IB · HL · Chemistry

6 hours 45 questions

Structured Questions

Functional Groups: Classification of Organic Compounds

Representing Formulas of Organic Compounds / Functional Groups / Homologous Series / IUPAC Nomenclature / Structural Isomers / Cis-Trans Isomers (HL) / Enantiomers (HL) / Mass Spectrometry (MS) Fragmentation Patterns (HL) / Infrared Spectra (IR) Interpretation (HL) / Proton NMR Spectroscopy (HL) / Peak Splitting in Proton NMR (HL) / Structural Analysis of Molecules (HL)

Easy (16 questions)	/102
Medium (16 questions)	/148
Hard (13 questions)	/97
Total Marks	**/347**

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Easy Questions

1 (a) Define the term hydrocarbon.

.....

(1 mark)

(b) State the general formula for the following hydrocarbon families.

Alkanes .....

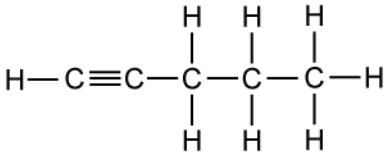
Alkenes .....

.....

.....

(2 marks)

(c) State the IUPAC name of the following hydrocarbon.



.....

(1 mark)

(d) A student stated that as the number of carbon atoms increases in an alkane, the boiling point increases. State if the student is correct and justify your answer.

(3 marks)

2 (a) Propanal and propanone have the same molecular formula, C_3H_6O, but have different structures. Draw the displayed structures of propanal and propanone.

.....

.....

(2 marks)

(b) State the type of isomerism that is exhibited by propanal and propanone.

.....

(1 mark)

(c) Butanone can be reduced to a secondary alcohol by $LiAlH_4$. State the name of this alcohol.

.....

(1 mark)

(d) State the general formula of an alcohol.

.....

(1 mark)

3 (a) Name the three possible isomers of C_5H_{12}.

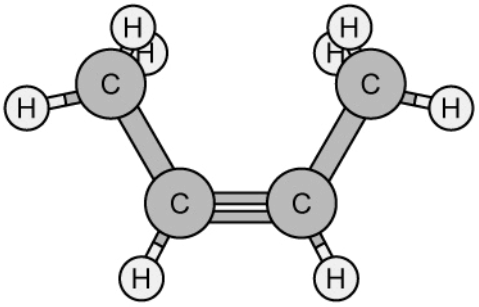
.....

.....

.....

(3 marks)

(b) Using IUPAC rules state the name of the molecule shown in the image below.



.....

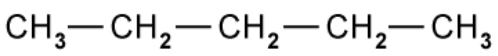
(1 mark)

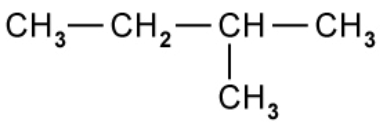
(c) Draw the sterochemical drawing of methane.

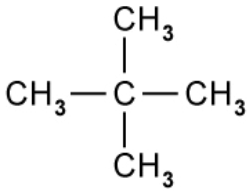
.....

(1 mark)

4 (a) Three isomers of pentane are shown below.

A 

B 

C 

Give the IUPAC names of isomers **B** and **C.**

.....

.....

(2 marks)

(b) Predict the number of different hydrogen environments in each of the isomers from part (a).

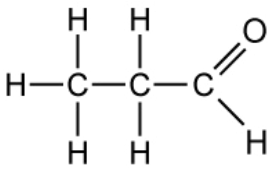
.....

.....

.....

(3 marks)

(c) The displayed formula of propanal is shown.



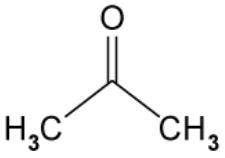
State the number of ^{1}H NMR signals that would appear in the ^{1}H NMR of propanal and state the ratio of the area under the peaks in which they would appear.

.....

.....

(2 marks)

(d) Propanal and propanone, shown below, both have the same molecular formula C_3H_6O.



Explain how propanone gives a different 1H NMR spectrum compared to propanal.

.....

.....

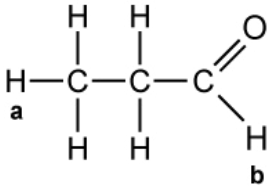
(2 marks)

Using section 21 of the data booklet, state the chemical shift for the ^1H NMR of propanone.

(e) .....

(1 mark)

5 (a) Using section 21 of the data booklet, state the chemical shift for hydrogens **a** and **b** in the ^{1}H NMR of propanal.



.....

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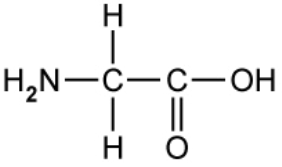
(2 marks)

(b) The structure of the amino acid glycine is shown below.



State the number of peaks found in the ^{1}H NMR spectrum of glycine.

.....

(1 mark)

(c) State the ratio of the areas under the hydrogen peaks for glycine.

.....

(1 mark)

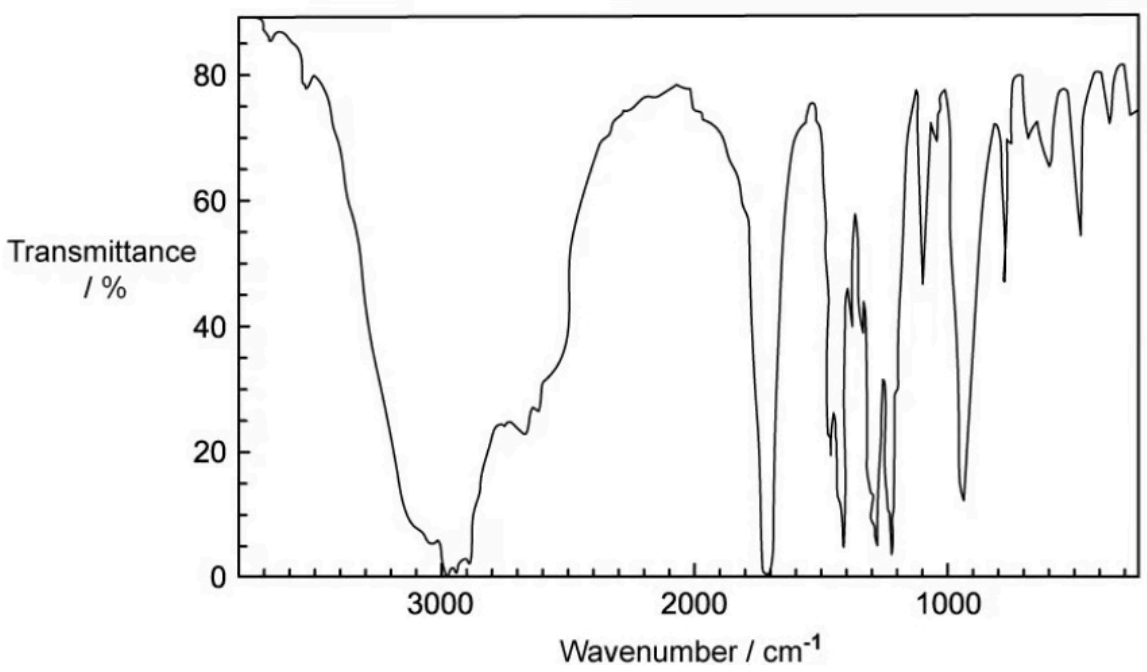
(d) The chemical shift for the protons in the NH_2 protons in glycine is 1.0 - 4.5 ppm.

Using section 21 of the data booklet, predict the other ^{1}H NMR chemical shifts for glycine.

.....

(1 mark)

6 (a) Under certain conditions, butan-1-ol can be oxidized to the compound with the infrared spectrum shown below.



Using section 20 of the data booklet, state the name of the compound that has produced the spectrum shown.

.....

(1 mark)

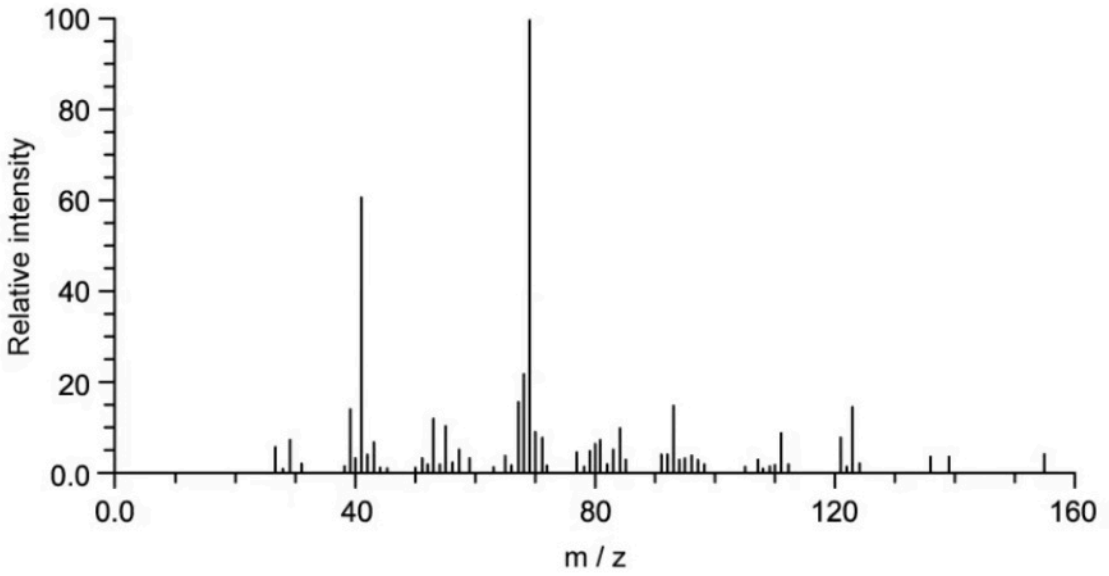
(b) State what the molecular (parent) ion, M^+ peak, in the mass spectrum of a hydrocarbon containing ^{12}C and ^{1}H represents.

.....

(1 mark)

7 (a) Geraniol is an organic molecule that contains alkene and alcohol functional groups.

The mass spectrum of geraniol is shown below.



i) State how this mass spectrum can be used to confirm the molar mass of geraniol.

[1]

ii) Give the formula of an ion that could be responsible for the peak at *m/ z* = 69.

[1]

.....

.....

(2 marks)

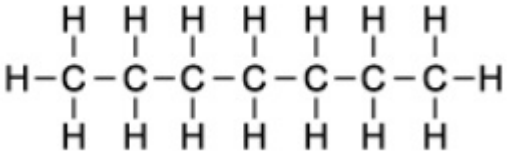
(b) A sample of propan-2-ol was heated under reflux with potassium dichromate(VI) acidified with sulfuric acid, and then the mixture was distilled.

Apart from the peaks due to the C—C and C—H bonds, what peak(s) would be present in the infrared spectrum of the distillate.

.....

(1 mark)

(c) The compound shown below can be analysed to obtain infrared and mass spectra.



Using section 22 of the data booklet, suggest the molecular formulae of the ions responsible for peaks in the mass spectrum with the following *m/z* values.

i) 15

[1]

ii) 100

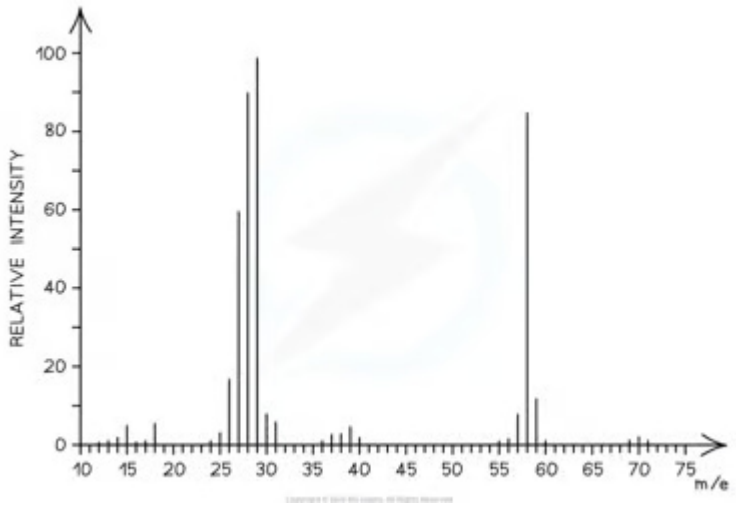
[1]

.....

.....

(2 marks)

(d) The mass spectrum shown below was obtained for propanal, CH_3CH_2CHO.



i) Use the mass spectrum to show that the empirical and the molecular formulae of the compound mentioned are the same.

[1]

ii) Using section 22 of the data booklet, suggest the species responsible for the peak at m/z = 29.

[1]

.....

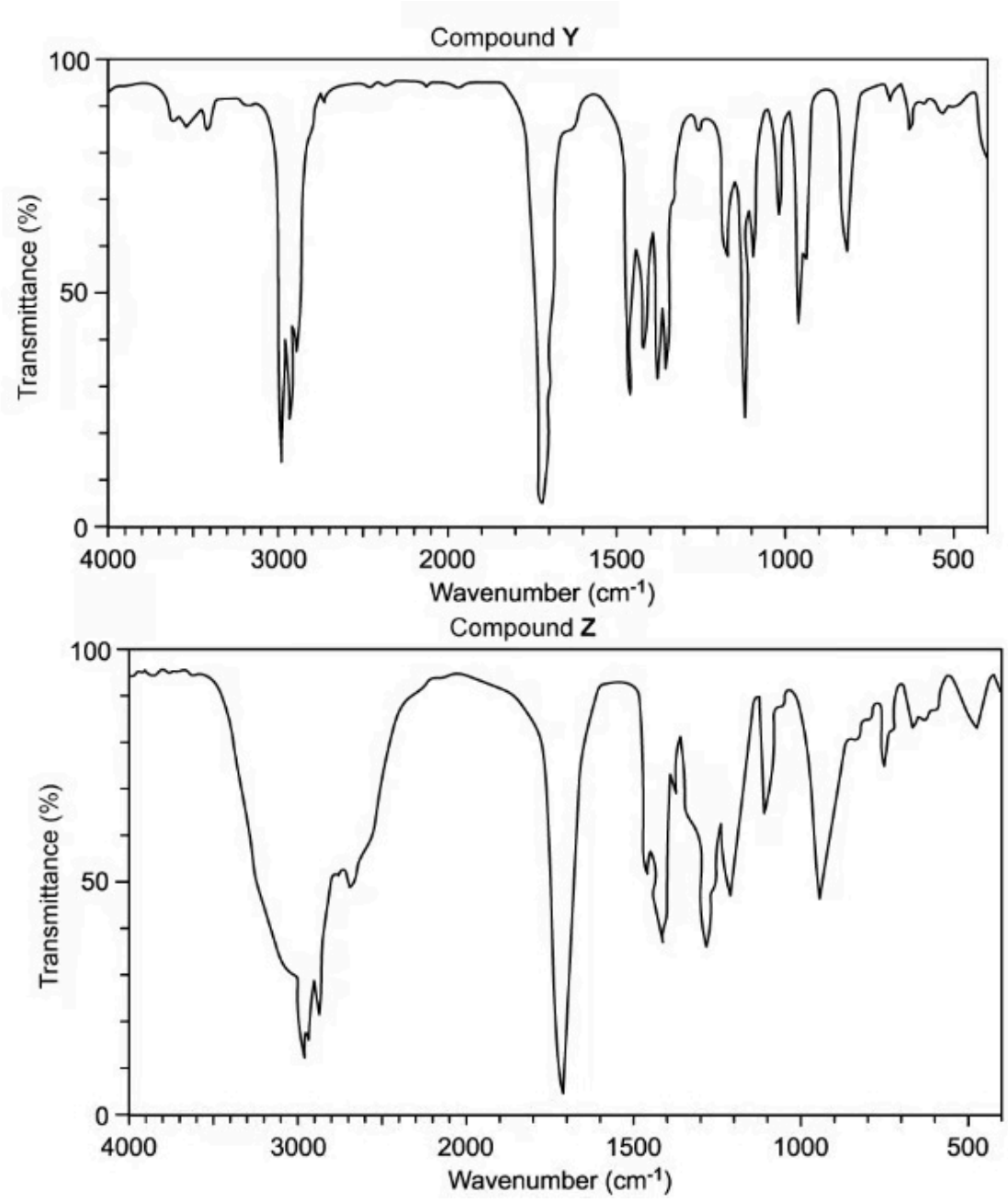
.....

(2 marks)

8 (a) This question is about some isomeric alcohols with the molecular formula $C_5H_{12}O$.

Some alcohols were heated with potassium dichromate(VI) and sulfuric acid. The organic compounds were separated from the reaction mixtures and purified.

The infrared spectra of two of these organic compounds are shown below.



Using section 20 of the data booklet, deduce the type of compound responsible for each spectrum.

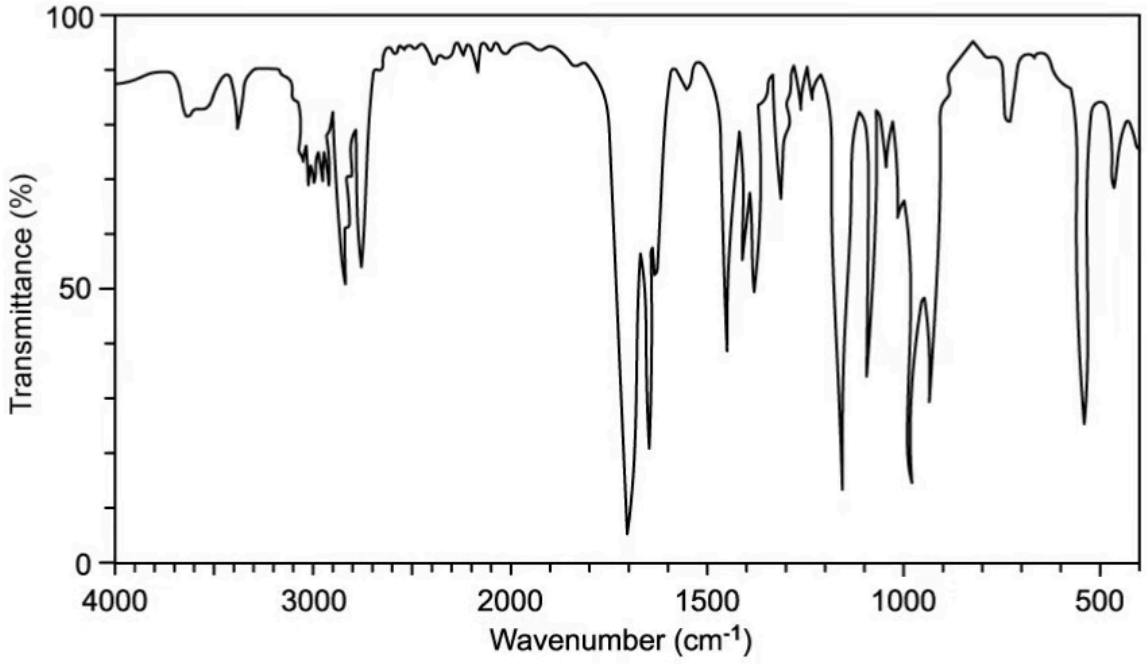
Include in your answer references to wavenumbers and their corresponding bonds.

(2 marks)

(b) State what is meant by the term '*fingerprint region*' on infrared spectra and explain how this can be used to identify primary, secondary and tertiary halogenoalkanes.

(2 marks)

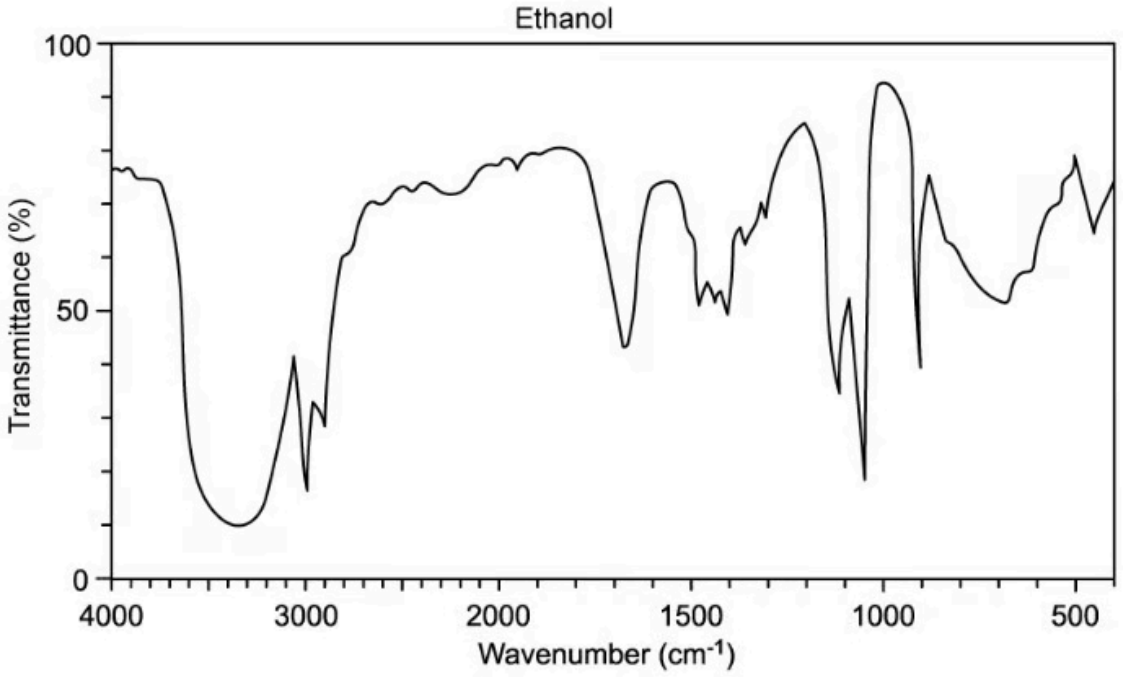
(c) The infrared spectrum a student obtained of an organic molecule which contains carbon, hydrogen and oxygen atoms is shown below.

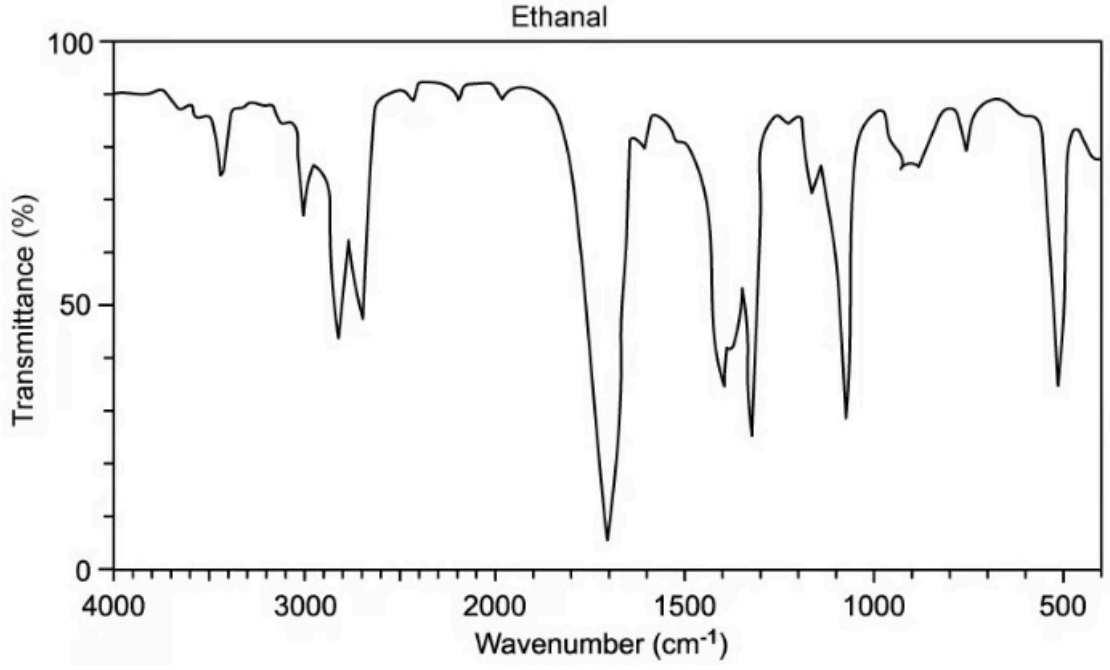


Use section 20 of the data booklet and information from the infrared spectrum to explain how the student deduced that the spectrum shows the presence of a carbonyl group.

(1 mark)

(d) In an experiment to prepare a sample of ethanal, CH_3CHO, ethanol, C_2H_5OH, is reacted with acidified potassium dichromate (VI) and the reaction mixture is distilled. The infrared spectra for ethanol and ethanal are shown below.





i) State the bonds that give rise to the absorption in the ethanol spectrum at 3400 cm^{-1} and the absorption in the ethanal spectrum at 1720 cm^{-1}.

[1]

ii) Explain why the absorption at 3400 cm^{-1} in the ethanol spectrum does not appear in the spectrum for ethanal.

[1]

.....

.....

(2 marks)

9 (a) Define the term *stereoisomers*.

.....

(1 mark)

(b) State the conditions needed for a compound to show cis-trans isomerism.

.....

.....

(2 marks)

10 (a) The chemical and physical properties of optical isomers are identical. However, there are some other differences that can be used to distinguish isomers from each other.
In terms of properties, state one difference between optical isomers.

.....

(1 mark)

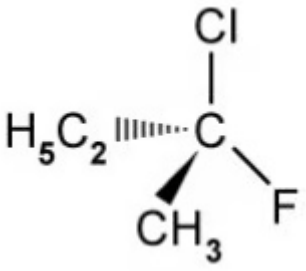
(b) Describe how you can detect optical activity in a sample.

.....

.....

(2 marks)

(c) The structure of one optical isomer of a chlorofluorocarbon is shown below.



Draw the structure of the other enantiomer.

.....

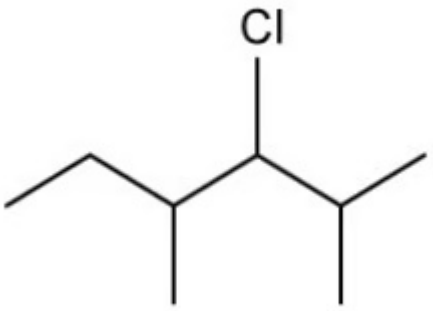
(1 mark)

11 (a) State what is meant by the term a chiral carbon.

.....

(1 mark)

(b) The skeletal structure of an organic compound is shown below.



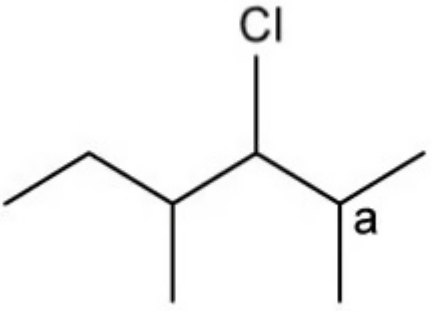
Identify the chiral carbons.

.....

.....

(2 marks)

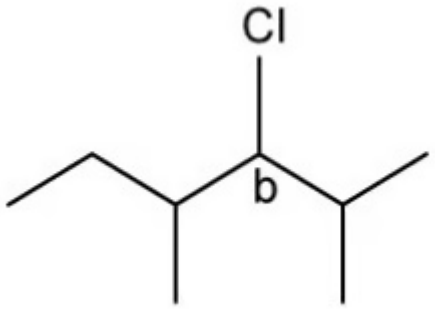
(c) Explain why carbon **a** cannot be a chiral carbon.



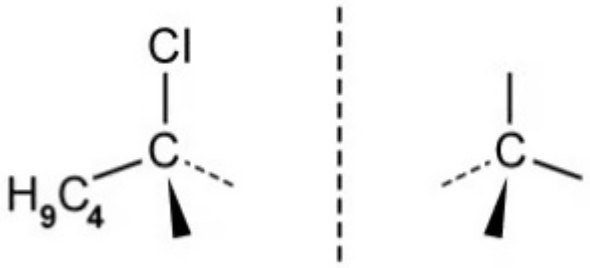
.....

(1 mark)

(d) The figure below identifies a different carbon, **b**, in the organic compounds structure.



Complete the figure below to show the 3D representations of the optical isomers formed at carbon **b**.



(2 marks)

12 (a) Define the term racemic mixture.

.....

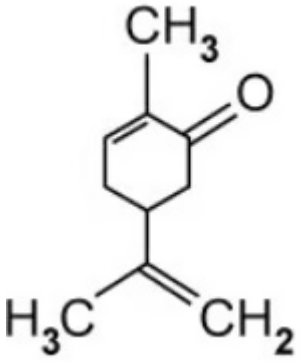
(1 mark)

(b) Describe the composition of enantiomers when a reaction mixture is optically active.

.....

(1 mark)

(c) Carvone is an optically active molecule which is found widely in plants, mostly in caraway seeds and spearmint leaves. The structure is shown below.



Mark on the diagram using an asterisk (*) the chiral carbon which causes this structure to exhibit optical isomerism.

.....

(1 mark)

(d) Draw the structure of the other optical isomer formed by carvone shown in part (c).

.....

(1 mark)

13 (a) Three important analytical techniques in the chemist's toolkit are Mass Spectrometry, MS, Infrared Spectroscopy, IR, and Nuclear Magnetic Resonance Spectroscopy, NMR.

For each technique identify the characteristic chemical information provided.

(3 marks)

(b) For each of the following, identify their significance in an ^{1}H NMR spectrum: number of peaks, area under each peak, chemical shift and splitting patterns.

(4 marks)

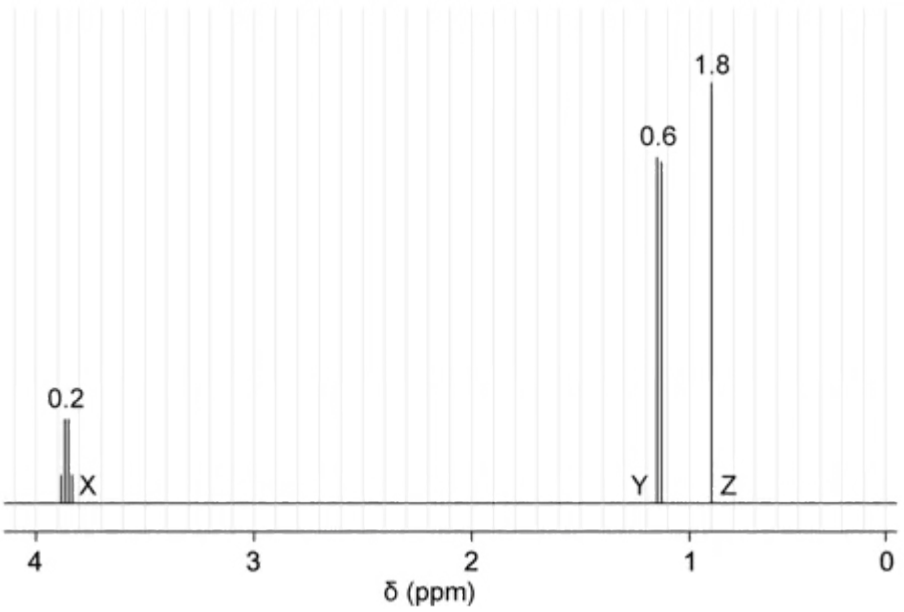
(c) ^{1}H NMR spectroscopy uses tetramethylsilane. State its formula and purpose in ^{1}H NMR spectroscopy.

(2 marks)

(d) State three advantages of using TMS in an ^{1}H NMR spectrum.

(3 marks)

14 (a) Part of the ^{1}H NMR spectrum of an organic compound is shown below:



Determine the number of unique hydrogen environments

.....

(1 mark)

(b) Deduce the whole number ratio of the hydrogen environments in the spectrum.

.....

(1 mark)

(c) State the splitting patterns present in the spectrum and suggest what information could be obtained from the patterns.

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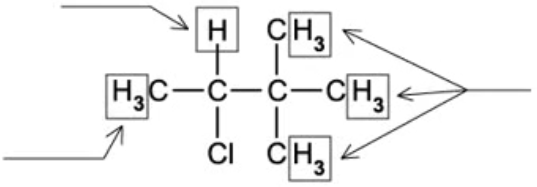
(4 marks)

(d) Assign peaks X, Y and Z to the correct location shown in the compound:



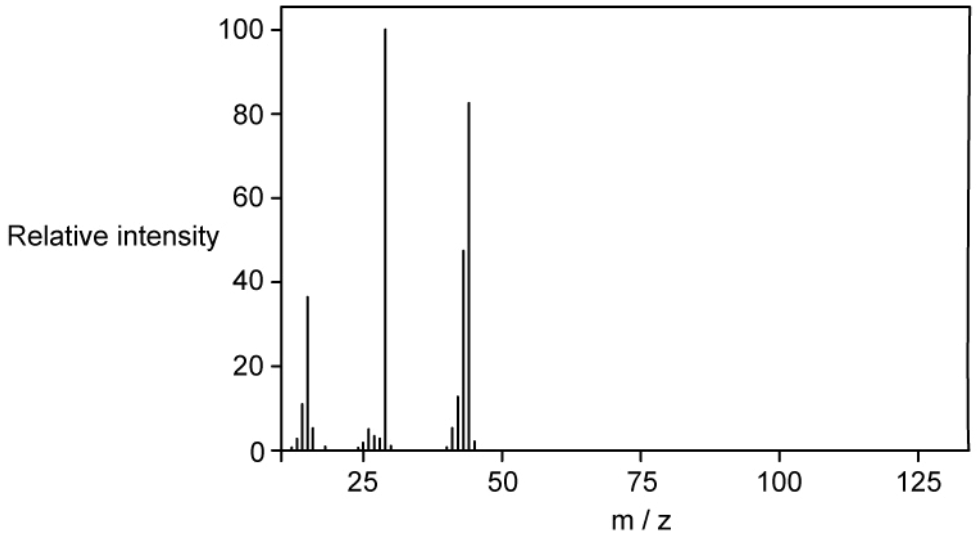
.....

.....

(2 marks)

15 (a) An organic molecule with molecular formula C_2H_4O is analysed using MS, IR and ^1H NMR. Use sectionS 20, 21 & 22 of the Data booklet to help you answer this question.

The MS is shown below:



Determine the relative molecular mass from the spectrum and account for the peak at *m/z* 29.

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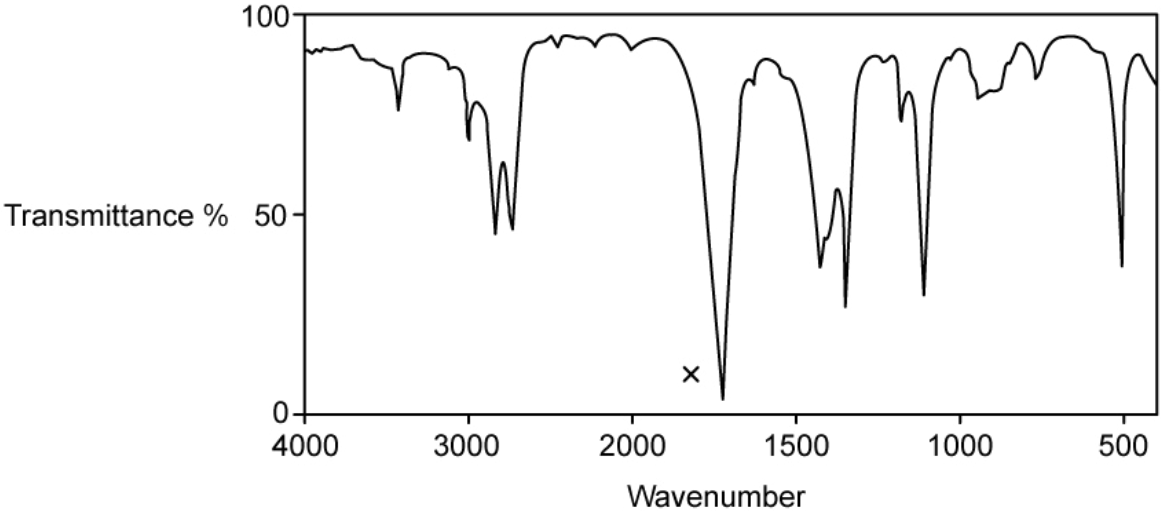
.....

(2 marks)

(b) The IR spectrum of the same compound is shown below.

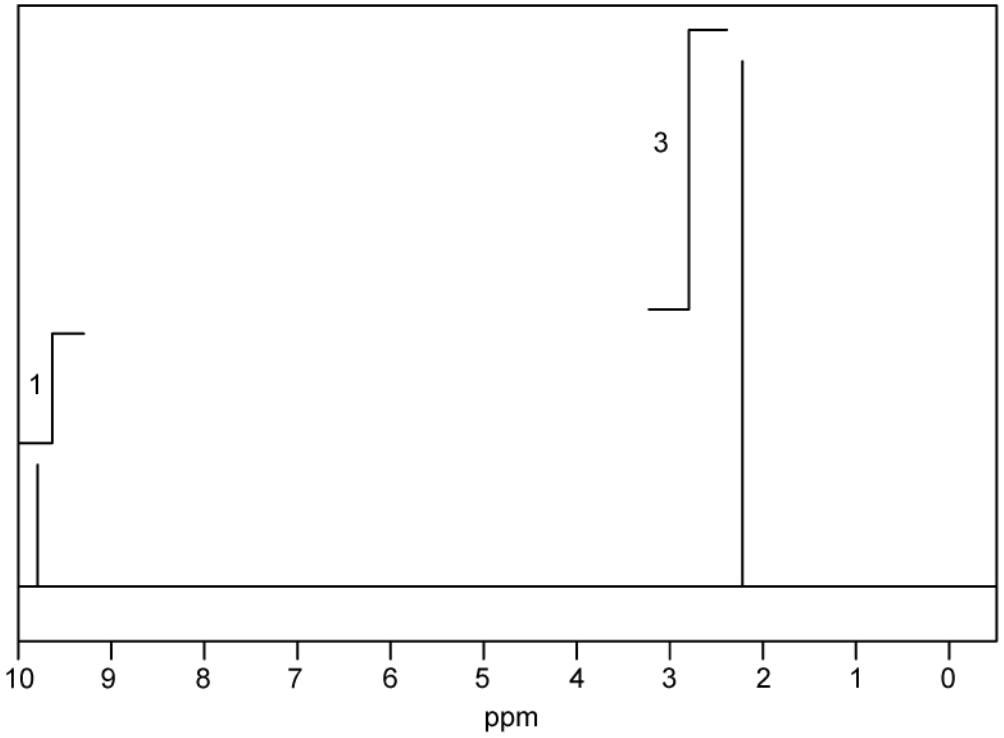


Identify the functional group responsible for the peak at X

.....

(1 mark)

(c) The ^{1}NMR spectrum of C_2H_4O is shown below:



Account for the peaks at 2.2 ppm and 9.8 ppm and their relative areas.

.....

.....

.....

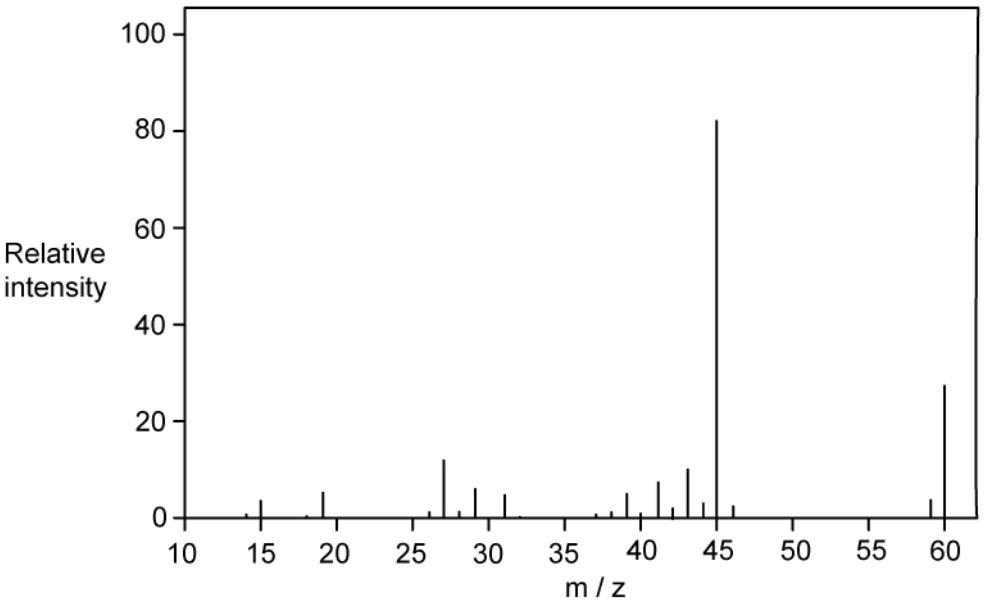
(3 marks)

(d) Deduce the displayed structure of this compound from the spectroscopic information.

.....

(1 mark)

16 (a) The MS of compound P is shown below. Compound P contains carbon, hydrogen and oxygen only. Use sections 20, 21 & 22 of the Data booklet to help you answer this question.



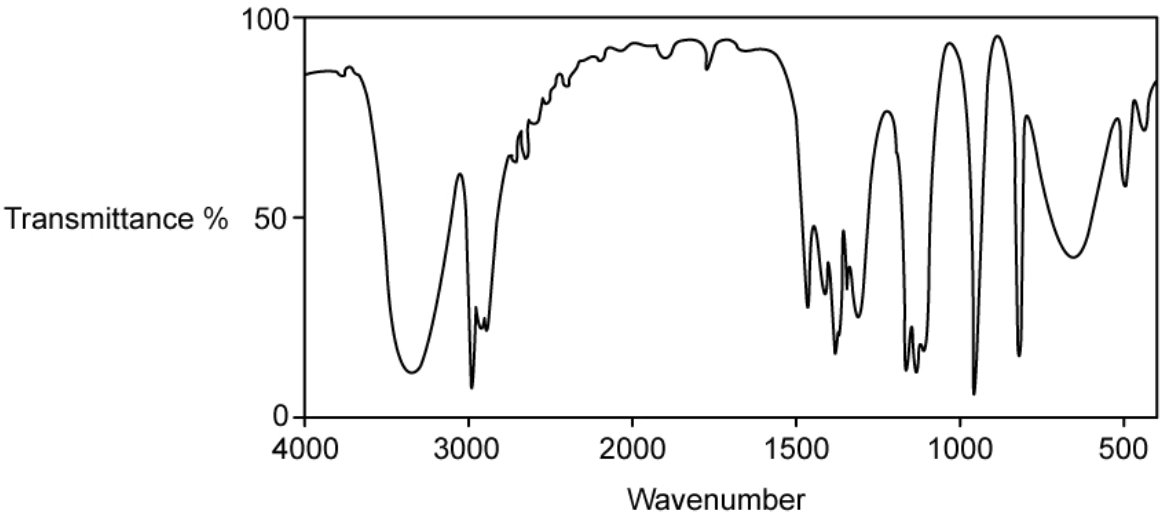
Determine the relative formula mass of P and account for the peak at *m/z* 45.

.....

.....

(2 marks)

(b) The IR spectrum of P is shown below.



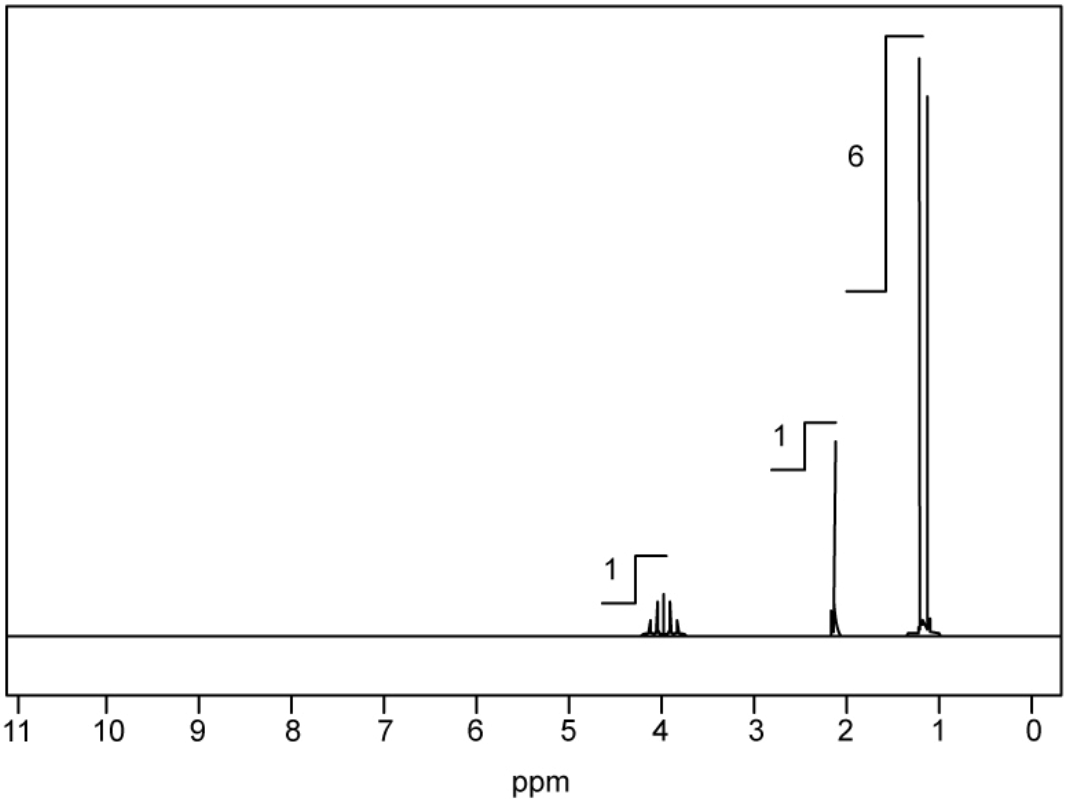
Use the spectrum and your answer to part a) to deduce a functional group that could be present in P.

.....

.....

(2 marks)

(c) The 1H NMR spectrum of P is shown below.



Deduce what information can be found from the spectrum.

(2 marks)

(d) A student suggests that P is propan-1-ol. Evaluate all the evidence from the spectra and determine whether the student is correct.

(4 marks)

Medium Questions

1 (a) Organic compounds are classified into families called a *homologous series*.

State three features of members belonging to the same *homologous series*.

.....

.....

.....

(3 marks)

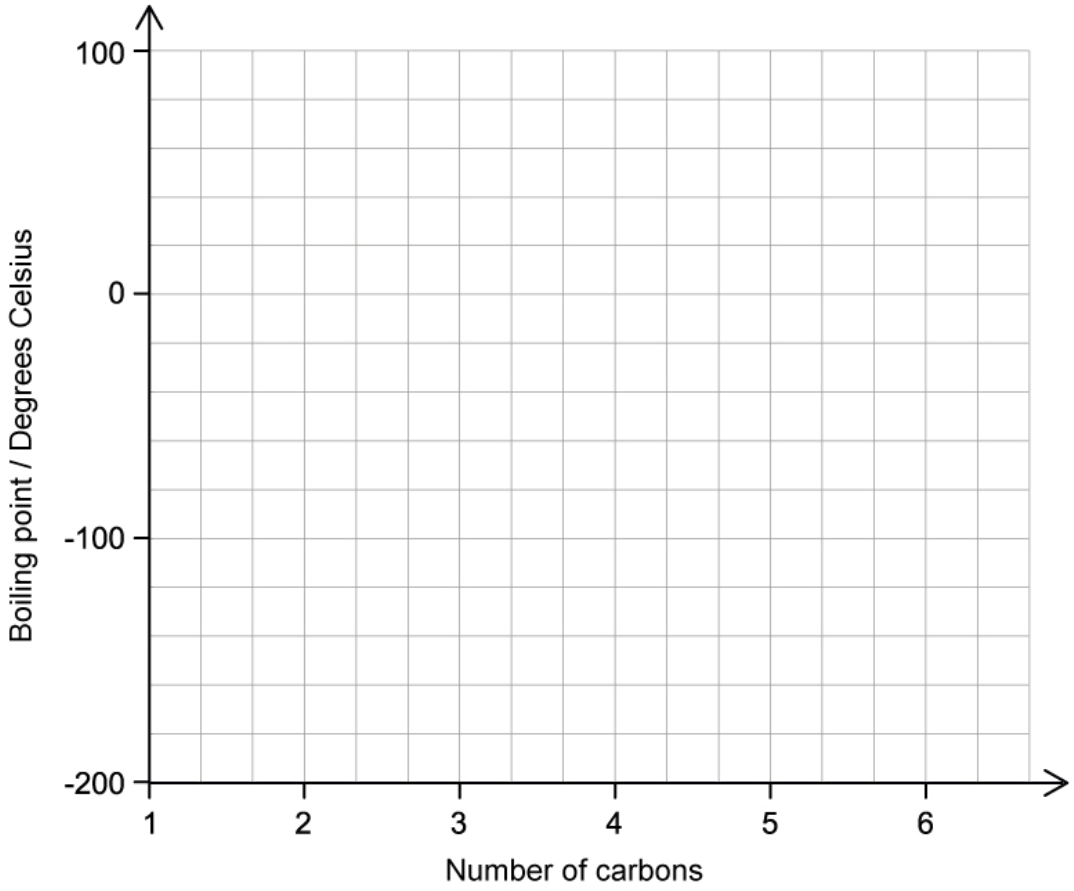
(b) **Table 1** shows the boiling points of the first five members of the alkane family.

Table 1

Alkane	Boiling point/ ^{o}C
methane	-162
ethane	-89
propane	-42
butane	-1
pentane	36

On the axes below in **Figure 1,** draw a graph of boiling point against the number of carbon atoms in the alkanes. Estimate the boiling point of the next member of the homologous series, hexane, C_6H_{14}, and show on your graph how you arrived at your estimated boiling point.

Figure 1



Estimated boiling point of hexane : _____ ^{o}C

(4 marks)

(c) State the general formula for an alkyne and give the molecular formula and name of the fifth member of the alkyne family.

(2 marks)

(d) The boiling point of ethyne, C_2H_2, is -84 ^oC.

State with, with a reason, whether the boiling point of ethyne would be expected to be higher or lower than the boiling point of ethane, C_2H_6.

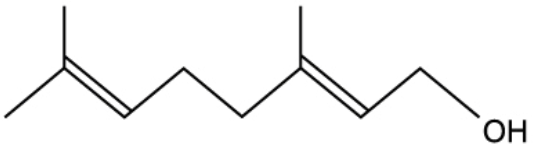
.....

.....

(2 marks)

2 (a) Geraniol is a colourless component of rose oil whose structure is shown in **Figure 1**.

Figure 1



i) State the names of the two functional groups found in geraniol.

[1]

ii) Deduce the molecular formula of geraniol.

[1]

iii) Draw the displayed formula of geraniol.

[1]

.....

.....

.....

(3 marks)

(b) Butan-2-ol is an organic compound used industrially to make butanone.

i) Draw the displayed structure of butan-2-ol.

[1]

ii) Draw the displayed structures of a positional isomer and a functional group isomer of butan-2-ol.

[2]

.....

.....

.....

(3 marks)

(c) Draw and name all the branched-chain isomers of butan-2-ol.

.....

.....

(2 marks)

(d) State, with a reason, the class of alcohols which butan-2-ol belongs to.

.....

(1 mark)

3 (a) The formulae of four organic compounds are given in **Table 1**. Write the names of the compounds in the second column.

Table 1

compound	name
$CH_3CH_2CH_2CH(OH)CH_3$	
$CH_3CH_2COCH_3$	
$CH_3CH_2CH_2OH$	
$CH_3CH_2CH_2CHO$	

.....

.....

(2 marks)

(b) Which of the compounds in part (a) are structural isomers of each other and what type of isomerism do they show?

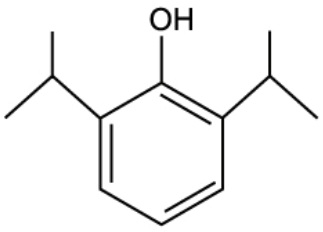
.....

.....

(2 marks)

(c) Propofol is a drug used to reduce consciousness during medical procedures. The skeletal structure of propofol is given in Figure 1.

Figure 1



i) Determine the empirical formula of propofol.

[1]

ii) Identify the number of positional isomers of propofol (not including propofol).

[1]

iii) State the names of two functional groups found in propofol.

[1]

.....

.....

.....

(3 marks)

(d) Valeric acid, $C_5H_{10}O_2$, is a straight chain carboxylic acid found in the plant *Valeriana officinalis*.

i) State the general formula for a carboxylic acid.

[1]

ii) Give the systematic name for valeric acid.

[1]

iii) Draw a condensed structural formula for valeric acid.

[1]

.....

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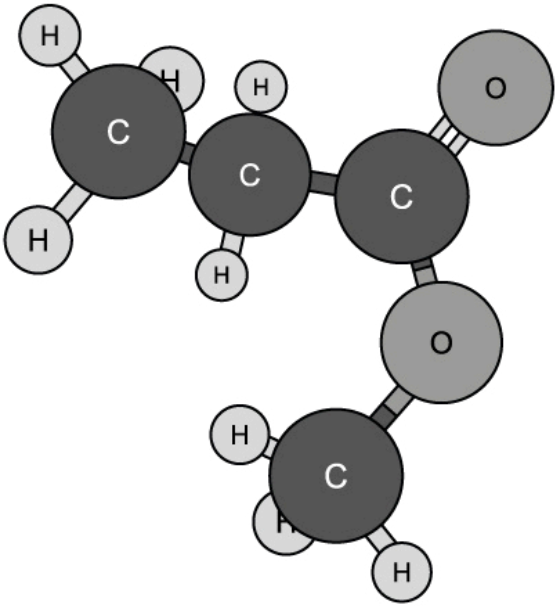
(3 marks)

4 (a) Draw and name all the possible isomers of C_6H_{14}.

(5 marks)

(b) **Figure 1** below shows a three-dimensional structure of a molecule.

Figure 1



i) Using IUPAC rules state the name of this molecule.

[1]

ii) Draw and name a functional group isomer of this molecule.

[1]

(2 marks)

5 (a) Often, scientists will use analytical techniques such as infrared spectroscopy to determine if a desired reaction has taken place. Outline how infrared spectroscopy generates useful information about an organic molecule.

.....

.....

(2 marks)

(b) A chemist uses infrared spectroscopy to distinguish between two organic molecules, a primary alcohol, and an aldehyde.

Use section 20 of the data booklet to state, with a reason, how the chemist could use the IR spectra produced to distinguish between these two molecules.

.....

.....

(2 marks)

(c) The chemist fully oxidized the alcohol from part (b) and used IR spectroscopy to prove that the reaction had taken place.

State how the chemist could use infrared spectroscopy to determine that the reaction had taken place. Use section 20 of the data booklet to support your answer.

.....

(1 mark)

6 (a) Toluene is a common organic chemical with many industrial and commercial applications. Toluene is also known as methylbenzene.

Draw the molecular structure of toluene.

.....

(1 mark)

(b) State the number of ^{1}H NMR signals that would be seen on the NMR spectrum of toluene and state the ratio of the area under the peaks in which they would appear.

.....

.....

(2 marks)

(c) Another derivative of benzene has the molecular formula C_8H_{10}.

Draw the structures of the four possible isomers of this derivative.

.....

.....

(2 marks)

(d) Infrared spectroscopy is a common analytical tool used in chemistry, to identify or distinguish between different organic compounds. These could be compounds such as toluene which contain a benzene ring, or any other organic compound. IR is often used alongside other analytical tools, such as mass spectrometry, to help identify the unknown.

An organic molecule, **J**, has the following composition by mass.

62.1% carbon

10.3% hydrogen

27.6% oxygen

In the mass spectrum of **J**, the molecular ion peak has a value of *m/z* = 116.

i) Use this information to determine the molecular formula of **J**.

[5]

ii) State how an IR spectrum could be used to prove that compound **J** is a carboxylic acid.

[2]

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(7 marks)

7 (a) The analytical instruments used for identification of organic compounds are constantly being improved.

Mass spectroscopy is one such analytical tool which provides key information used to identify an unknown compound.

An unknown compound has the empirical formula C_2H_4O, and its mass spectrum has a molecular ion peak at *m/z* 84.

Deduce the molecular formula of the compound.

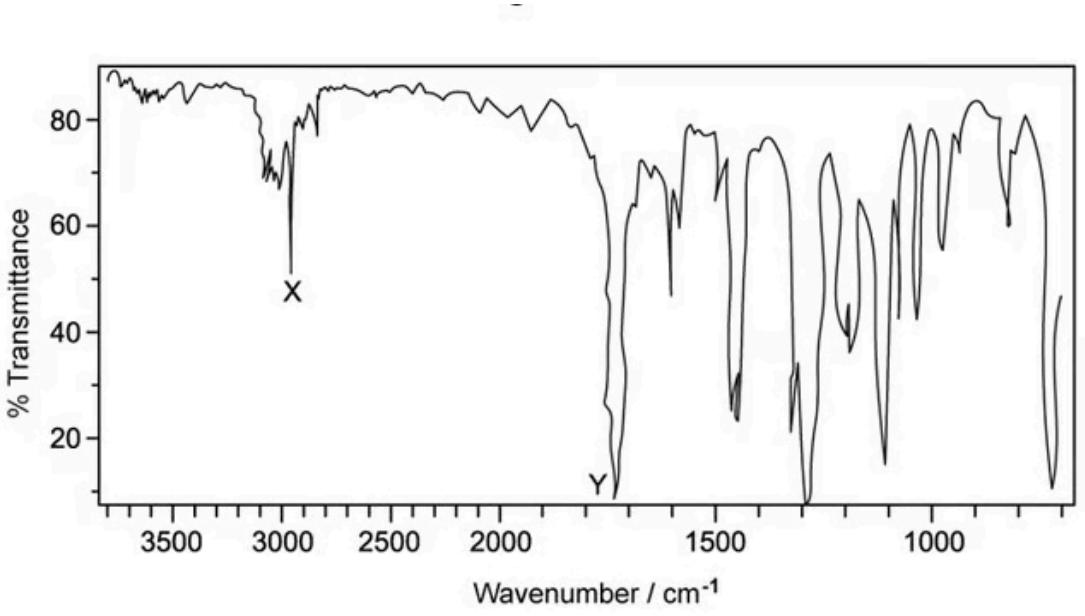
.....

(1 mark)

(b) **Figure 1** below shows the IR spectrum of the unknown compound in part (a).

Identify the bonds which are causing peak X and peak Y on the spectrum, using section 20 of the data booklet.

Figure 1



.....

(1 mark)

(c) The unknown compound is a carboxylic acid. Deduce the two possible carboxylic acid structural isomers.

(2 marks)

(d) For each of the isomers drawn in part (c), state the number of signals which would be seen in an ^{1}H NMR spectrum and the ratio of the areas under the peaks.

(4 marks)

8 (a) A group of students are asked to distinguish between four samples of different organic compounds.

The four samples are as follows:

- A primary alcohol
- A tertiary alcohol
- An aldehyde
- A carboxylic acid

Describe how the group of students could distinguish between the two different alcohols.

.....

.....

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(3 marks)

(b) One of the students wanted to distinguish between three compounds using mass spectrometry alone. The three compounds are shown below in **Figure 1** and the mass spectrum for one of the compounds is shown in **Figure 2**.

Figure 1

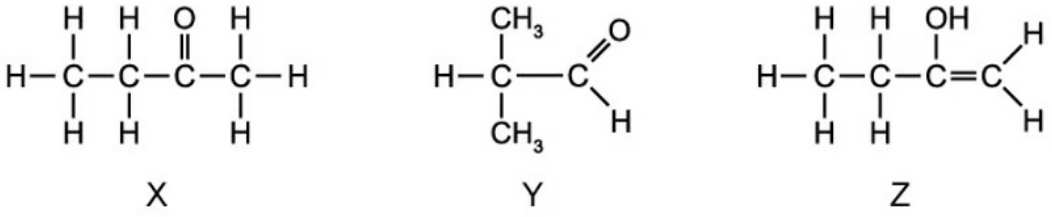
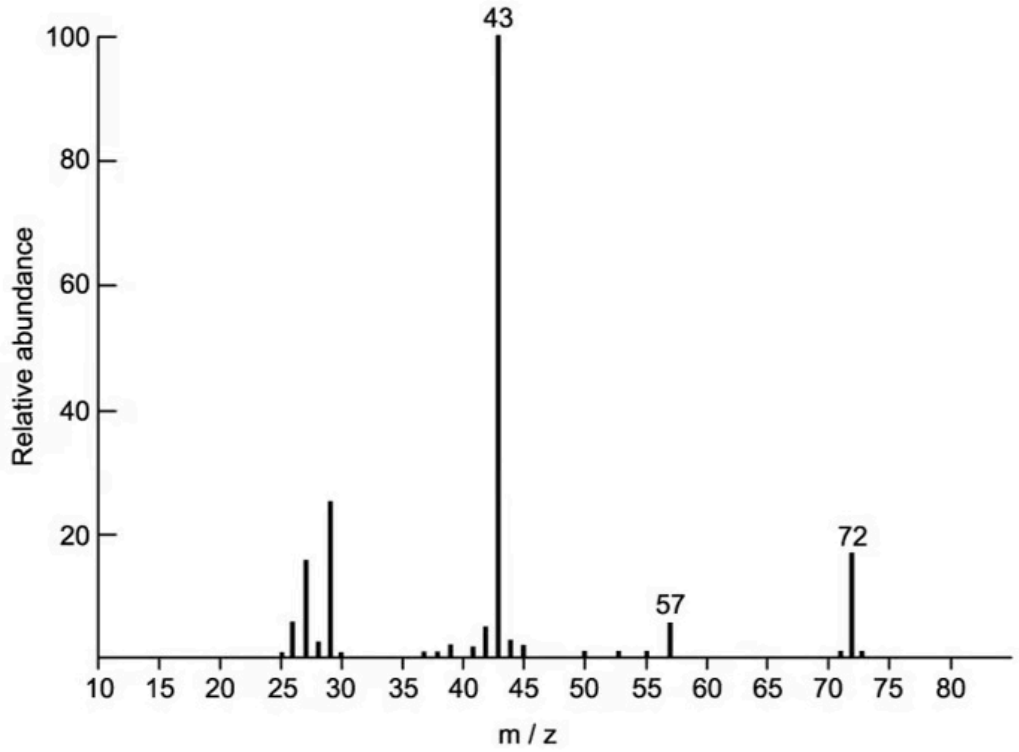


Figure 2



Explain, using **Figure 2**, why determining the exact mass using mass spectrometry alone would not help in distinguishing between the samples of X, Y and Z shown in **Figure 1**.

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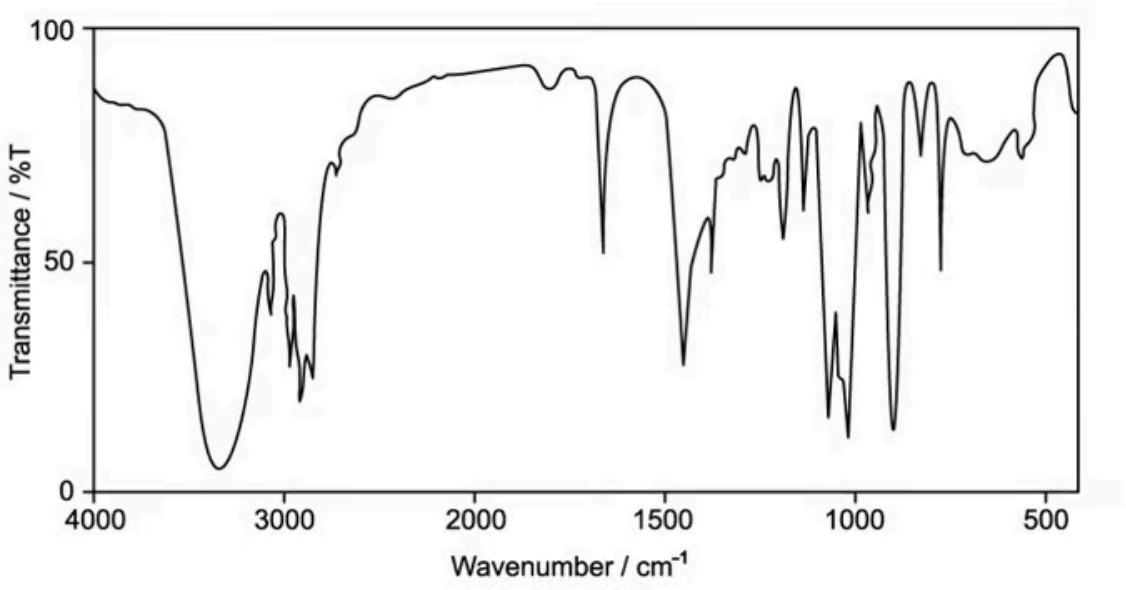
(3 marks)

(c) The three compounds from **Figure 1** in part (b) were analysed using IR spectroscopy. The spectrum of one of the compounds is shown below:

Figure 3



Identify which of the three compounds X, Y or Z this spectrum belongs to. Justify your choice.

.....

.....

(2 marks)

(d) State, with a reason, how infrared spectroscopy would be used to distinguish between the compounds X and Y from **Figure 1** in part (b).

.....

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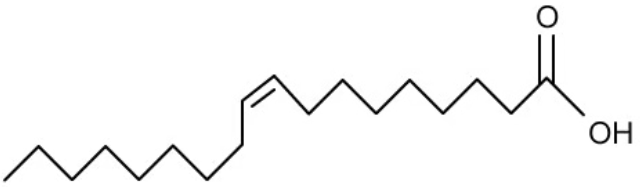
(2 marks)

9 (a) A molecule of oleic acid is shown.



Oleic acid

Oleic acid is a fatty acid which occurs naturally in different animals and plants.

Oleic acid exhibits *stereoisomerism*. Explain the meaning of this term and identify why oleic acid has stereoisomers.

.....

.....

(2 marks)

(b) Crotonic acid is another fatty acid which has a similar structure to oleic acid. The molecular formula of crotonic acid is $C_4H_6O_2$.

i) State the empirical formula of crotonic acid.

[1]

ii) Crotonic acid has a carboxylic acid functional group. Draw the displayed formula of the positional and branch-chain isomers of crotonic acid.

[2]

iii) Identify which of the isomers you have drawn shows *E / Z* isomerism.

[1]

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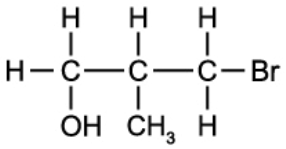
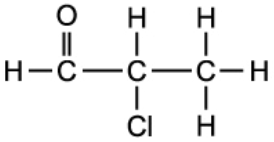
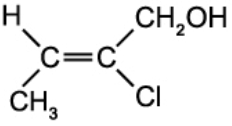
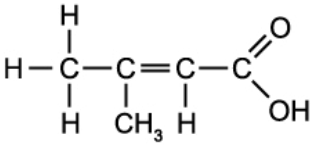
(4 marks)

10 (a) A chemist is analysing a collection of organic compounds. The structural formulae of these compounds are shown.

Compound	Structural Formula	IUPAC Name
1		
2		
3		
4		

Give the IUPAC name for the compounds to complete the table.

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(4 marks)

(b) This question refers to the compounds in the table in part (a)

i) Identify the compounds which have chain isomers and draw their isomers.

[3]

ii) State the empirical formula of compound **3.**

[1]

iii) Does compound 4 exhibit stereoisomerism? Explain your answer.

[1]

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(5 marks)

11 (a) 2-methylbut-2-ene can be converted into 2-methylbutan-2-ol, a liquid that smells of camphor.

State the reagents needed to convert 2-methylbut-2-ene into 2-methylbutan-2-ol.

.....

.....

(2 marks)

(b) The reaction in part (a) produces a small amount of an isomeric co-product, **X**, which is optically active.

i) State the meaning of *optical activity.*

[1]

ii) Draw the structure of **X**.

[1]

.....

.....

(2 marks)

(c) What does optical activity indicate about the structure of **X**?

.....

(1 mark)

(d) Explain how optical activity can be detected using a polarimeter

.....

.....

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(3 marks)

12 (a) Dichloroethene exists as two stereoisomers. Draw the structures of these isomers.

(1 mark)

(b) Explain why dichloroethene has stereoisomers.

(1 mark)

(c) Draw the structures of the stereoisomers of 1-bromo-1-chloroethane, C_2H_4BrCl, and show the relationship between them.

(1 mark)

(d) Explain the differences in chemical and physical properties between the isomers of C_2H_4BrCl

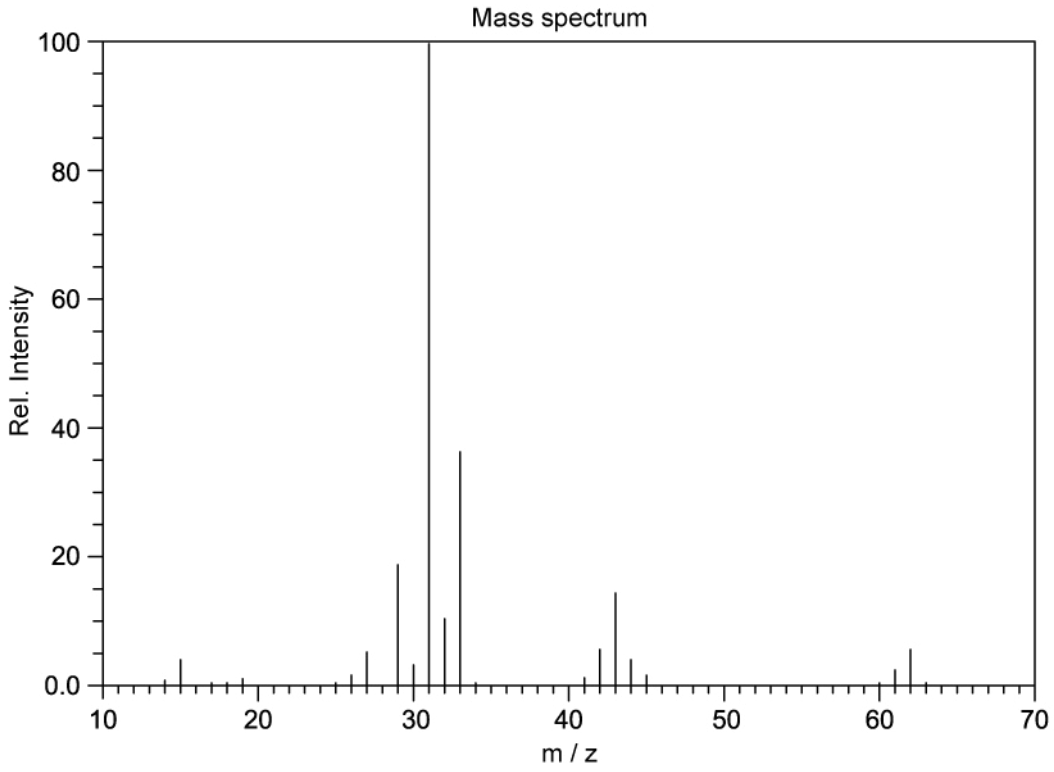
(3 marks)

13 (a) Ethane-1,2-diol, $C_2H_6O_2$, can be distinguished from ethanedioic acid,$C_2H_2O_4$, by a number of analytic techniques including MS, IR and NMR

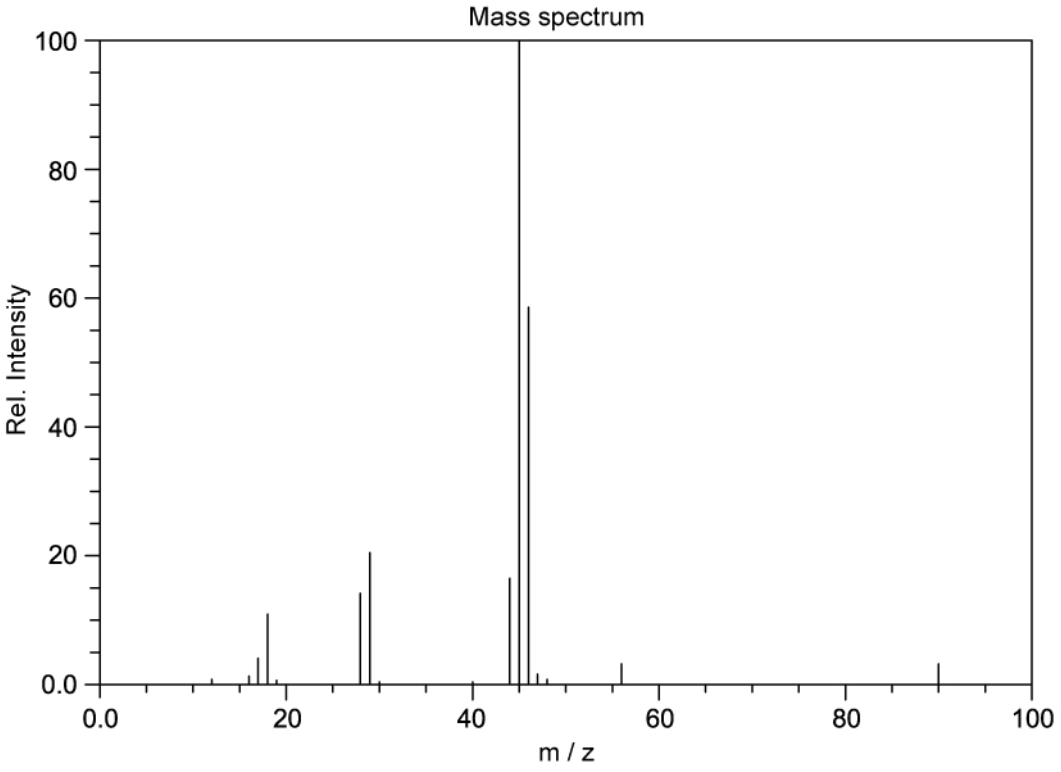
The MS of these molecules is shown below.

Which spectrum belongs to each molecule? Justify your answer.

Spectrum **A**



Spectrum **B**



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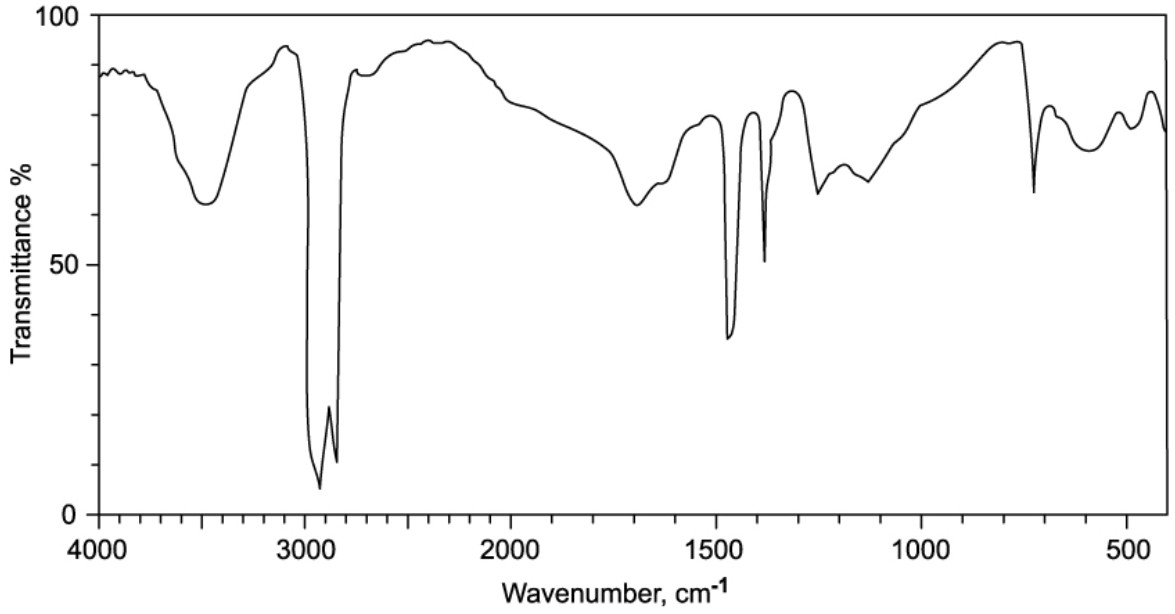
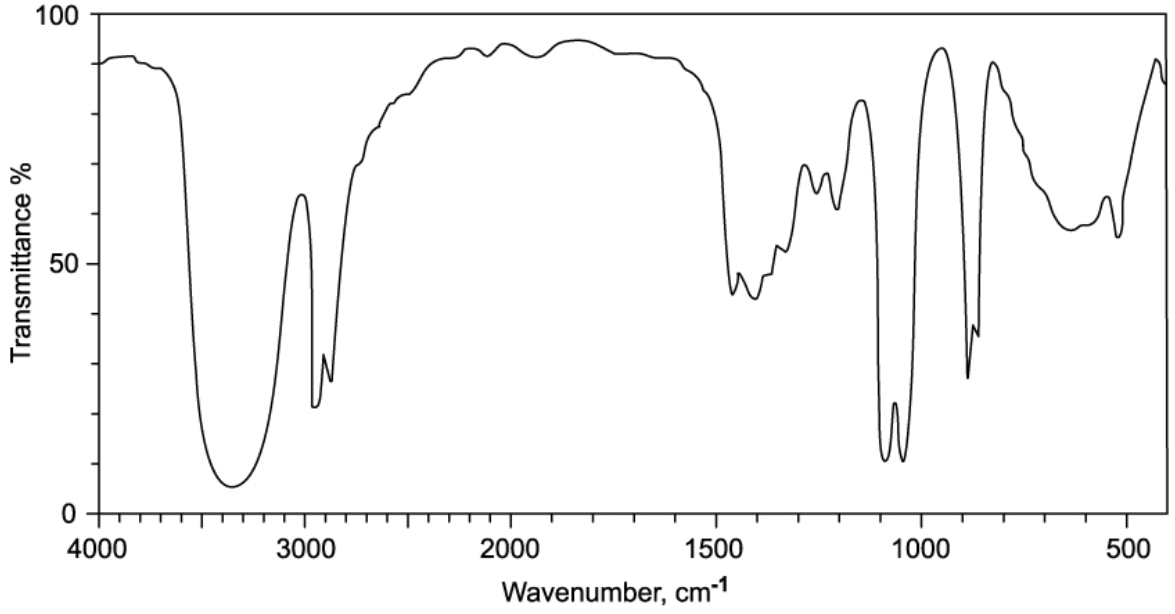
(2 marks)

(b) The IR spectra of ethane-1,2-diol, $C_2H_6O_2$, and ethanedioic acid dihydrate, $C_2H_2O_4.2H_2O$, are shown in spectrum **C** and **D**. Use Section 20 of the Data Booklet to answer this question.

Spectrum **C**



Spectrum **D**



Which spectrum belongs to each molecule? Justify your answer.

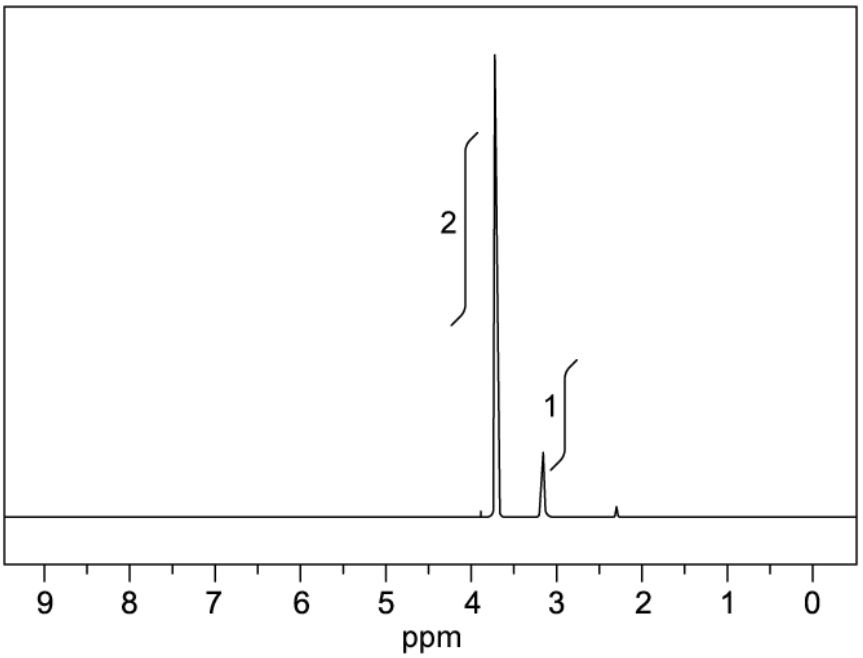
.....

.....

(2 marks)

(c) The ^{1}H NMR spectrum of ethane-1,2-diol is shown in spectrum **E**. Explain the significance of the spectrum.

Spectrum **E**



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(3 marks)

(d) Predict the number of ^{1}H NMR signals and splitting pattern for ethanedioic acid.

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.....

(2 marks)

14 (a) During the production of a ^{1}H NMR spectrum, tetramethylsilane (TMS) is mixed with the sample.

i) Draw the structural formula of TMS.

[1]

ii) State two reasons why this chemical is suitable to be used as the standard reference compound.

[2]

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(3 marks)

(b) Predict the number of peaks in the ^{1}H NMR spectrum of 1,3-dichlorobenzene.

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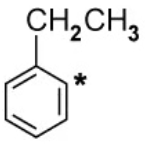
(1 mark)

(c) The structural formula of ethylbenzene is shown below in **Figure 1**.

Figure 1



i) Predict the number of peaks in the ^{1}H NMR spectrum of ethylbenzene.

[1]

ii) One of the hydrogen atoms in the structure of ethylbenzene shown above is labelled with an asterisk (*).
Use Section 21 from the Data Booklet to suggest a range of **δ** values for the peak due to this proton in the ^{1}H NMR spectrum of ethylbenzene.

[1]

.....

.....

(2 marks)

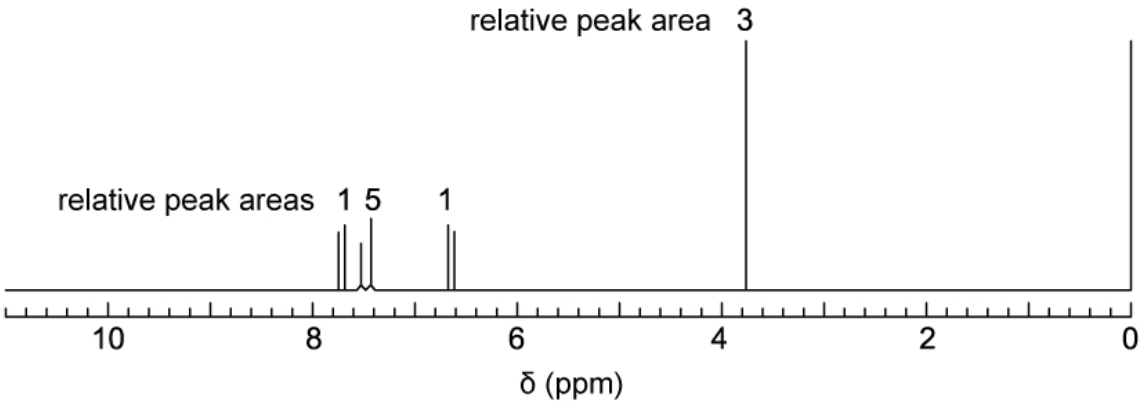
(d) Predict the splitting patterns of the signals due to the ethyl group found in the ^{1}H NMR spectrum of ethylbenzene.

.....

(1 mark)

15 (a) Methyl cinnamate, $C_{10}H_{10}O_2$, is a white crystalline solid used in the perfume industry. A sample of methyl cinnamate was analysed by ^1H NMR spectroscopy.

A simplified spectrum is shown below.

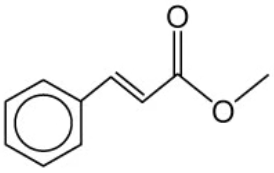


i) Name the compound responsible for the peak at a chemical shift of 0 ppm. State its purpose.

[2]

ii) Identify the proton environment that causes the peak at a chemical shift of 3.8 ppm by circling it on the structure of methyl cinnamate shown. Justify your answer.

[3]



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(5 marks)

(b) This question is about the use of ^{1}H NMR spectroscopy to distinguish between isomers of $C_6H_{12}O_2$.

Draw the two esters with formula $C_6H_{12}O_2$ that each have only two peaks, both singlets, in their ^{1}H NMR spectra. The relative peak areas are 3:1 for both esters.

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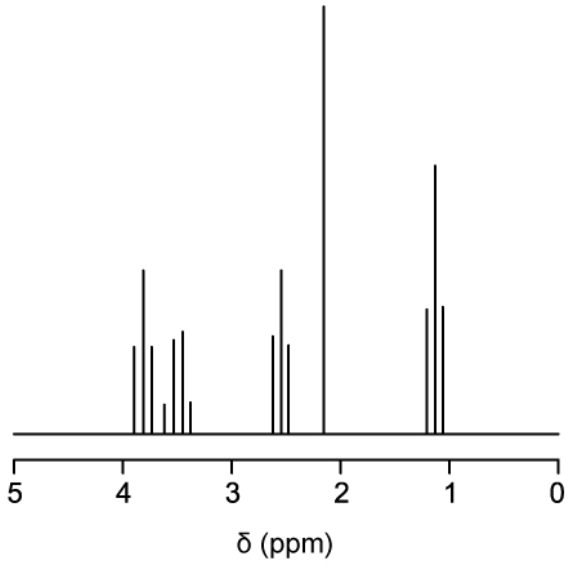
(2 marks)

(c) The high resolution ^{1}H NMR spectrum of another isomer of $C_6H_{12}O_2$ is shown below.



The integration values for the peaks in the ^{1}H NMR spectrum of this isomer, are given below.

Chemical shift, δ/ppm	3.8	3.5	2.6	2.2	1.2
Integration value	0.6	0.6	0.6	0.9	0.9
Splitting pattern	triplet	quartet	triplet	singlet	triplet

i) Deduce the simplest ratio of the relative numbers of protons in each environment in the isomer.

[1]

ii) Use Section 21 from the Data Booklet and the information given to deduce the part of the isomer that causes the signal at δ= 3.5 and the part of the structure at the isomer that causes the signal at δ=1.2. Explain why the splitting patterns of these peaks are produced.

[4]

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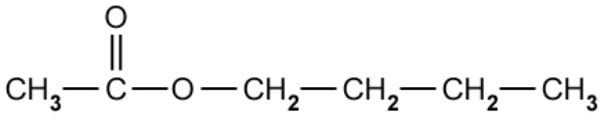
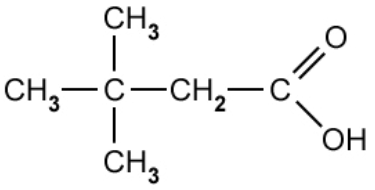
(5 marks)

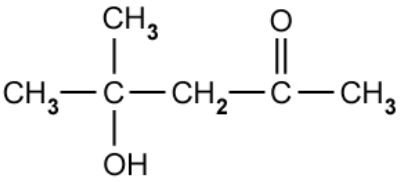
(d) Four isomers of $C_6H_{12}O_2$ are shown below.



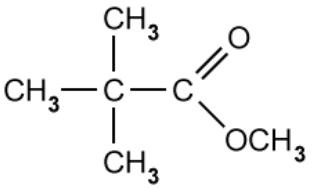
A



B

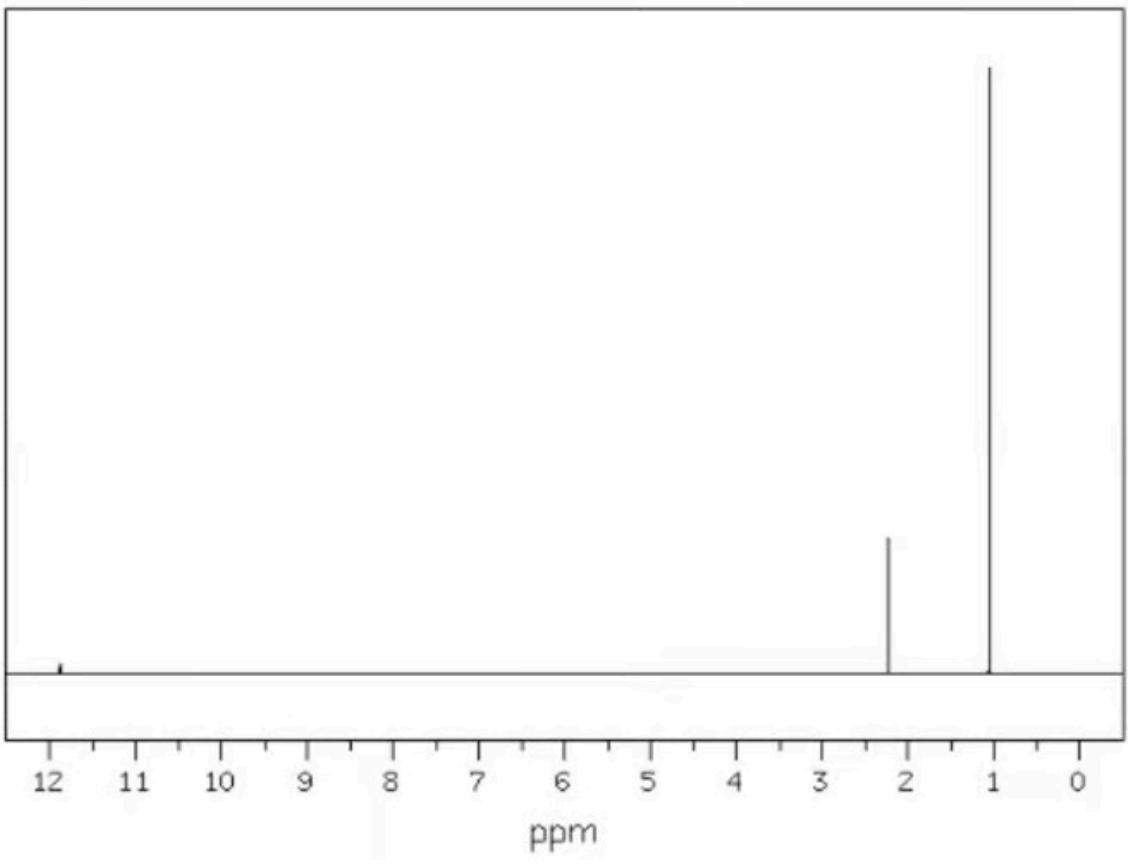


C



D

Which isomer matches the ^{1}H NMR spectrum below? Justify your choice.



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(2 marks)

16 (a) An isomer with the molecular formula $C_5H_{10}O_2$ was analysed by infrared spectroscopy, to confirm it was a carboxylic acid.

i) Give the wavenumbers of **two** characteristic absorptions for a carboxylic acid. Indicate the bond responsible for each absorption. Suggest why one of the absorptions is broad.

[3]

ii) The ^1H NMR spectrum of this isomer contains only two peaks with the integration ratio 9:1. Using this information from the spectra, deduce the structure of the isomer.

[1]

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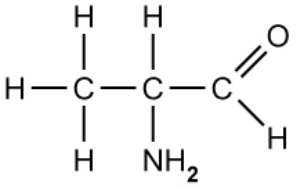
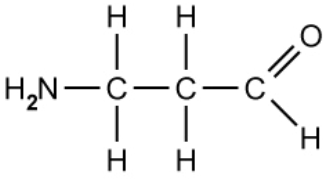
(4 marks)

(b) This question is about two aldehydes, 2-aminopropanal and 3-aminopropanal.



2-aminopropanal



3-aminopropanal

Explain how ^1H NMR spectra can be used to distinguish between these two aldehydes. You need to reference the splitting patterns and integration pattern in your answer.

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(5 marks)

(c) Suggest how the two isomers in part b) could be distinguished using mass spectroscopy.

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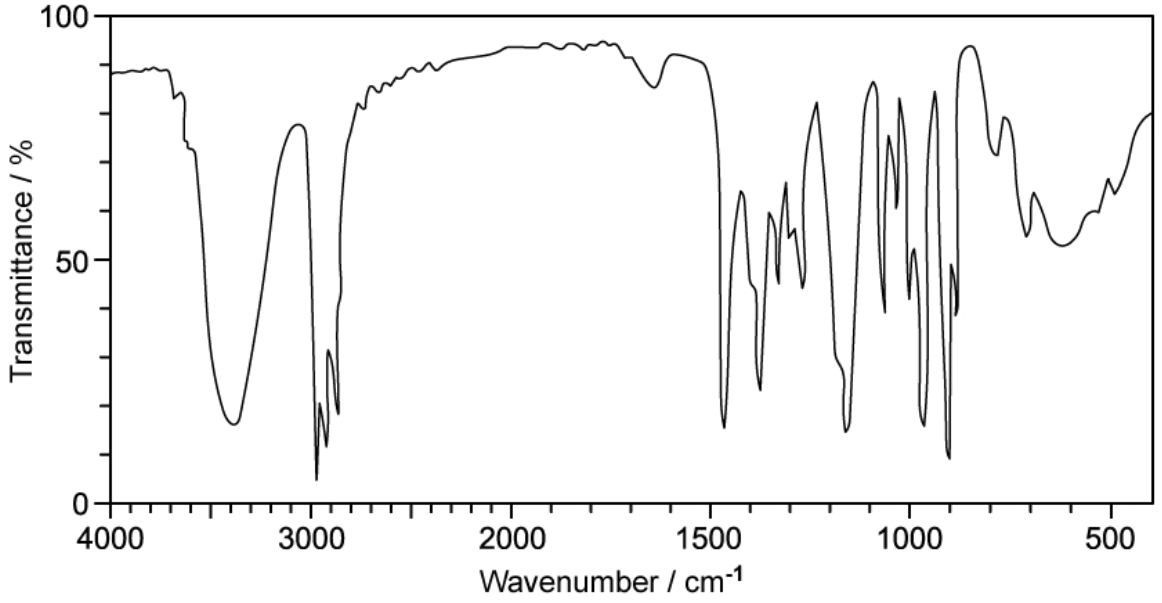
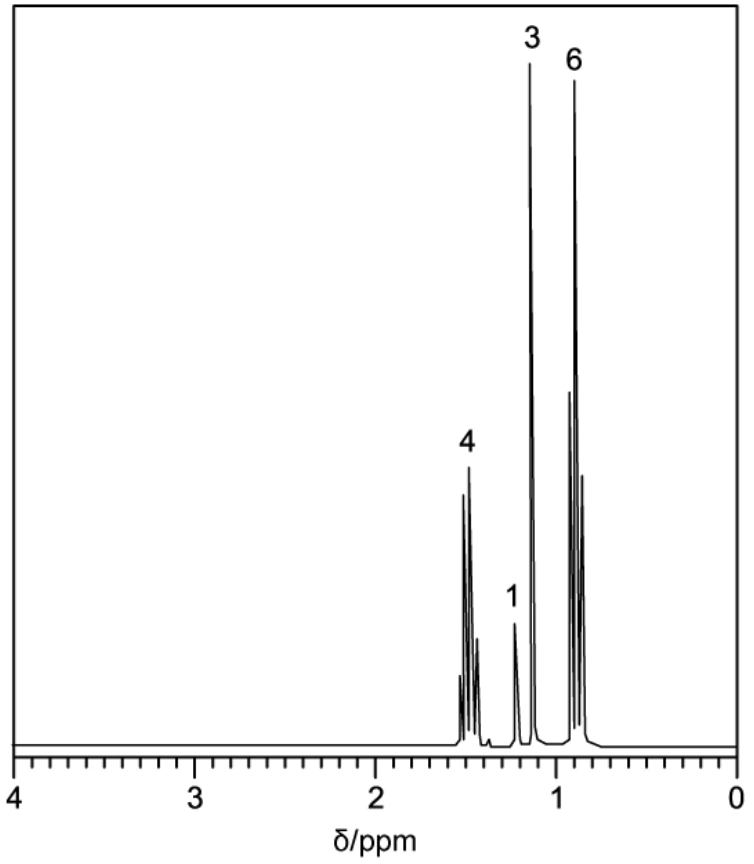
(1 mark)

(d) A compound **X** has a molecular formula of $C_6H_{14}O$. The infrared spectrum and ^1H NMR spectrum of compound **X** are shown below.





Using Sections 20 and 21 from the Data Booklet, deduce the structure of compound **X**. Justify each of your deductions.

(7 marks)

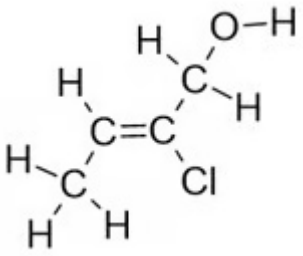
Hard Questions

1 (a) State the IUPAC names for the isomers of $C_5H_{12}O$ that are primary alcohols.

(4 marks)

(b) State the IUPAC name for the following primary alcohols.

i)



[1]

ii) $CH_2(Br)CH(CH_3)CH_2OH$

[1]

(2 marks)

(c) Draw the displayed formula for a straight chain isomer of $CH_2(Br)CH(CH_3)CH_2OH$.

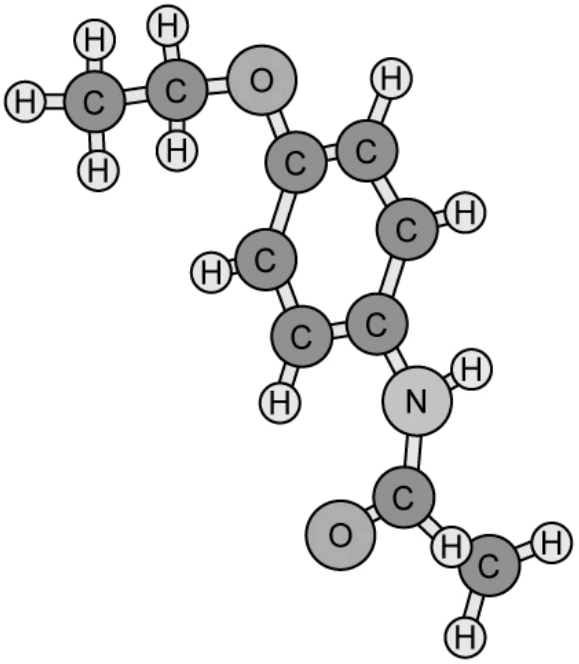
(1 mark)

(d) The empirical formula of the compound in part b) i).

.....

(1 mark)

2 (a) Phenacetin is a pain killer though the use of this was banned as it was found to cause harm to kidney function.



Deduce the molecular formula of phenacetin.

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(1 mark)

(b) Identify the names of the three functional groups present in phenacetin.

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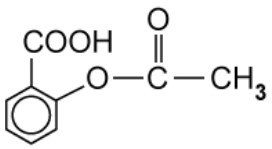
(3 marks)

(c) Aspirin is a common pain killer and has the following structure.

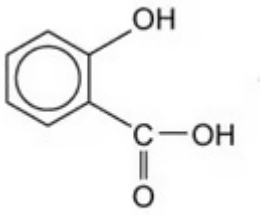


State the empirical formula of aspirin.

.....

(1 mark)

(d) Aspirin is formed from ethanoic anhydride and compound A. State the IUPAC name of compound **A**.



Compound A

.....

(1 mark)

Deduce the number of isomers of C_6H_{14}.

3 (a) .....

(1 mark)

State the IUPAC name of **two** branched isomers of C_6H_{14}.

.....

(b) .....

(2 marks)

Draw the displayed formula of a possible isomer of C_6H_{12} that does **not** contain a π bond.

(c) .....

(1 mark)

(d) State the IUPAC names of two branched isomers of C_5H_{10} that contain a π bond.

.....

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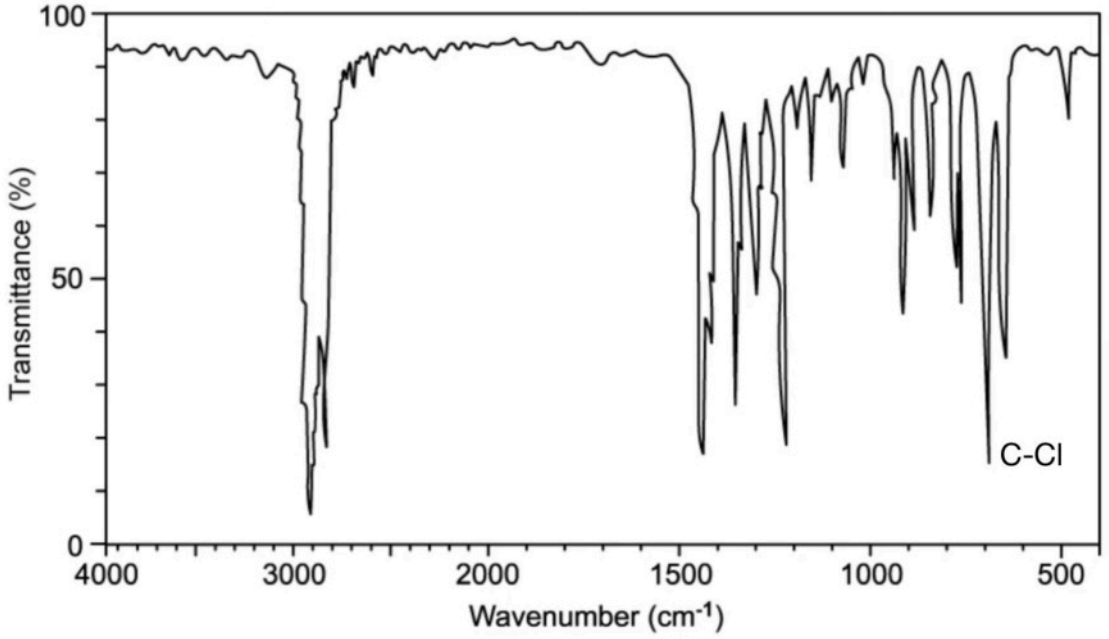
(3 marks)

4 (a) An alcohol can be prepared by hydrolysing the halogenoalkane $C_2H_5CHBClCH_3$ with aqueous sodium hydroxide. The infrared spectrum for $C_2H_5CHClCH_3$ is shown below with the C–Cl bond absorption labelled.



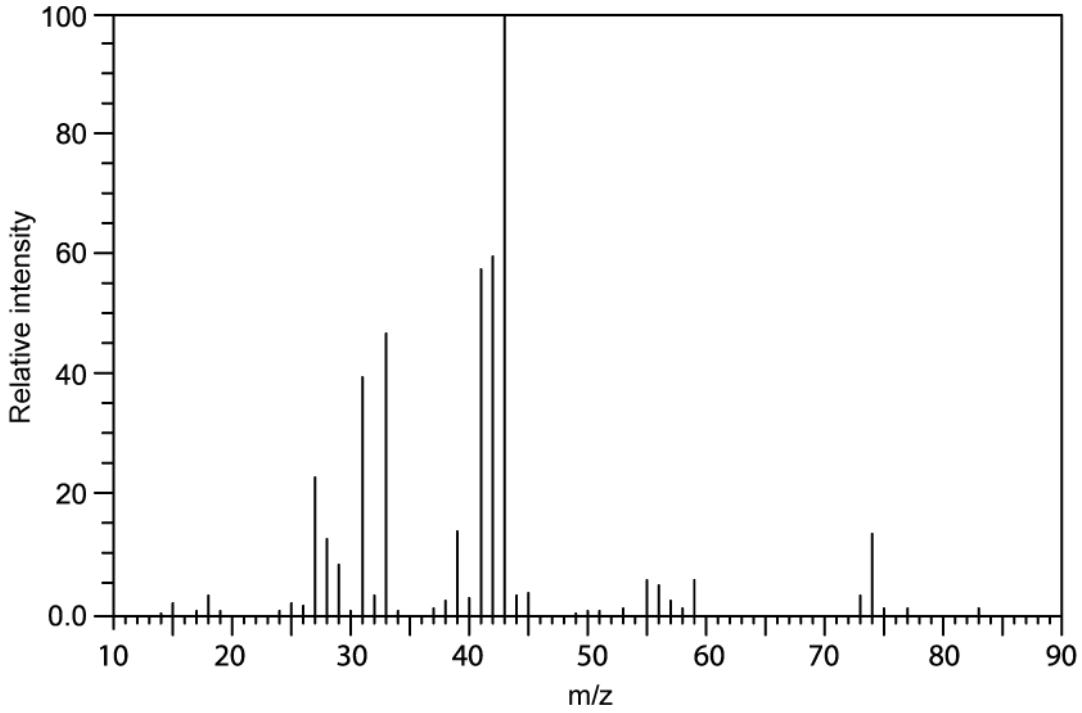
Using section 20 of the data booklet deduce how IR spectroscopy will change as a result of the above reaction.

.....

.....

(2 marks)

(b) The mass spectrum of $(CH_3)_2CHCH_2OH$ is shown below.



Deduce which ion is responsible for the peak with the greatest relative intensity.

.....

(1 mark)

(c) Alcohol **X** has the following percentage composition by mass. Carbon = 68.2%, hydrogen = 13.6%, oxygen = 18.2%. The molecular ion peak in the mass spectrum for alcohol **X** occurs at *m/z* = 88.

i) Use this information and section 6 of the data booklet to show that the molecular formula for alcohol **X** is $C_5H_{12}O$. Include your working.

[2]

ii) When alcohol **X** is oxidised, a carboxylic acid can be formed. State what information this gives about alcohol **X**.

[1]

.....

.....

.....

(3 marks)

(d) The mass spectrum of alcohol **X** has a major peak at *m/z* = 45.

i) Draw the structure of the species that could give this peak.

[1]

ii) Alcohol **X** has a branched chain. Deduce the structural formula and IUPAC name of alcohol **X**. Justify your answer.

[2]

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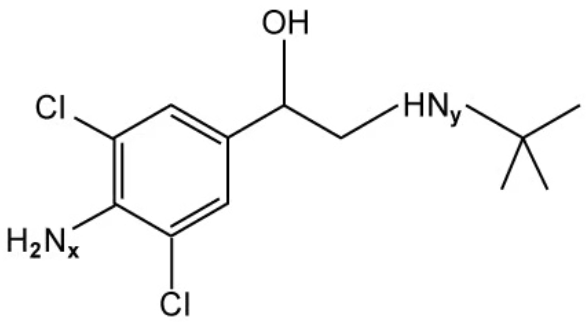
(3 marks)

5 (a) Clenbuterol, shown below, is considered a performance enhancing drug and is believed to increase short term work rate and cardiovascular output.



Deduce the functional groups marked *x* and *y* and state to which class they belong to.

.....

.....

(2 marks)

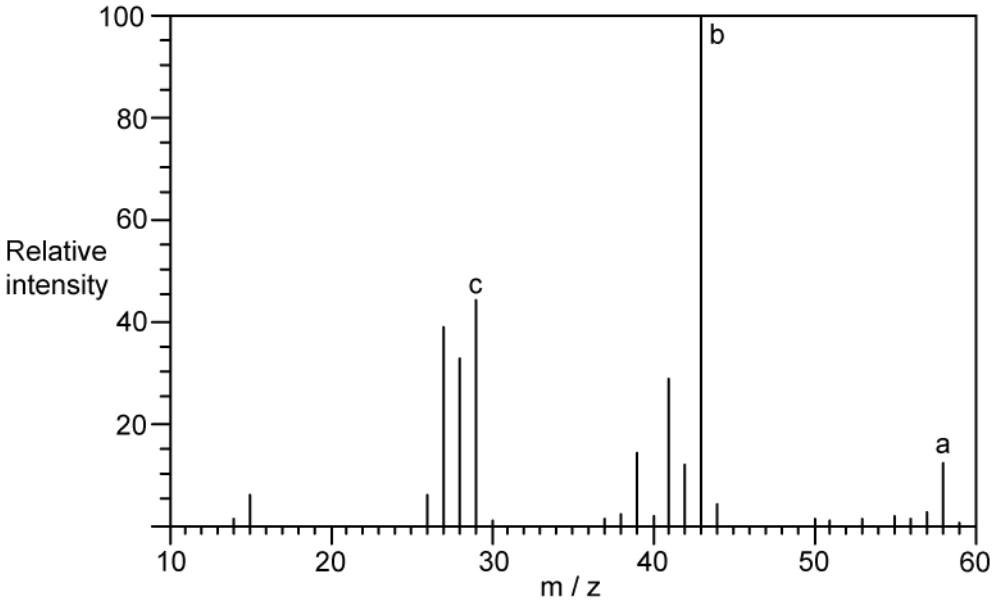
(b) Determine the *m/z* value of the molecular ion, M^+, of clenbuterol. Justify your answer.

.....

.....

(2 marks)

(c) Two students, **P** and **Q**, were provided with the mass spectrum of an alkane, shown in below. Student **P** analysed peaks **a** and **b** and concluded that the alkane was one of two structures. Student **Q** analysed peaks **a**, **b** and **c** and was able to identify one possible alkane structure.



i) Deduce which fragments of the alkane correspond to peaks **a**, **b** and **c**.

[3]

ii) Suggest why the two students obtained different conclusions.

[2]

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(5 marks)

6 (a) Four samples containing isomeric alcohols with molecular formula $C_4H_{10}O$, were studied using ^1H NMR spectroscopy

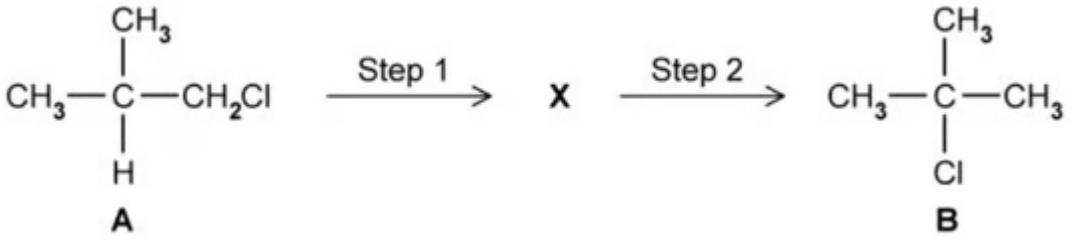
Draw structural formulas of the alcohols and deduce the number of peaks in the NMR spectrum of each alcohol

(4 marks)

(b) Two of the alcohols produce the same number of peaks in an ^1H NMR spectrum. Suggest how they may be distinguished, by further spectroscopy analysis.

(2 marks)

(c) Compound A can be converted into compound B via an intermediate species.

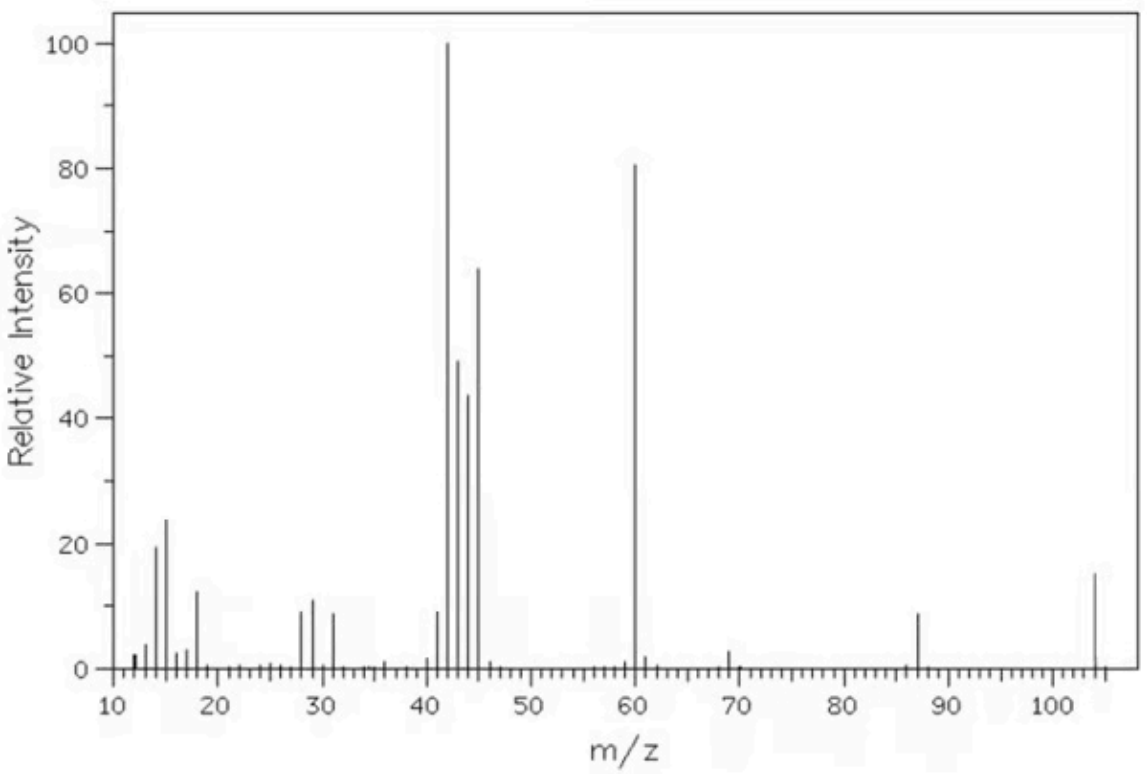


Suggest how you would be able to determine the difference between Compounds **A** and **B** by analysis of their ^1H NMR spectra.

(2 marks)

7 (a) Malonic acid, $C_3H_4O_4$, is naturally occurring and found in many fruits and vegetables. It contains only carbon, hydrogen and oxygen.

The MS of malonic acid is show below.



Determine the relative molecular mass of malonic acid from the spectrum and account for the peak at *m/z* 45, using section 22 of the Data booklet to support your answer.

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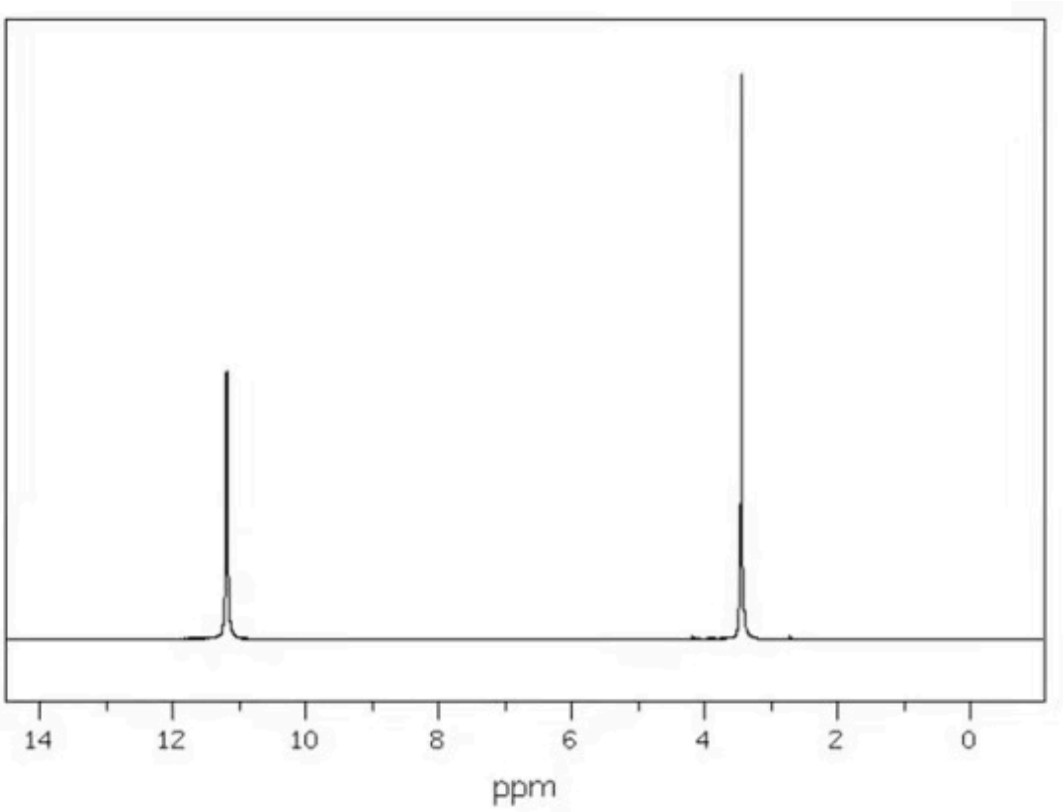
(2 marks)

(b) The ^1H NMR spectrum of malonic acid is shown below. Use section 21 of the Data booklet to help you with this question.



Suggest the identity of the proton environments seen in the spectrum and comment on the type of signals shown.

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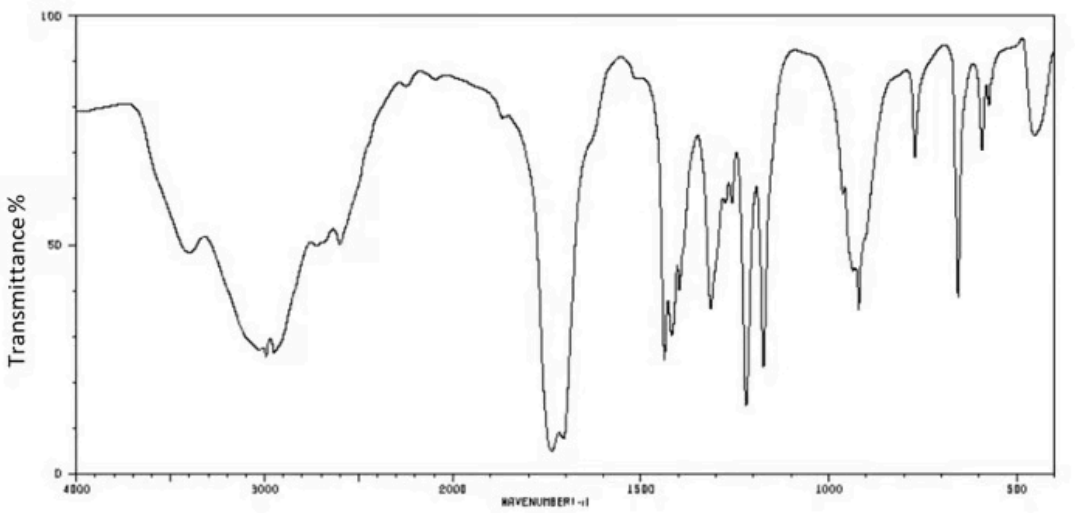
(3 marks)

(c) The IR spectrum of malonic acid is shown below:



i) Identify two characteristic peaks and bonds that can be found in the spectrum of malonic acid.

[2]

ii) Explain how the spectrum can be used to distinguish malonic acid from ethanoic acid.

[1]

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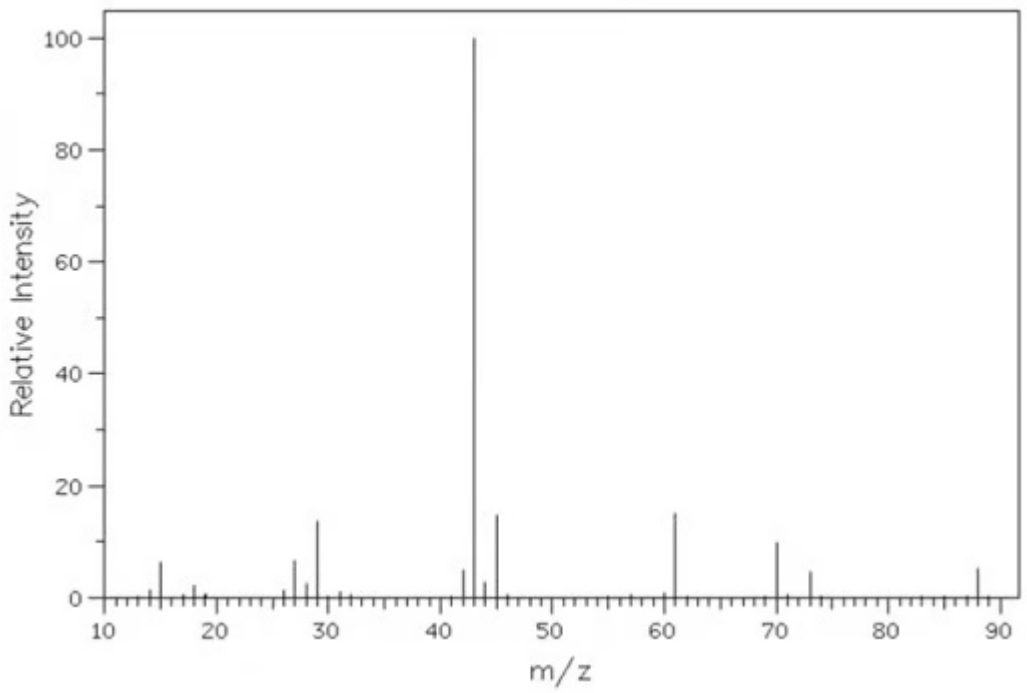
(3 marks)

(d) Draw a displayed structure for malonic acid.

.....

(1 mark)

8 (a) An organic compound, **Q**, of molecular formula $C_xH_yO_z$, has the following MS. Use section 22 of the Data booklet to help you answer this question.



i) Determine the relative molecular mass of **Q** and account for the peaks at *m/z* 15 and *m/z* 29.

[2]

ii) Comment on the size of the peak at *m/z* 43.

[1]

iii) Write an equation for the formation of the fragment at m/z 29.

[1]

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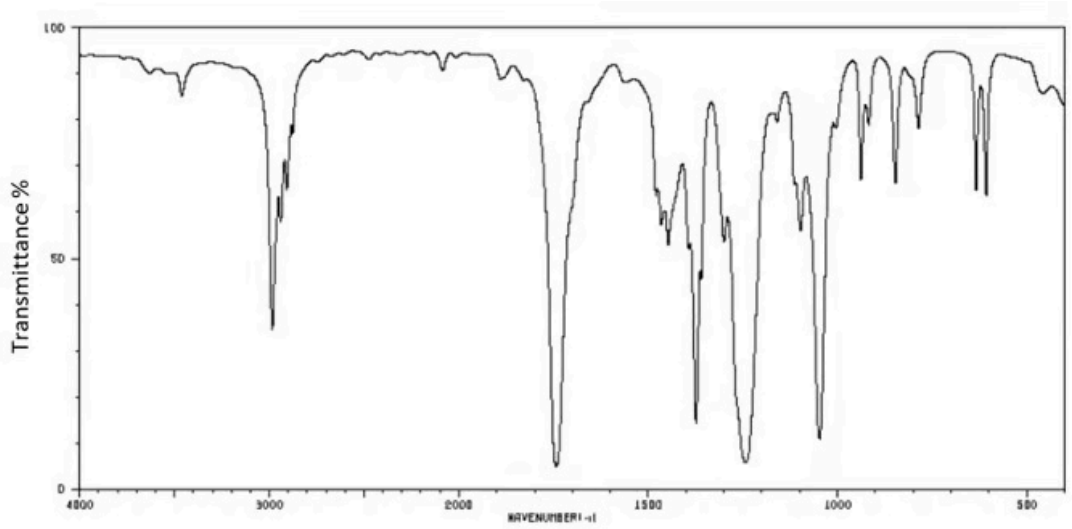
(4 marks)

(b) The IR spectrum of **Q** is shown below.

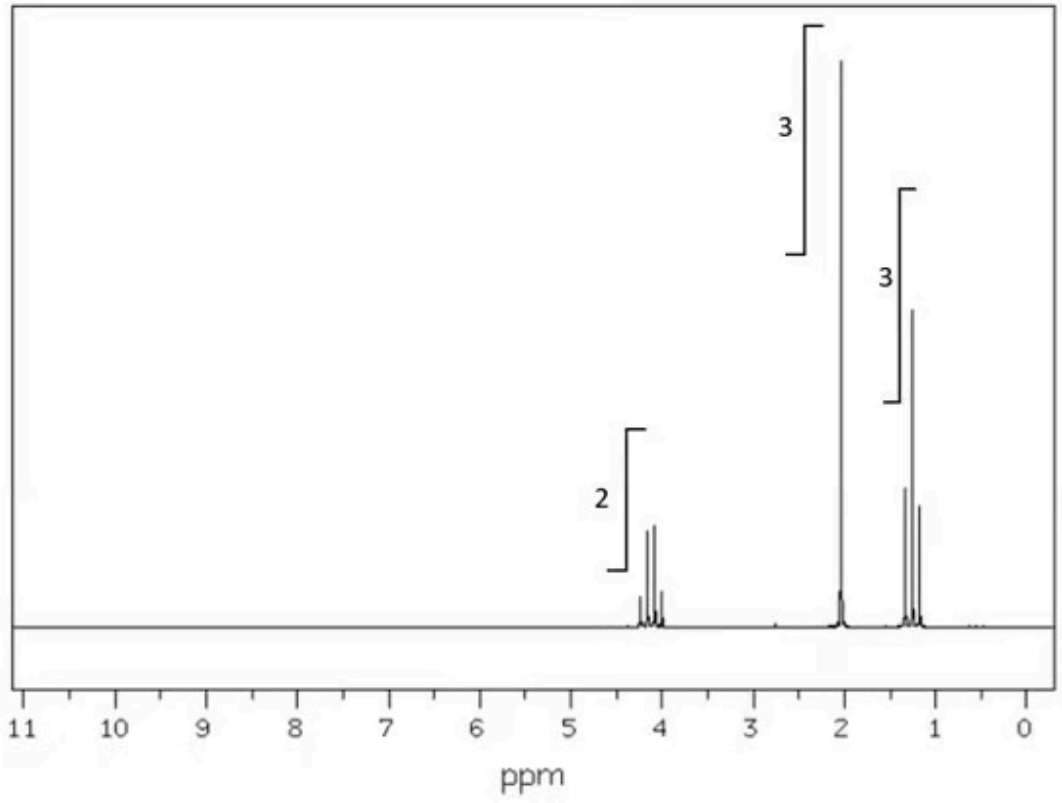


Suggest which functional group(s) could be present in **Q**.

.....

(1 mark)

(c) The ^{1}H NMR spectrum of **Q** is shown below.



Explain the relative peak heights and splitting patterns.

(5 marks)

(d) Suggest the identity of **Q**, giving your reasons.

(3 marks)

9 (a) Compound **A**, has molecular formula C_5H_{10} and occurs as 6 isomers. The table below shows the number of signals in the NMR spectrum of each isomer.

Isomer	Number of ^{1}H NMR signals
A	1
B	5
C	5
D	5
E	5
F	4

Suggest a structure for **A** and **F**.

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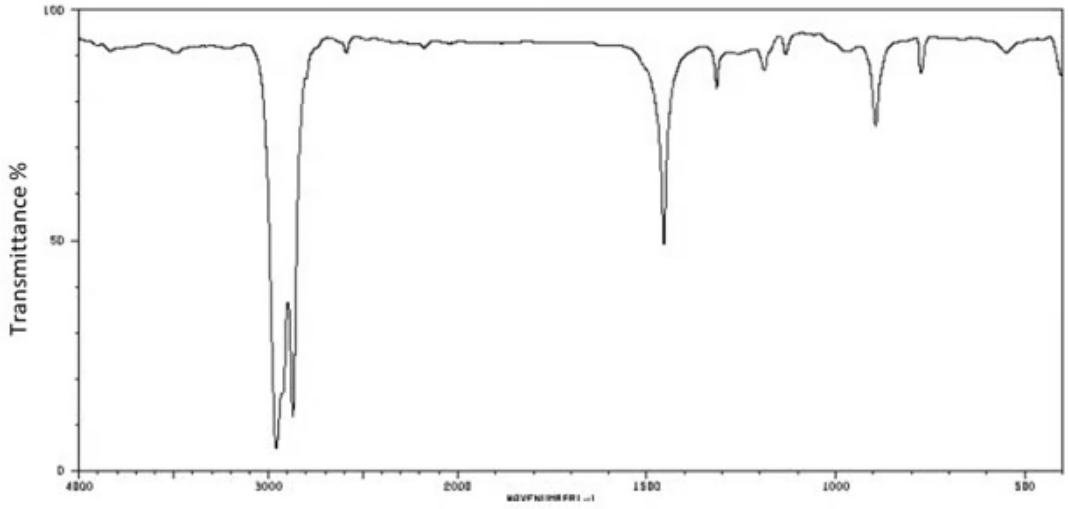
(2 marks)

(b) The IR spectrum of **A** is shown below.



How does this spectrum distinguish **A** from the other isomers?

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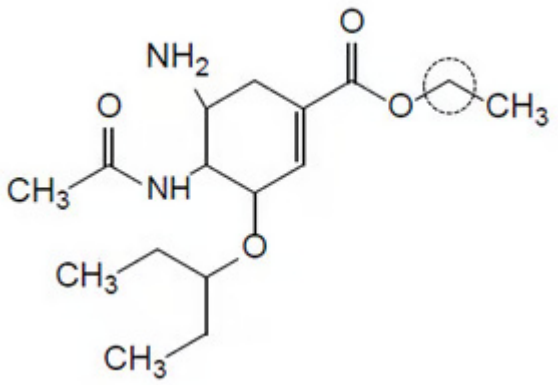
(3 marks)

10 (a) Oseltamivir is a drug used to treat and prevent influenza A and influenza B.



Predict the number of different proton environments in the molecule.

.....

(1 mark)

(b) Predict the chemical shift and the splitting pattern seen for the hydrogens on the carbon atom circled in the diagram. Use section 21 of the Data booklet.

.....

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(2 marks)

(c) Predict three absorptions you would expect to see in the IR spectrum of oseltamivir. Use section 20 of the data booklet.

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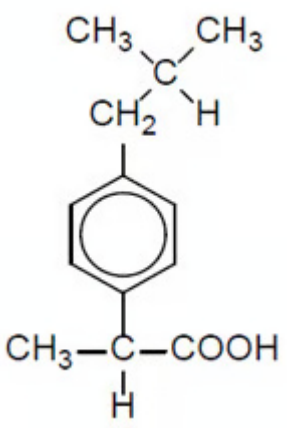
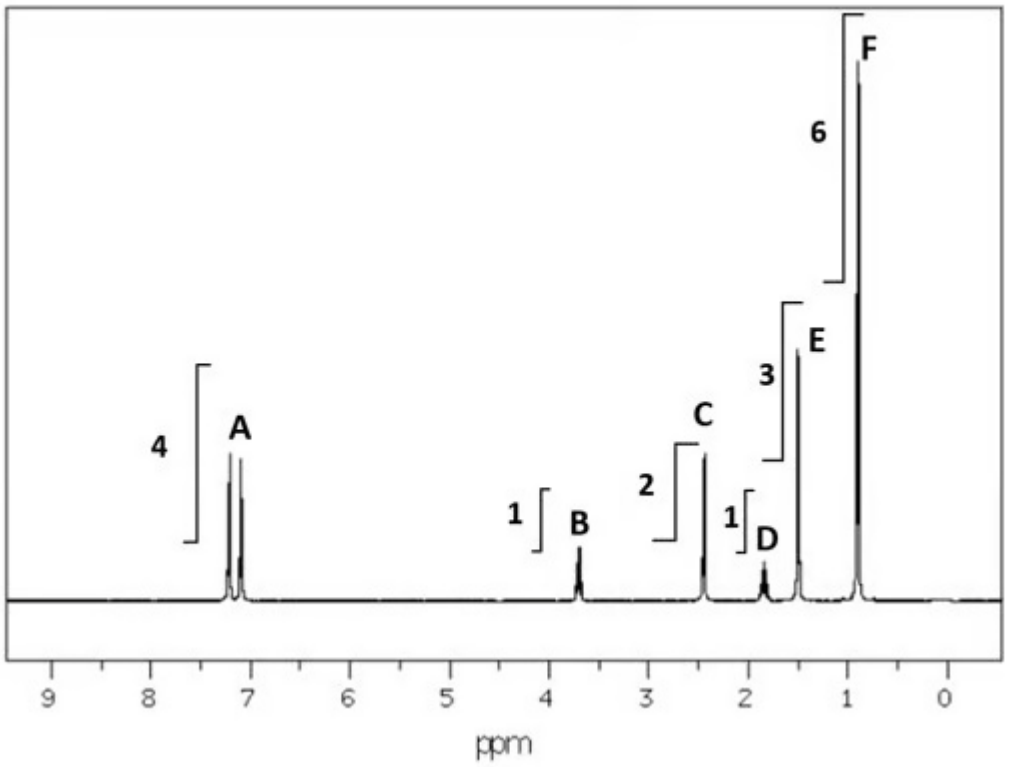
(3 marks)

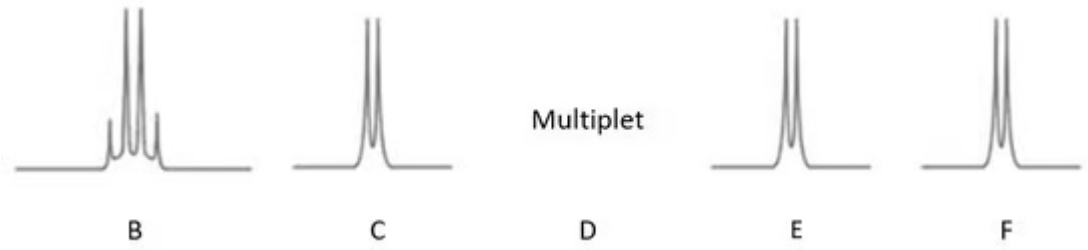
11 (a) Ibuprofen is an important painkilling drug. The structure is:



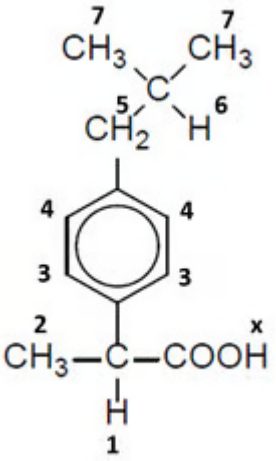
Part of the low resolution ^{1}H NMR spectrum is shown below.



The high resolution expansion of the peaks in **B**-**F** is:



The protons responsible for the peaks are numbered 1-7:



Complete the table to show the assignment of the missing peaks.

Peak	H atoms responsible
A	3 & 4
B	
C	
D	
E	
F	
Off spectrum	x

(3 marks)

(b) A sample of ibuprofen shows strong absorptions at 1716 cm^{-1} and 3345 cm^{-1} in an IR spectrum. Suggest the bonds responsible for these absorptions using section 20 of the data booklet.

.....

.....

(2 marks)

(c) A sample of ibuprofen rotates plane polarised light. Identify the feature in ibuprofen responsible for this.

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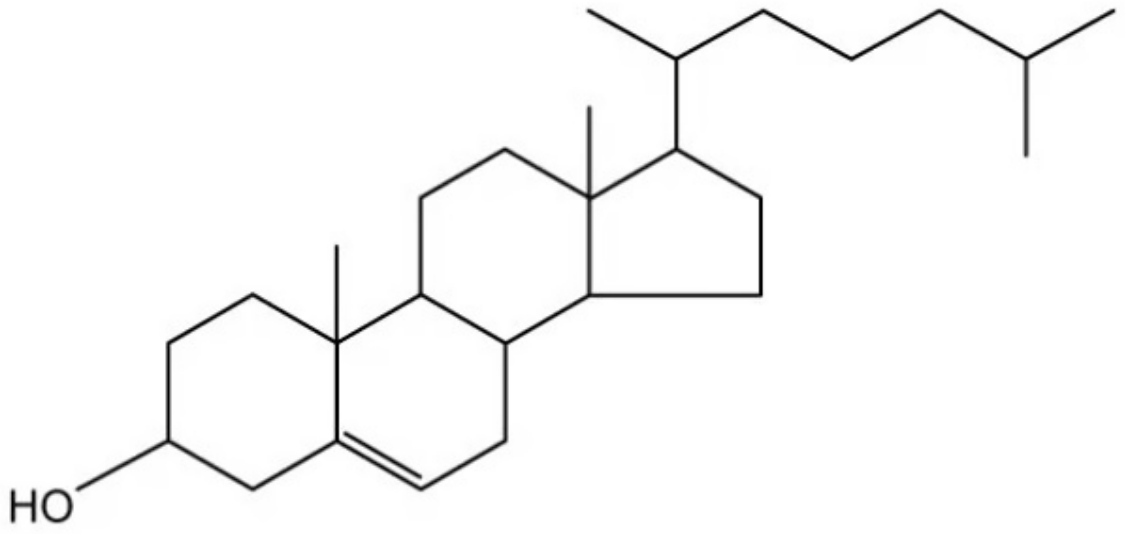
(1 mark)

12 (a) Cholesterol, shown below, is a fatty chemical used by the body to build healthy cells.



State the number of chiral carbons in the cholesterol structure.

.....

(1 mark)

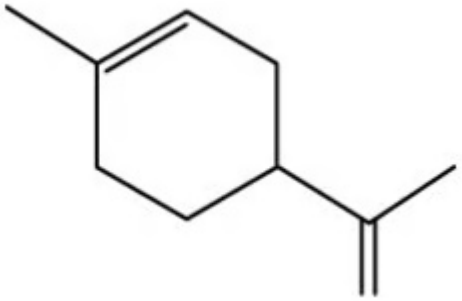
(b) A student suggested that cholesterol could be tested with plane polarised light to show that it contains chiral centres.

Is the student correct? Justify your answer.

.....

(1 mark)

(c) Limonene, shown below, is a naturally occurring hydrocarbon with the molecular formula $C_{10}H_{16}$ and is commonly found in the rinds of citrus fruits such as grapefruit, lemon, lime and oranges.



Limonene exists as a pair of enantiomers; one enantiomer is responsible for a strong orange smell while the other is thought to smell like lemons.

Draw 3D representations of the two enantiomers of limonene.

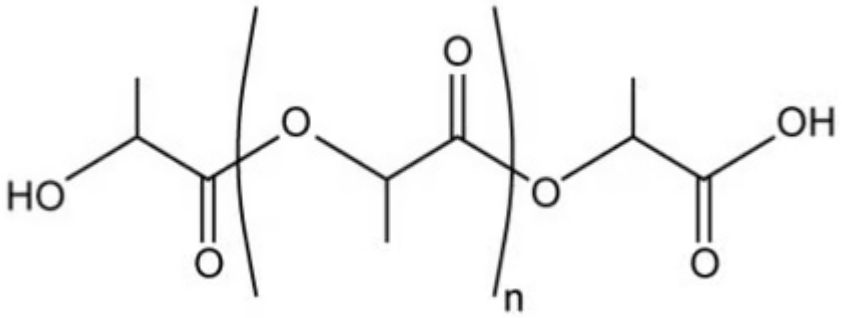
(2 marks)

13 (a) Lactic acid has the molecular formula of $C_3H_6O_3$, and the structural formula of $CH_3CHOHCOOH$.

Illustrate the types of isomerism shown by $C_3H_6O_3$.

(4 marks)

(b) The general structure of polylactic acid is shown below:



Draw **two** possible structures formed from two repeating units.

Your answer should keep the main polymer chain in the same plane but show the 3D representation of the chiral carbons.

(2 marks)

(c) State, why the polymer formed from the uncontrolled condensation polymerisation of lactic acid, is not a racemate.

(1 mark)