



Questions

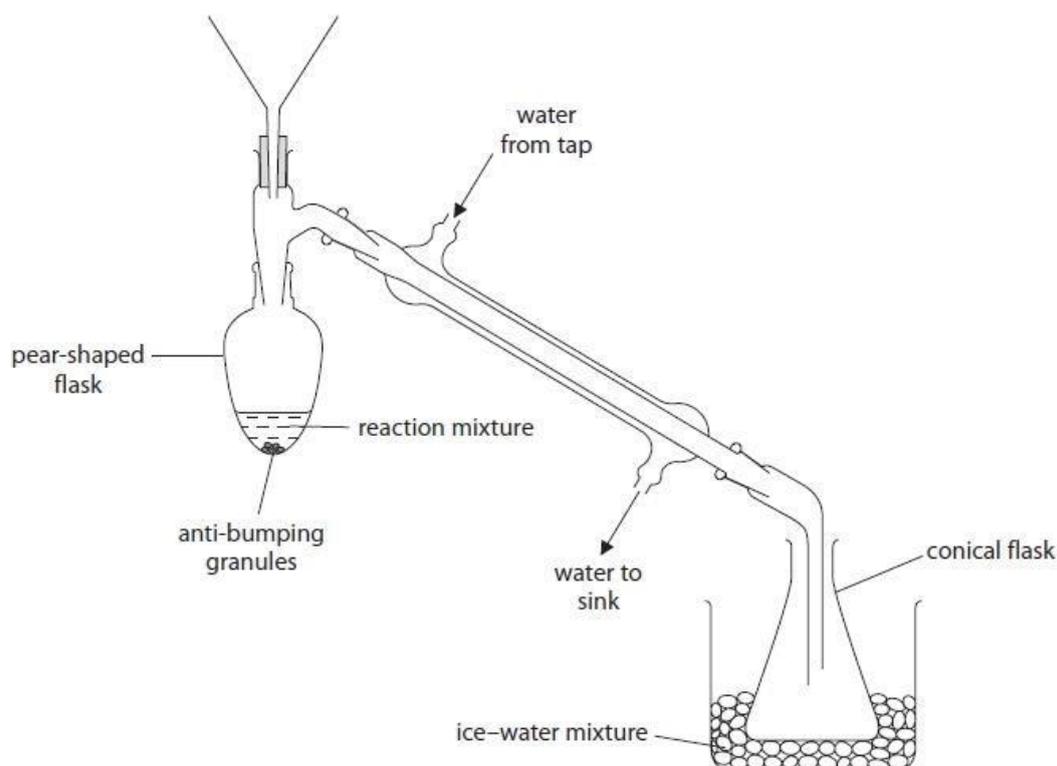
Q1.

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.

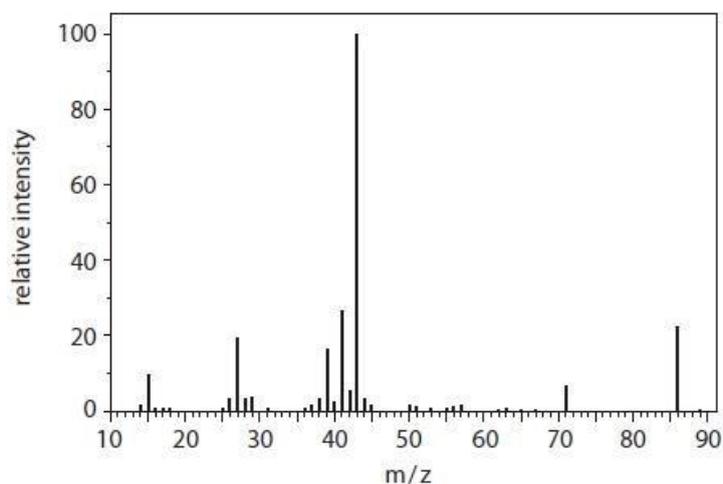
The student sets up the apparatus as shown in the diagram. You may assume that all the equipment is suitably clamped.

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.



(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)



Q2.

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

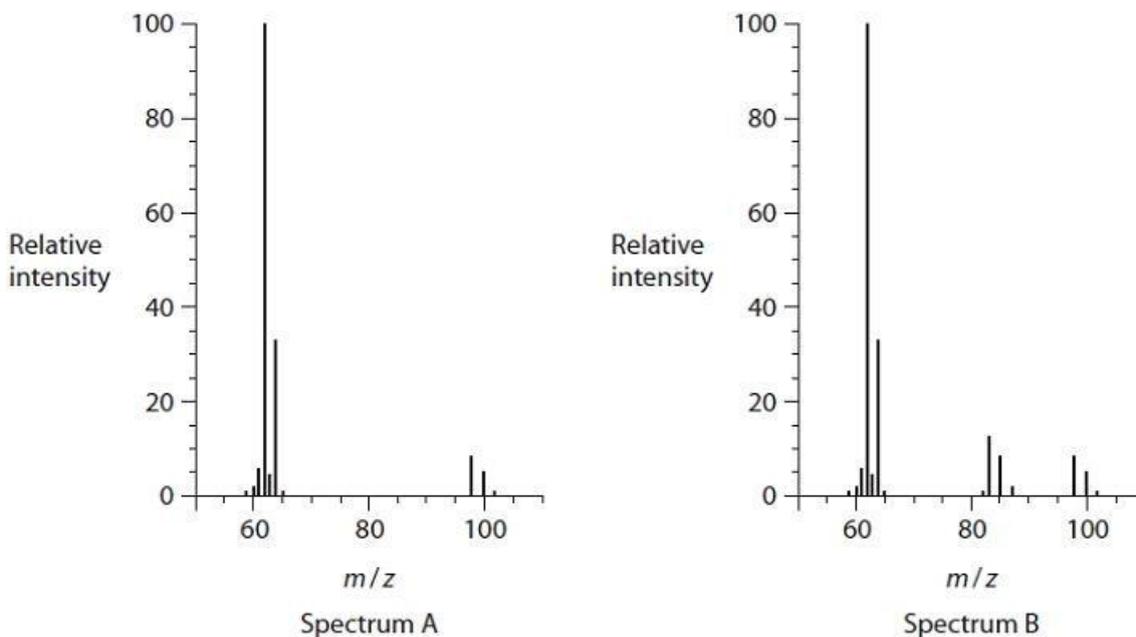
(iii) Further reactions of chloroethane result in the formation of small amounts of the isomers 1,1-dichloroethane and 1,2-dichloroethane.

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

(3)



(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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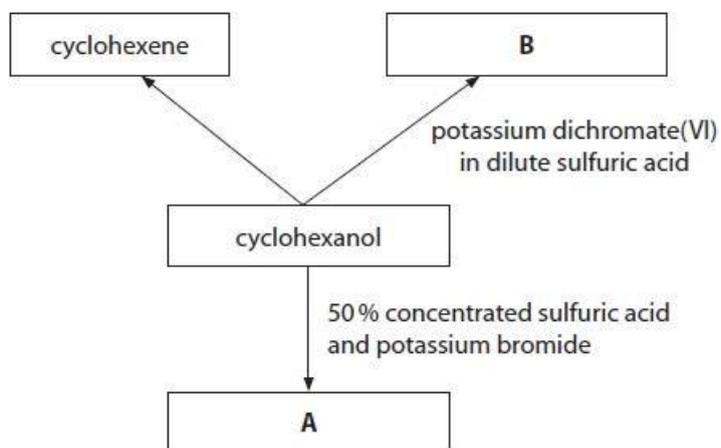
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(Total for question = 10 marks)



Q3.

This question is about some reactions of cyclohexanol.



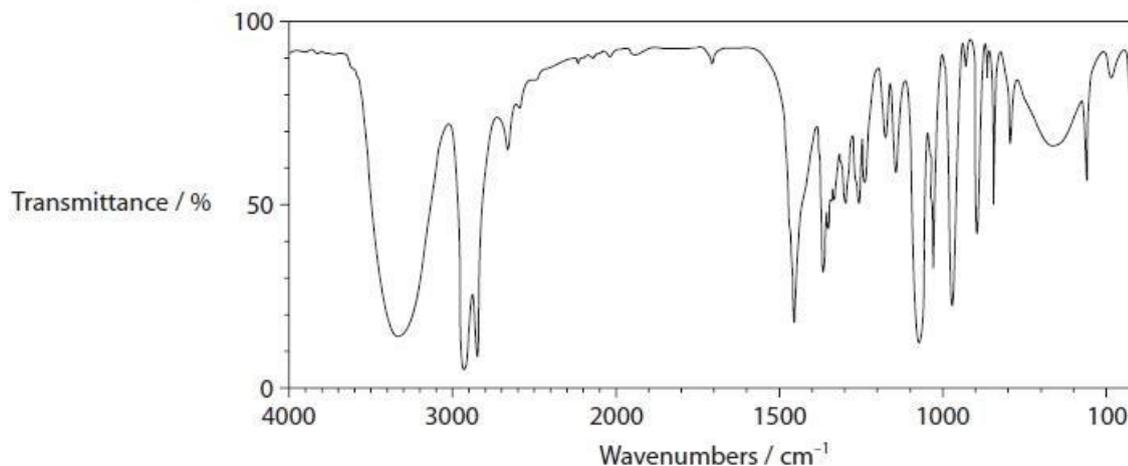
(i) Give the name **and** displayed formula of compound **B**.

(2)

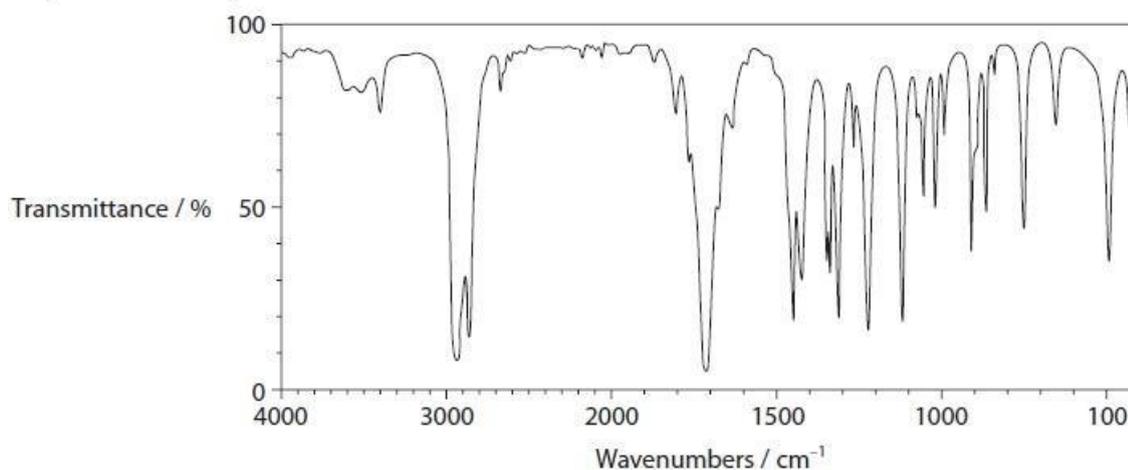


(ii) The infrared (IR) spectra of cyclohexanol and compound **B** are shown.

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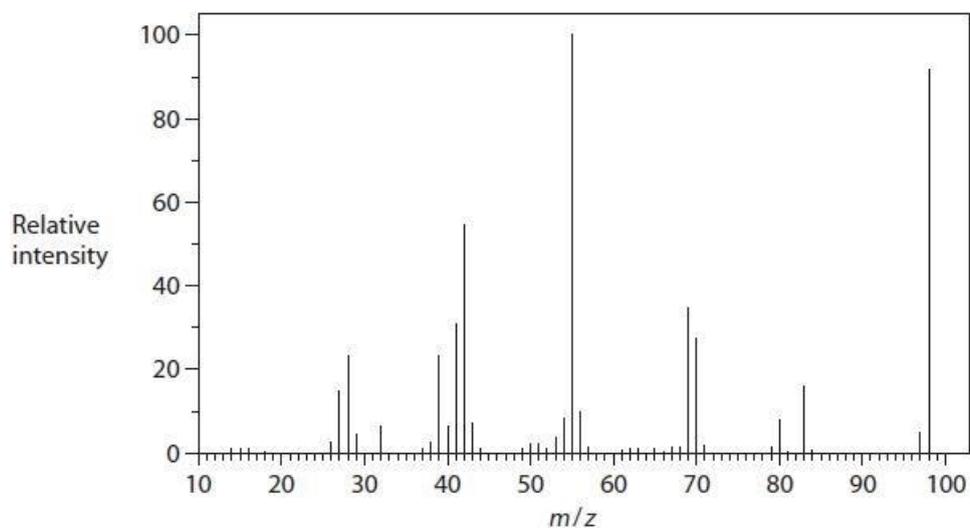
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(iii) The mass spectrum of compound **B** is shown.



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)



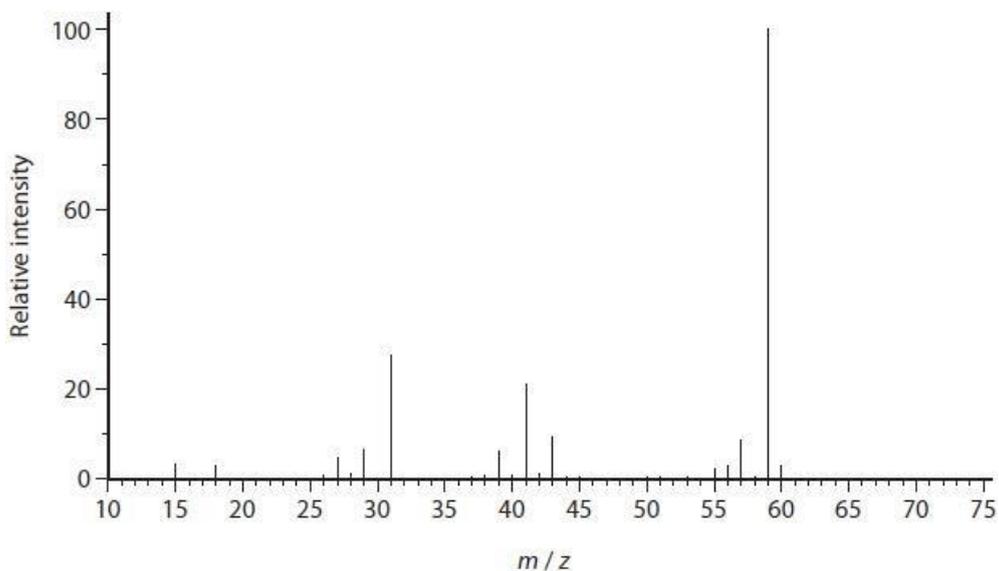
Q4.

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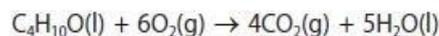
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(ii) Write the formula for a species that could be responsible for the peak at $m/z = 59$.

(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)



Q5.

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



(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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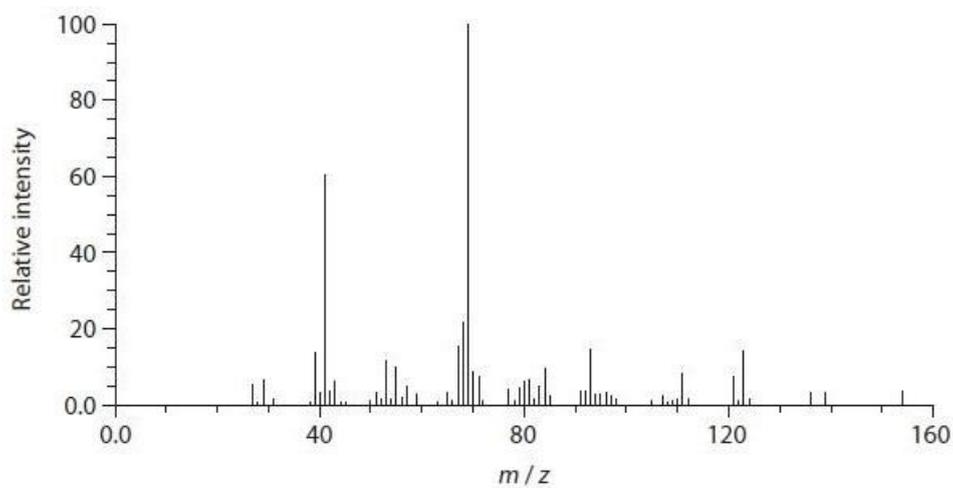
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(Total for question = 9 marks)



Q6.

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)

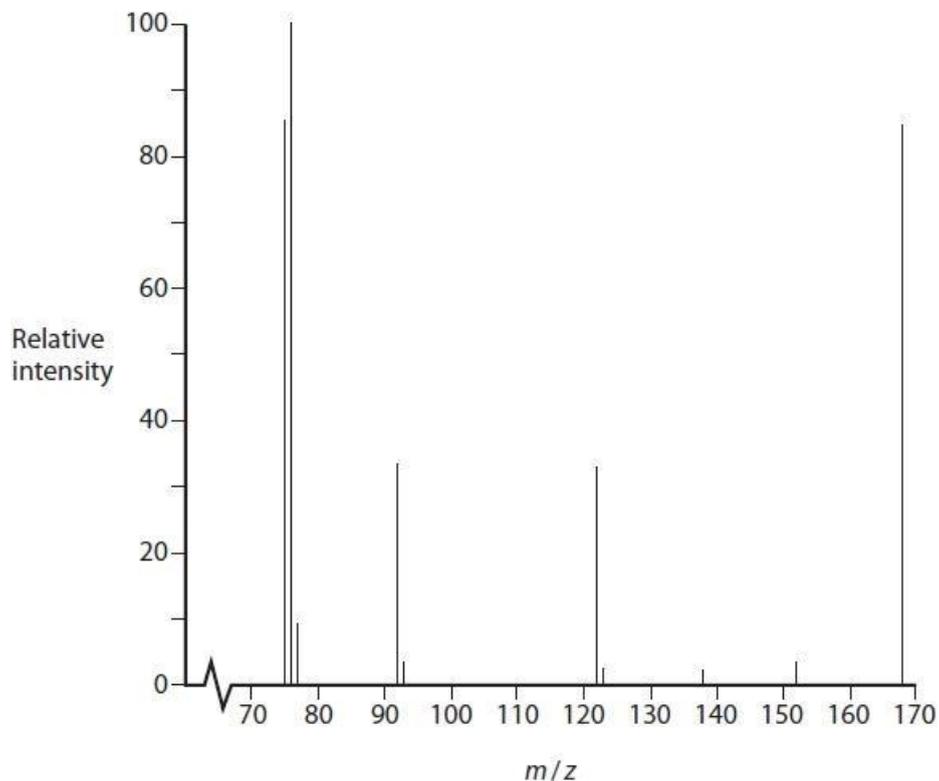
(Total for question = 2 marks)



Q7.

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)



Q8.

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.

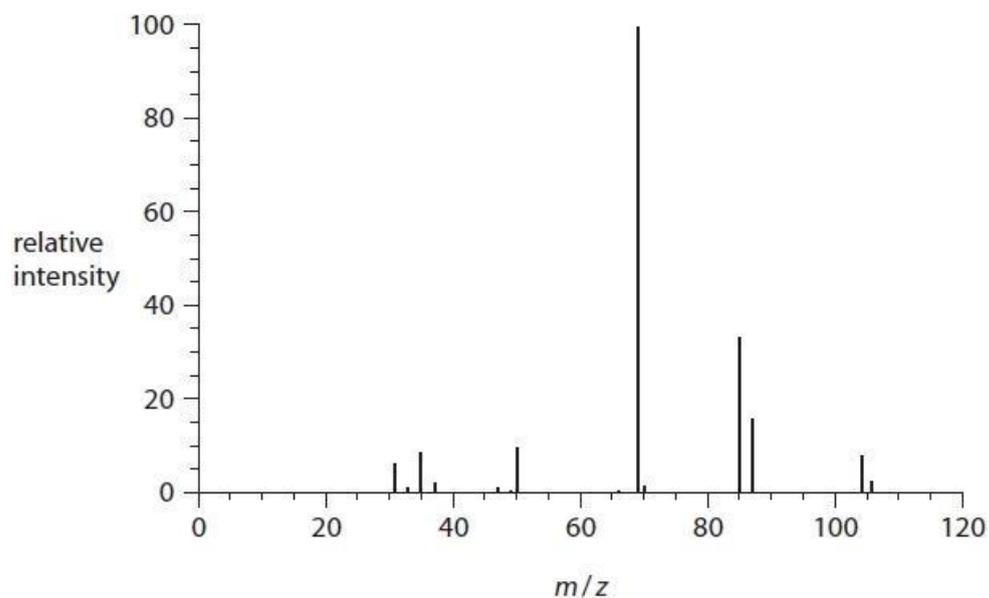
(i) A different refrigerant contains 34.0% chlorine and 54.5% fluorine by mass, with the remainder carbon.

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)

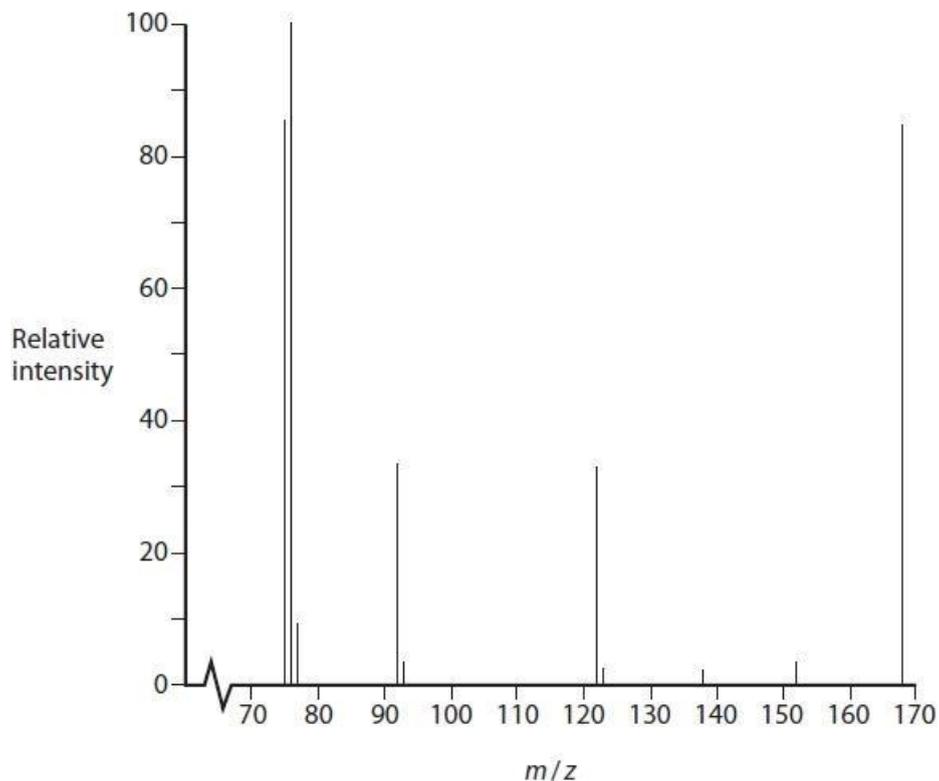
(Total for question = 5 marks)



Q9.

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)



(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).

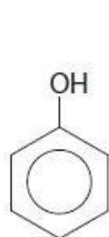
(3)

(Total for question = 6 marks)

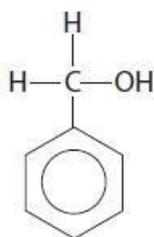


Q10.

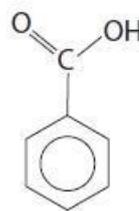
This is a question about the analysis of three aromatic substances with —OH groups.



phenol



phenylmethanol



benzoic acid

Spectroscopy is an effective means of distinguishing between molecules.

- (i) Compare and contrast the infrared spectra of phenol, phenylmethanol and benzoic acid. Include relevant bonds and their wavenumber ranges using the Data Booklet.

(5)

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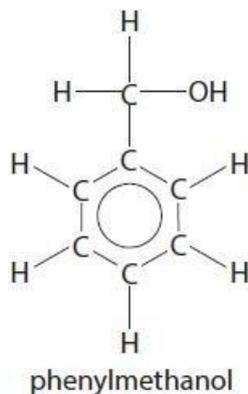
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(ii) Predict the number of peaks present, and their chemical shifts, in the ^{13}C nuclear magnetic resonance (NMR) spectrum of phenylmethanol.

Use the information in the Data Booklet to help you.

(3)



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(iii) Give the formula of a fragment ion, with its m/z value, that you would expect to be present in the mass spectrum of benzoic acid but **not** in the mass spectrum of phenol or the mass spectrum of phenylmethanol.

(2)

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(Total for question = 10 marks)



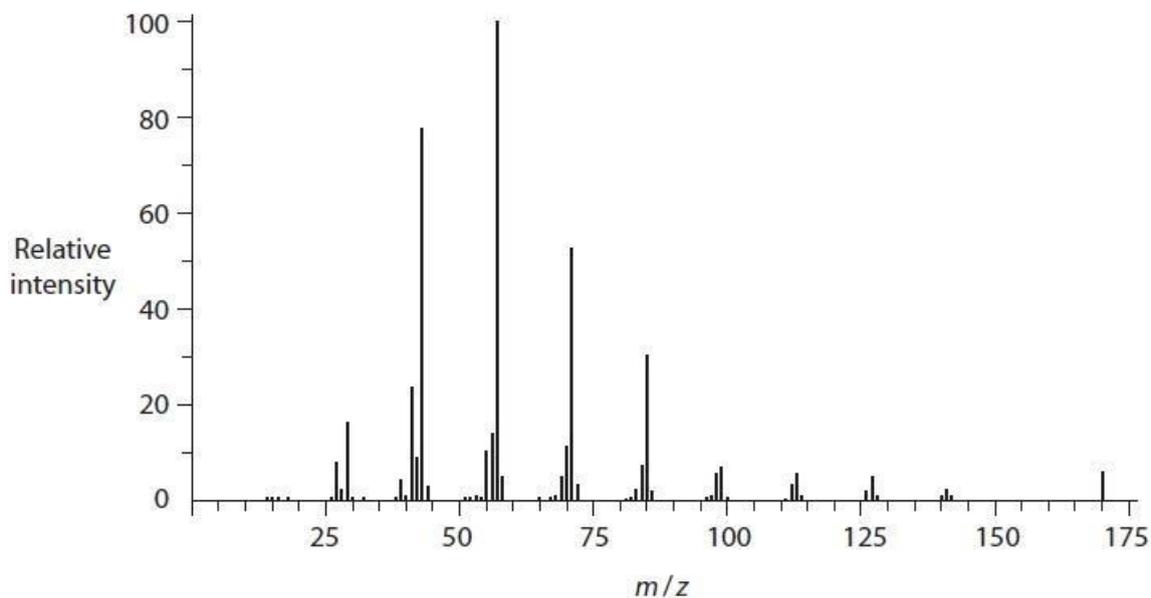
Q11.

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)