IB · DP · Chemistry

2 hours 15 questions

Structured Questions: Paper 2

21.1 Spectroscopic Identification of Organic compounds

Easy (5 questions)	/43
Medium (5 questions)	/56
Hard (5 questions)	/40
Total Marks	**/139**

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Easy Questions

1 (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)

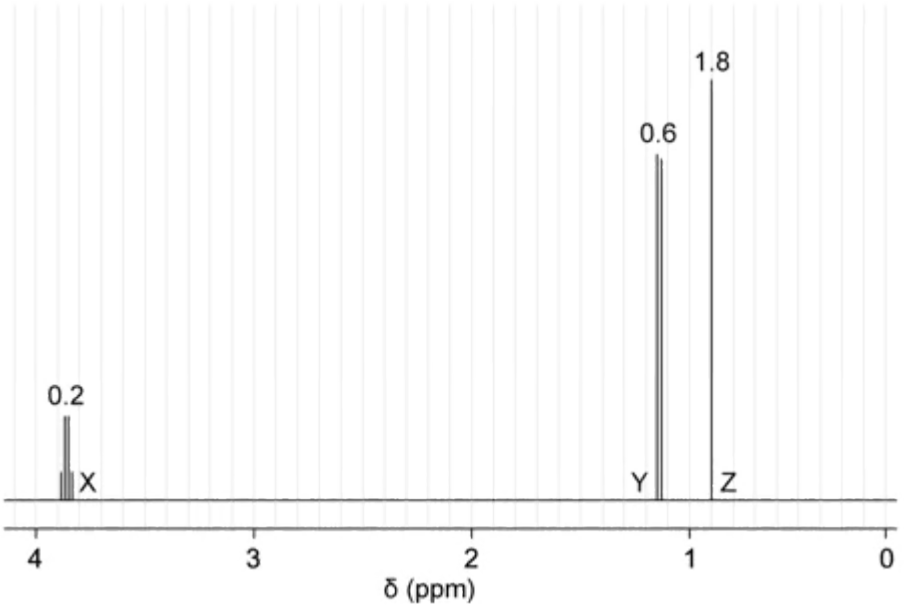
(c) ^{1}H NMR spectroscopy uses tetramethylsilane. State its formula and purpose in ^{1}H NMR spectroscopy.

(2 marks)

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

(3 marks)

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



Determine the number of unique hydrogen environments

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(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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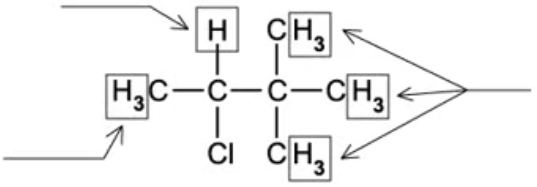
(4 marks)

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



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(2 marks)

3 (a) Outline what chemical information can be obtained about inorganic ionic substances and complex organic molecules from X-ray crystallography studies.

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(2 marks)

(b) Explain why X-ray crystallography is not very useful for compounds containing hydrogen.

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(2 marks)

(c) Suggest another limitation of X-ray crystallography for organic compounds.

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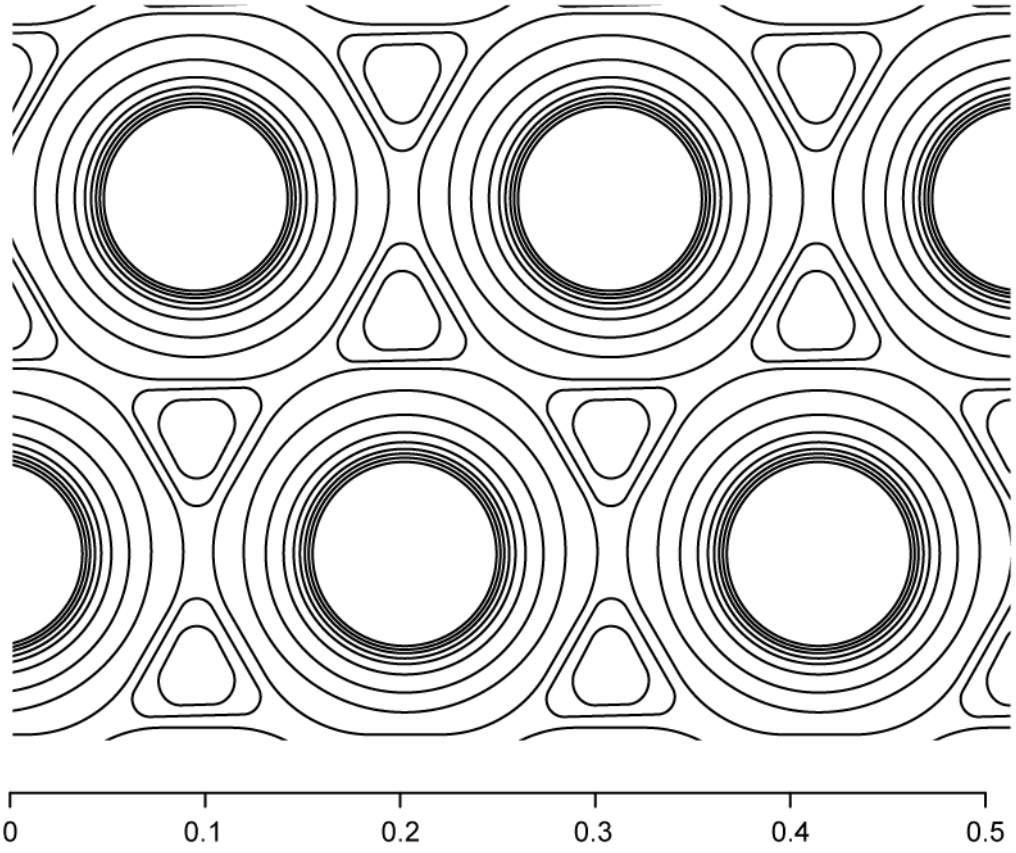
(1 mark)

(d) An electron density map obtain from the X-ray crystallography of copper metal is shown below:



Use the diagram to estimate the radius of a copper atom. The units are nm.

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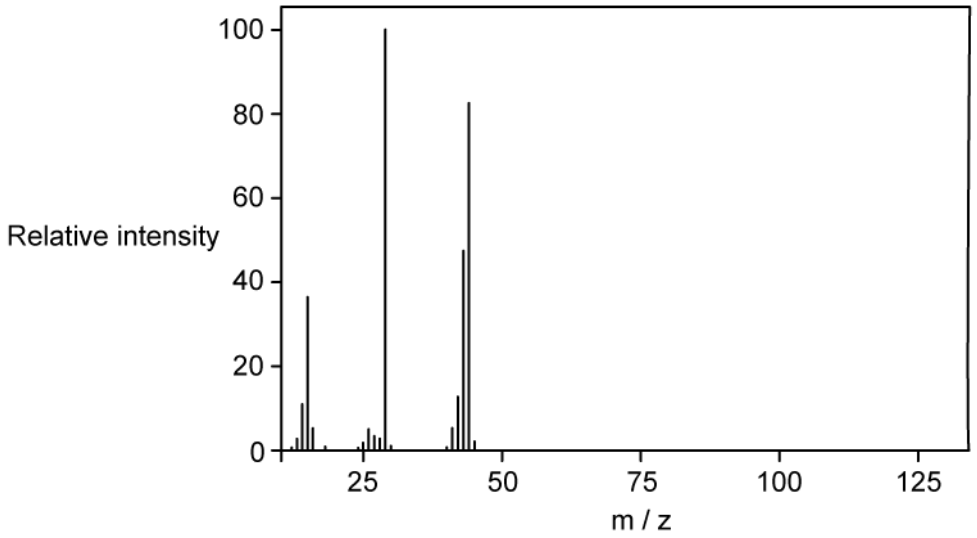
(1 mark)

4 (a) An organic molecule with molecular formula C_2H_4O is analysed using MS, IR and ^1H NMR. Use section 26, 27 & 28 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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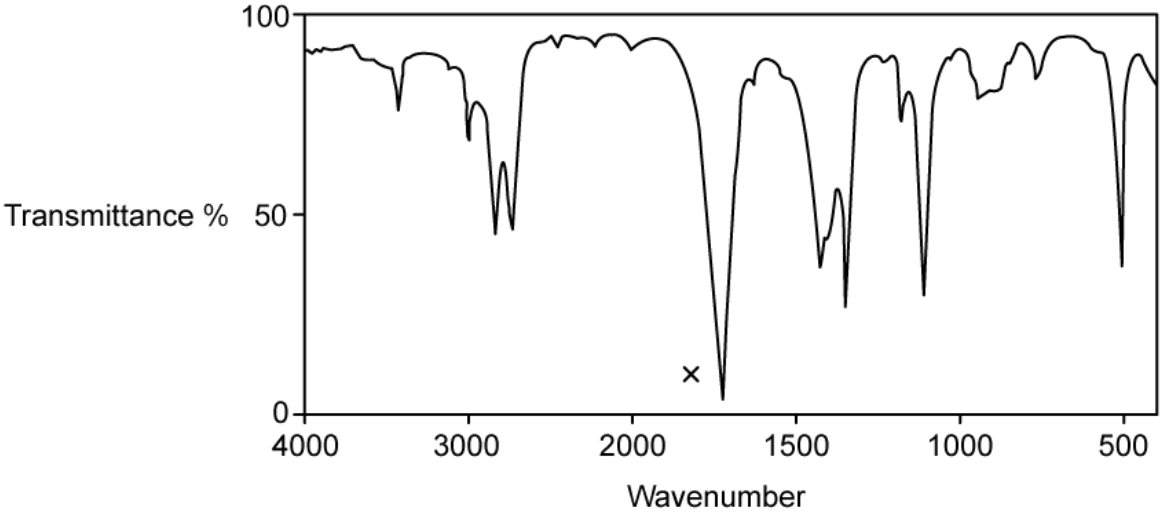
(2 marks)

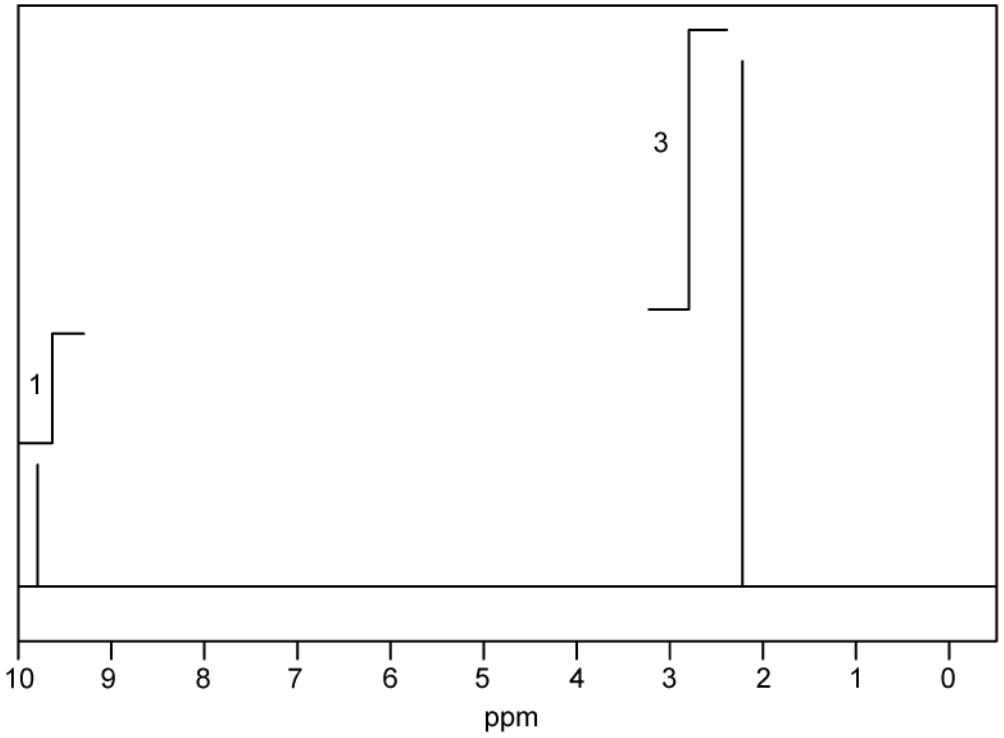
(b) The IR spectrum of the same compound is shown below.



Identify the functional group responsible for the peak at X

(1 mark)

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



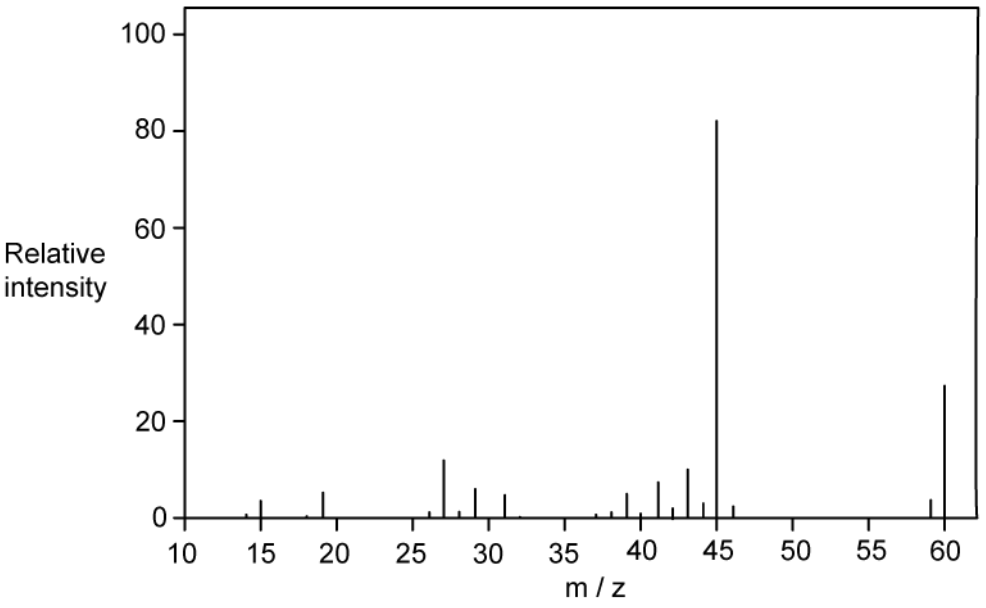
Account for the peaks at 2.2 ppm and 9.8 ppm and their relative areas.

(3 marks)

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

(1 mark)

5 (a) The MS of compound P is shown below. Compound P contains carbon, hydrogen and oxygen only. Use section 26, 27 & 28 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.

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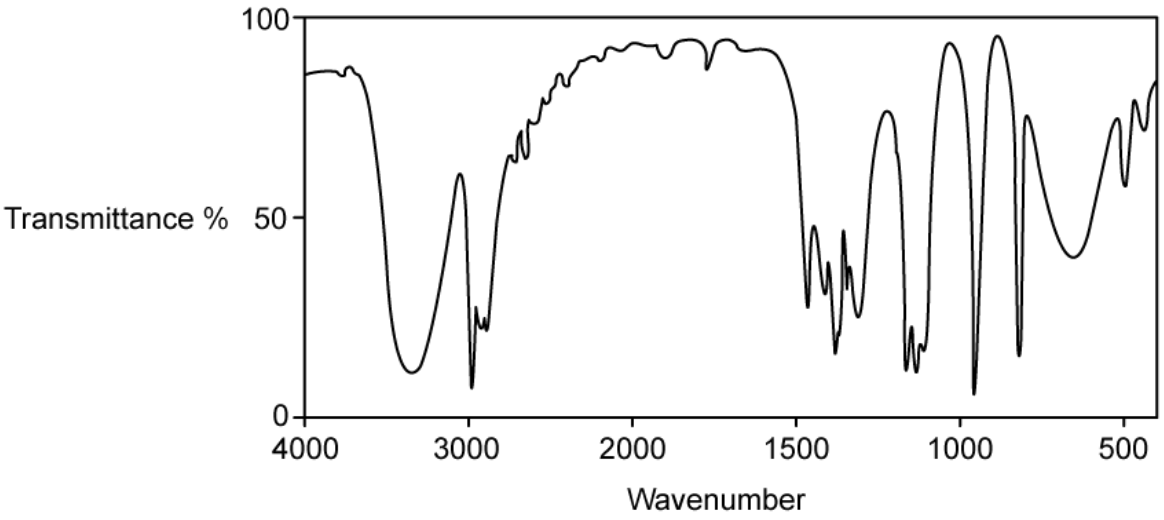
(2 marks)

(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.

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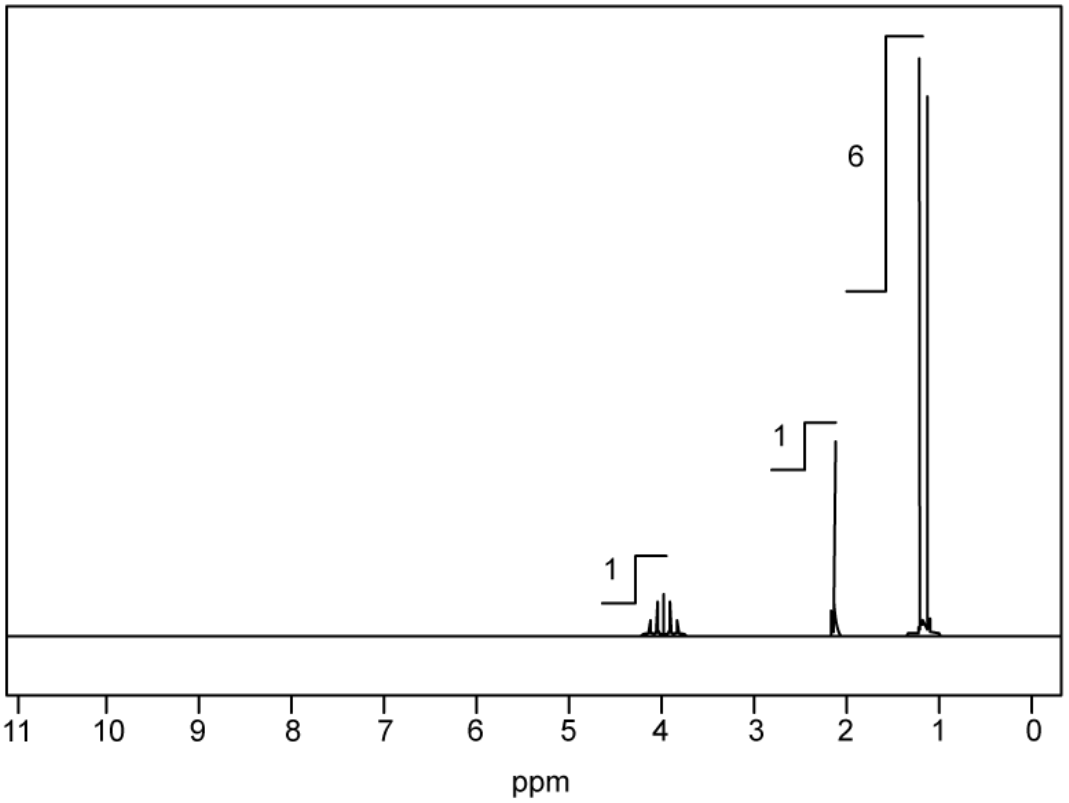
(2 marks)

(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)

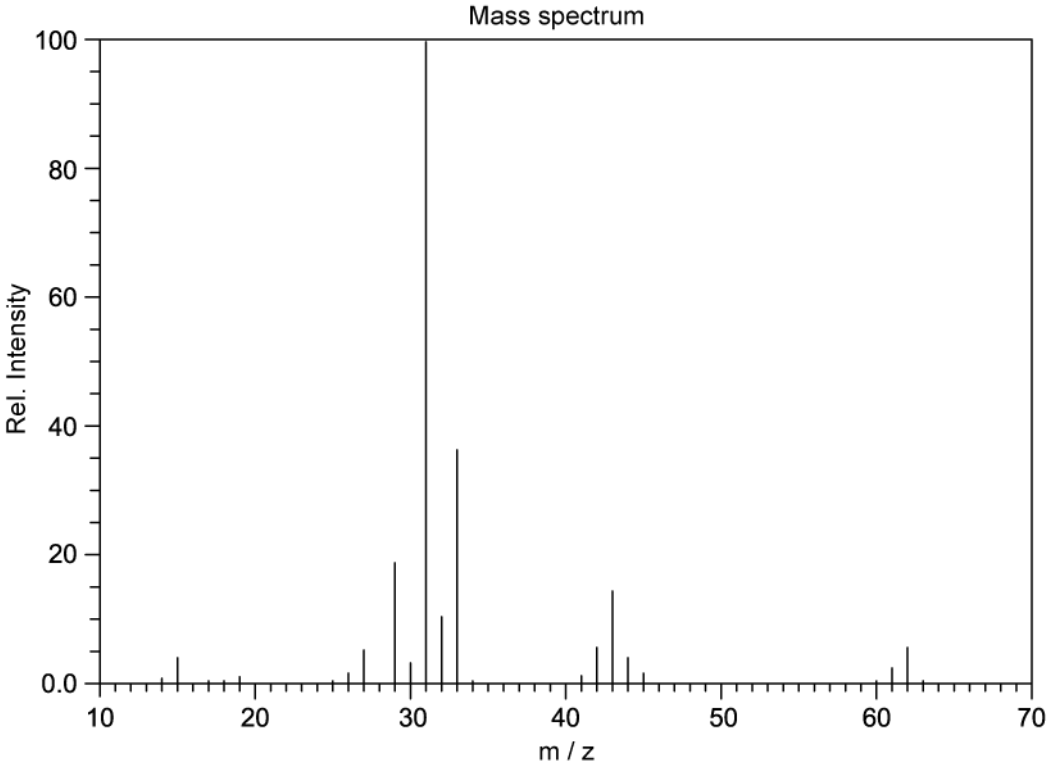
Medium Questions

1 (a) 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

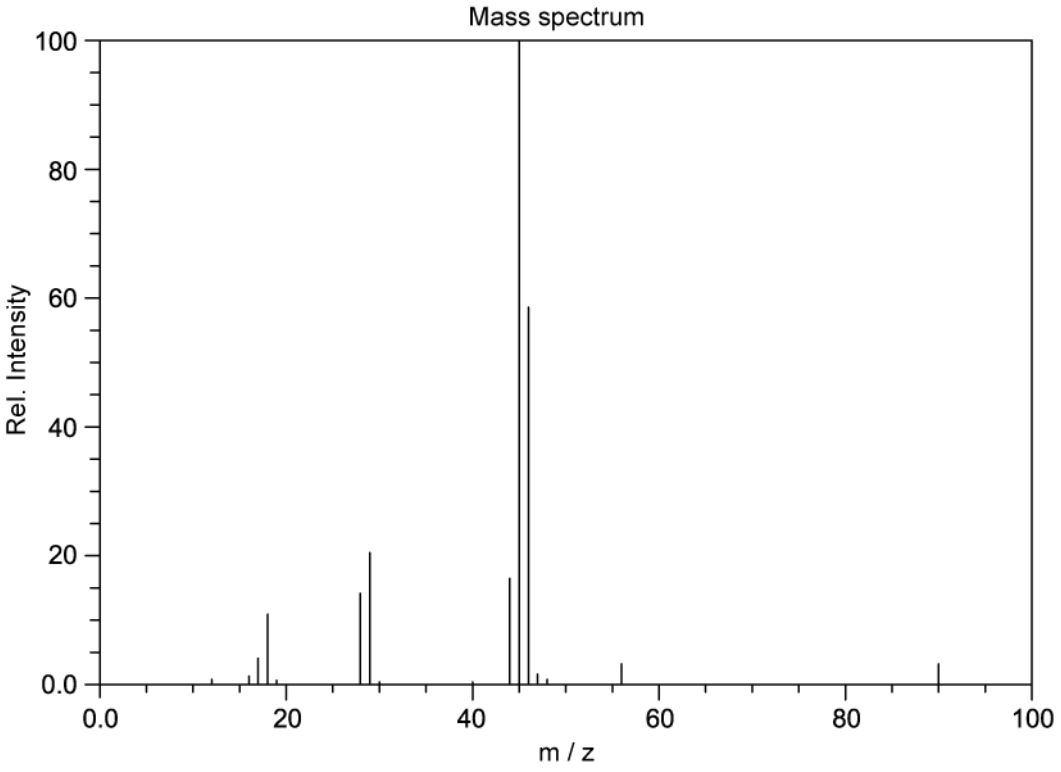
The MS of these molecules is shown below.

Which spectrum belongs to each molecule? Justify your answer.

Spectrum **A**



Spectrum **B**



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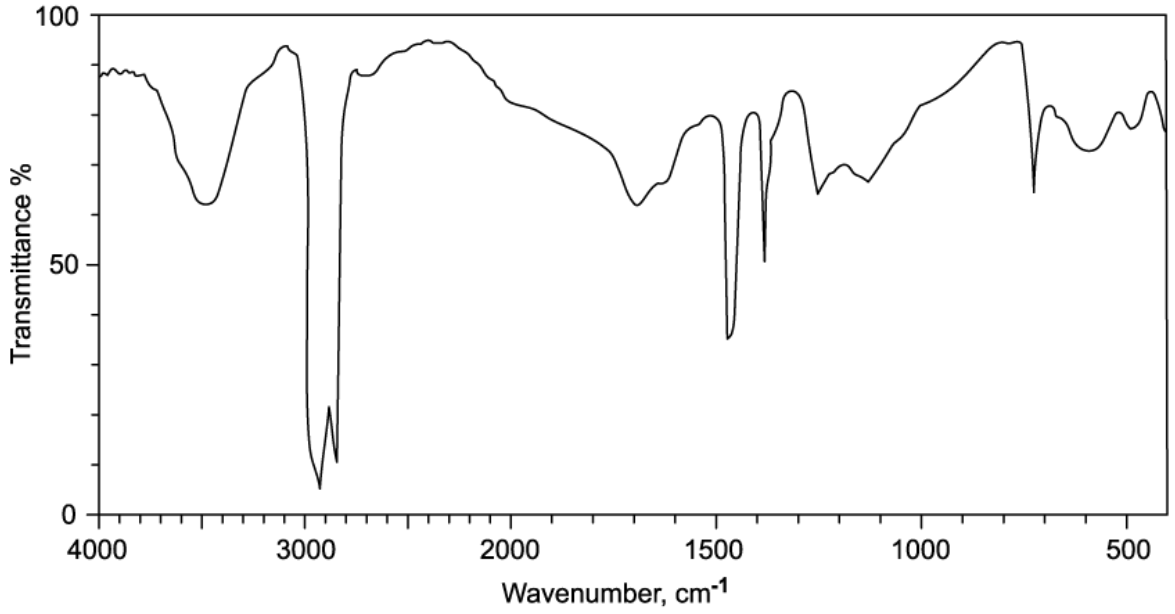
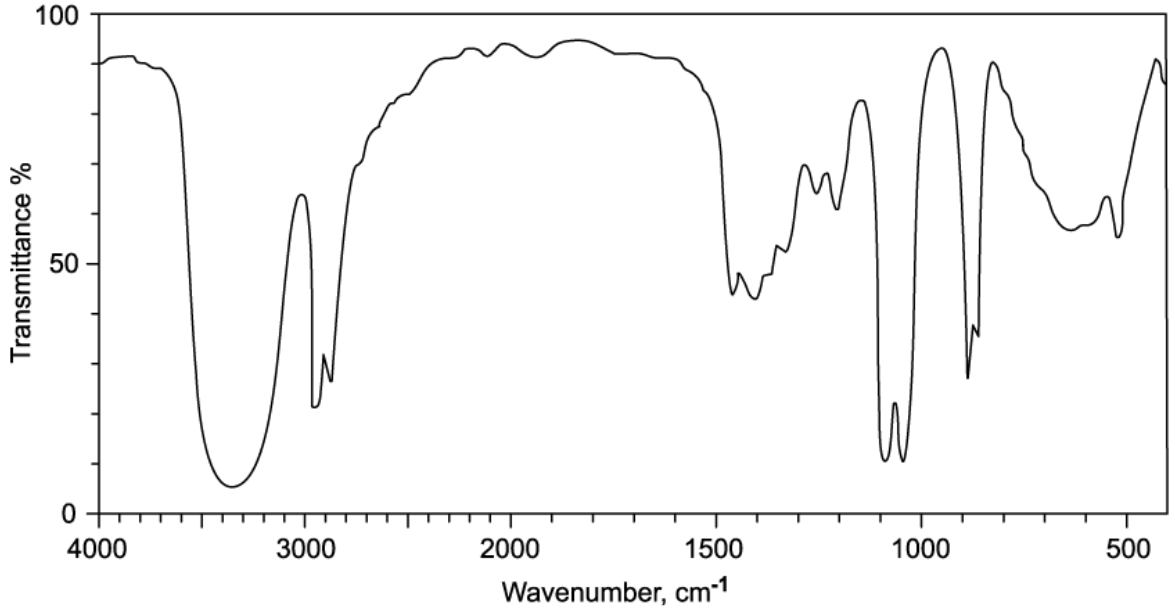
(2 marks)

(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 26 of the Data Booklet to answer this question.

Spectrum **C**



Spectrum **D**



Which spectrum belongs to each molecule? Justify your answer.

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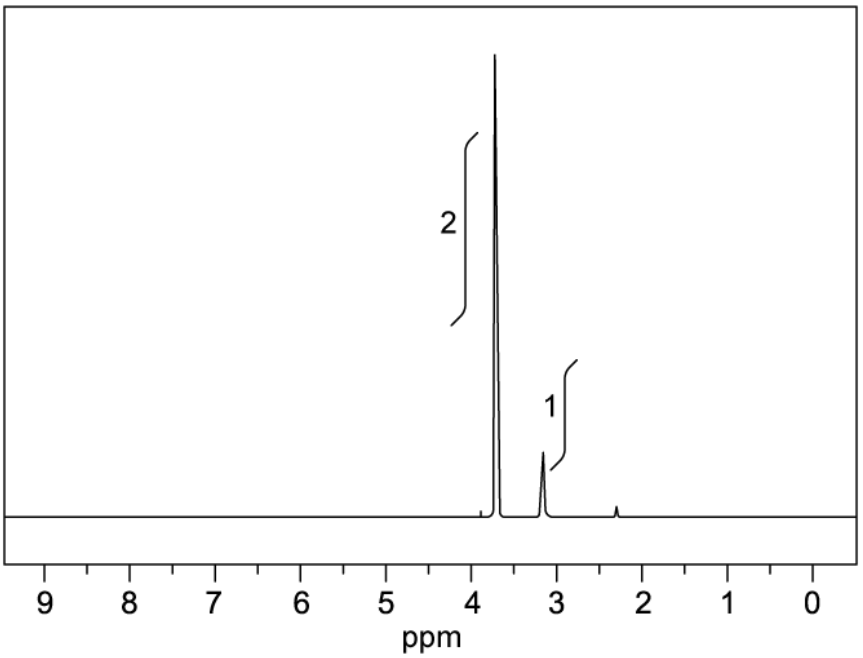
(2 marks)

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

Spectrum **E**



(3 marks)

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

(2 marks)

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

i) Draw the structural formula of TMS.

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

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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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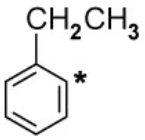
(1 mark)

(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

ii) One of the hydrogen atoms in the structure of ethylbenzene shown above is labelled with an asterisk (*).
Use Section 27 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.

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(2 marks)

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

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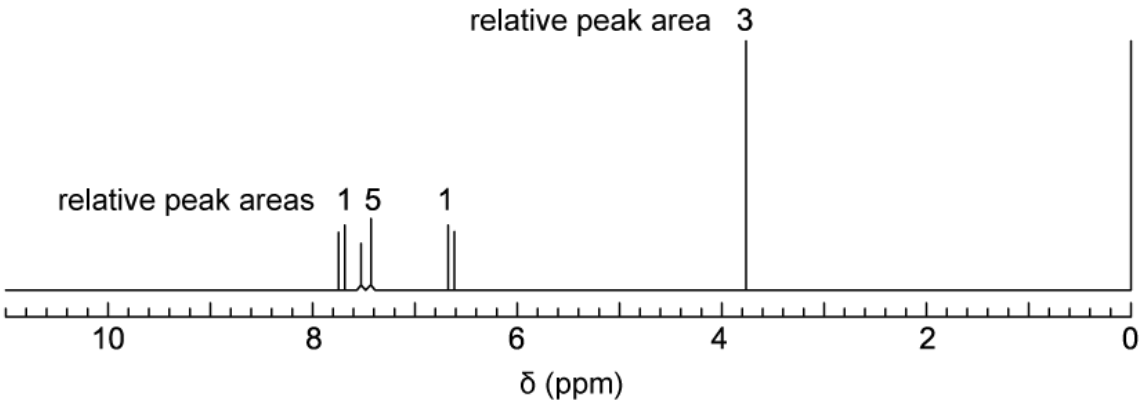
(1 mark)

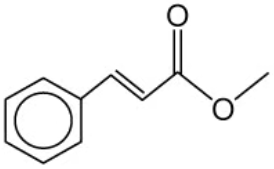
3 (a) Methyl cinnamate, $C_{10}H_{10}O_2$, is a white crystalline solid used in the perfume industry. A sample of methyl cinnamate was analysed by ^1H NMR spectroscopy.

A simplified spectrum is shown below.



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

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.



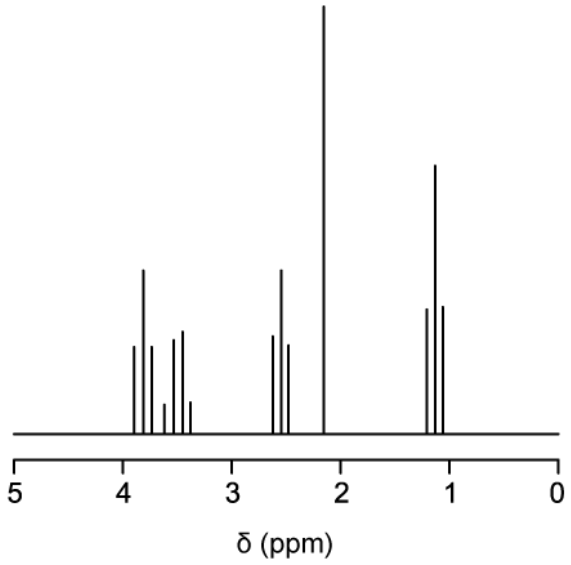
(5 marks)

(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.

(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

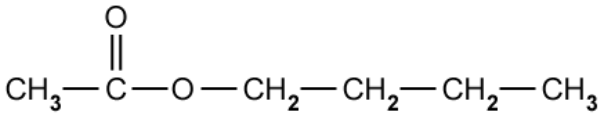
i) Deduce the simplest ratio of the relative numbers of protons in each environment in the isomer.

ii) Use Section 27 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.

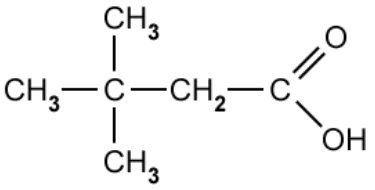
Explain why the splitting patterns of these peaks are produced.

(5 marks)

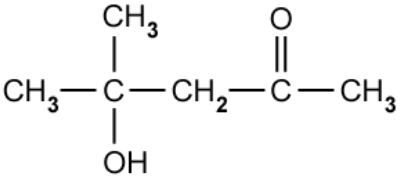
(d) Four isomers of $C_6H_{12}O_2$ are shown below.



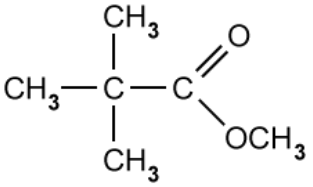
A



B

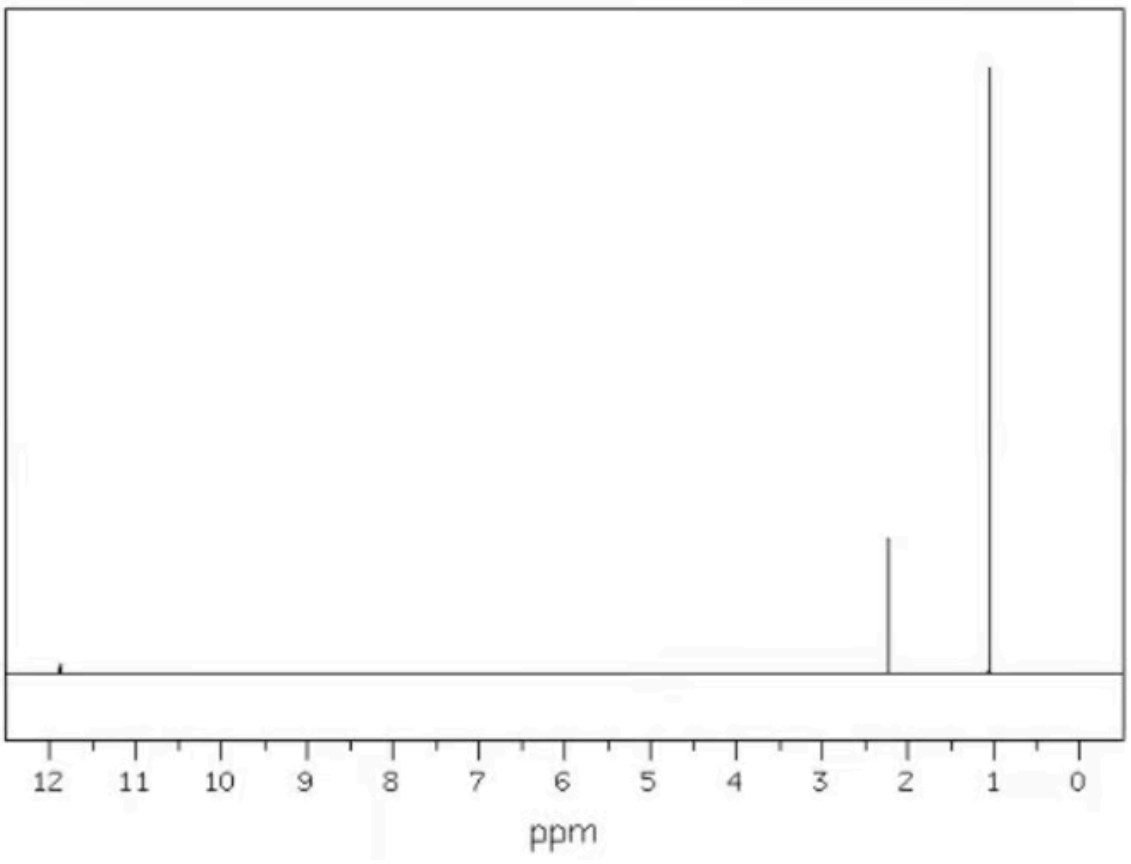


C



D

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



(2 marks)

4 (a) X- ray crystallography is a spectroscopy technique use to determine structural Information. State **two** pieces of information found by this technique.

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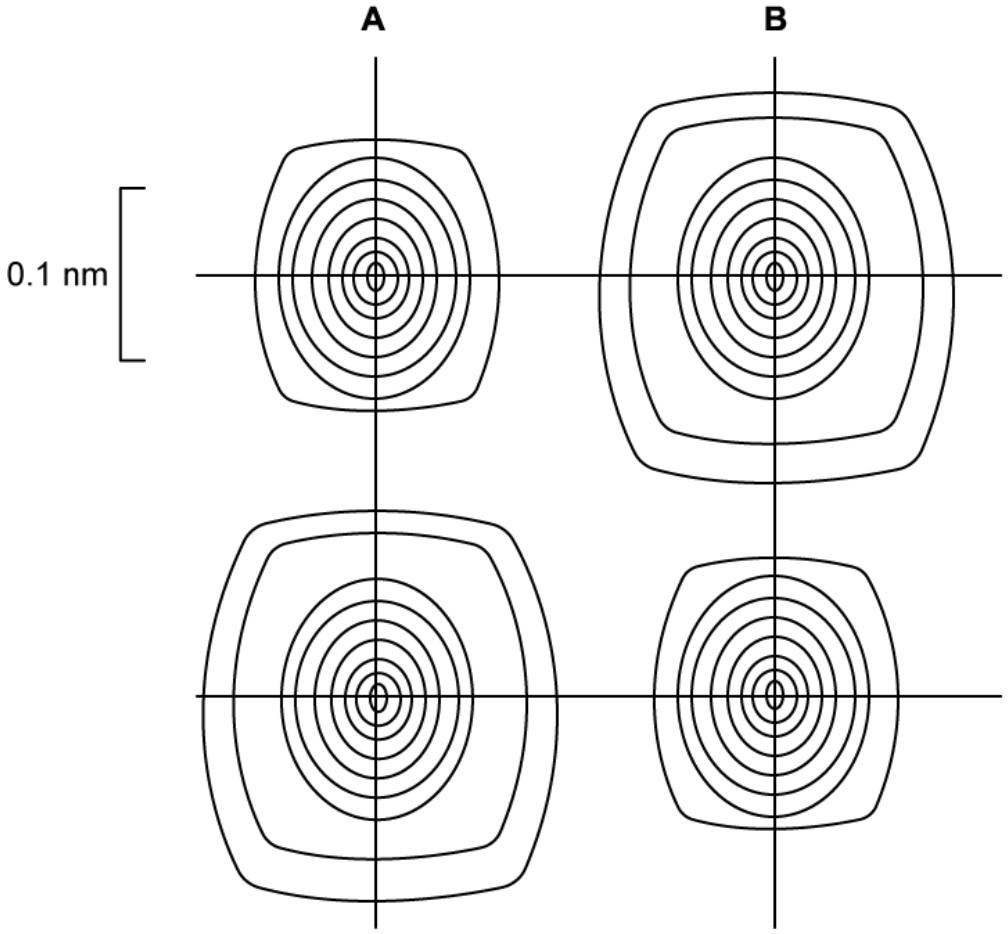
(1 mark)

(b) X ray crystallography enables chemists to produce electron density maps for substances, such as sodium chloride, shown below.



Estimate the interionic bond length and state which of the two patterns, **A** or **B**, belongs to the chloride ion.

.....

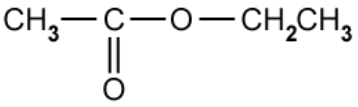
.....

(2 marks)

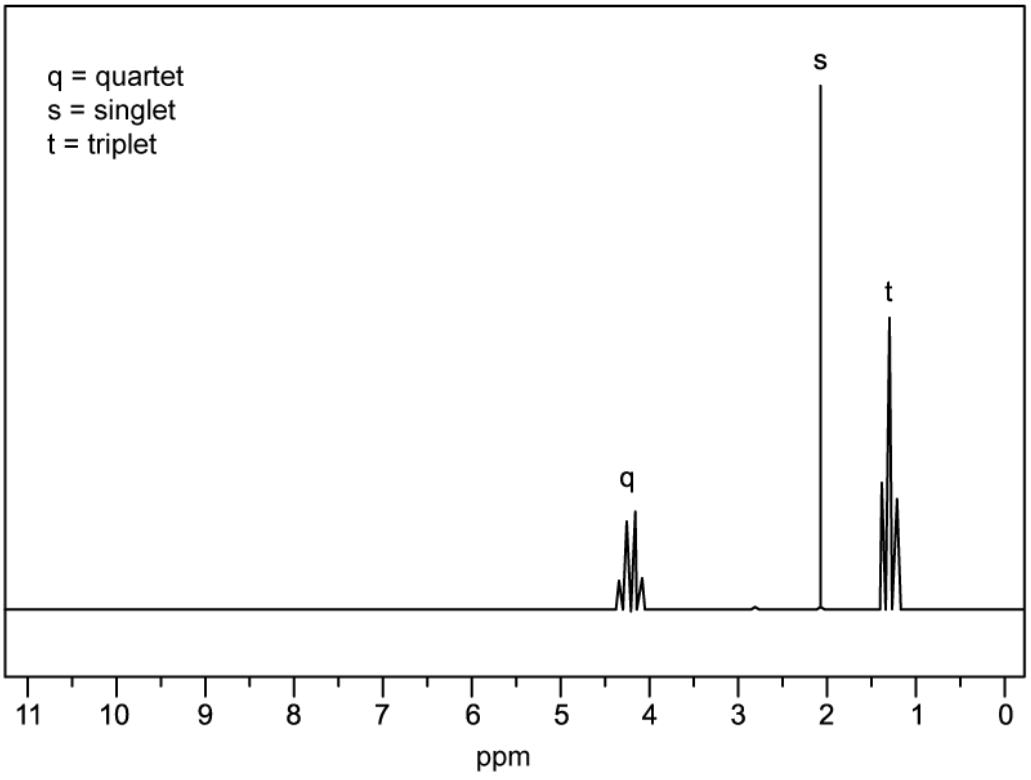
(c) Using Sections 26 & 27 of the Data Booklet and other sources, state three pieces of different spectroscopic evidence that would give structural information to identify benzene.

(3 marks)

(d) The ester shown below was analysed by high resolution ^{1}H NMR spectroscopy.



The ^{1}H NMR spectrum shown was produced for this ester.



Explain the splitting pattern marked on the spectrum.

(3 marks)

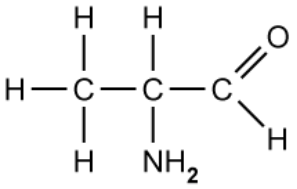
5 (a) An isomer with the molecular formula $C_5H_{10}O_2$ was analysed by infrared spectroscopy, to confirm it was a carboxylic acid.

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.

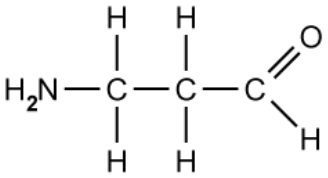
ii) The ^1H NMR spectrum of this isomer contains only two peaks with the integration ratio 9:1. Using this information from the spectra, deduce the structure of the isomer.

(4 marks)

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



2-aminopropanal



3-aminopropanal

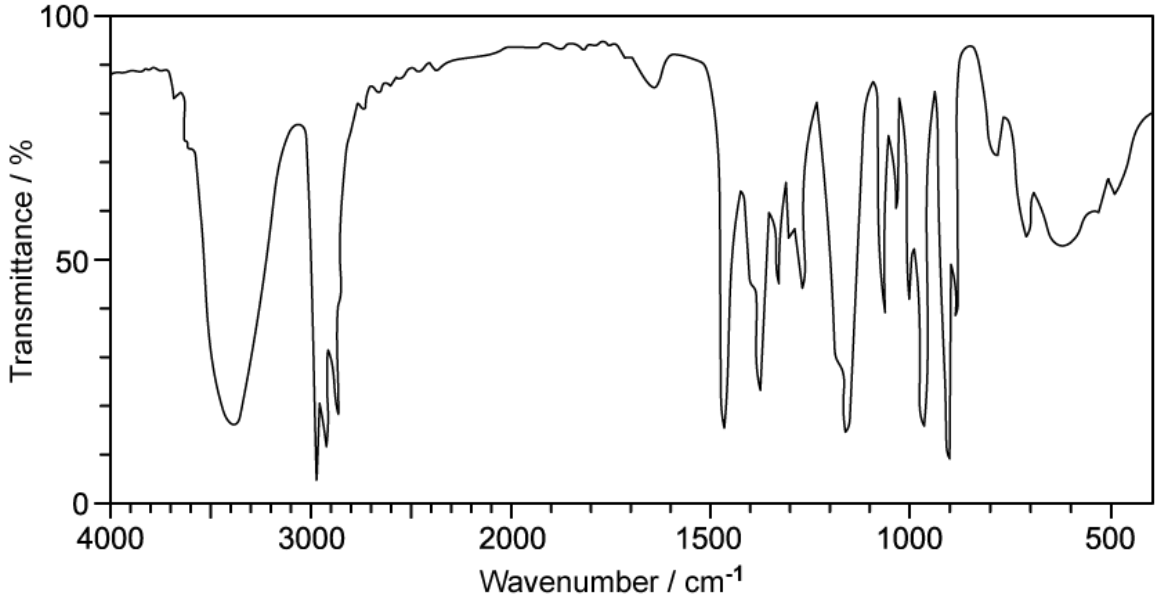
Explain how ^1H NMR spectra can be used to distinguish between these two aldehydes. You need to reference the splitting patterns and integration pattern in your answer.

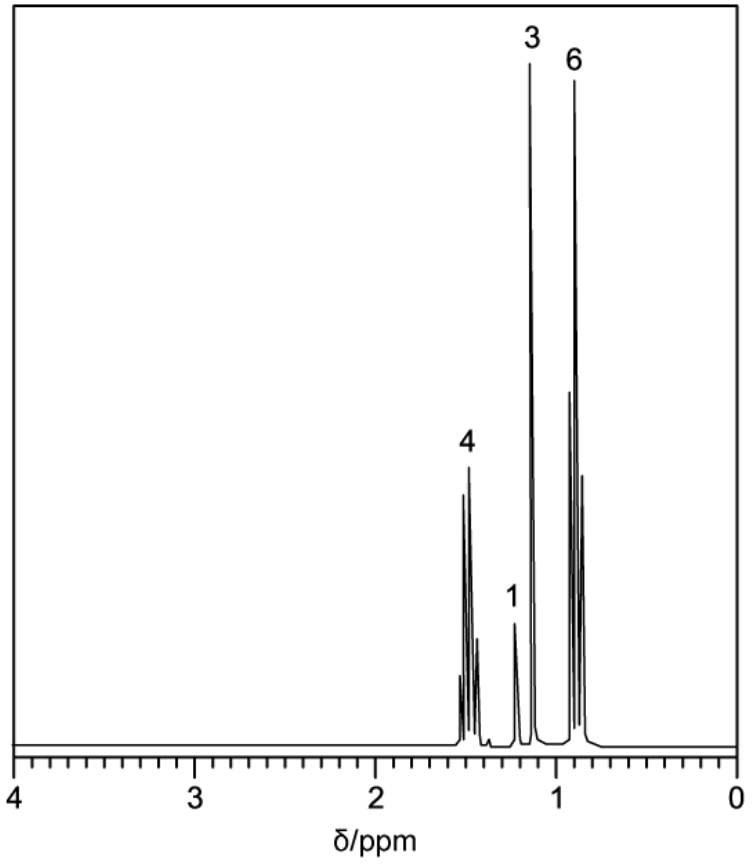
(5 marks)

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

(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.





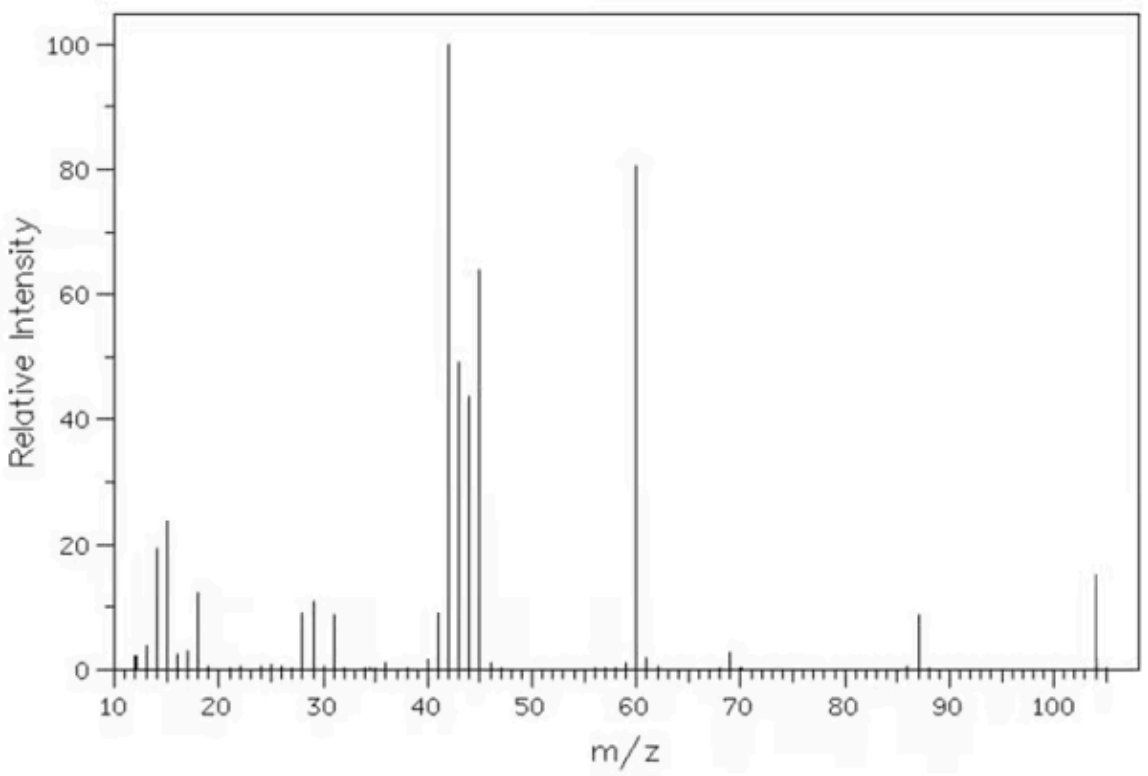
Use Section 26 from the Data Booklet, deduce the structure of compound **X**. Justify each of your deductions.

(7 marks)

Hard Questions

1 (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 28 of the Data booklet to support your answer.

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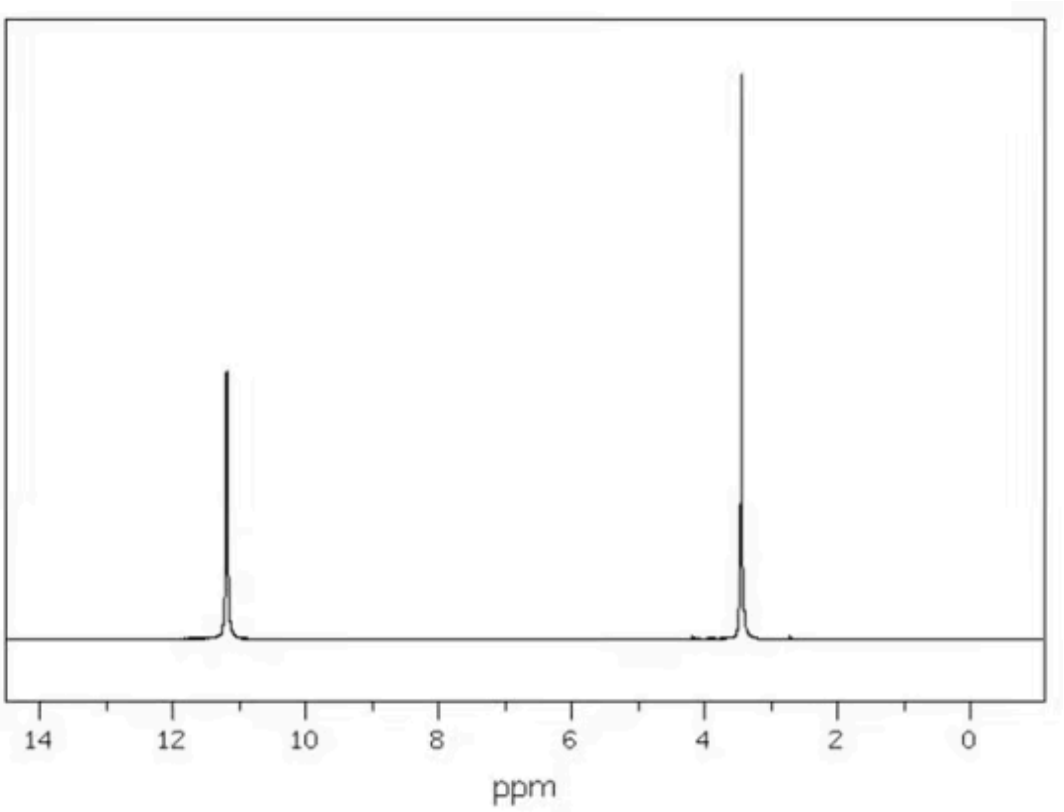
(2 marks)

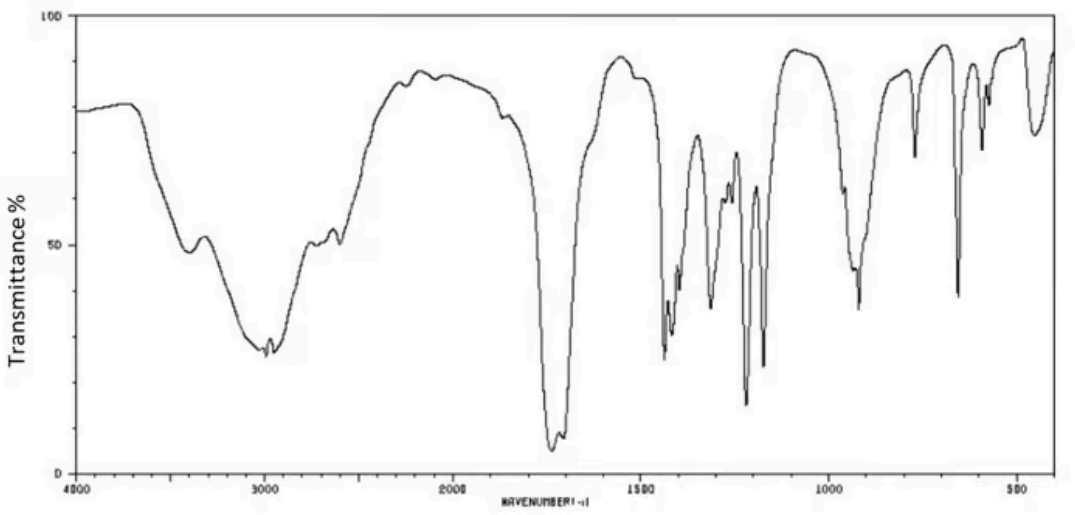
(b) The ^1H NMR spectrum of malonic acid is shown below. Use section 27 of the Data booklet to help you with this question.



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

(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.

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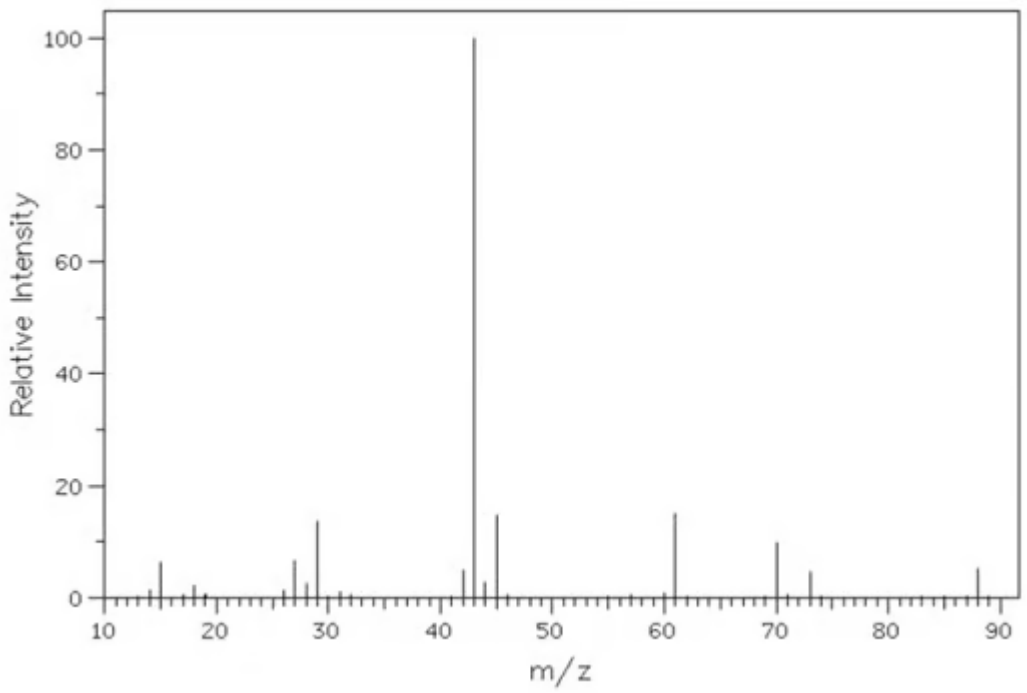
(1 mark)

2 (a) An organic compound, Q, of molecular formula $C_xH_yO_z$, has the following MS. Use section 28 of the Data booklet to help you answer this question.



i) Determine the relative molecular mass of Q and account for the peaks at 15 and 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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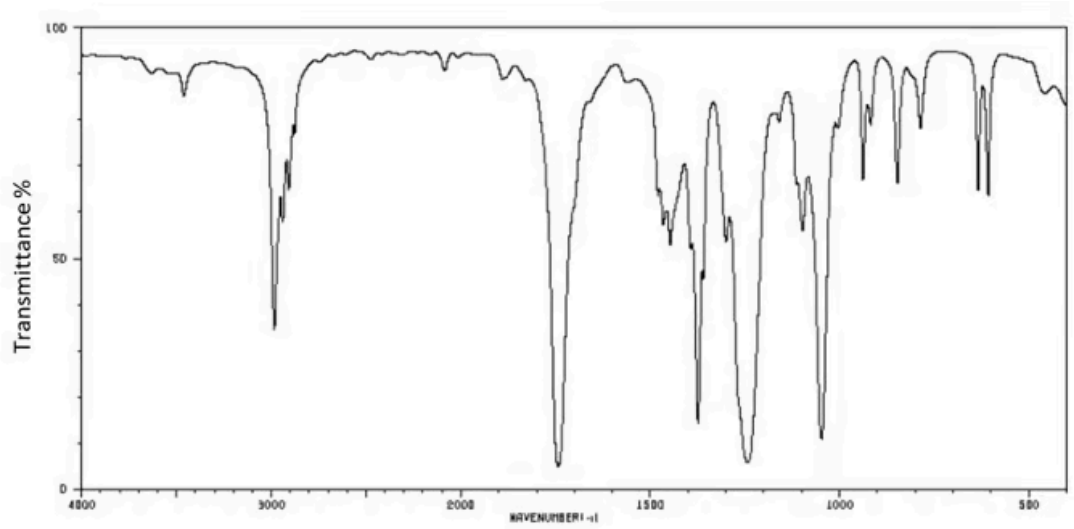
(4 marks)

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



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

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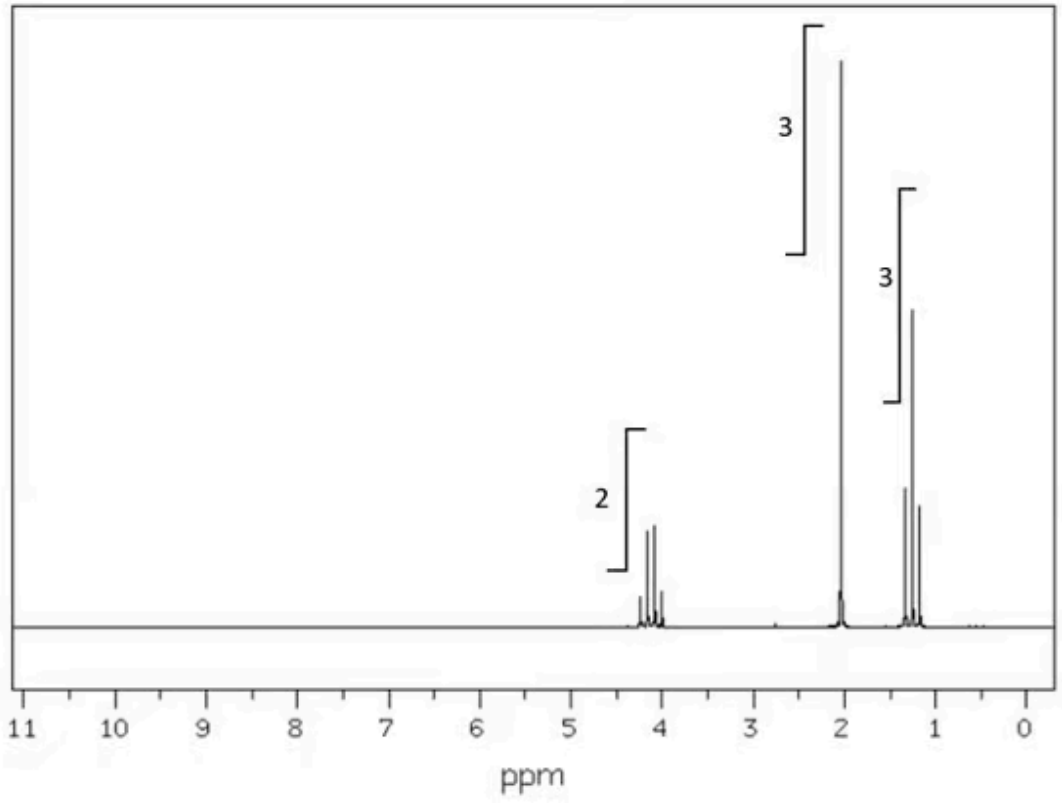
(1 mark)

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



Explain the relative peaks heights and splitting patterns

(5 marks)

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

(3 marks)

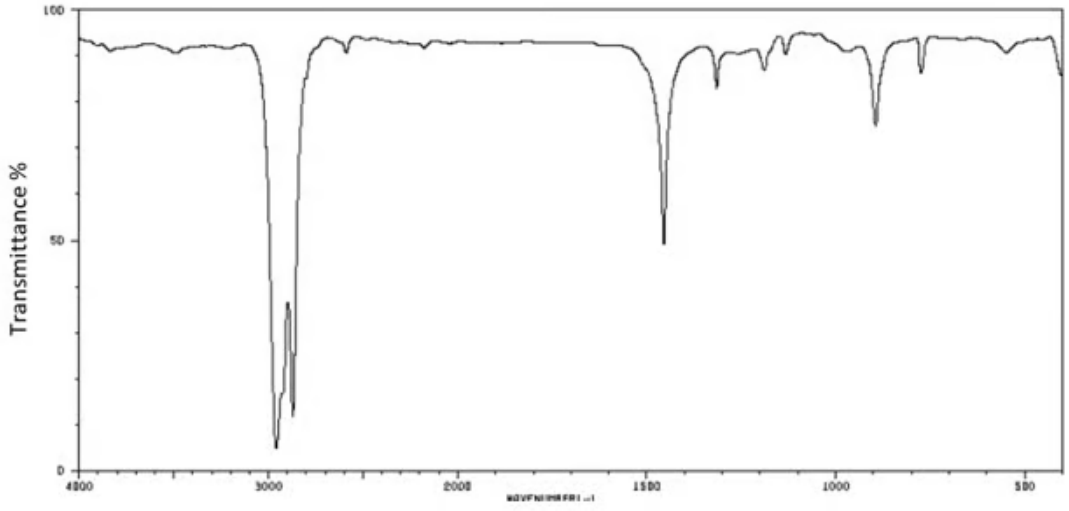
3 (a) Compound A, has molecular formula C_5H_{10} and occurs as 6 isomers. The table below shows the number of signals in the NMR spectrum of each isomer.

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

Suggest a structure for A and F.

(2 marks)

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



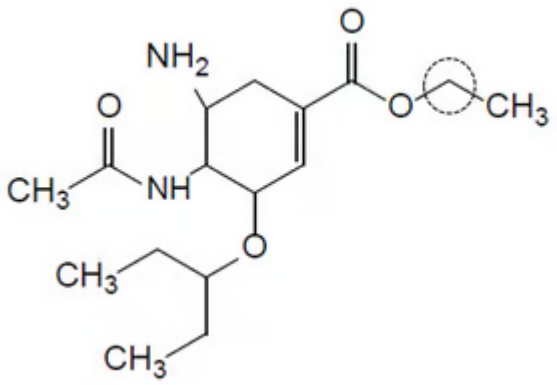
How does this spectrum distinguish A from the other isomers?

(3 marks)

(c) Evaluate whether X-ray crystallography could distinguish between the isomers of A.

(1 mark)

4 (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)

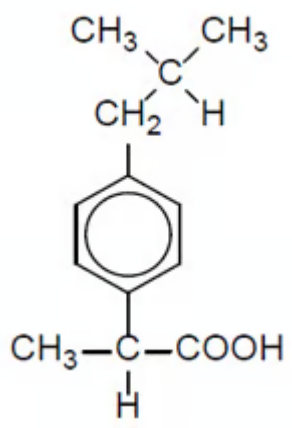
(b) Predict the chemical shift and the splitting pattern seen for the hydrogens on the carbon atom circled in the diagram. Use section 27 of the Data booklet.

(2 marks)

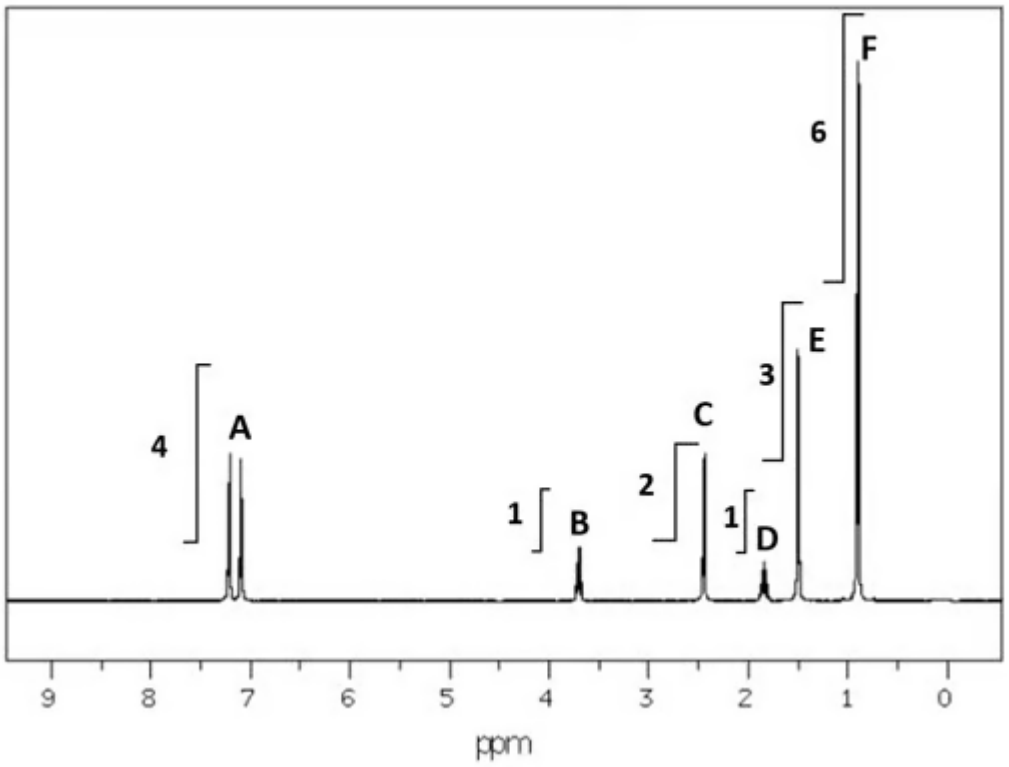
(c) Predict three absorptions you would expect to see in the IR spectrum of oseltamivir. Use section 26 of the data booklet.

(3 marks)

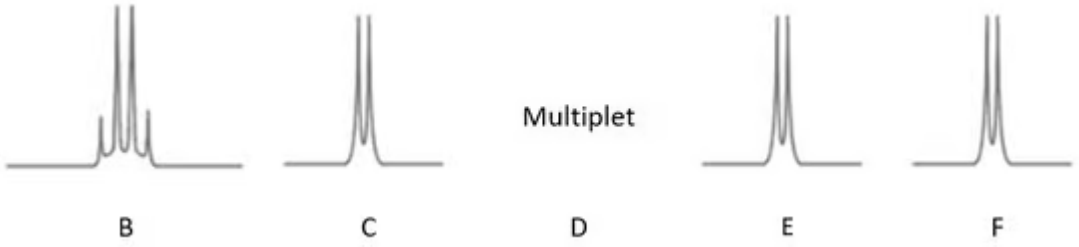
5 (a) Ibuprofen is an important painkilling drug. The structure is:



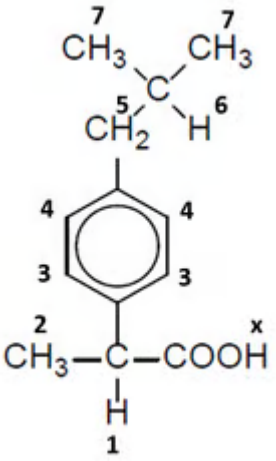
Part of the low resolution ^{1}H NMR spectrum is shown below.



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 26 of the data booklet.

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(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)