

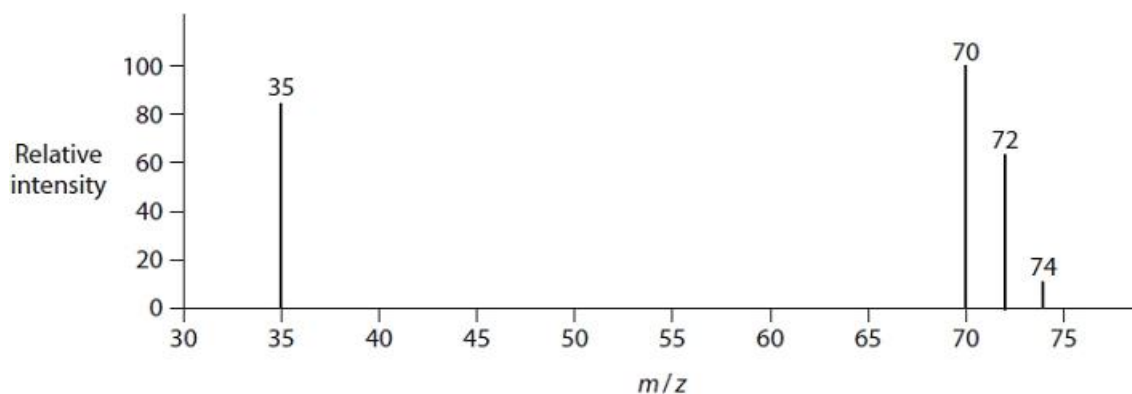
Questions

Q1.

This question is about isotopes, mass spectra and hydrocarbons.

The diagram shows the mass spectrum of a sample of chlorine with one peak missing.

Chlorine has two isotopes, ^{35}Cl and ^{37}Cl , and a relative atomic mass of 35.5



(i) The relative abundance of the isotope ^{35}Cl is 75.5 %.

The relative peak height of this isotope is 82.5 in the mass spectrum.

Calculate the relative peak height of the missing peak caused by the isotope ^{37}Cl .

(2)

(ii) Give a reason for the presence of the three peaks at 70, 72 and 74.

(1)

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(iii) Explain, using calculations, why there is an approximate ratio of 9 : 6 : 1 for the peak heights corresponding to the m/z values of 70, 72 and 74.

(3)

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(Total for question = 6 marks)

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Q2.

A phosphorus atom has mass number 31.

Phosphorus has one naturally occurring isotope with mass number 31.

Chlorine exists as two isotopes with mass numbers 35 and 37.

Give the formulae and mass/charge ratio of the ions responsible for the molecular ion peaks in the mass spectrum of phosphorus(III) chloride, PCl_3 .

(2)

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(Total for question = 2 marks)

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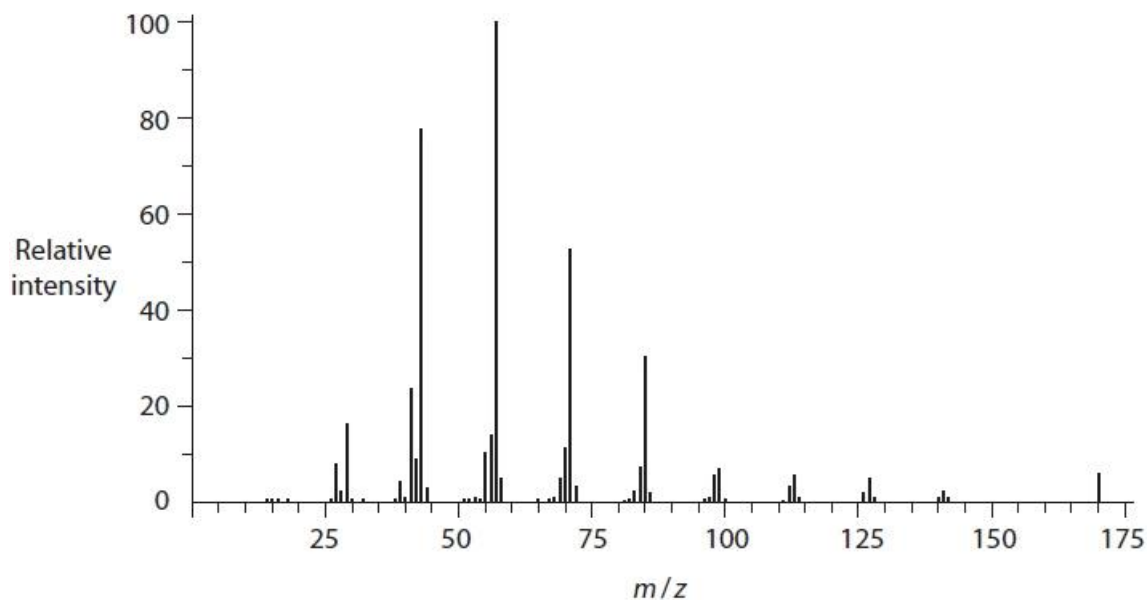
Q3.

This question is about isotopes, mass spectra and hydrocarbons.

The mass spectrum of a hydrocarbon, **B**, which has a molecular formula C_xH_y , is shown.

(i) Determine the relative molecular mass of compound **B**.

(1)



Relative molecular mass of compound **B** is

(ii) Deduce the molecular formula of hydrocarbon **B**.

(1)

(Total for question = 2 marks)

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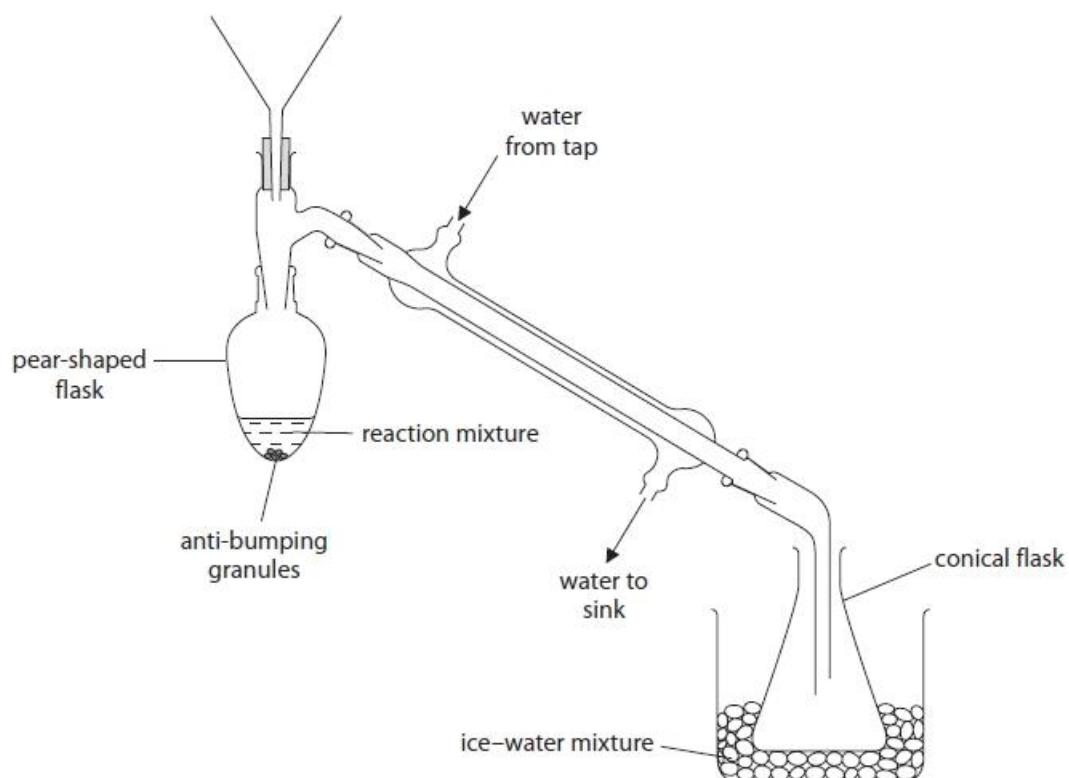
Q4.

This question is about the preparation of a sample of the ketone, 3-methylbutan-2-one.

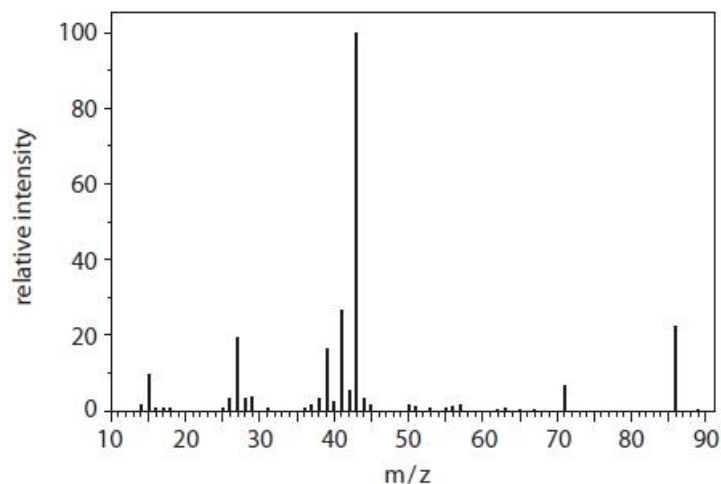
A student's research suggested that 3-methylbutan-2-one may be prepared by oxidising 3-methylbutan-2-ol with acidified potassium dichromate(VI) solution.

The student sets up the apparatus as shown in the diagram. You may assume that all the equipment is suitably clamped.

The student adds dilute sulfuric acid to the pear-shaped flask. A mixture of potassium dichromate(VI) and 3-methylbutan-2-ol is then added slowly to the dilute sulfuric acid in the flask.



The mass spectrum of pure 3-methylbutan-2-one is shown.



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(i) State how you would find the molar mass of 3-methylbutan-2-one from the mass spectrum.

(1)

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(ii) The mass spectrum shows a peak at $m/z = 43$.

Draw the **displayed** formulae of two fragment **ions** that might be responsible for this peak.

(2)

(Total for question = 3 marks)

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Q5.

Answer the question with a cross in the box you think is correct . If you change your mind about an answer, put a line through the box and then mark your new answer with a cross .

This question is about the analysis of organic compounds.

X is an organic compound.

(i) The accurate relative atomic masses, A_r , of the four elements that could make up **X** are shown in the table.

Element	A_r
hydrogen, H	1.0078
carbon, C	12.0000
nitrogen, N	14.0031
oxygen, O	15.9949

X gives a molecular ion peak at $m/z = 100.0522$ on its mass spectrum.
Which is the molecular formula of **X**?

(1)

- A** C_7H_{16}
 B $C_6H_{12}O$
 C $C_6H_{14}N$
 D $C_5H_8O_2$

(ii) The infrared spectrum of **X** contains major absorption wavenumber ranges at 3300–2500 cm^{-1} , 1725–1700 cm^{-1} and 1669–1645 cm^{-1} .

Identify the two functional groups in **X**.

(2)

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(iii) **X** has an unbranched carbon chain and does **not** exhibit geometric isomerism.

Draw the **skeletal formula** of **X**.

(1)

(Total for question = 4 marks)

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Q6.

Ethane can also be converted into chloroethane.

(i) Give the reagent and condition required to convert ethane into chloroethane.

(1)

Reagent

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Condition

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(ii) What is the mechanism and type of reaction by which ethane is converted into chloroethane?

(1)

- A** electrophilic addition
- B** free radical addition
- C** free radical substitution
- D** nucleophilic substitution

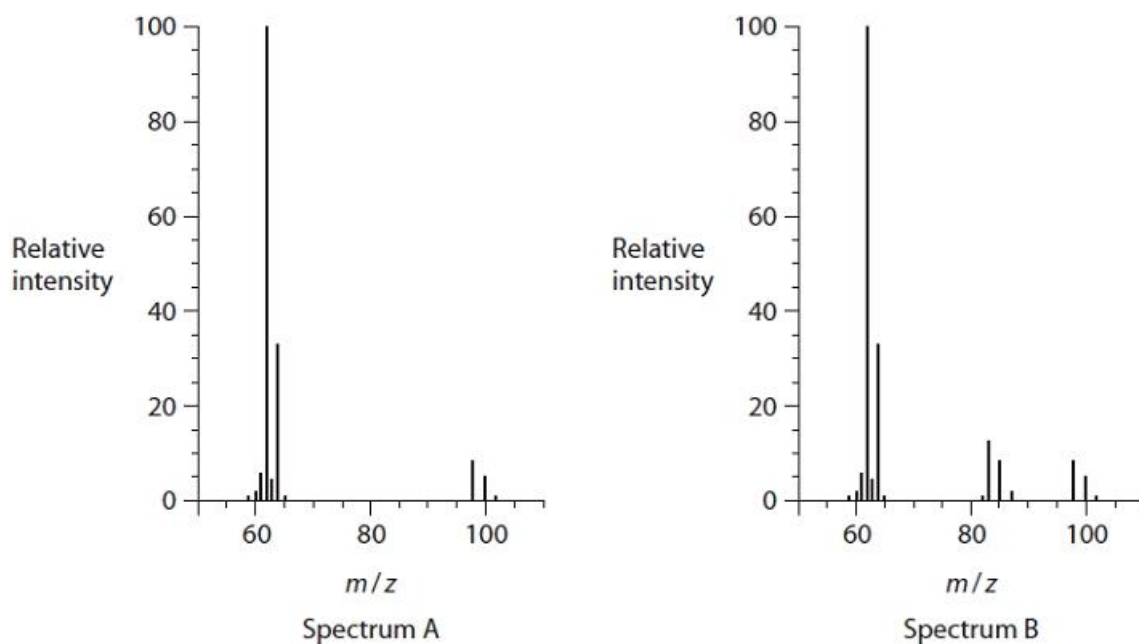
(iii) Further reactions of chloroethane result in the formation of small amounts of the isomers 1,1-dichloroethane and 1,2-dichloroethane.

Write equations to show the formation of these products.
Curly arrows are not required.

(3)

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(iv) The mass spectra of the two isomers of dichloroethane are shown.



Deduce the molecular formulae of the species responsible for the molecular ion peaks at m/z 98, 100 and 102.

The molecular formulae for the species producing these peaks are the same in both spectra.

(2)

(v) State why in both spectra the peaks at 98, 100 and 102 have different relative intensities.

(1)

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(vi) Explain how the presence of the peaks at 83, 85 and 87 in Spectrum B allows the identification of the isomer responsible for this spectrum.

(2)

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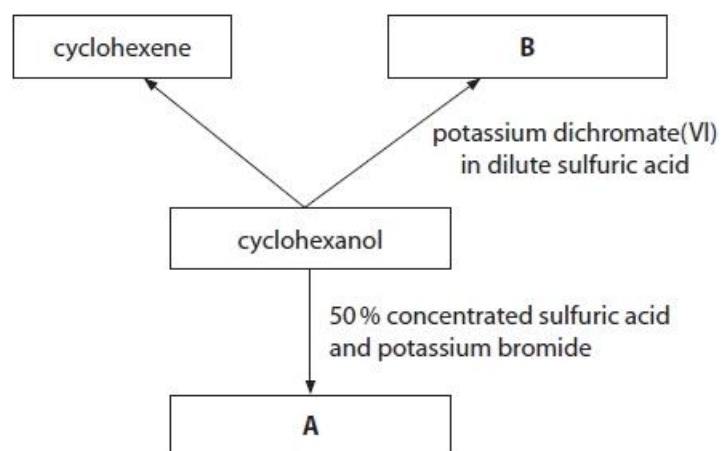
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(Total for question = 10 marks)

Q7.

This question is about some reactions of cyclohexanol.



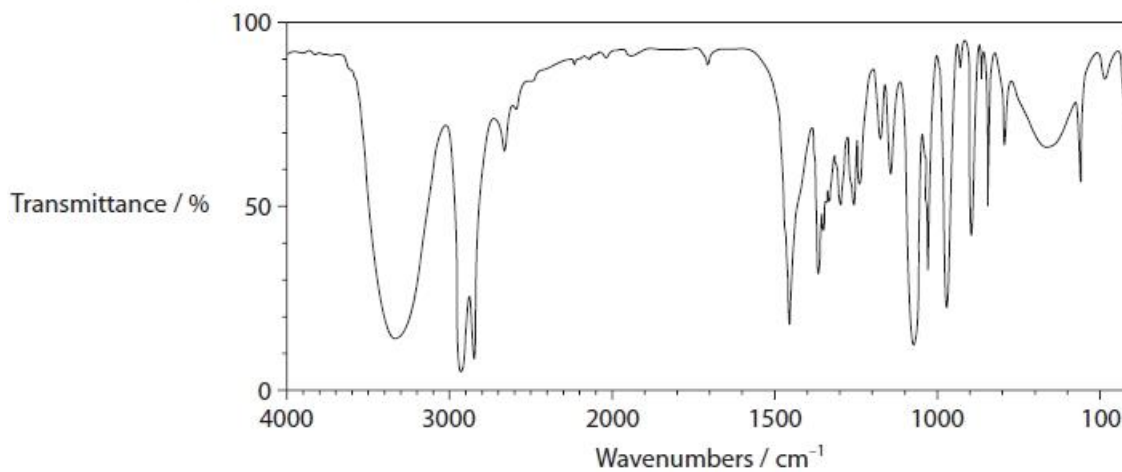
(i) Give the name **and** displayed formula of compound **B**.

(2)

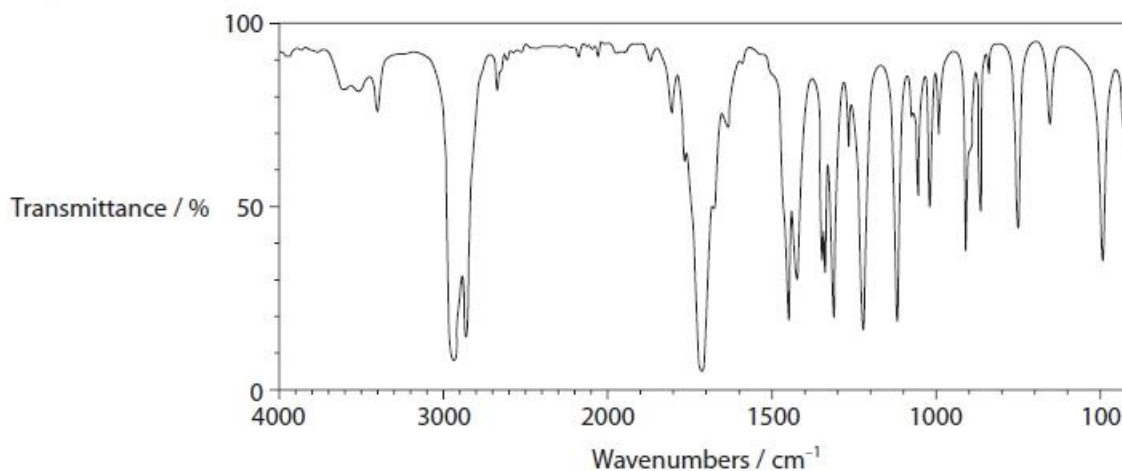
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(ii) The infrared (IR) spectra of cyclohexanol and compound **B** are shown.

IR Spectrum of cyclohexanol



IR Spectrum of compound **B**



Identify the bonds, using **both** IR spectra, that help to confirm the reaction of cyclohexanol to produce compound **B**.

Your answer must include the wavenumber ranges of any relevant bonds.

(2)

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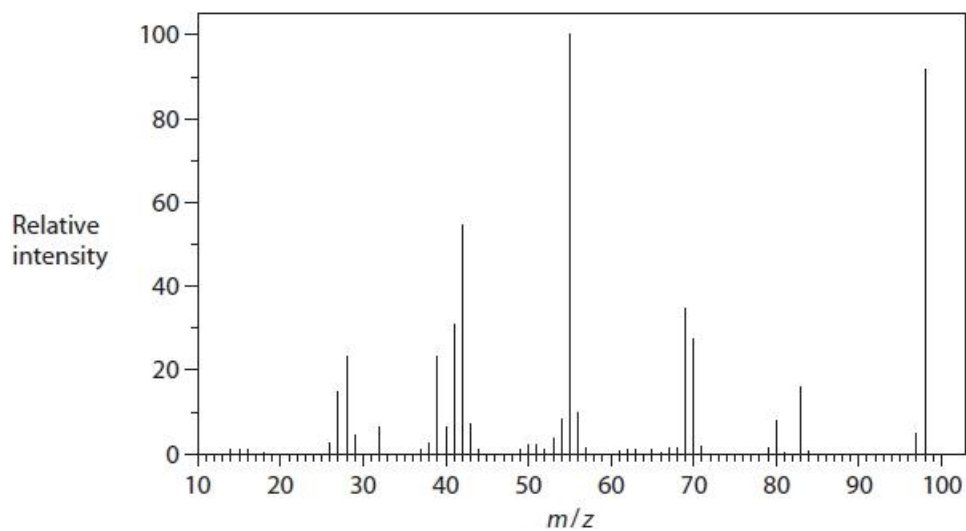
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(iii) The mass spectrum of compound **B** is shown.



Deduce the relative molecular mass of compound **B** using the mass spectrum. Justify your answer.

(1)

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(iv) In the mass spectrum of cyclohexanol, there is a peak at $m/z = 83$.

Give the formula of a fragment that could be responsible for this peak.

(2)

(Total for question = 7 marks)

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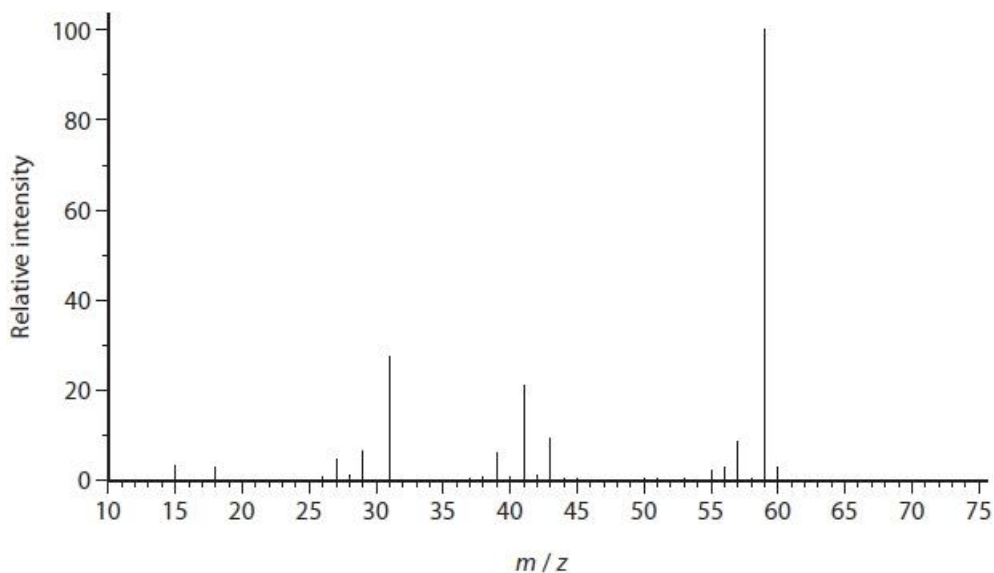
Q8.

This question is about 2-methylpropan-2-ol.

(a) Draw the fully **displayed** formula of 2-methylpropan-2-ol.

(1)

(b) The mass spectrum of 2-methylpropan-2-ol is shown.



(i) The relative molecular mass of 2-methylpropan-2-ol is 74.

Give a possible reason why there is no molecular ion peak in the mass spectrum of 2-methylpropan-2-ol.

(1)

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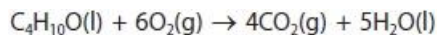
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(ii) Write the formula for a species that could be responsible for the peak at $m/z = 59$.

(1)

(c) The equation for the complete combustion of 2-methylpropan-2-ol is



(i) Using the bond enthalpies shown in the table, calculate a value for the enthalpy change, in kJ mol^{-1} , for the complete combustion of 2-methylpropan-2-ol.

(4)

Bond	Mean bond enthalpy / kJ mol^{-1}
C—C	347
C—H	413
C—O	358
O—H	464
O=O	498
C=O	805

(ii) 2-methylpropan-2-ol burns in air with a smoky flame.

Explain how burning with a smoky flame affects the value of the experimentally determined enthalpy change of combustion.

(2)

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(iii) A Data Book value for the enthalpy change of combustion of 2-methylpropan-2-ol is $-2643.8 \text{ kJ mol}^{-1}$.

Give the main reason for the difference between this value and your answer to part (c)(i).

(1)

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(Total for question = 10 marks)

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Q9.

This question is about the identification of an alcohol, **X**.

(a) Alcohol **X** has the following percentage composition by mass:

carbon, C = 68.2%

hydrogen, H = 13.6%

oxygen, O = 18.2%

The molecular ion peak in the mass spectrum for alcohol **X** occurs at $m/z = 88$.
Use all of these data to show that the molecular formula for alcohol **X** is $C_5H_{12}O$. Include your working.

(2)

(b) (i) When alcohol **X** is oxidised, a carboxylic acid is formed.

State what information this gives about alcohol **X**.

(1)

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(ii) Draw the **displayed** formulae of the four possible structural isomers that could be alcohol **X**.

(3)

Alcohol 1	Alcohol 2
Alcohol 3	Alcohol 4

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- (iii) The mass spectrum of alcohol **X** has a major peak at $m/z = 45$.
Draw the structure of the species that could give this peak.

(1)

- (iv) Alcohol **X** has a branched chain.
Identify alcohol **X**, explaining your reasoning.

(2)

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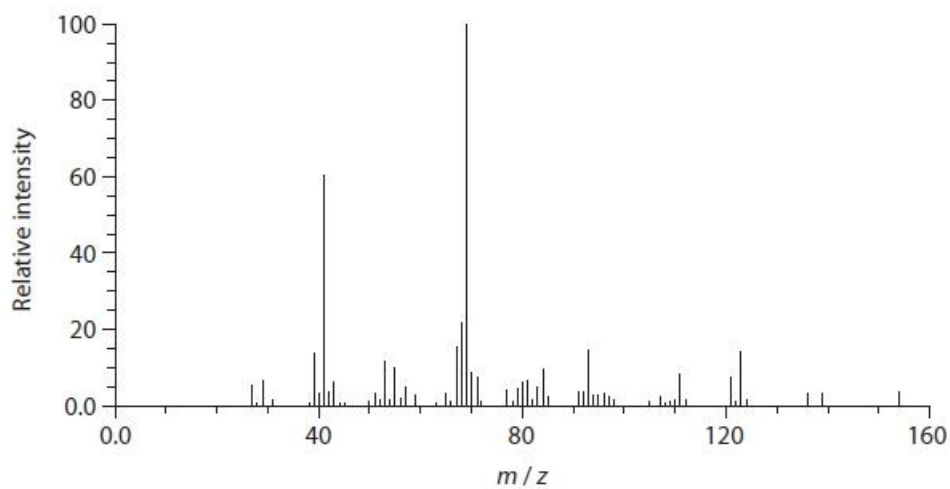
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(Total for question = 9 marks)

Q10.

The mass spectrum of geraniol is shown.



(i) Show that this mass spectrum can be used to confirm the molar mass of geraniol.

(1)

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(ii) Identify an ion that could be responsible for the peak at $m/z = 69$.

(1)

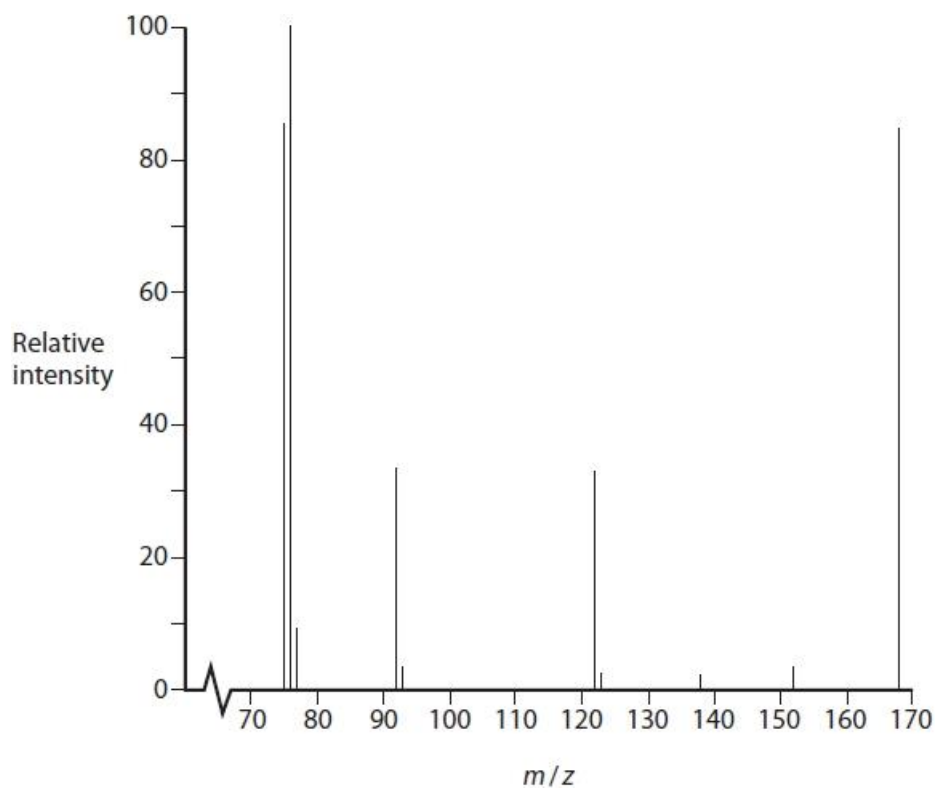
(Total for question = 2 marks)

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Q11.

Organic compound **D** contains the elements carbon, hydrogen, oxygen and nitrogen only.

Part of the mass spectrum of **D** is shown.



Deduce the molecular formula of **D**. Justify your answer.

(2)

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(Total for question = 2 marks)

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Q12.

This question is about organic compounds containing fluorine and chlorine.

The use of chlorofluorocarbons as refrigerants has ceased due to concerns about their effects on the ozone layer. One such compound is dichlorodifluoromethane.

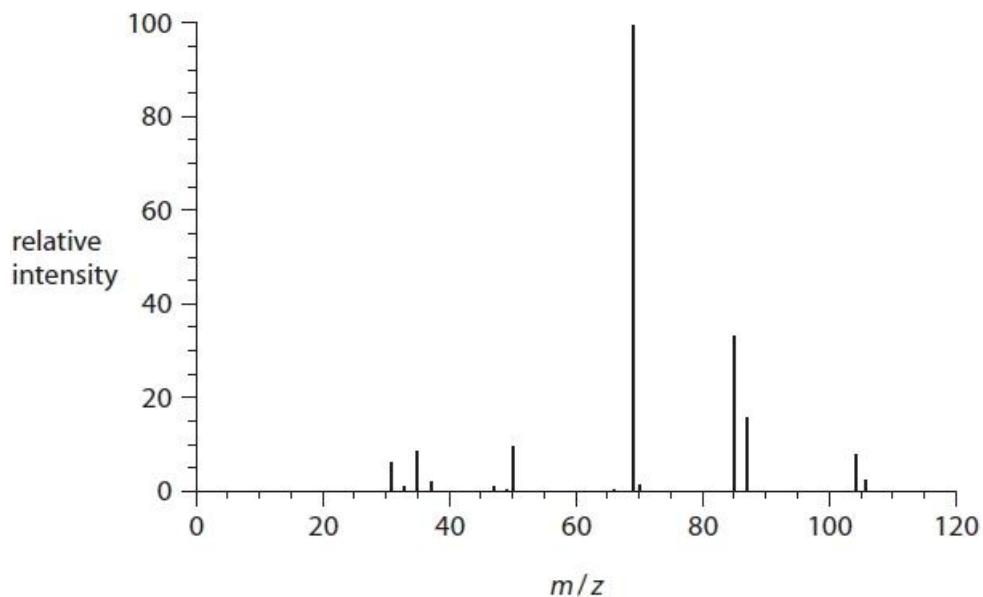
(i) A different refrigerant contains 34.0% chlorine and 54.5% fluorine by mass, with the remainder carbon.

Calculate the empirical formula of this compound.

(3)

(ii) Use the mass spectrum to show that the empirical and the molecular formulae of this compound are the same.

(1)



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(iii) Suggest the species responsible for the peak at $m/z = 69$.

(1)

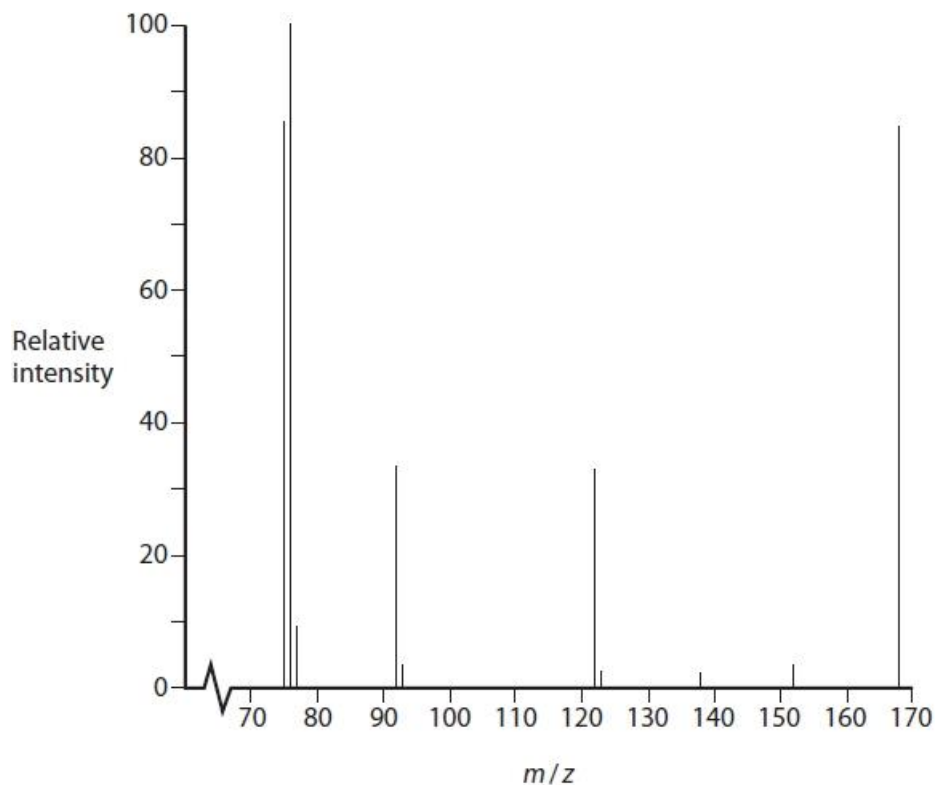
(Total for question = 5 marks)

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Q13.

Organic compound **D** contains the elements carbon, hydrogen, oxygen and nitrogen only.

Part of the mass spectrum of **D** is shown.



Compound **D** contains a benzene ring.

(i) Give the molecular formula of the species that causes the peak at $m/z = 76$ in the mass spectrum of **D**.

.....

(1)

(ii) Draw the structures of the **three** possible isomers of **D** containing a benzene ring.

(2)

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(iii) The ^{13}C NMR spectrum of compound **D** has four peaks.

Identify the structure of **D**. Justify your answer by labelling the different carbon environments in **all** the structures drawn in (ii).

(3)

(Total for question = 6 marks)