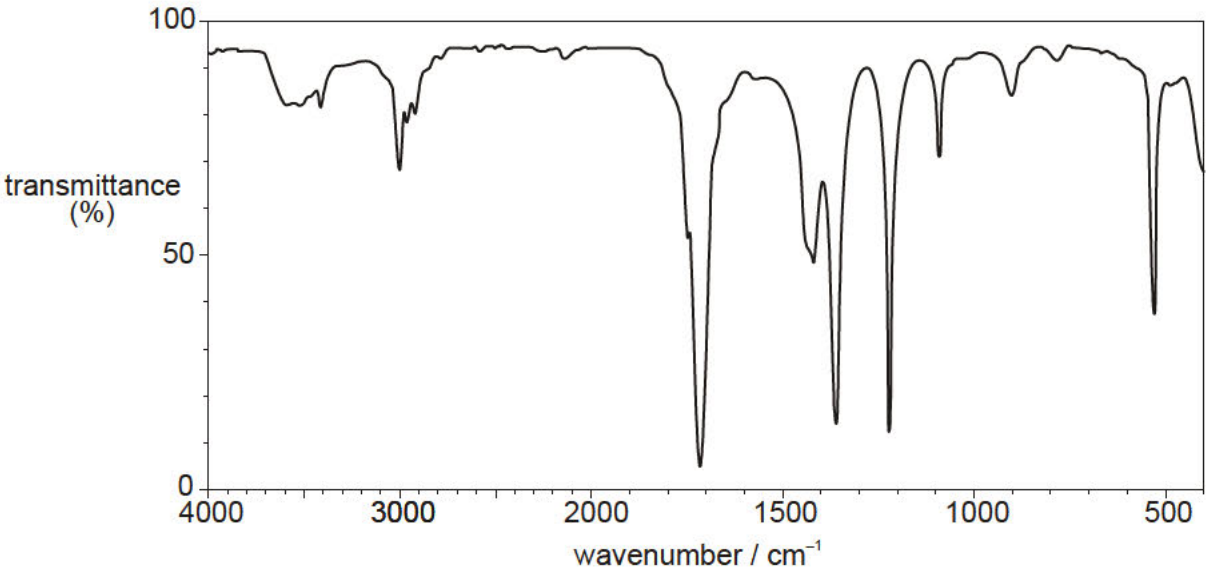
butan-2-ol	**ethane-1,2-diol**
2-methylpentan-3-ol	**2-methylpropan-2-ol**
propan-1-ol	**propan-2-ol**

A student oxidises alcohol **E** by heating under reflux with excess acidified potassium dichromate(VI). An organic product **F** is isolated.

The mass spectrum of the alcohol **E** is shown below.



The infrared spectrum of the organic product **F** is shown below.



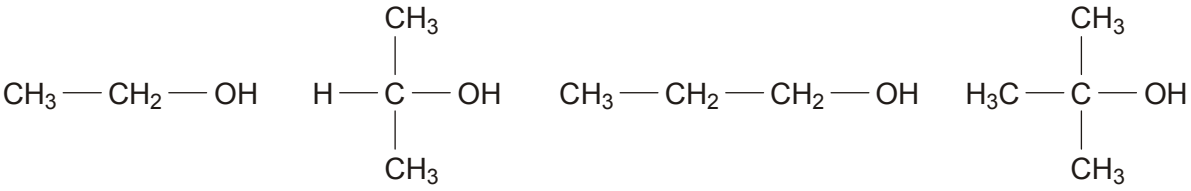
- Name **or** draw the structures of the alcohol **E** and the organic product **F**.
- Write an equation for the reaction of alcohol **E** with acidified potassium dichromate(VI).

Use [O] to represent the oxidising agent, acidified potassium dichromate(VI).

In your answer, you should make clear how each structure fits with the information given above.

[Total 7 marks]

2. Alcohols **A**, **B**, **C** and **D** are shown below.



A **B** **C** **D**

(a) Compound **A** is ethanol, a very useful alcohol.

Identify the two main methods used in the industrial production of ethanol. Write an equation for each method.

method 1 .....

.....

equation .....

.....

method 2 .....

.....

equation .....

[4]

(b) A student heated each alcohol, **A**–**D**, with acidified potassium dichromate(VI) as the oxidising agent. With alcohols **A**, **B** and **C**, the colour turned from orange to green.

(i) Identify the organic product and write a balanced equation for the reaction of alcohol **B** with acidified potassium dichromate(VI).

Use [O] to represent the oxidising agent, acidified potassium dichromate(VI).

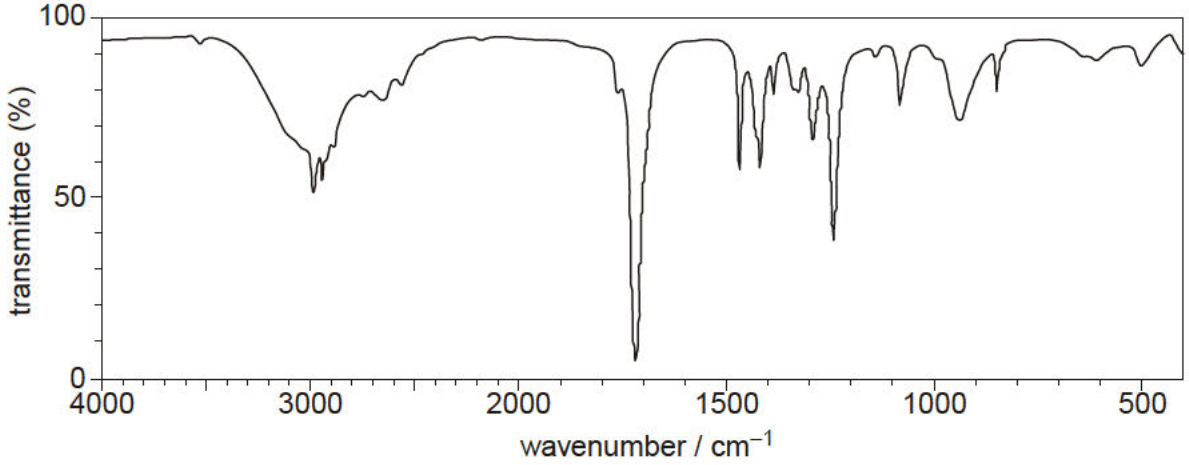
organic product:

balanced equation:

[2]

(ii) The organic product obtained from **C** was analysed by infrared (IR) spectroscopy.

The IR spectrum of the product is shown below.



wavenumber / cm^{-1}

Use your *Data Sheet* to identify the organic product. Explain your reasoning.

organic product:

reasoning .....

.....

.....

[3]

(c) The student heated alcohol **D** with ethanoic acid in the presence of an acid catalyst. An organic product **E** was formed with a fruity smell.

(i) Name alcohol **D**.

.....

[1]

(ii) Name the functional group in the organic product **E**.

.....

[1]

(iii) Draw the structure of the organic product **E**.

[2]

[Total 13 marks]

3. A student carried out an investigation to compare the rates of hydrolysis of 1-iodopropane and 1-bromopropane. The student heated hot aqueous sodium hydroxide with each halogenoalkane and found that 1-iodopropane was hydrolysed faster.

The equation for the reaction with 1-iodopropane is shown below.

$$CH_3CH_2CH_2I + OH^- \rightarrow CH_3CH_2CH_2OH + I^-$$

(a) (i) Outline the mechanism for this hydrolysis of 1-iodopropane.

Show curly arrows and relevant dipoles.

[3]

(ii) State the name of this type of mechanism.

.....

[1]

(b) Explain why 1-iodopropane is hydrolysed faster than 1-bromopropane.

.....

.....

.....

.....

[2]

[Total 6 marks]

4. An analytical chemist was provided with a compound **J** which has an unbranched carbon skeleton. After analysis, the chemist obtained the following results.

type of analysis	**evidence**
infrared spectroscopy	broad absorption at 3350 cm^{-1}
percentage composition by mass	C, 70.59%; H, 13.72%; O, 15.69%
mass spectrometry	molecular ion peak at m/z = 102.0

Use this information to suggest all the possible structures for the **unbranched** compound **J.**

In your answer you should make clear how your explanation is linked to the evidence.

.....

.....

.....

.....

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.....

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.....

.....

[Total 8 marks]

5. Bromobutane, $CH_3CH_2CH_2CH_2Br$, can be reacted with hot aqueous sodium hydroxide to prepare butan-1-ol.

$$CH_3CH_2CH_2CH_2Br + OH^- \rightarrow CH_3CH_2CH_2CH_2OH + Br^-$$

The butan-1-ol produced can be analysed by mass spectrometry.

(i) Predict **two** fragment ions that you would expect to see in the mass spectrum of butan-1-ol and state the *m*/*z* value of each ion.

.....

.....

[2]

(ii) State a use of mass spectrometry outside of the laboratory.

.....

[1]

[Total 3 marks]

6. Compound **X** is an atmospheric pollutant emitted from fuel combustion of petrol and diesel vehicles. Compound **X** is a potent human carcinogen.

- Analysis of compound **X** showed the following percentage composition by mass: C, 88.89%; H, 11.1%.
- Mass spectrometry showed a molecular ion peak at *m/z* = 54.
- Compound **X** reacts with H2 in the presence of a nickel catalyst in a 1 : 2 molar ratio.

Analyse and interpret this information to determine a possible structure for compound **X**.

Show all your working.

[Total 5 marks]

7. (a) Butan-1-ol can be oxidised to form butanal.

(i) State a suitable oxidising mixture for this reaction.

.....

[2]

(ii) State the colour change you would see during this oxidation.

from ..... to .....

[1]

(b) A sample of the butanal from (a) was analysed using infra-red spectroscopy. The infra-red spectrum contained an absorption in the region 1680–1750 cm^{-1} but did **not** contain a broad absorption in the region 2500–3300 cm^{-1}.

Refer to the Data Sheet for Chemistry provided.

(i) What does the absorption in the region 1680–1750 cm^{-1} indicate?

.....

[1]

(ii) What does the absence of a broad absorption in the region 2500–3300 cm^{-1} indicate?

.....

[1]

(iii) The reaction in (a) was carried out using distillation and **not** reflux.

Explain why.

.....

.....

[2]

[Total 7 marks]

8. Compound **E** can be oxidised to form a carboxylic acid.

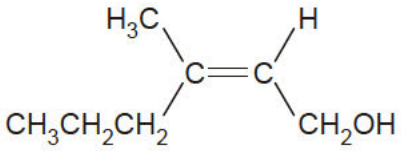
(i) State a suitable oxidising mixture for this reaction.

.....

[2]

(ii) Write a balanced equation for this oxidation of compound **E**.

Use [O] to represent the oxidising mixture.



compound **E**

[3]

(iii) Explain how compound **E** and the carboxylic acid could be distinguished by infra-red spectroscopy.

.....

.....

[1]

[Total 6 marks]

9. (a) When ethanol is heated with acidified potassium dichromate(VI) solution, it can be oxidised to form either ethanal, CH_3CHO (Fig. 1), or ethanoic acid, CH_3COOH (Fig. 2).

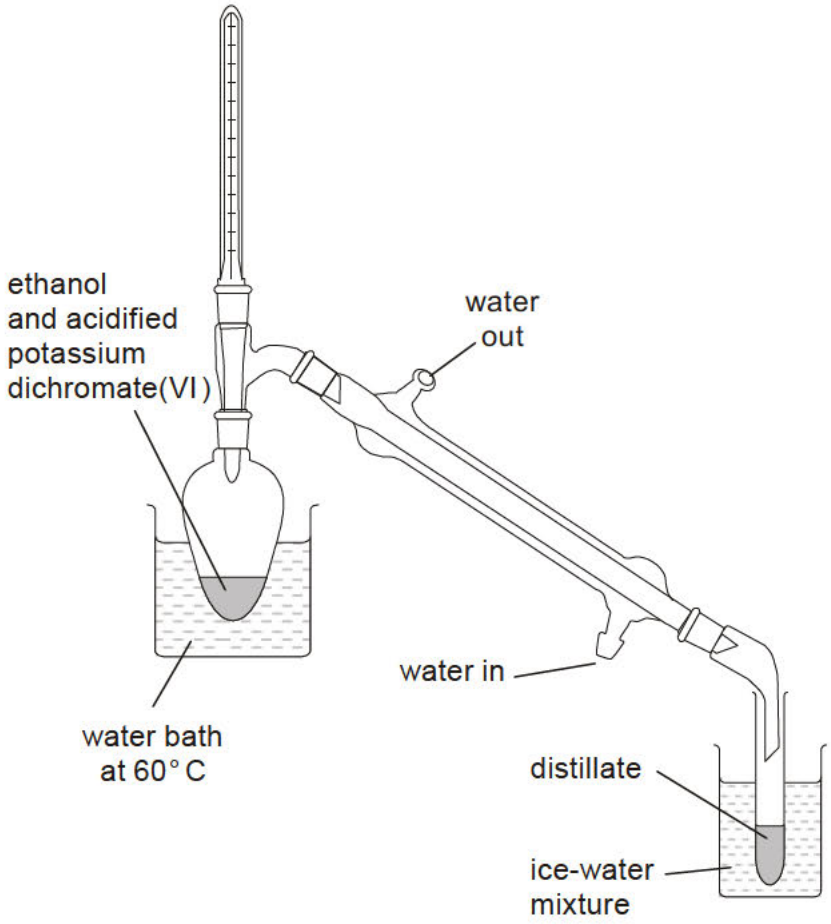


Fig. 1

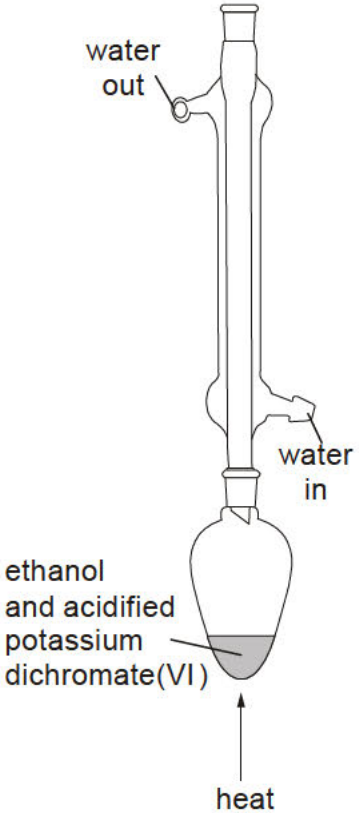


Fig. 2

The boiling points of ethanol, ethanal and ethanoic acid are given in the table below.

	CH_3CH_2OH	CH_3CHO	CH_3COOH
boiling point/ °C	78	21	118

Use this table of boiling points to explain

(i) why the organic product is likely to be ethanal if the apparatus shown in Fig. 1 is used,

.....

.....

[2]

(ii) why the organic product is likely to be ethanoic acid if the apparatus shown in Fig. 2 is used.

.....

.....

[2]

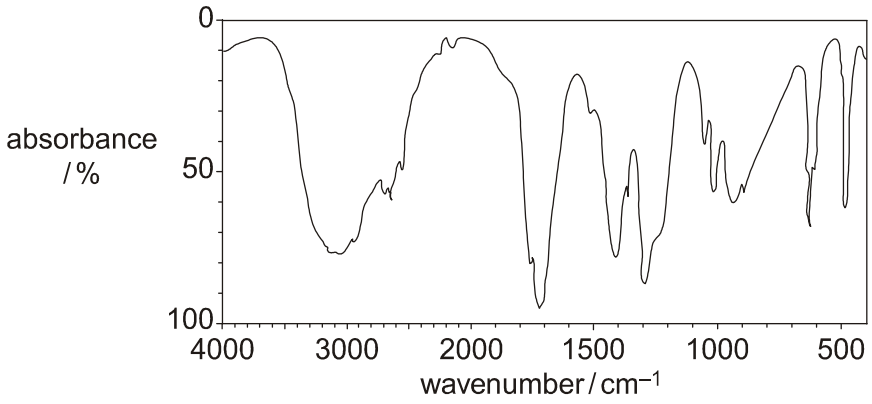
(b) Write a balanced equation for the oxidation of ethanol to ethanoic acid. Use (O) to represent the oxidising agent.

.....

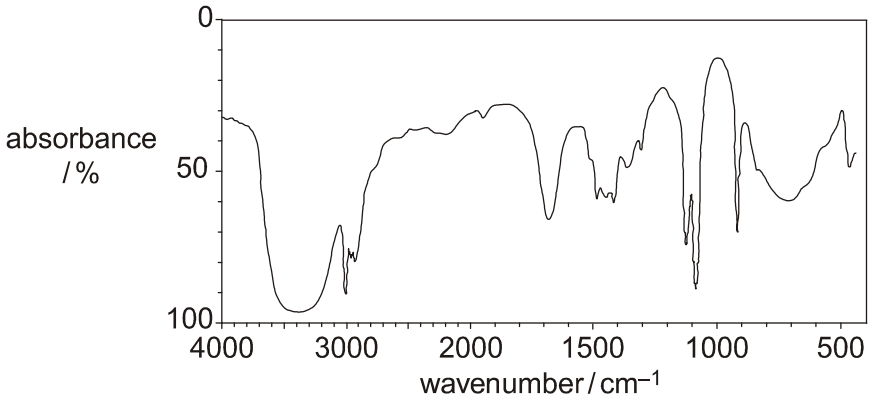
[2]

(c) The ethanal collected using the apparatus shown in Fig. 1 was analysed by infra-red spectroscopy. Use your *Data Sheet* to justify which of the three spectra shown below is most likely to be that of ethanal.

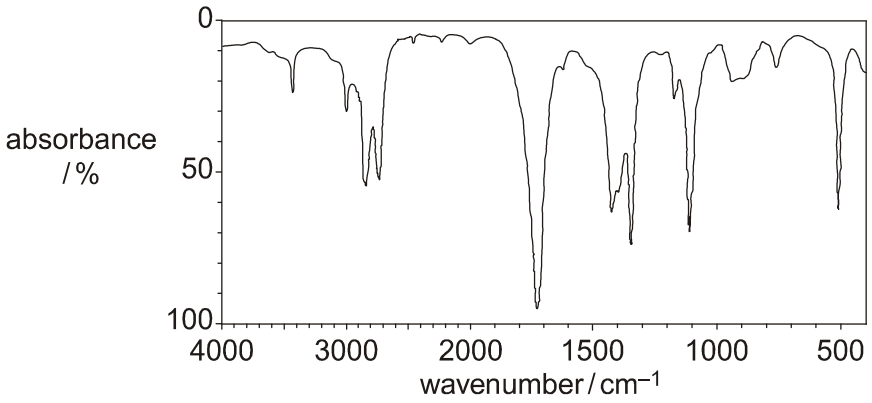
spectrum **A**



spectrum **B**



spectrum **C**



The organic product collected when using the apparatus shown in Fig. 1 is most likely to be that shown by spectrum ..... because.....

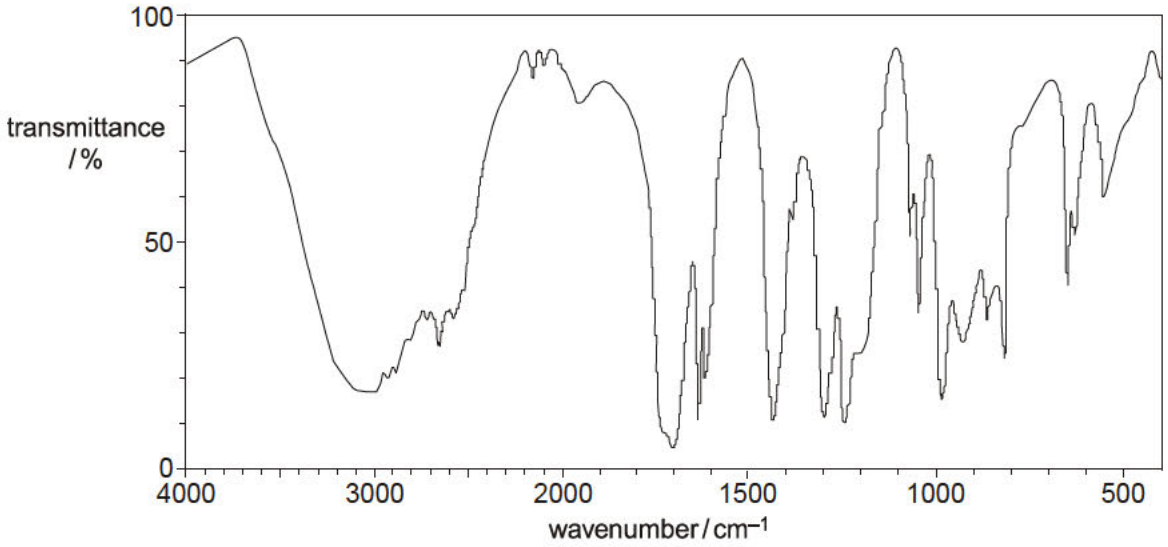
.....

.....

[3]

[Total 9 marks]

10. A sample of prop-2-en-1-ol was oxidised and an infra-red spectrum of the organic product was obtained.



By referring to your Data Sheet, decide whether acrolein, CH_2==CHCHO, or acrylic acid, CH_2==CHCOOH, was formed.

The infra-red spectrum above is of .....

because .....

.....

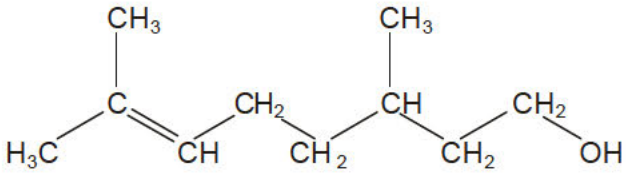
.....

.....

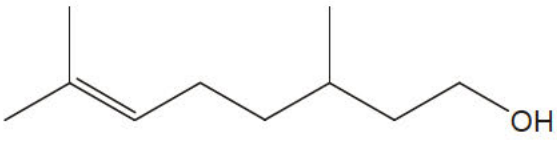
.....

[Total 3 marks]

11. Citronellol, $C_{10}H_{20}O$, occurs naturally in both rose and geranium oils. The structural and skeletal formulae of citronellol are shown below.



structural formula



skeletal formula

(a) Name the **two** functional groups present in citronellol.

…… and .....

[2]

(b) The functional groups in citronellol can be identified either by chemical tests or by infrared spectroscopy.

(i) State which of the two functional groups you named in (a) is:

1 identified when bromine is added to citronellol, ...

2 more easily identified from the infra-red spectrum. .....

[1]

(ii) State what you would **see** when bromine is added to citronellol.

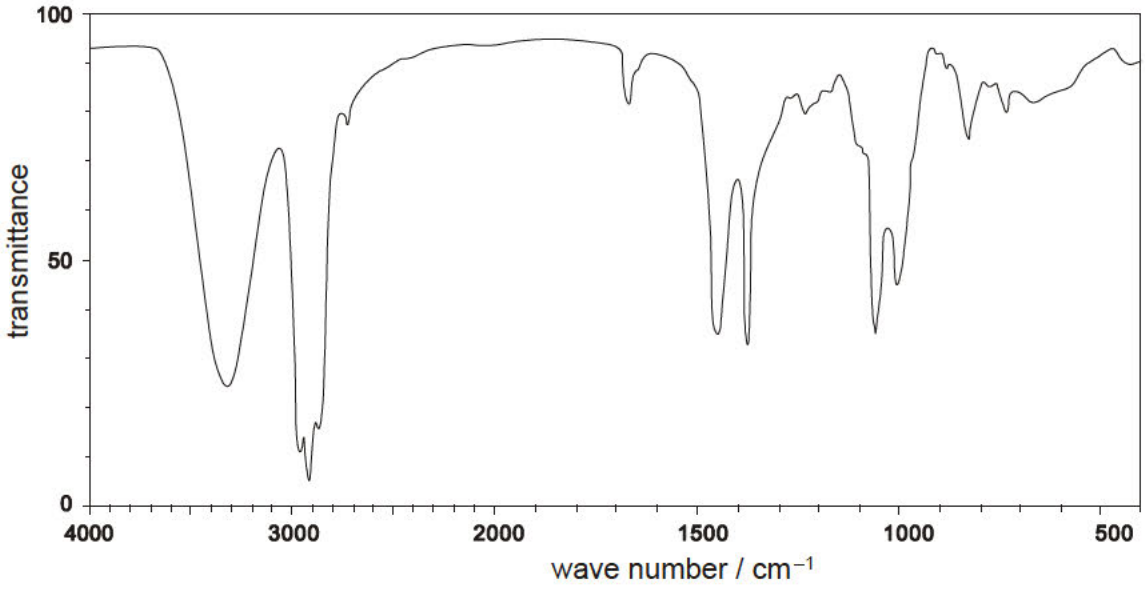
.....

[1]

(iii) Draw the skeletal formula of the organic product formed when bromine is added to citronellol.

[1]

(iv) The infra-red spectrum of citronellol is shown below. Mark on this spectrum, with the letter **X**, the absorption that confirms the presence of the functional group that is most easily identified from this spectrum.



[1]

(c) Reaction of a sample of citronellol, $C_{10}H_{20}O$, with hydrogen in the presence of a catalyst results in the formation of a saturated compound **C**.

(i) Suggest a catalyst for this reaction.

.....

[1]

(ii) Determine the molecular formula of the saturated compound **C**.

.....

[1]

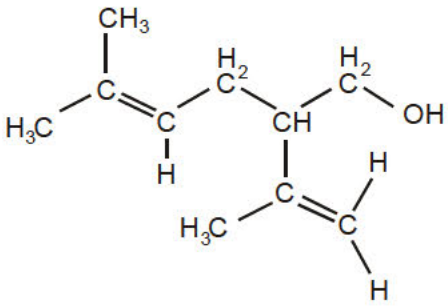
(iii) Construct a balanced equation for this reaction.

.....

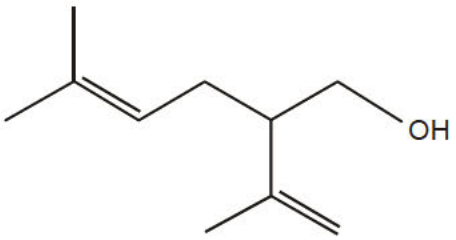
[1]

[Total 9 marks]

12. Lavandulol, $C_{10}H_{18}O$, is a fragrant oil which is found in lavender. The structural and the skeletal formulae of lavandulol are shown below.



structural formula



skeletal formula

(a) (i) Identify **two** different functional groups in lavandulol.

..... and .....

[2]

(ii) Why does lavandulol **not** have *cis-trans* isomerism?

.....

.....

[1]

(b) Lavandulol, $C_{10}H_{18}O$, also reacts with bromine to form a saturated organic product.

State what you would see in this reaction and deduce the molecular formula of the organic product.

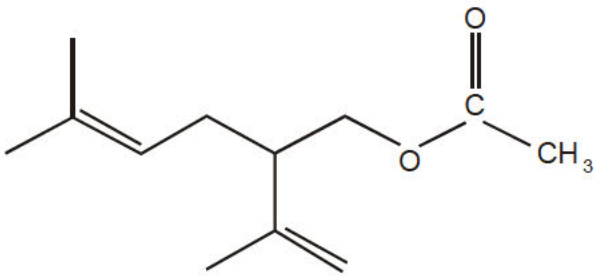
observation .....

[1]

molecular formula .....

[2]

(c) Lavandulol could be converted into an ester **X**, which is also found in lavender oil.



ester **X**

State a reagent and a catalyst that could be used to form ester **X** from lavandulol.

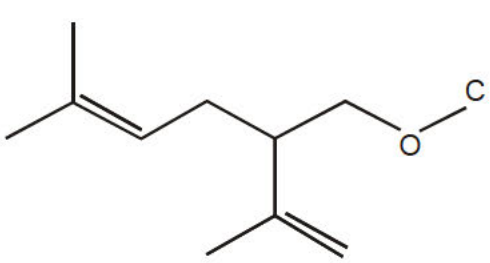
reagent .....

[1]

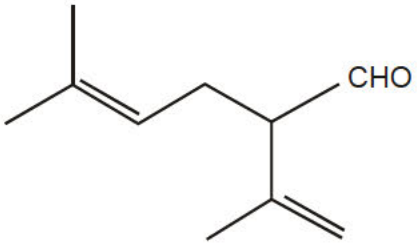
catalyst .....

[1]

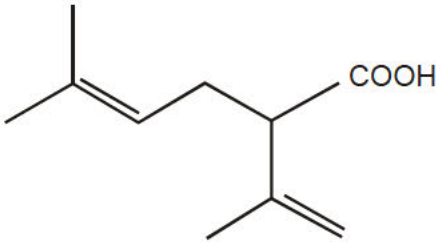
(d) Lavanduloi can be oxidised to produce either compound **Y** or compound **Z**.



lavandulol
$C_{10}H_{18}O$



compound **Y**
$C_{10}H_{16}O$



compound **Z**
$C_{10}H_{16}O_2$

(i) Write a balanced equation for the oxidation of lavandulol to produce compound **Z**. Use the molecular formulae given above and use [O] to represent the oxidising agent.

.....

[2]

(ii) An infra-red spectrum of either compound **Y** or compound **Z** was obtained and was found to contain an absorption between 1680 – 1750 cm^{-1}. However, there was no broad absorption between 2500 – 3300 cm^{-1}.

By referring to your *Data Sheet*, use this information to deduce whether the infra-red spectrum was of compound **Y** or of compound **Z**. Show your reasoning.

The infra-red spectrum was of compound ..... because .....

.....

.....

.....

[2]

[Total 12 marks]