

# Identification of 10 Compounds by Combined Modern Analytical Techniques **ANSWERS**

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NMR



MS



IR



# Introduction

In each of these problems, you are given a range of information and spectra about 10 unknown compounds.

For each compound, it is recommended that you begin by using the **% composition data** to work out the **empirical formula**.

The **mass spectrum** will then allow you to determine the **molecular formula**. Don't forget the **m+1 peak!** This is caused by some of the molecules (at least 1 in 100) having **<sup>13</sup>C atoms** in them. The more carbon atoms the molecule has, the greater the relative size of this peak to the m<sup>+</sup> peak. (It's a simple probability thing!)

Try to get as much from the **molecular formula** as you can! Think about levels of saturation (C to H ratio). For example, if you have a hydrocarbon with general formula C<sub>n</sub>H<sub>2n+2</sub> then you know that the compound is saturated and aliphatic. Very high carbon to hydrogen ratios (around 1:1) suggest that the compound is aromatic (an arene). Also, check to see if there are 2 oxygens present. This would suggest an ester or carboxylic acid. This isn't guaranteed but a good starting point.

You should now have some clues as to the possible functional groups that the compound could contain. The **infra-red spectrum** will help confirm the identity of some functional groups. This is especially useful for identifying the presence of **-OH** (alcohols and carboxylic acids) and **C=O** (aldehydes, ketones, carboxylic acids and amides).

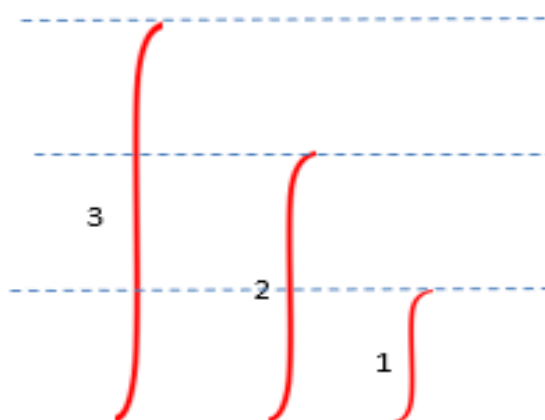
The **<sup>1</sup>H** and **<sup>13</sup>C NMR spectra** should confirm the arrangement of the **H** and **C** atoms in the molecule.

## Integration.

For the **<sup>1</sup>H NMR** you will see an integration curve for each peak or multiplet.

The **relative heights** of these integration lines gives you the **relative number of hydrogens** represented by that peak.

Measure the heights of the **red integration lines** and then find the ratio of their heights.

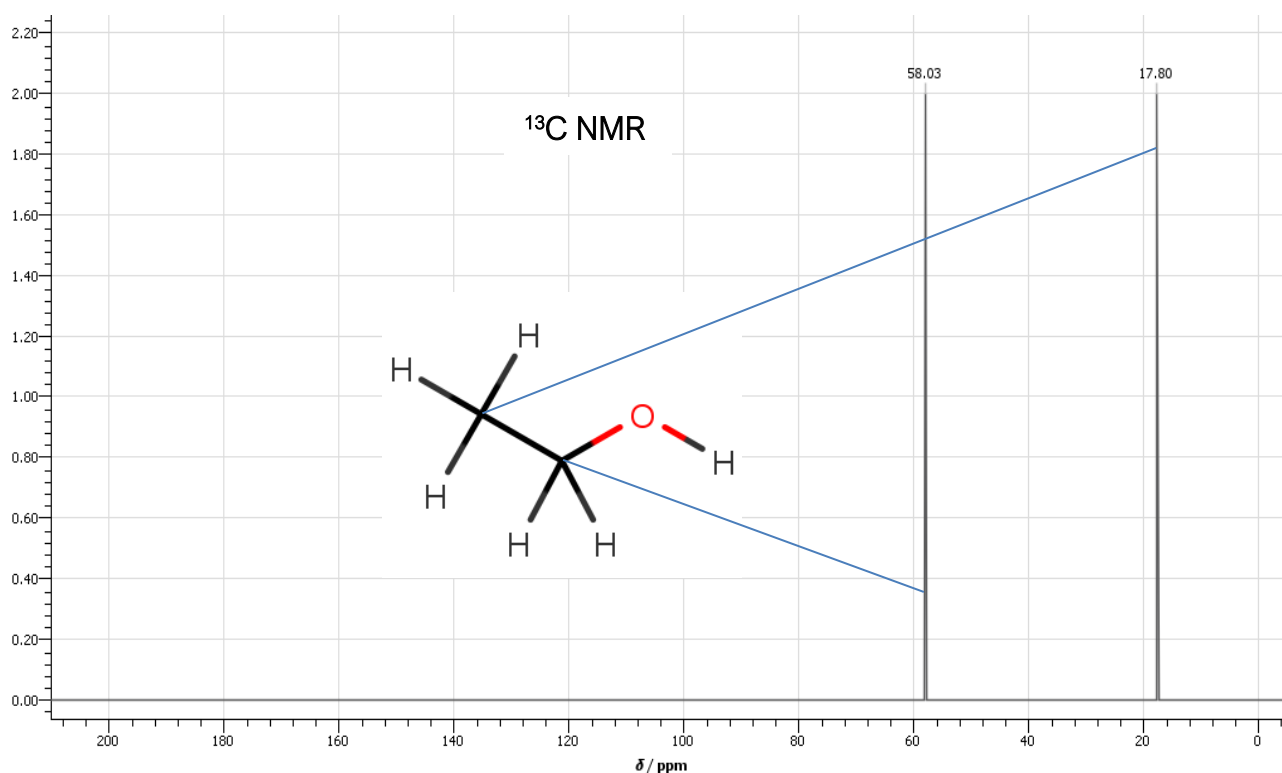
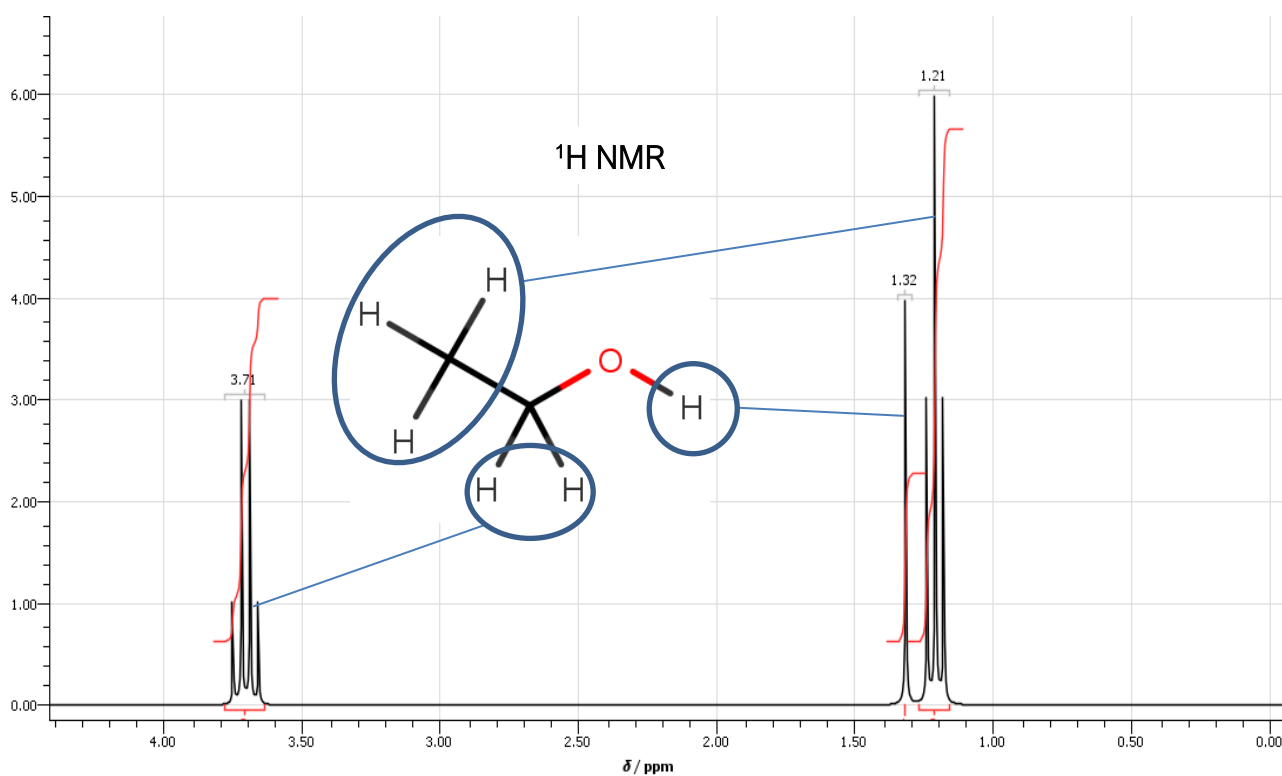


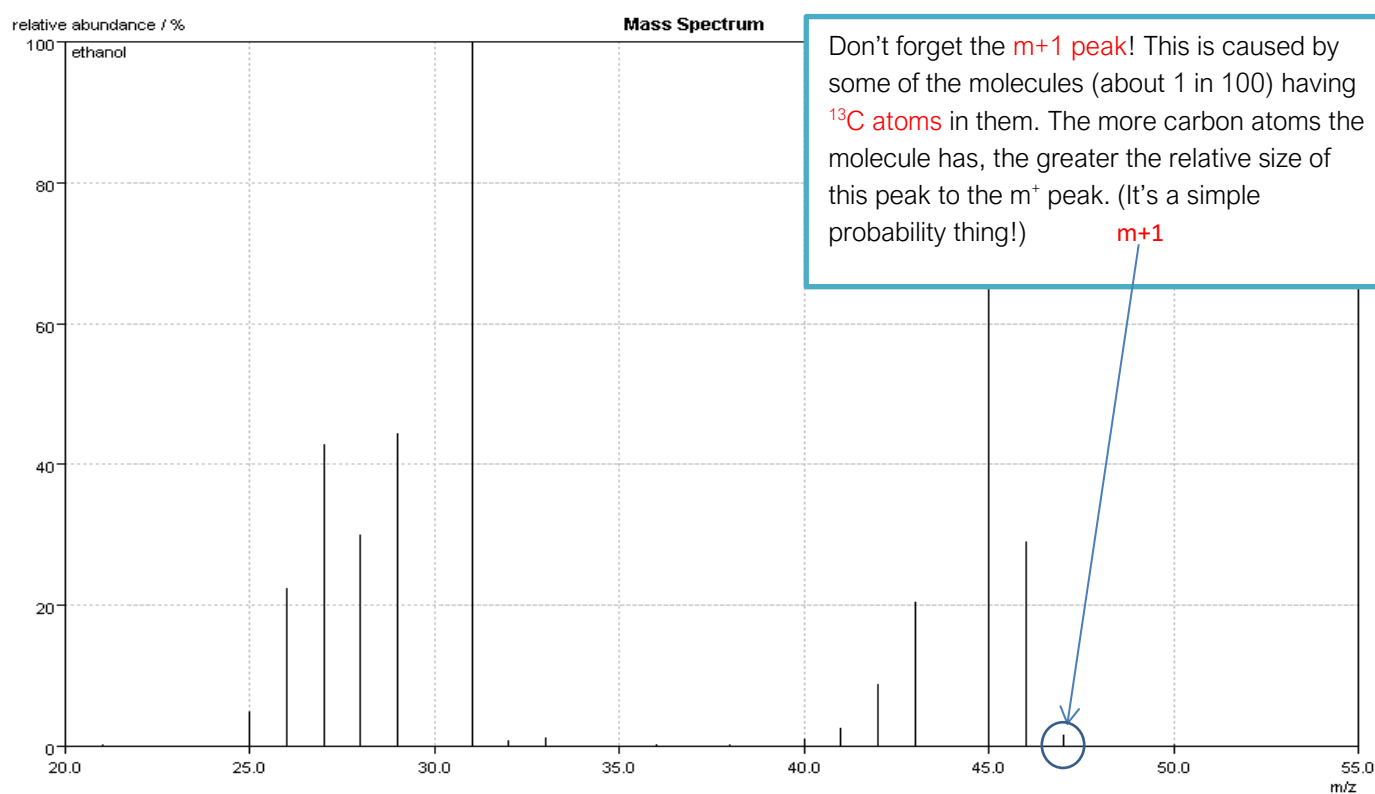
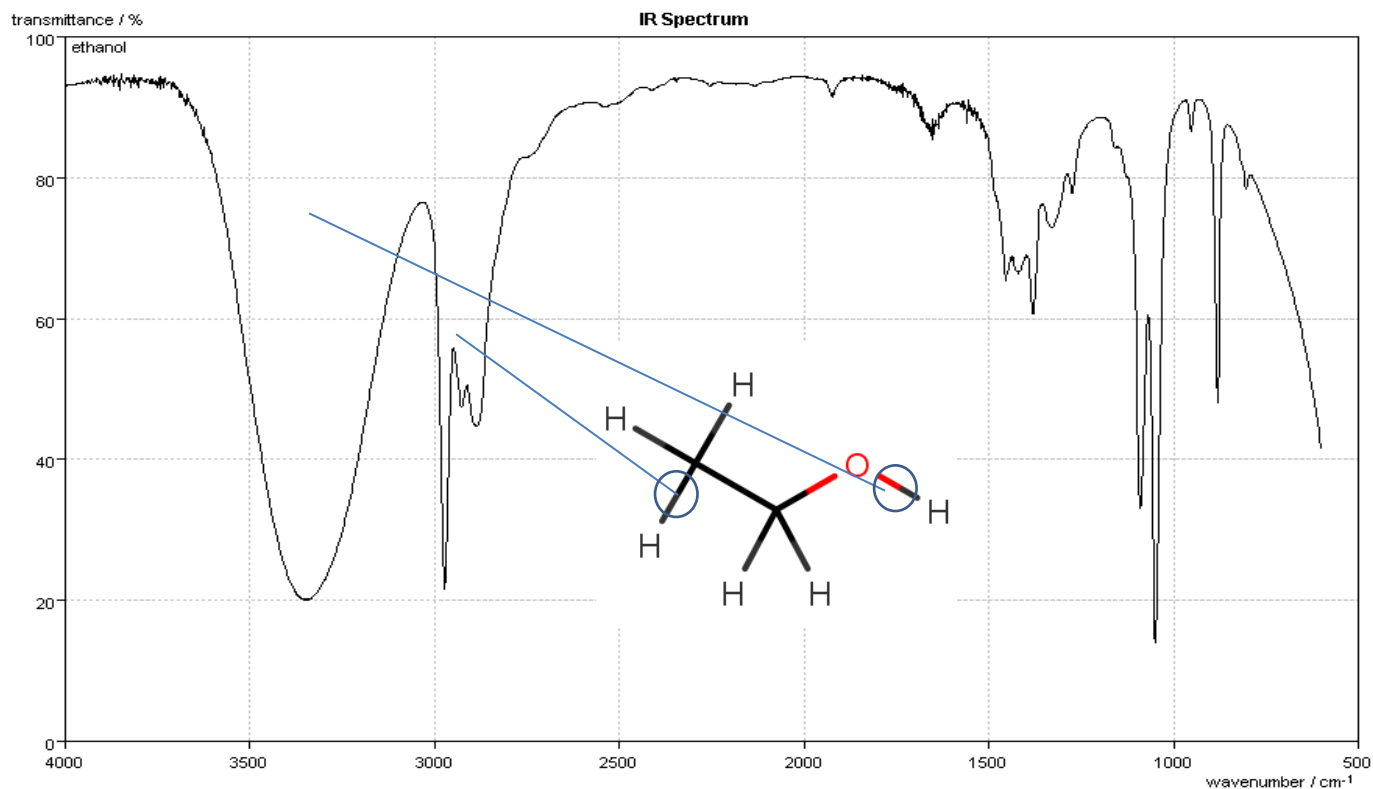
## Compound 1 ANSWERS

description: Colourless volatile liquid

composition: C 52.17%; H 13.04%; O 34.78%

molecular formula:  $C_2H_5OH$  ethanol





### Further Information:

Colourless liquid that mixes completely with water to form a neutral solution.

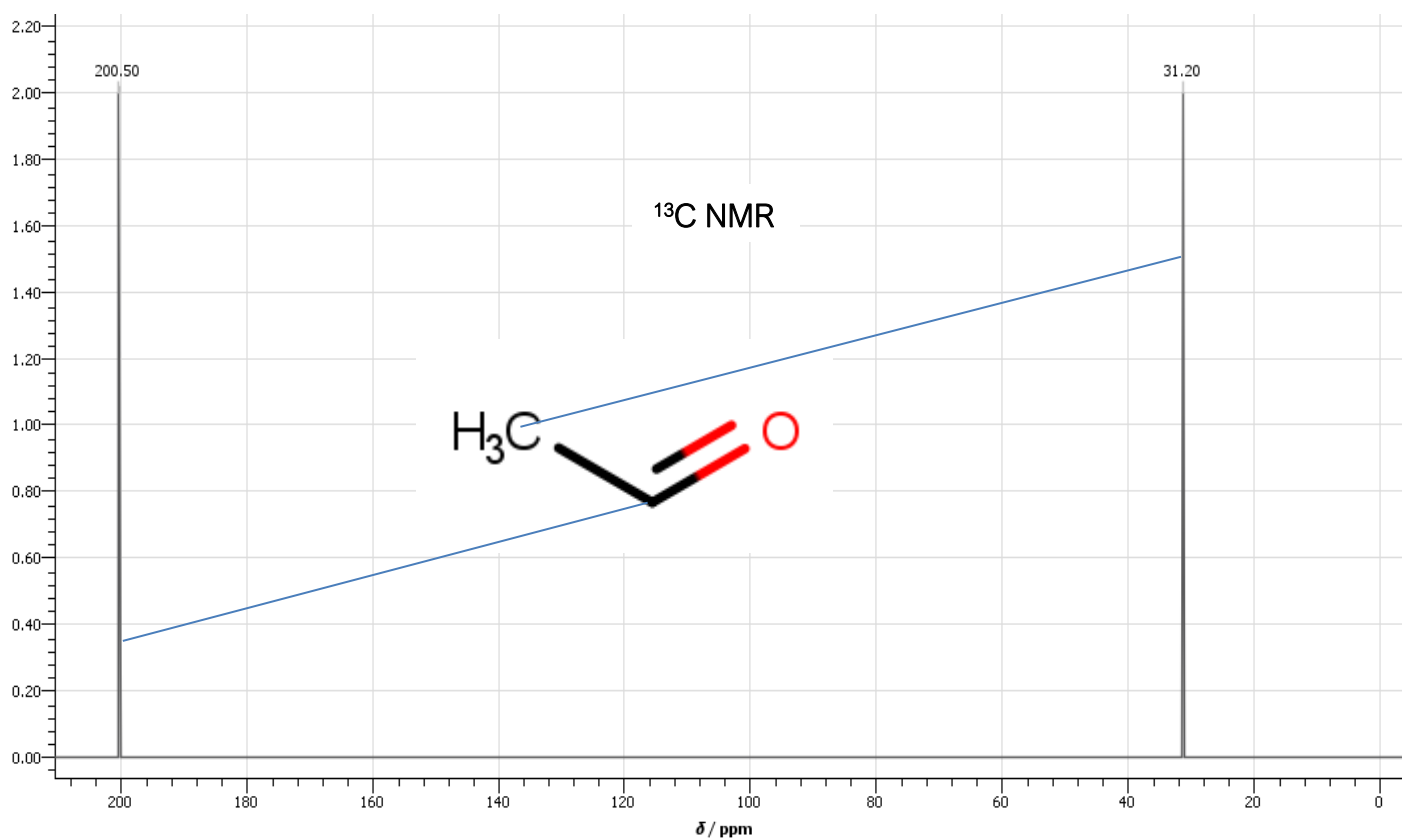
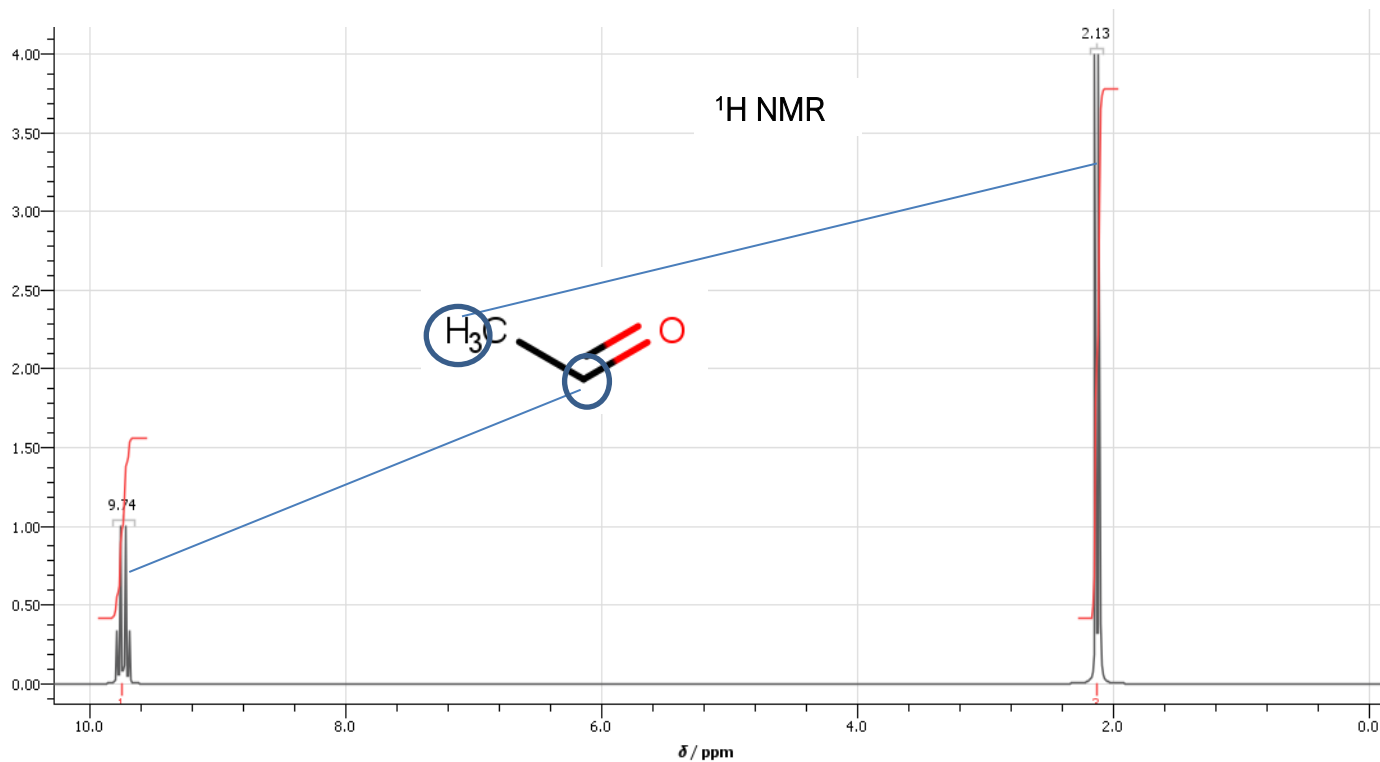
Compound reacts readily with acidified dichromate solution to give two oxidation products.

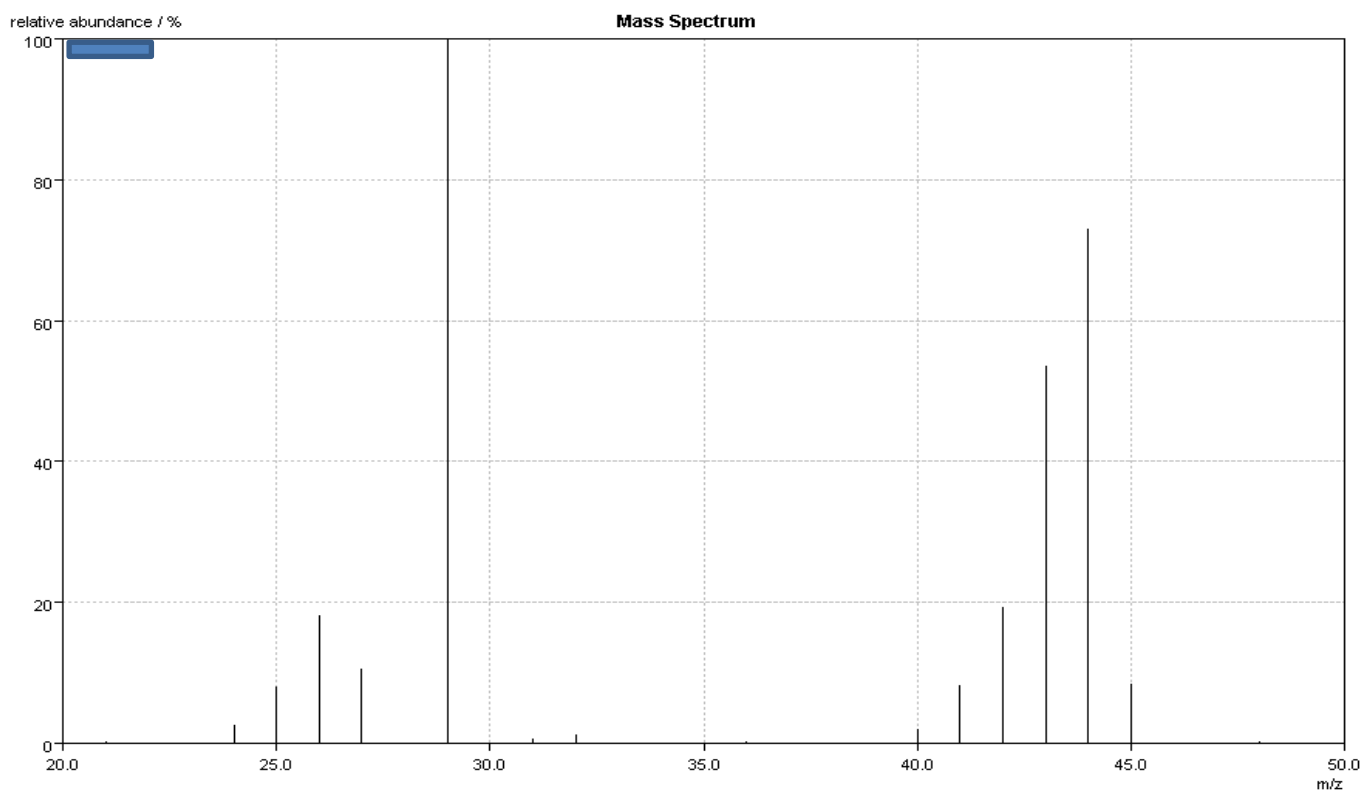
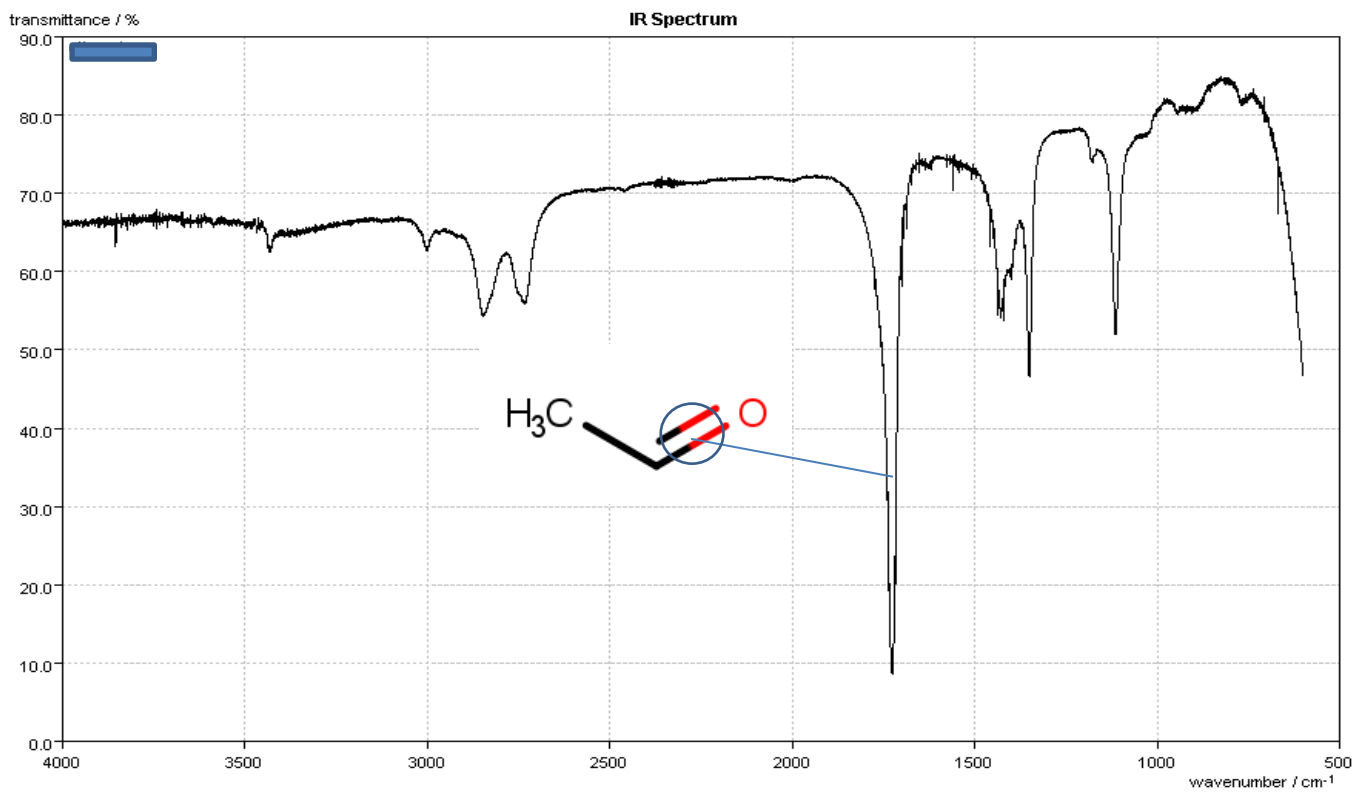
## Compound 2 ANSWERS

description: colourless volatile liquid

composition: C 54.55% H 9.09% O 36.36%

molecular formula:  $C_2H_4O$  ethanal





### Further Information:

Compound reacts with 2,4-dinitrophenylhydrazine (Brady's Reagent) to give an intensely coloured precipitate.

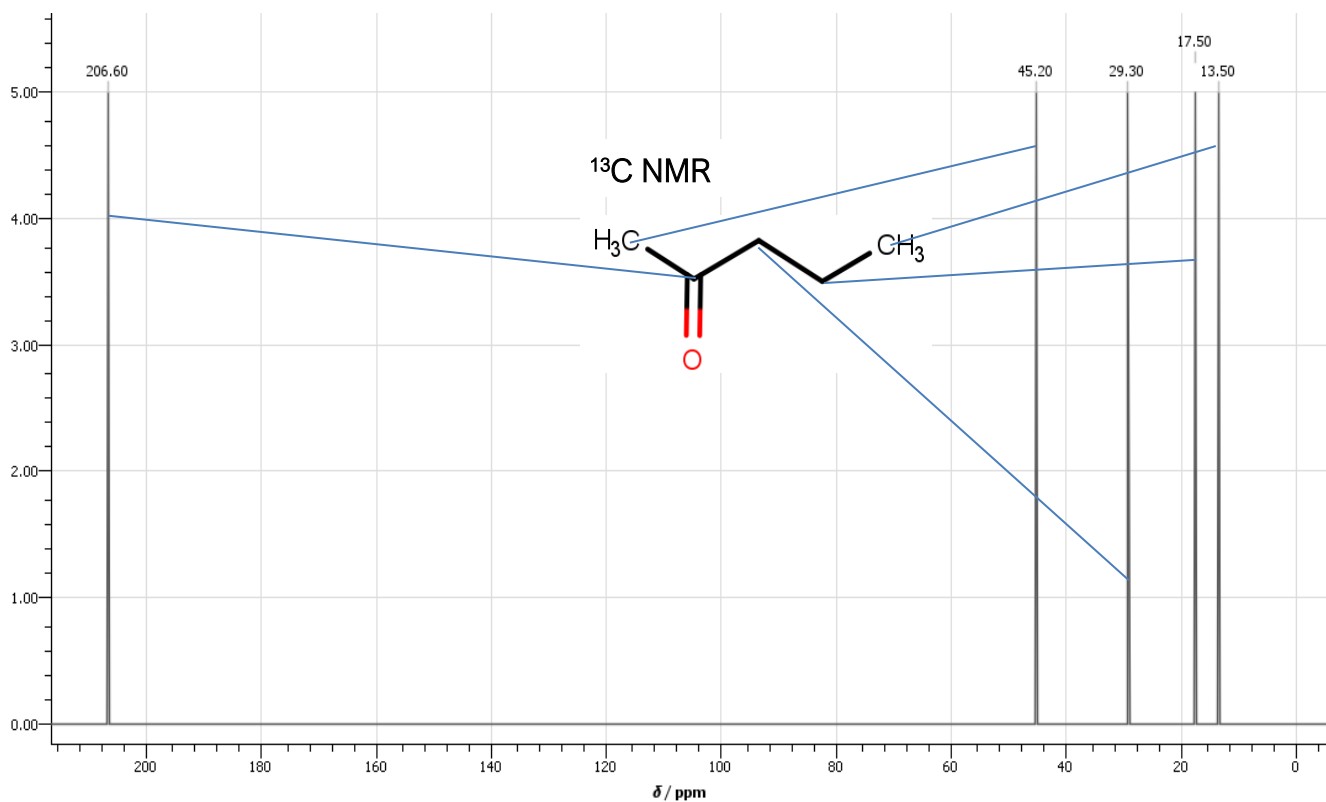
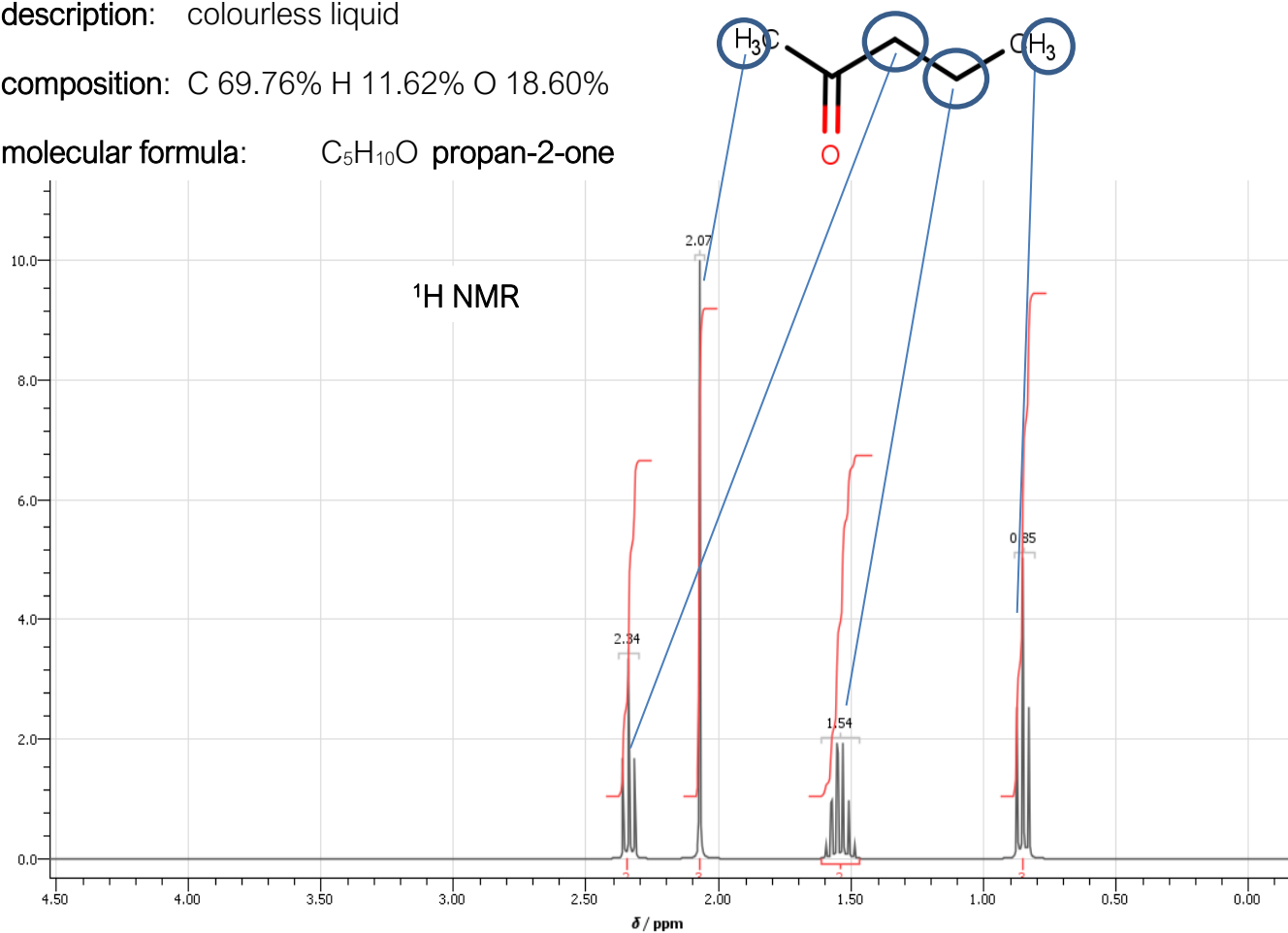
Compound reacts with Tollens' reagent to give a silver mirror.

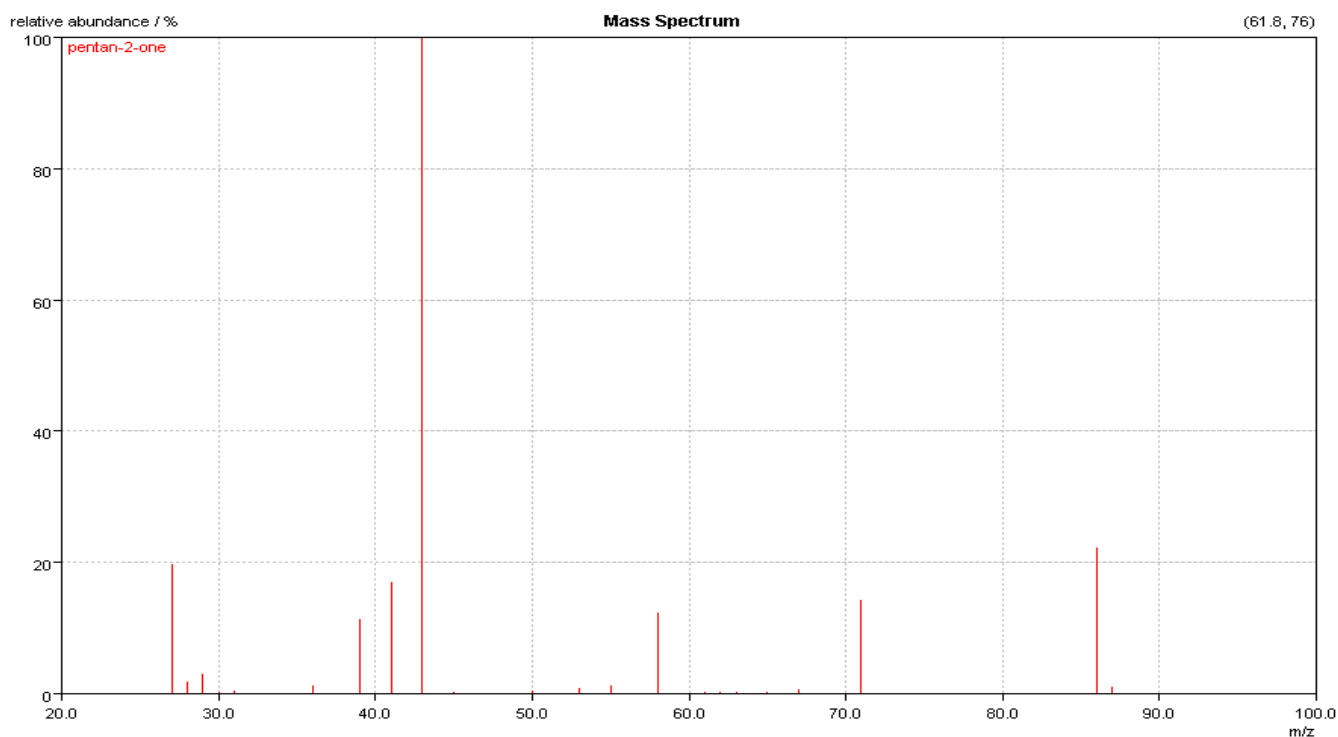
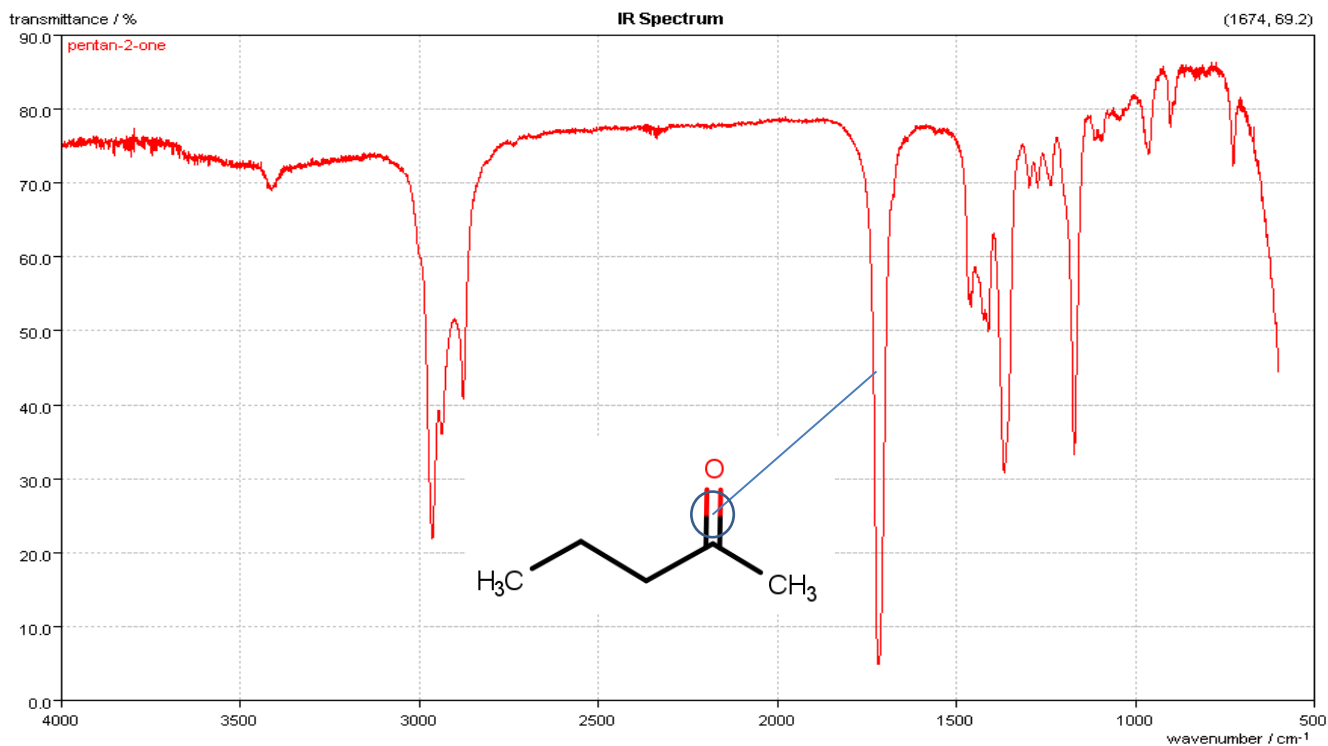
## Compound 3 ANSWERS

description: colourless liquid

composition: C 69.76% H 11.62% O 18.60%

molecular formula:  $C_5H_{10}O$  propan-2-one





### Further Information: :

Compound reacts with 2,4-dinitrophenylhydrazine (Brady's Reagent) to give an intensely coloured precipitate.

Compound reacts readily with NaBH<sub>4</sub> to produce a secondary alcohol.

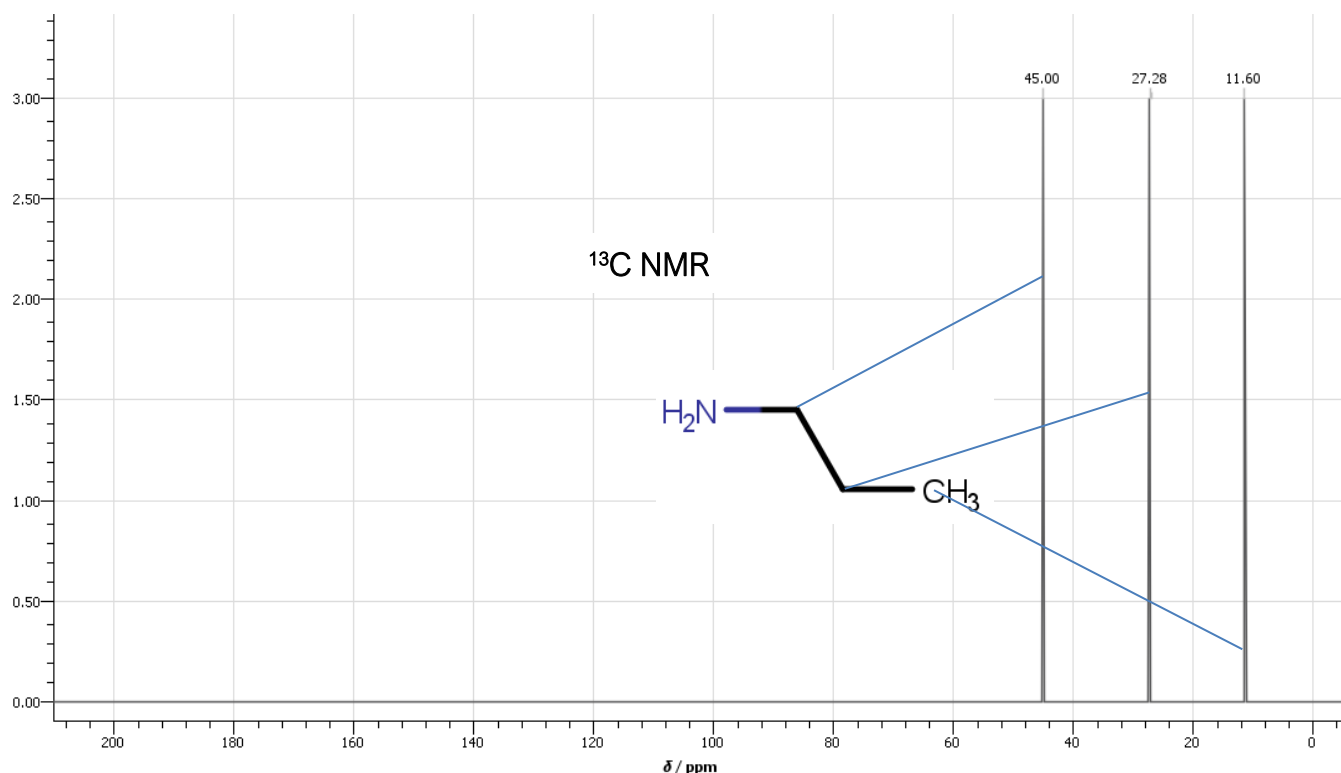
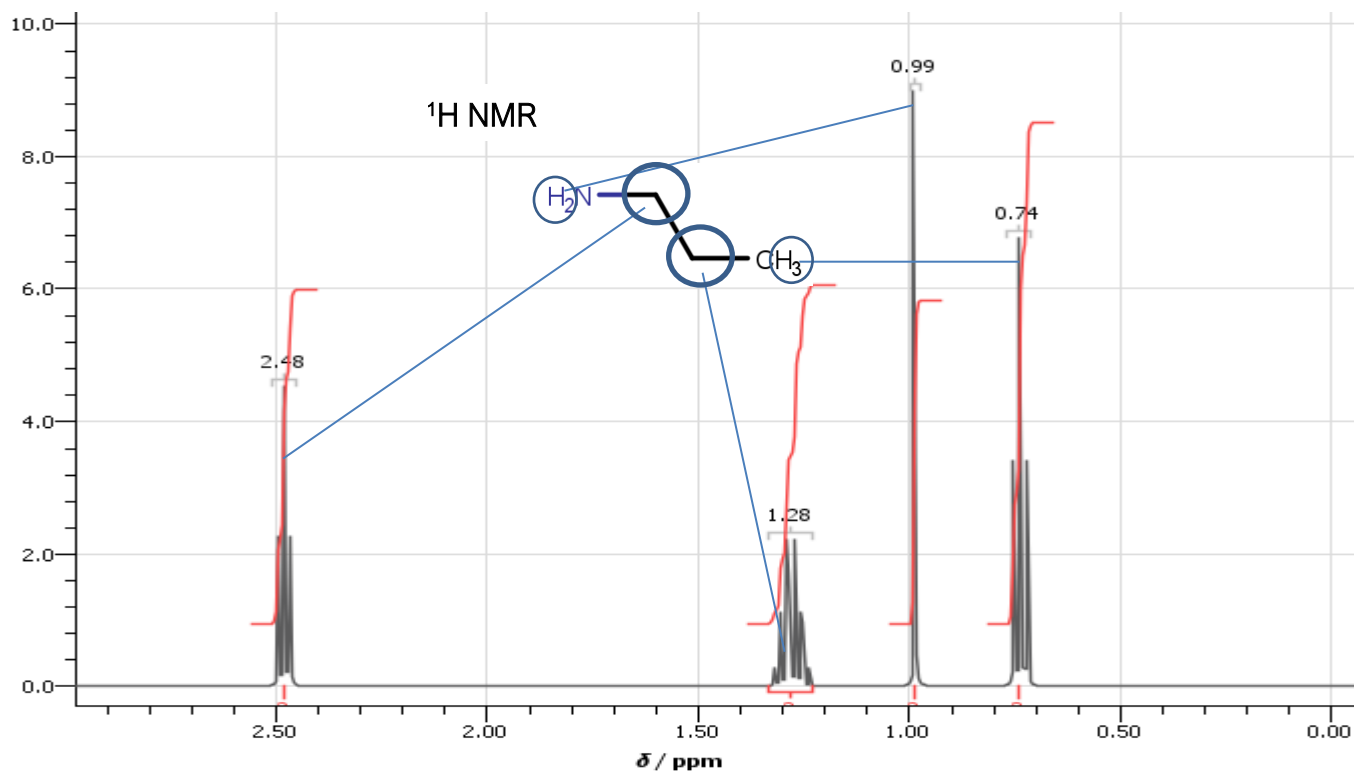
Compound does not react with Tollens' reagent.

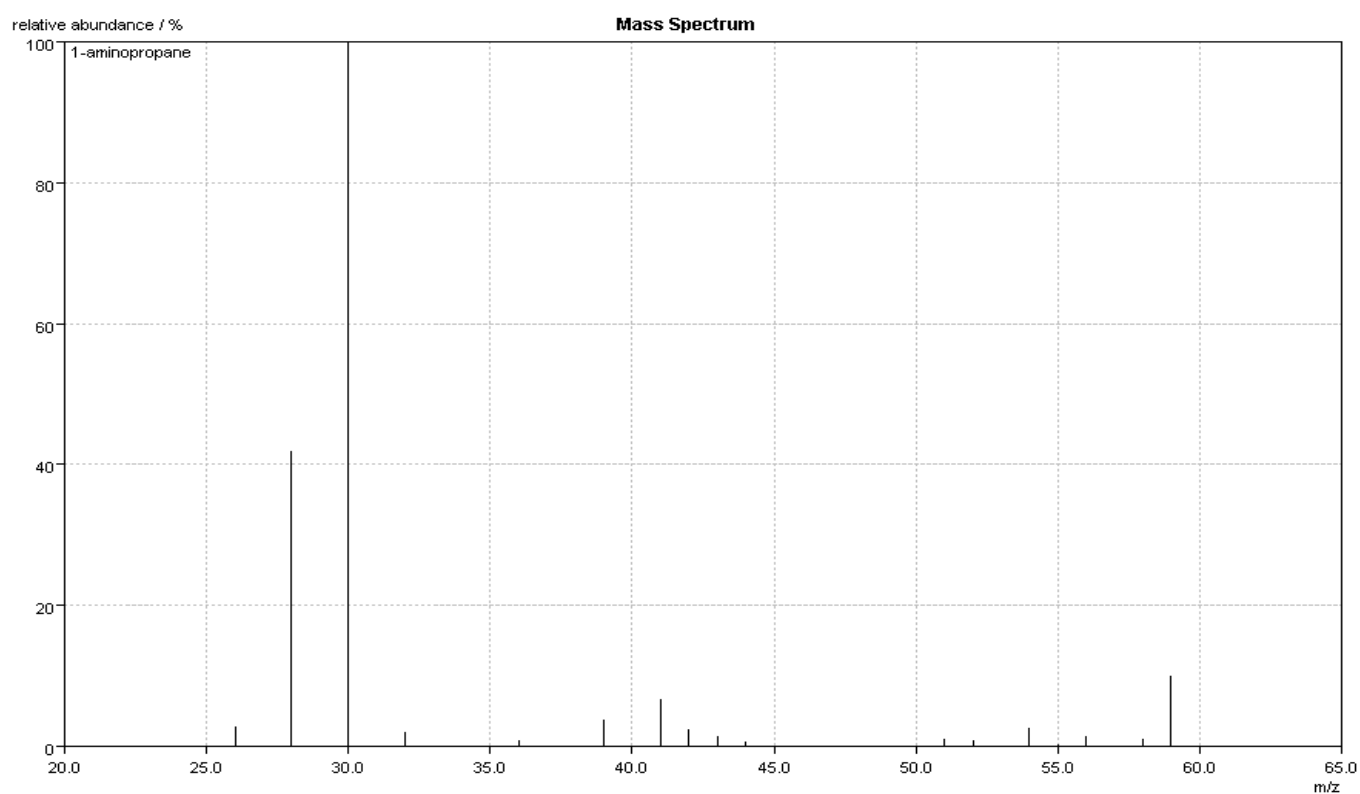
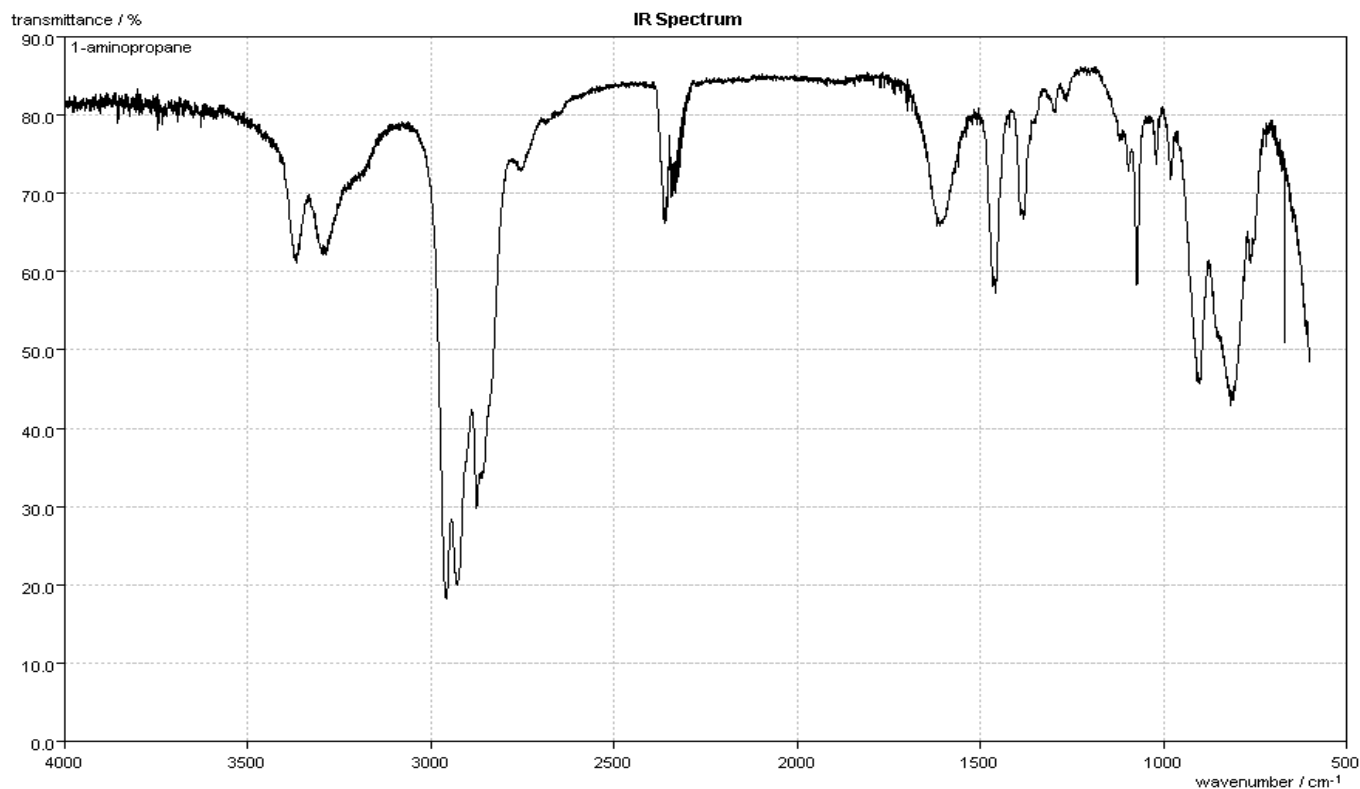
## Compound 4 ANSWERS

description: colourless liquid

composition: C 61.02%; H 15.25%; N 23.73%

molecular formula:  $C_3H_7NH_2$  1-aminopropane





### Further Information:

Compound has a fishy smell.

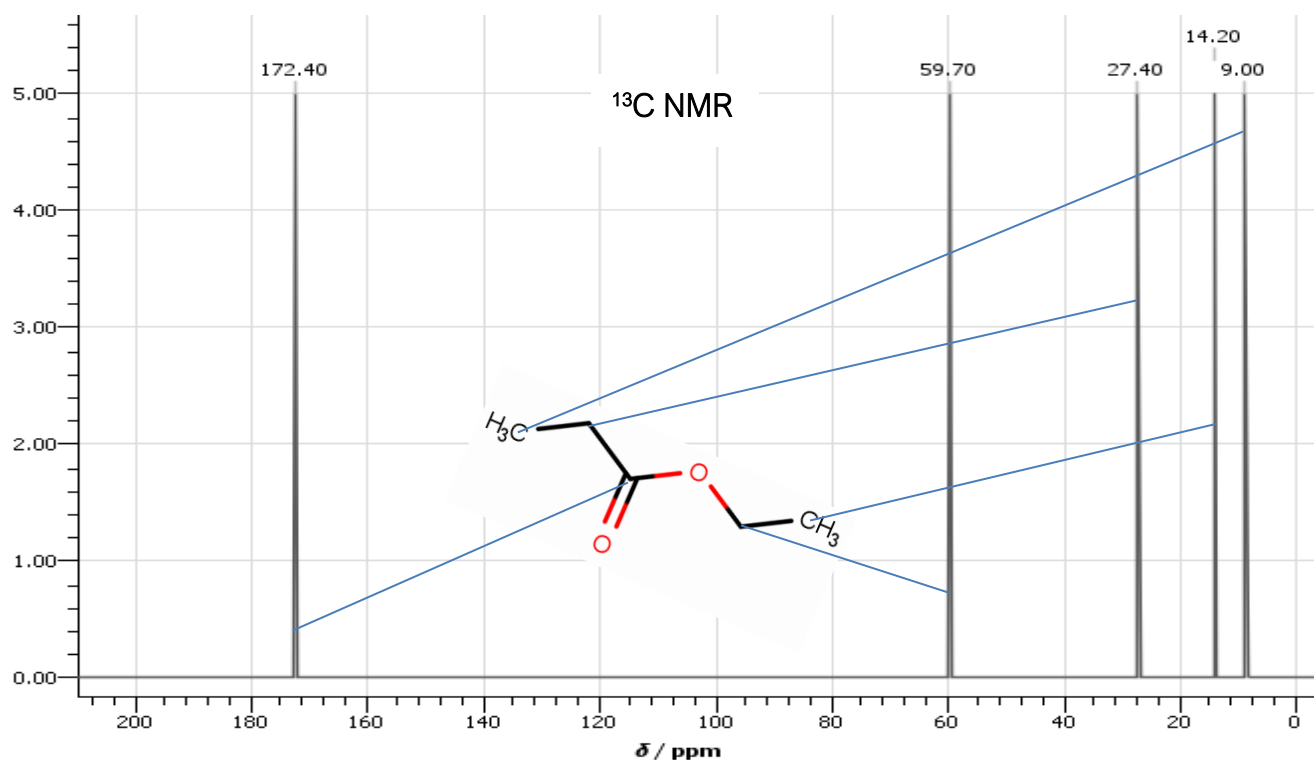
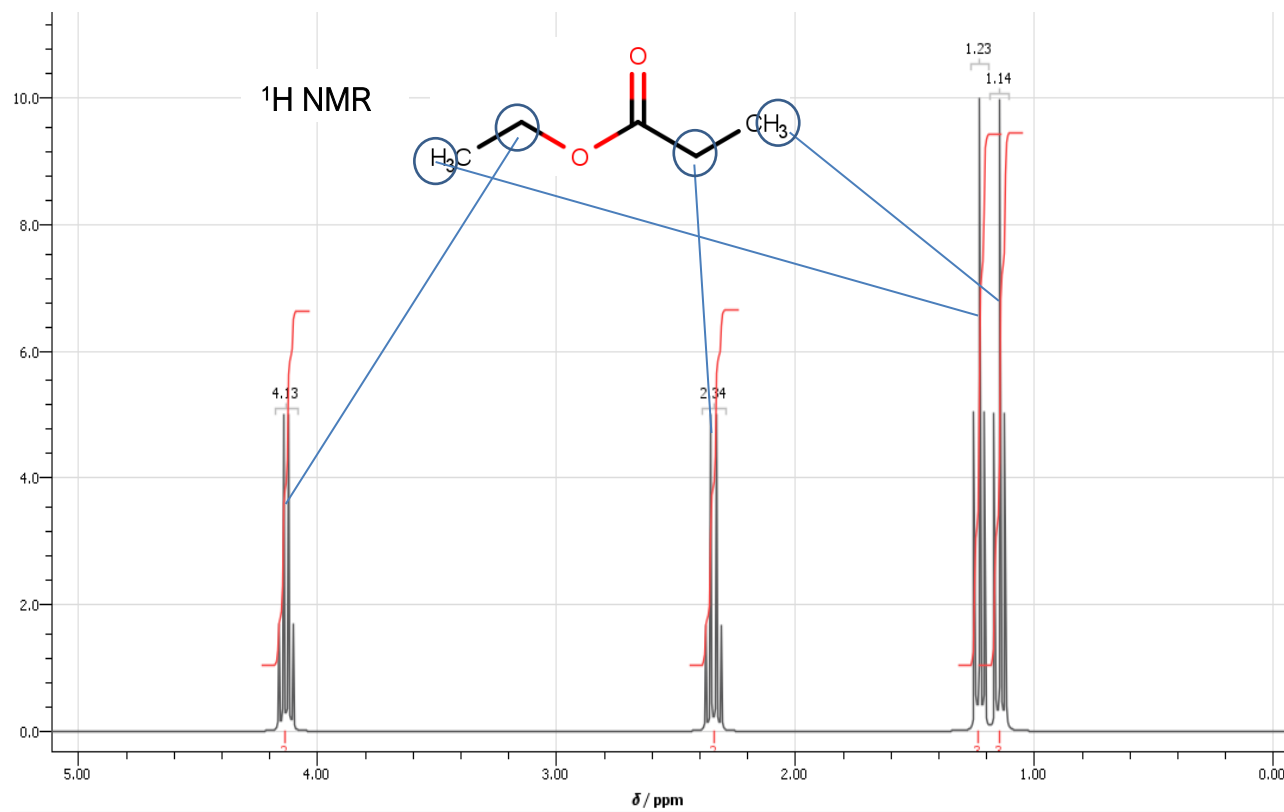
Compound dissolves in water to form an alkaline solution and reacts with hydrochloric acid to form a salt.

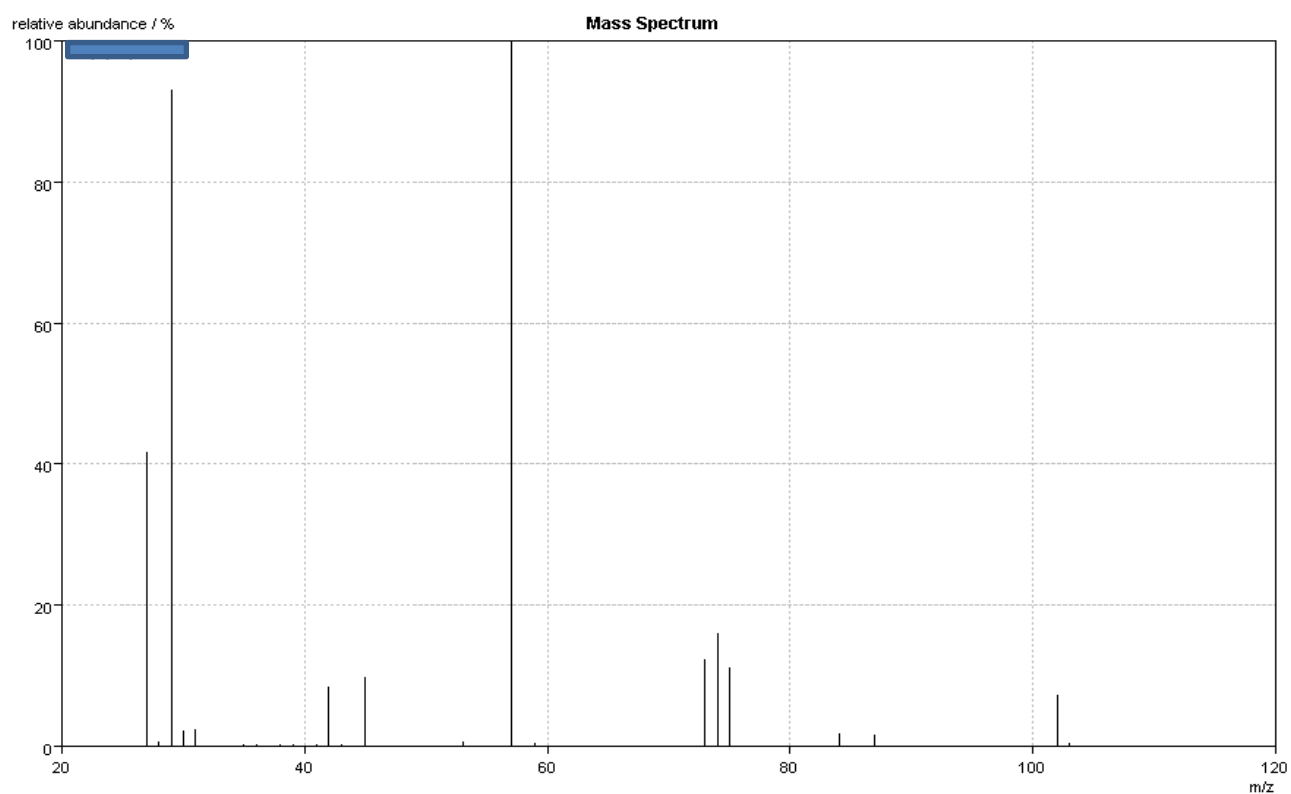
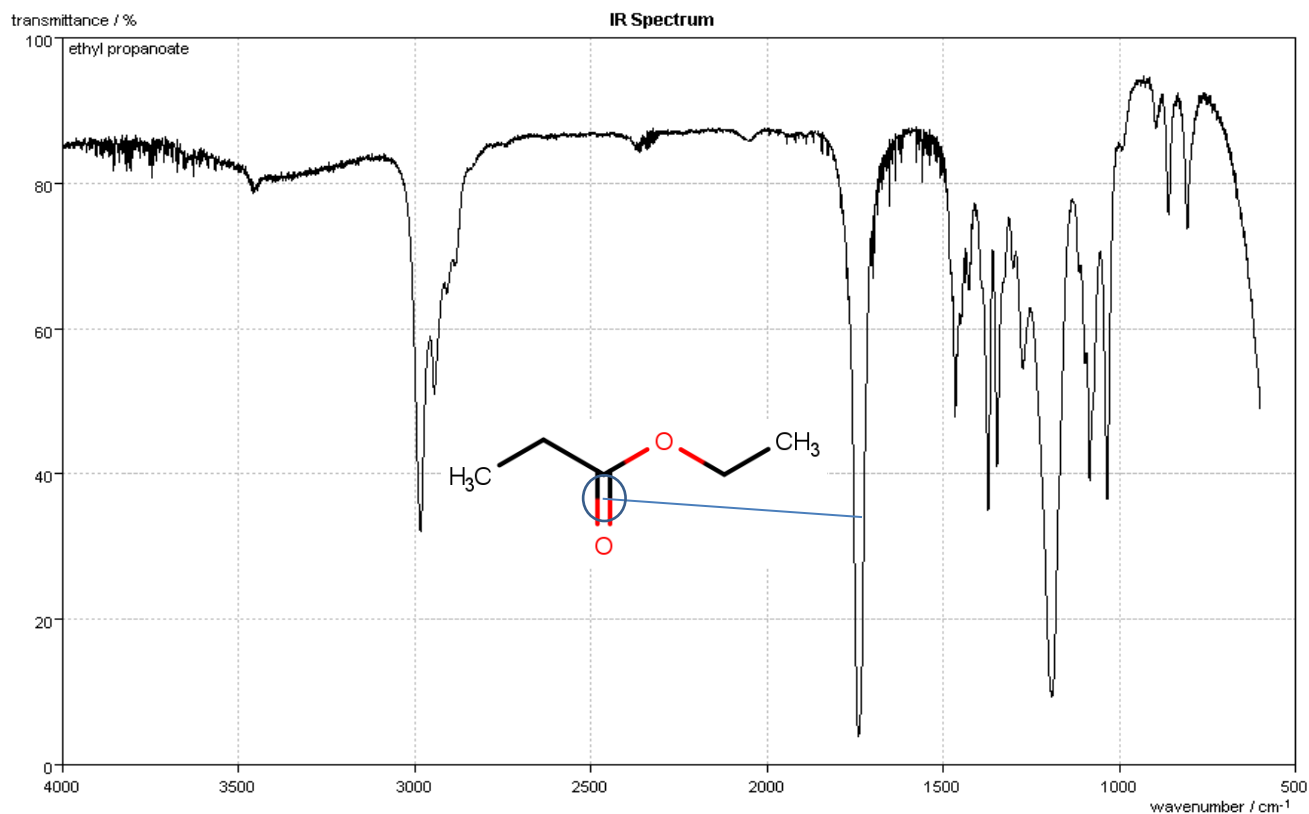
## Compound 5 ANSWERS

description: Colourless liquid

composition: C 58.80% H 9.87% O 31.33%

molecular formula:  $C_5H_{10}O_2$  ethyl propanoate





### Further Information:

Compound has a fruity smell.

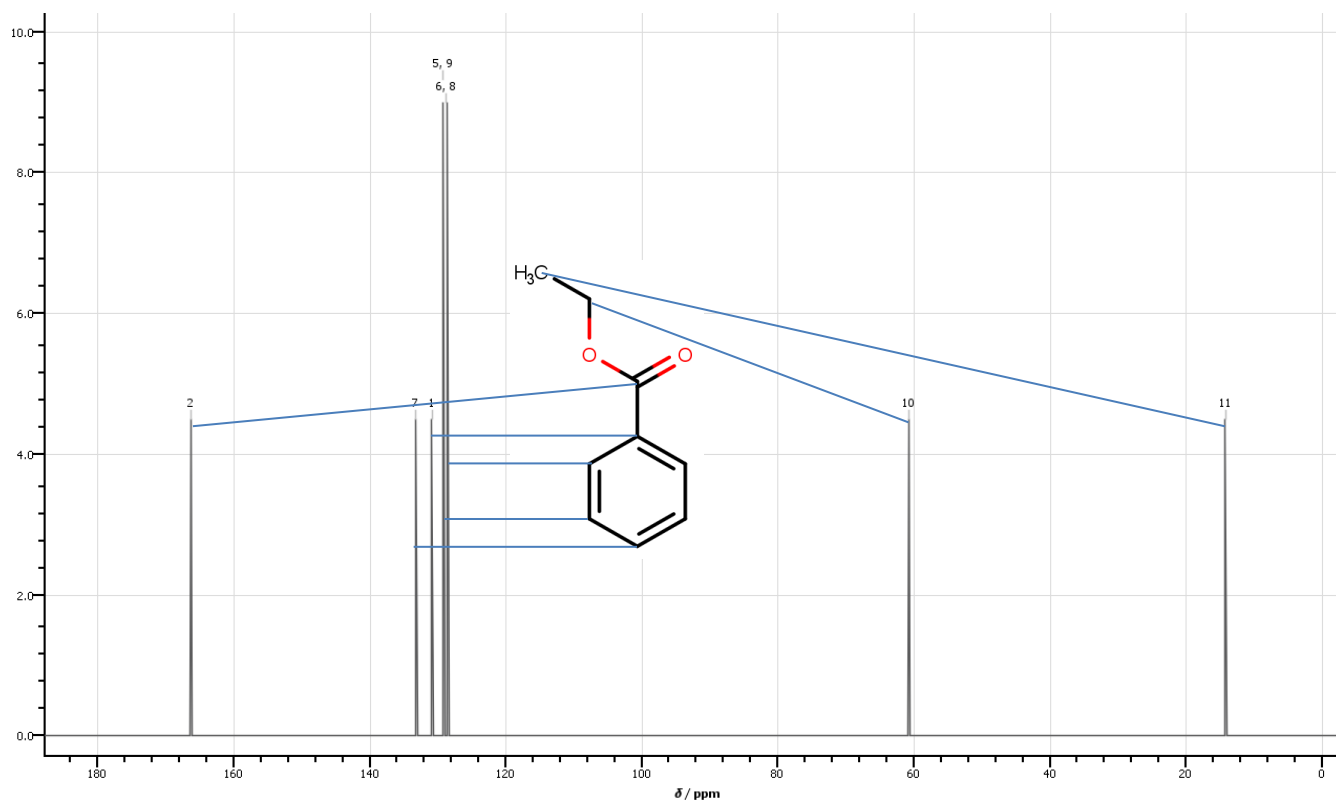
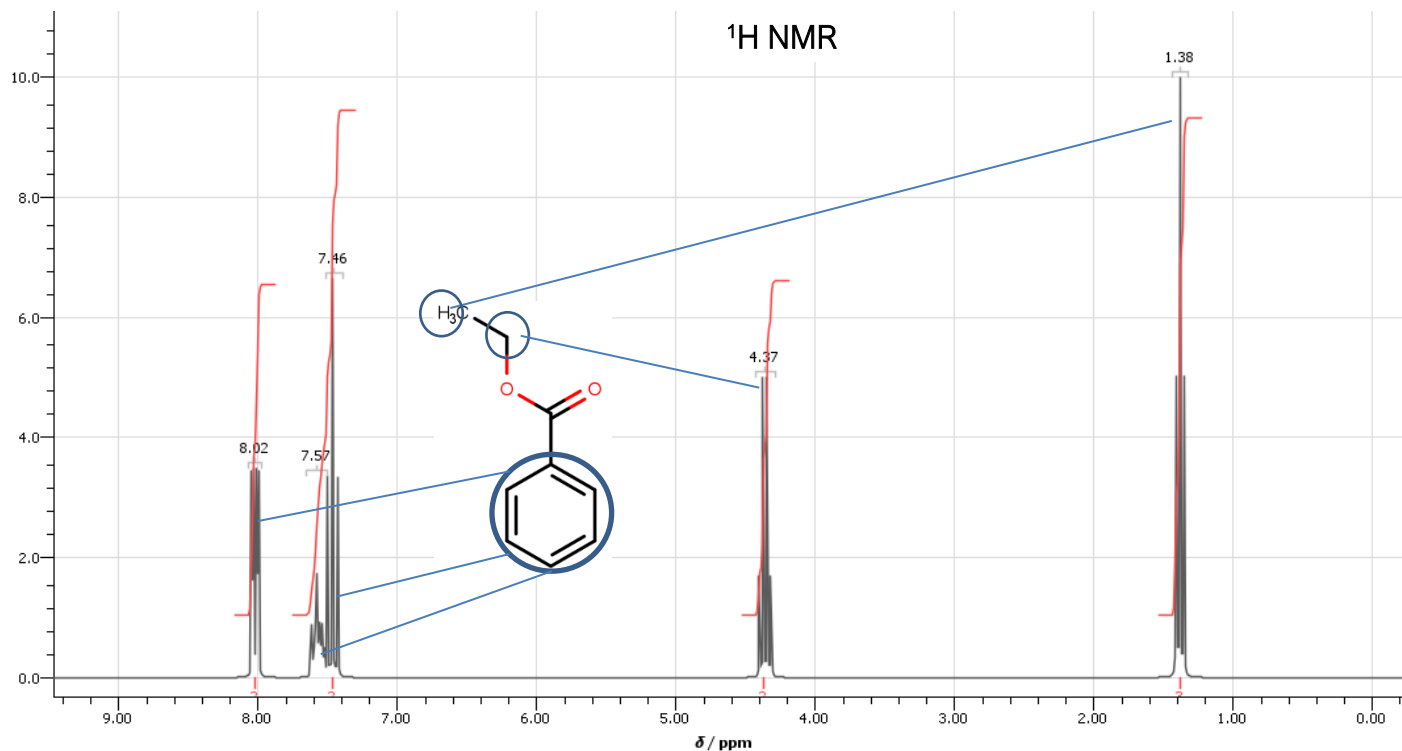
Compound hydrolyses in aqueous hydroxide to give sodium propanoate as one of two products.

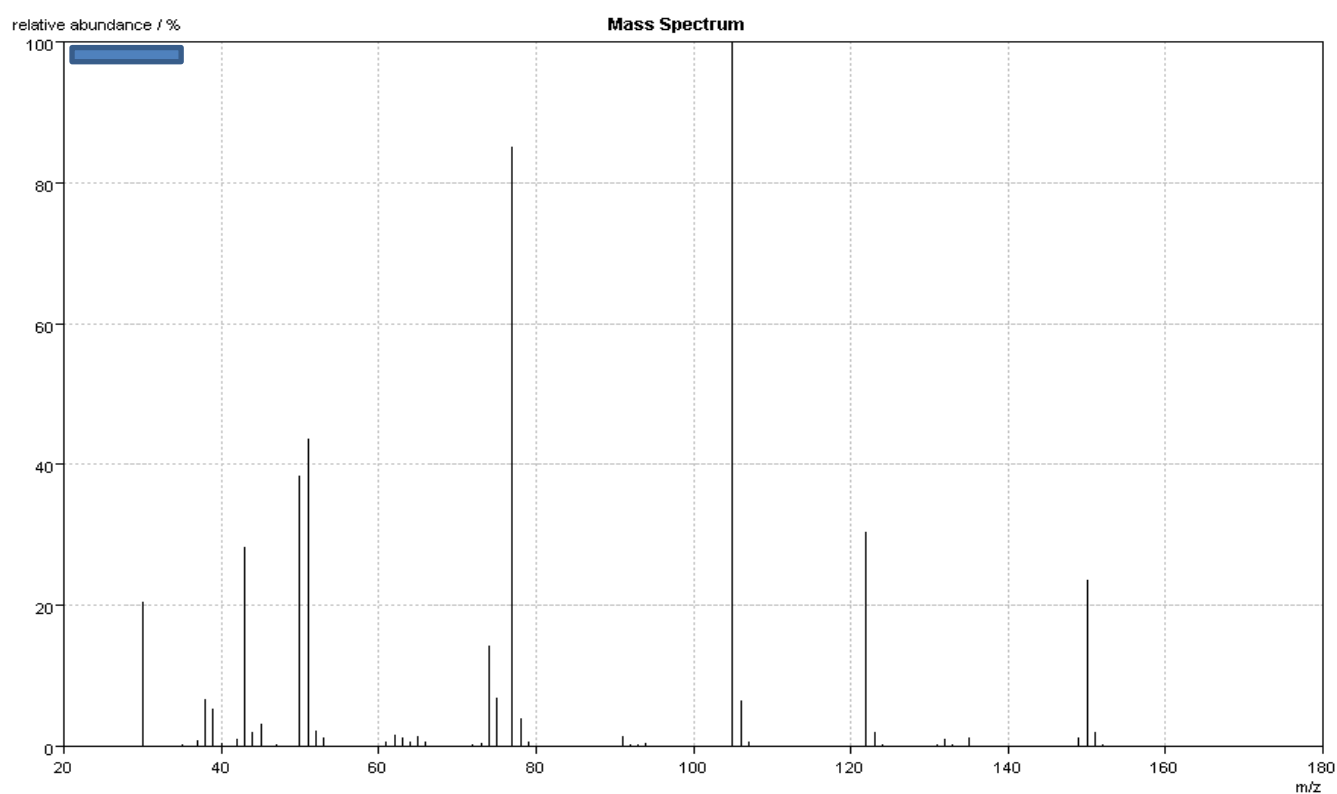
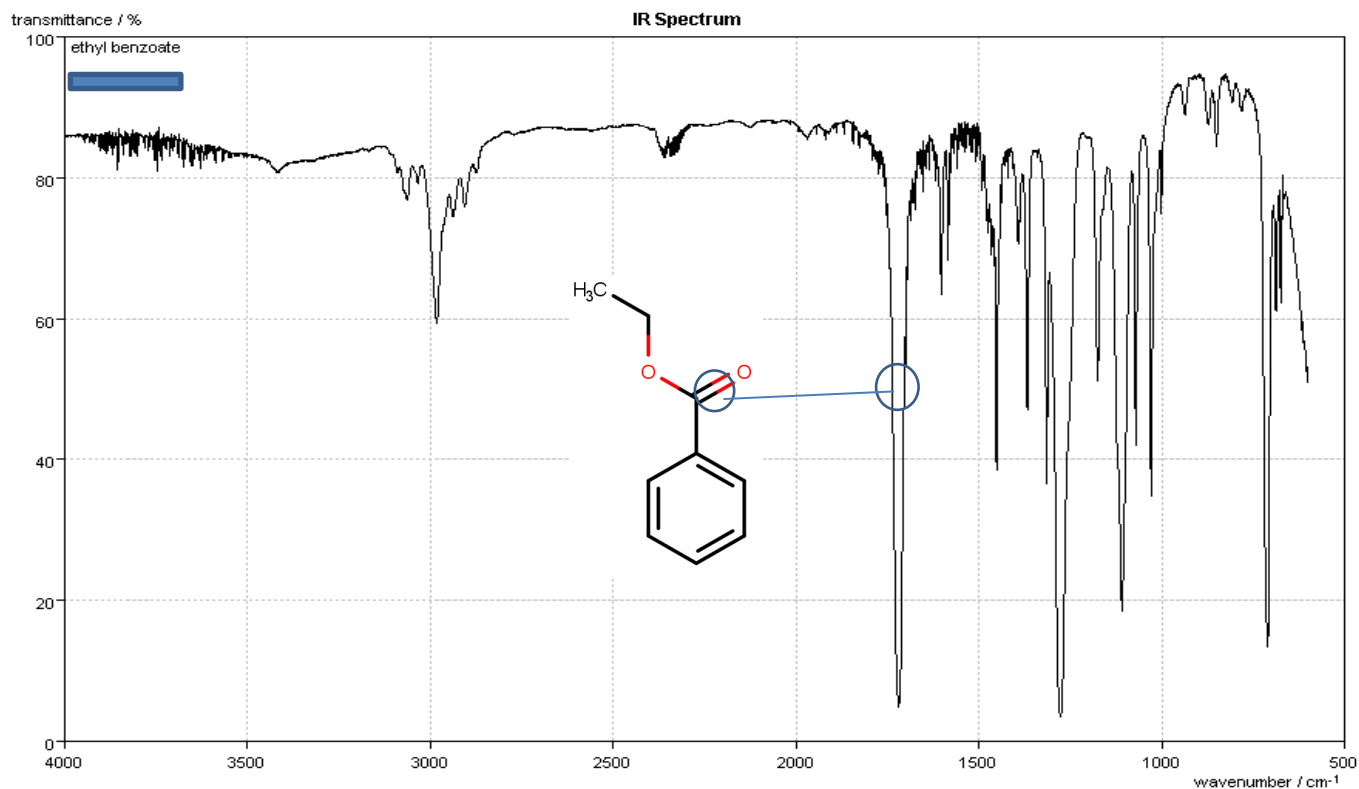
## Compound 6 ANSWERS

description: Colourless liquid

composition: C 71.98% H 6.71% O 21.31%

molecular formula:  $C_9H_{10}O_2$  ethyl benzoate





### Further Information:

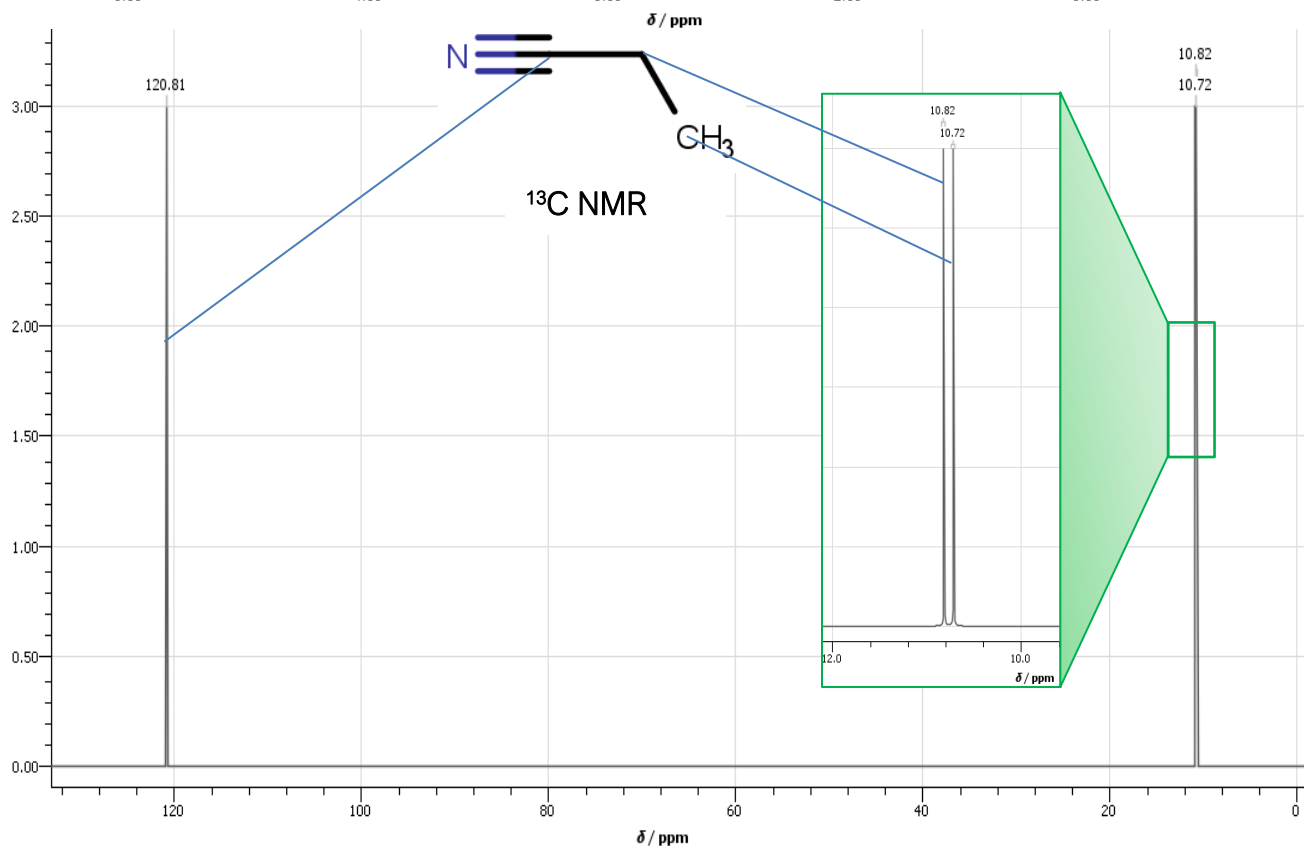
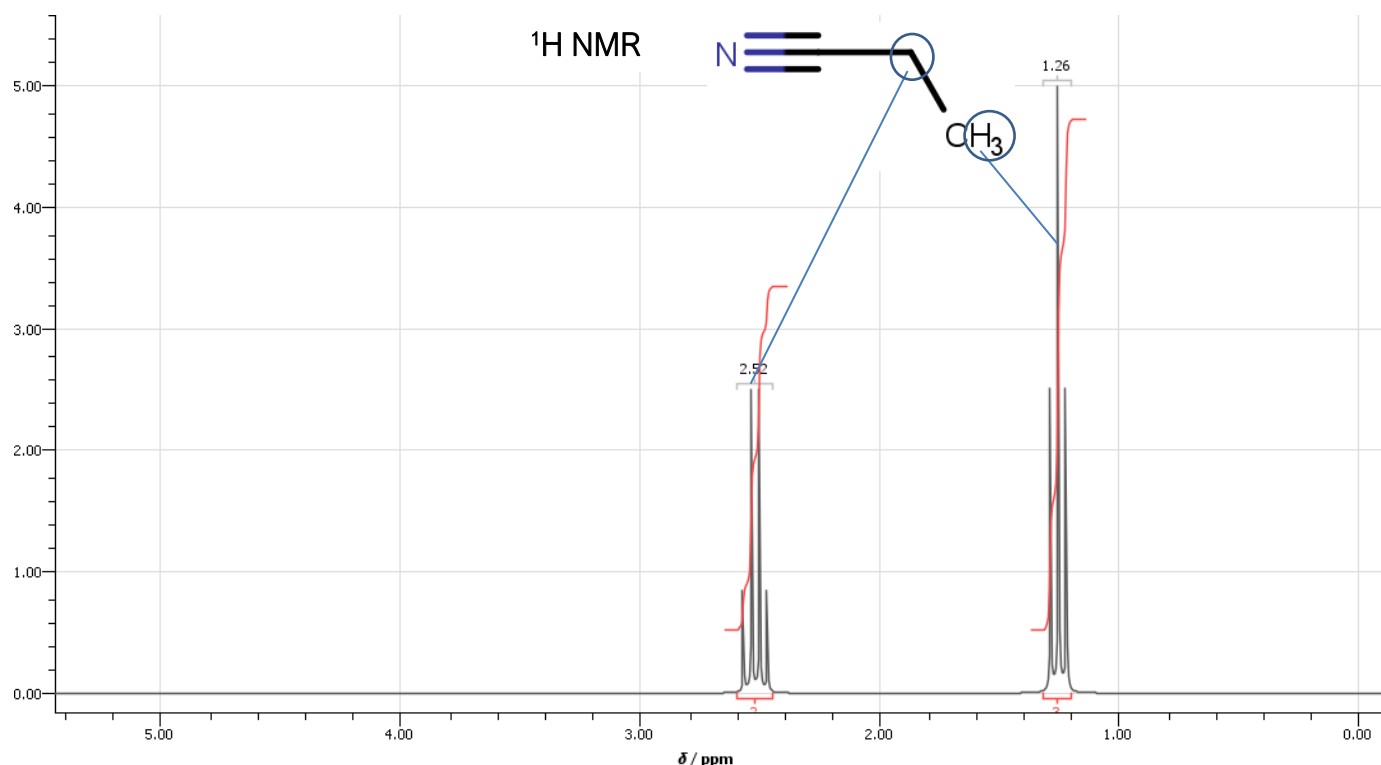
Compound hydrolyses in aqueous hydrochloric acid to give ethanol as one of two products.

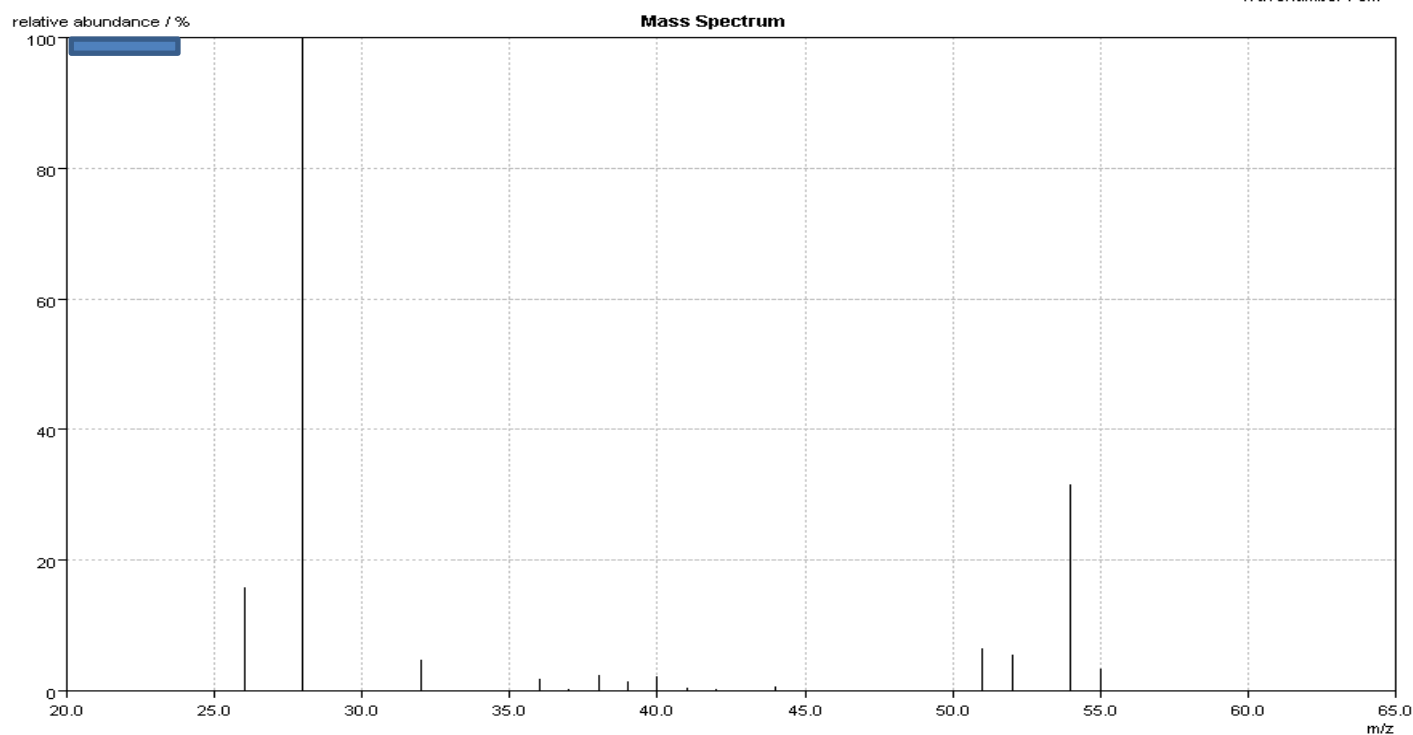
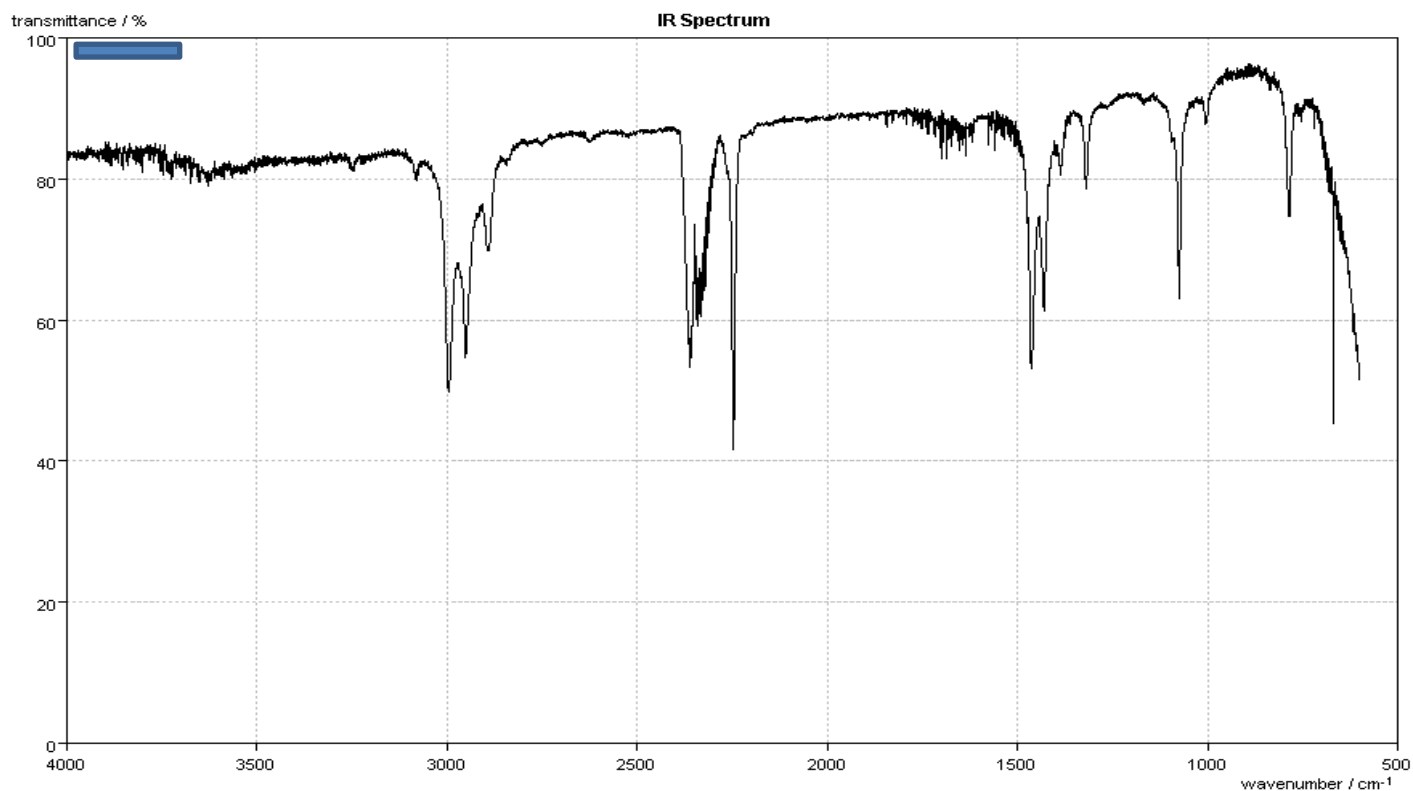
## Compound 7 ANSWERS

description: colourless liquid

composition: C 65.42%; H 9.15%; N 25.43%

molecular formula:  $C_3H_5N$  propanenitrile





#### Further Information:

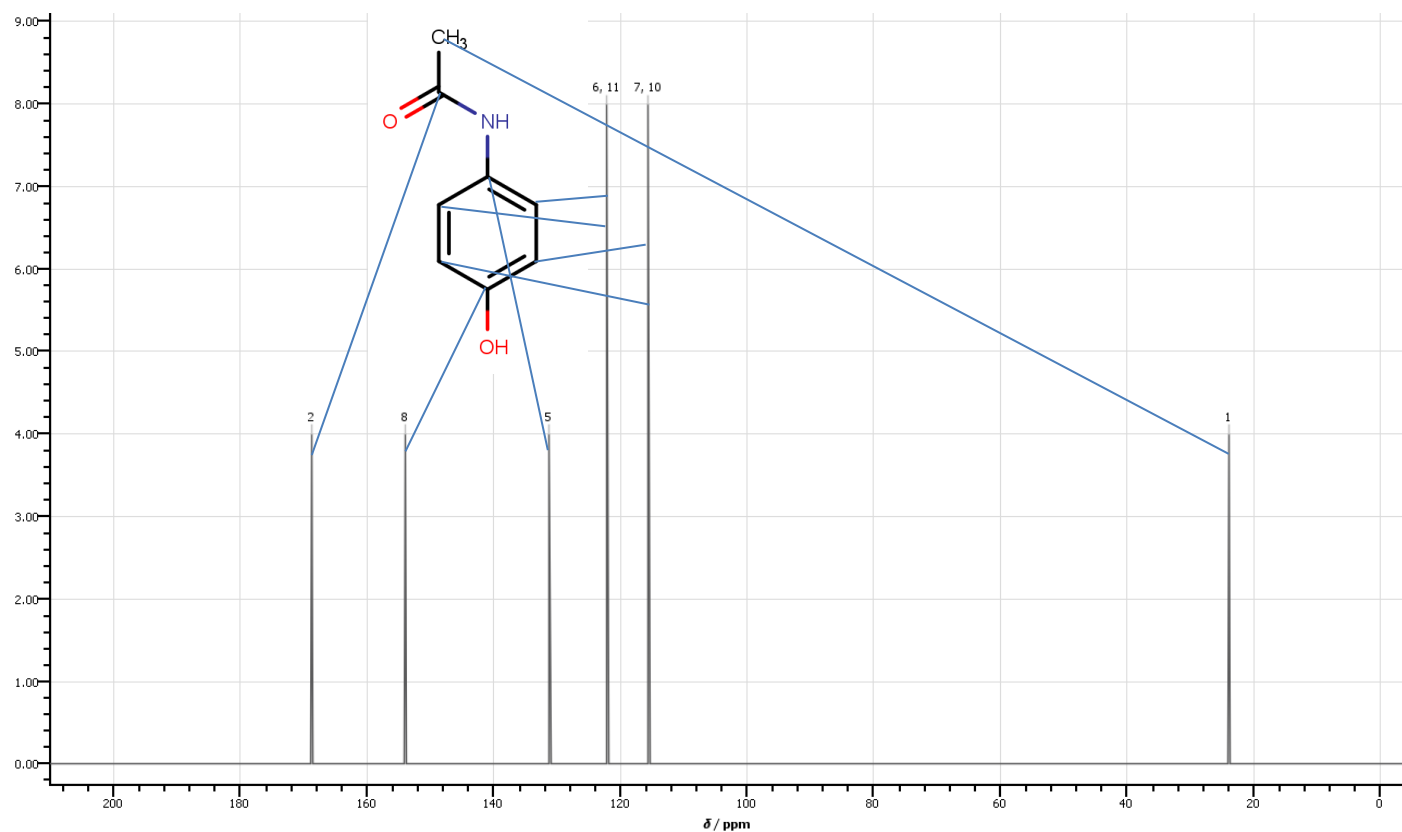
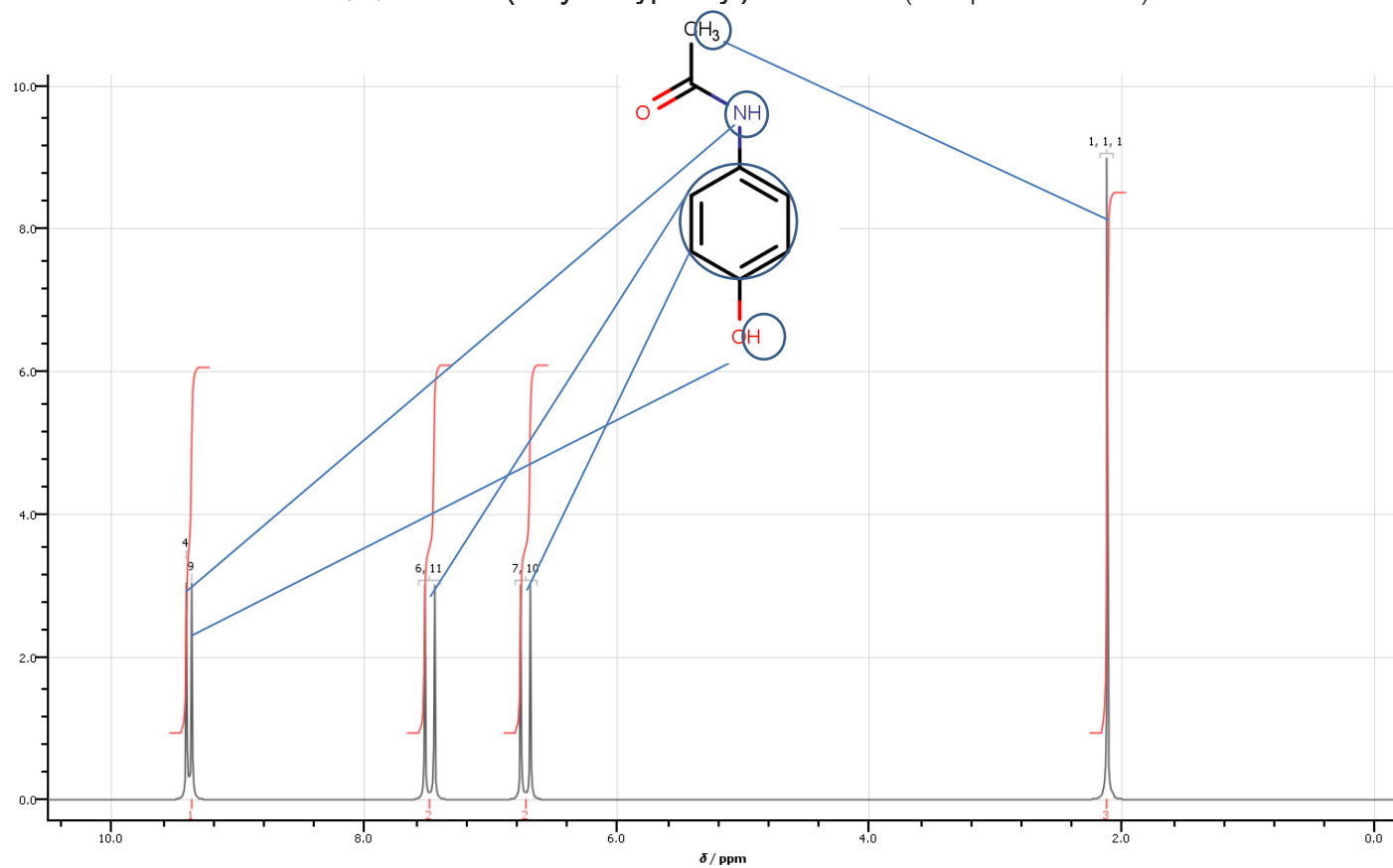
Compound dissolves in water to give a neutral, mildly poisonous solution.

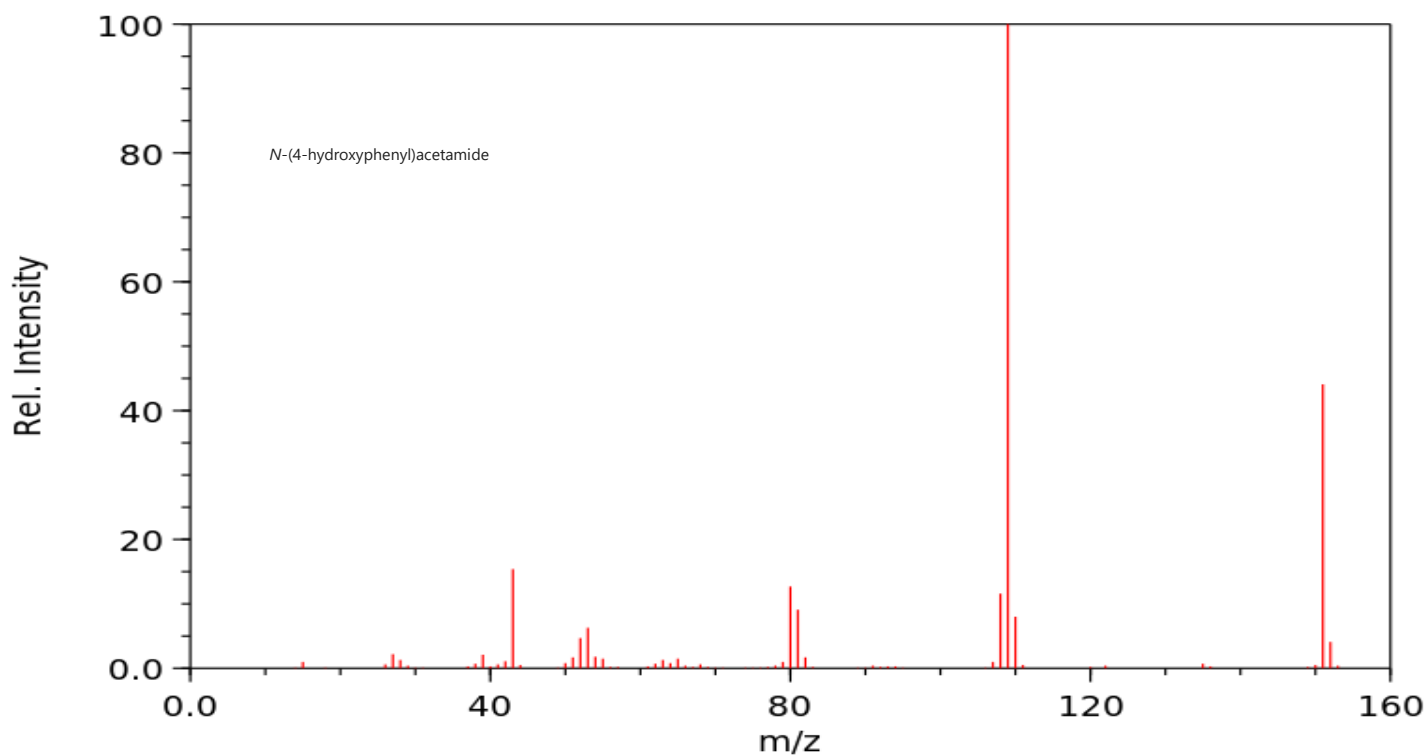
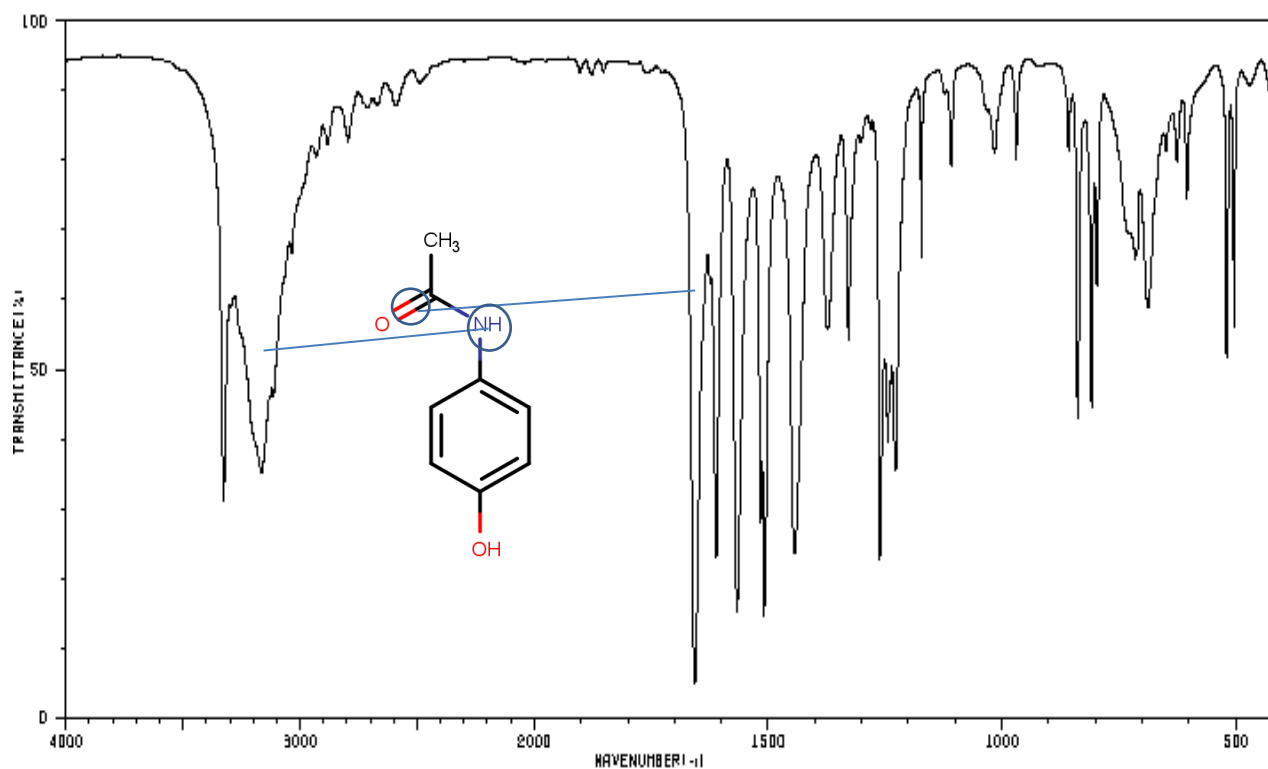
# Compound 8 ANSWERS

Description: white crystalline solid

Composition: C 63.56%; H 6.00%; N 9.27%; O 21.17%

Molecular formula:  $C_8H_9NO_2$  N-(4-hydroxyphenyl)acetamide (aka paracetamol)





#### Further Information:

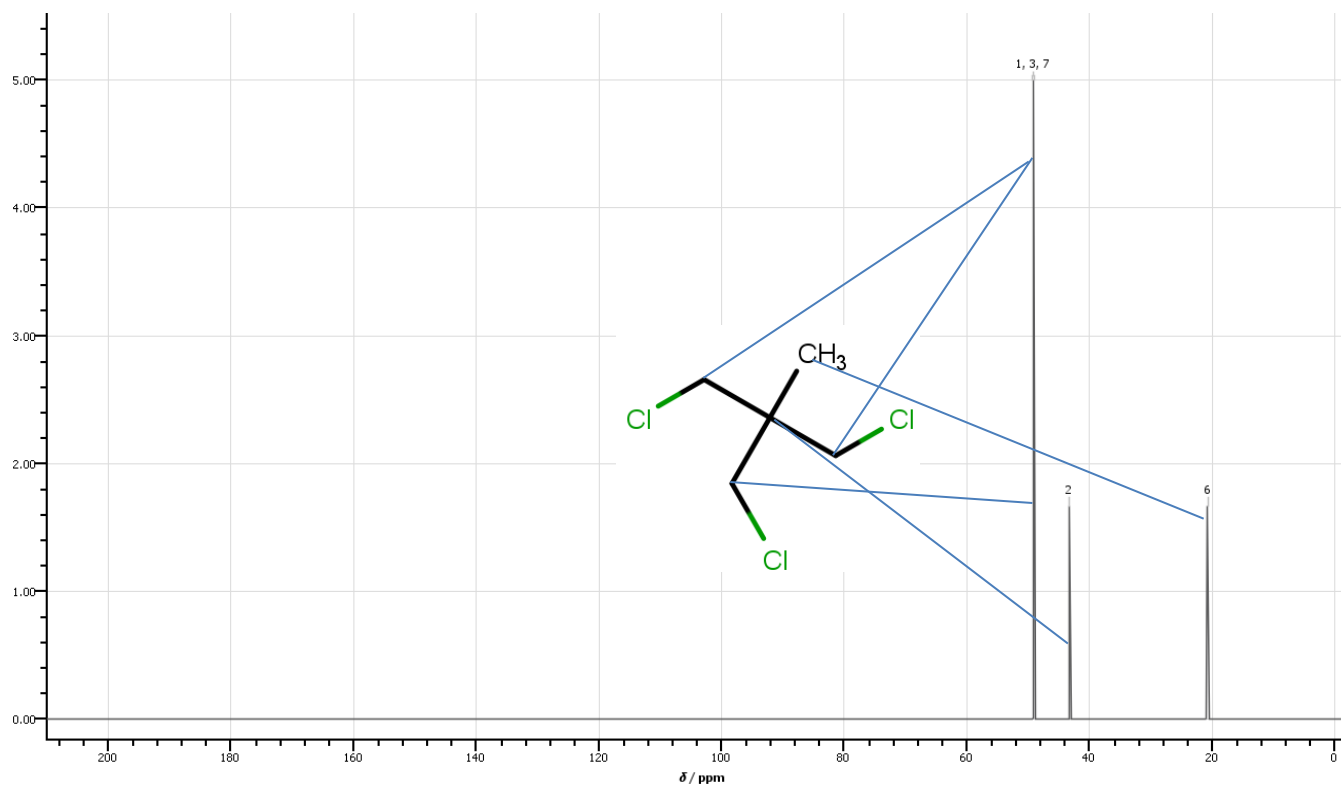
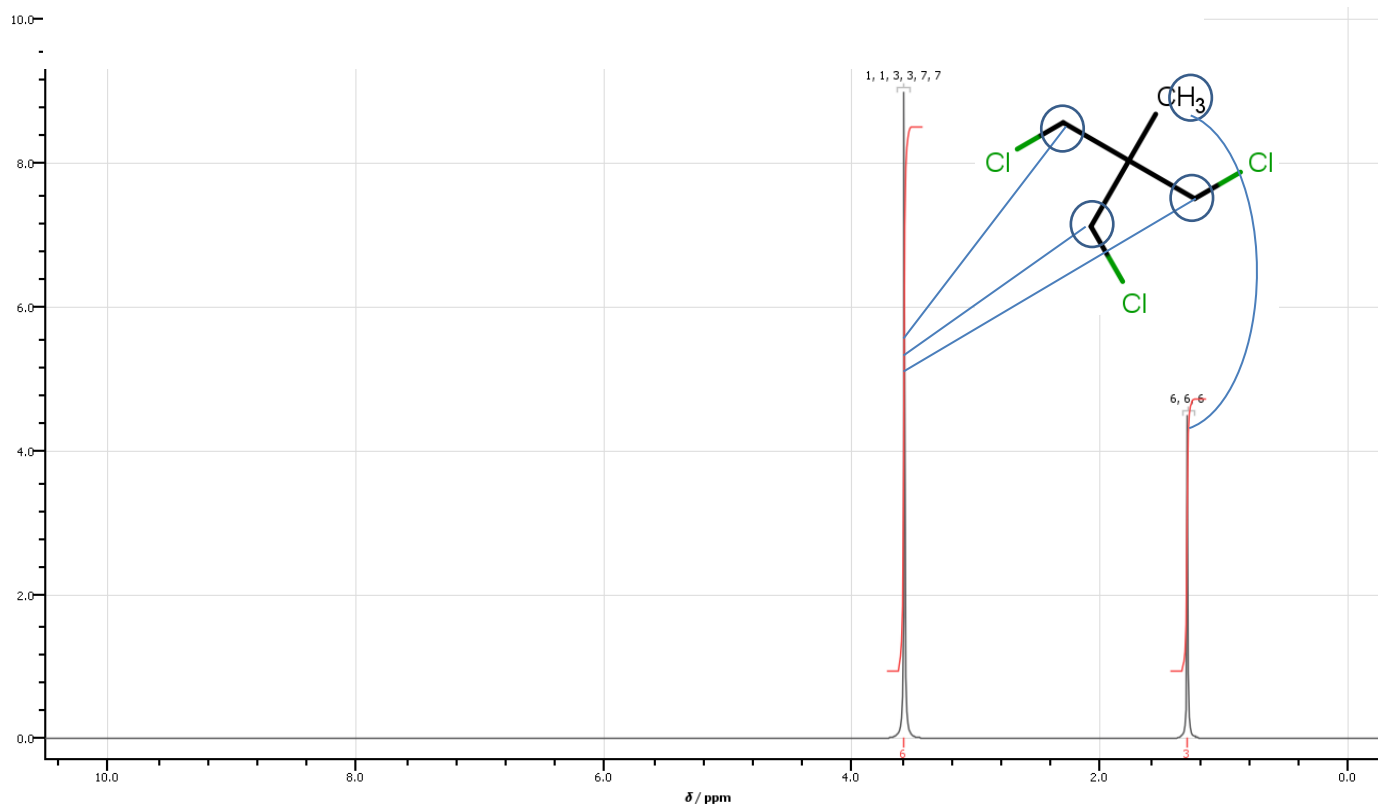
Compound can be hydrolysed in boiling hydrochloric acid or sodium hydroxide solution to produce, ethanoic acid or sodium ethanoate respectively, as one of the products

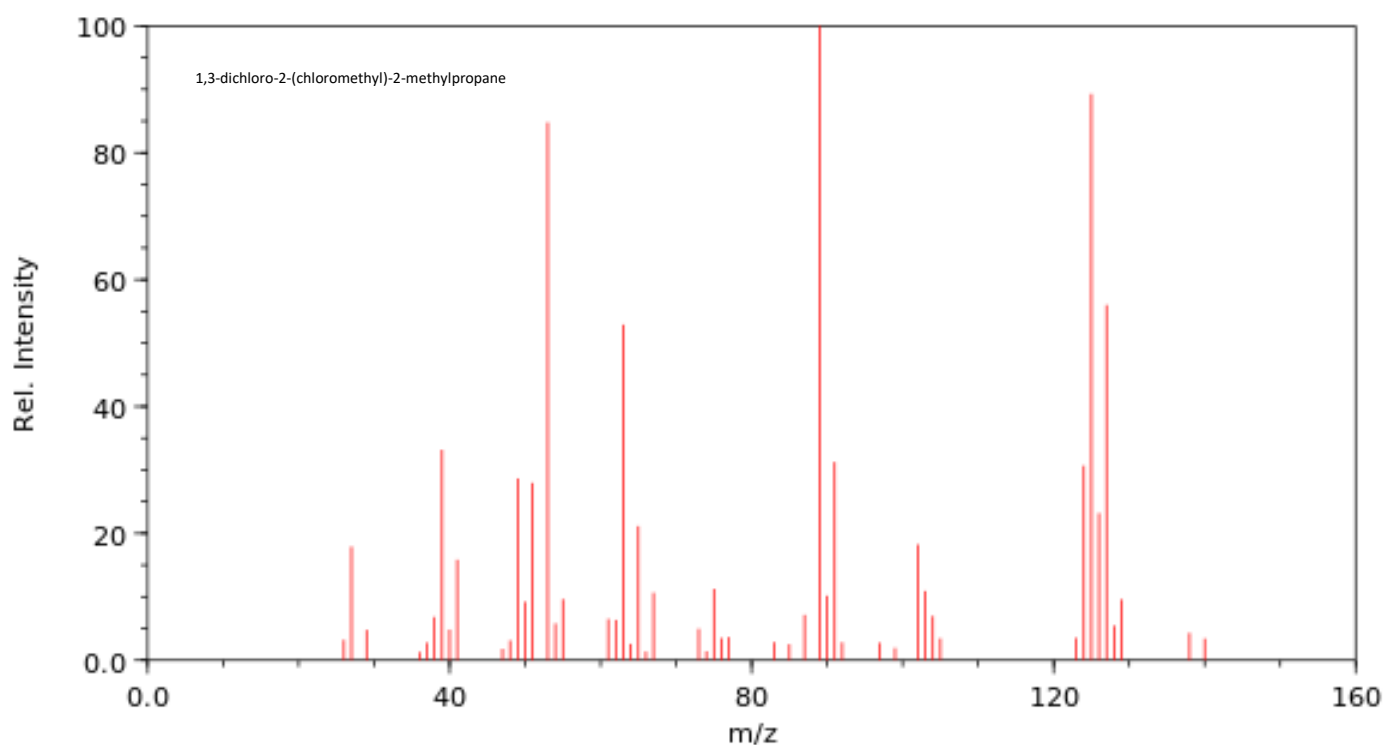
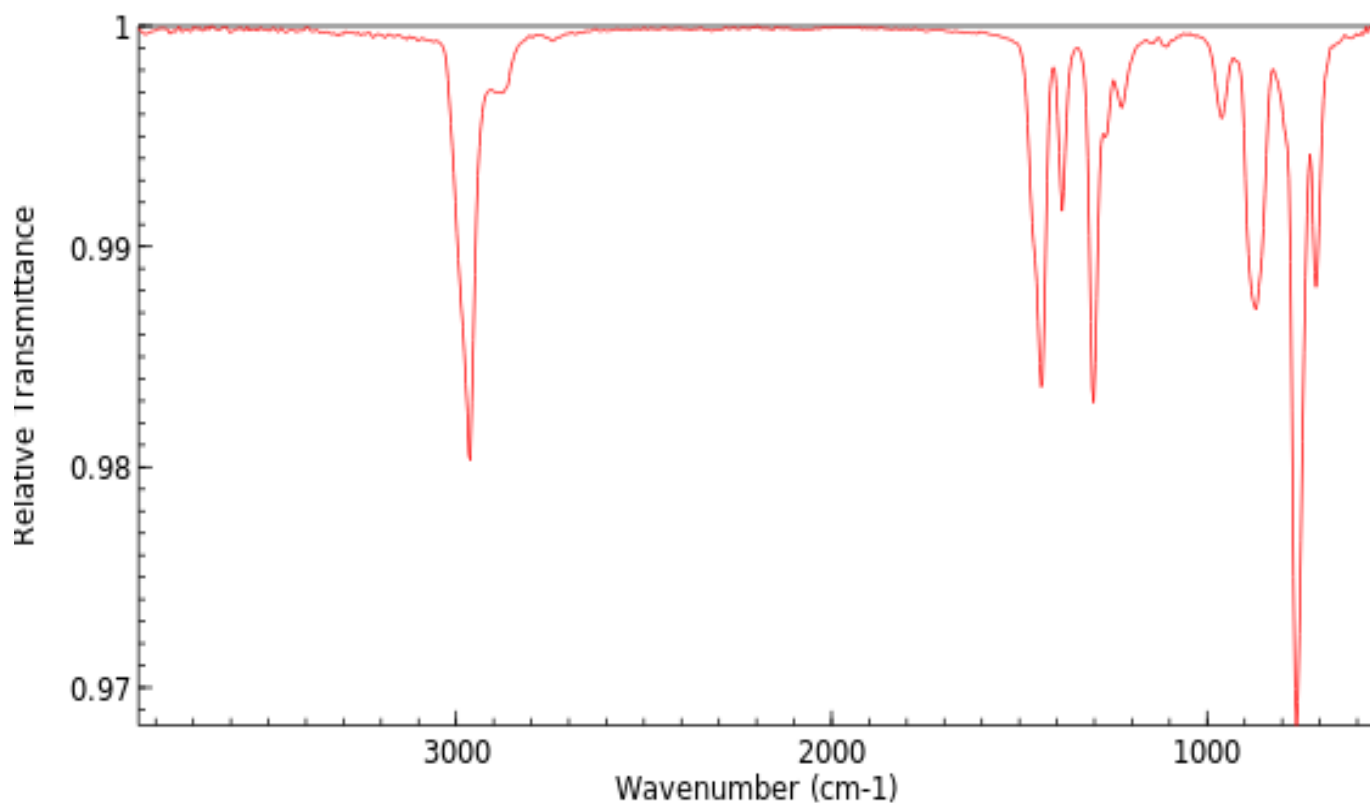
Compound is a pain killer and anti-pyretic. It is also moderately hepatotoxic.

Compound 9 **ANSWERS**

description: Colourless volatile liquid

composition: C 34.22%; H 5.17%; Cl 60.61%

molecular formula:  $C_5H_9Cl_3$  1,3-dichloro-2-(chloromethyl)-2-methylpropane



#### Further Information:

Compound is immiscible (insoluble) in water.

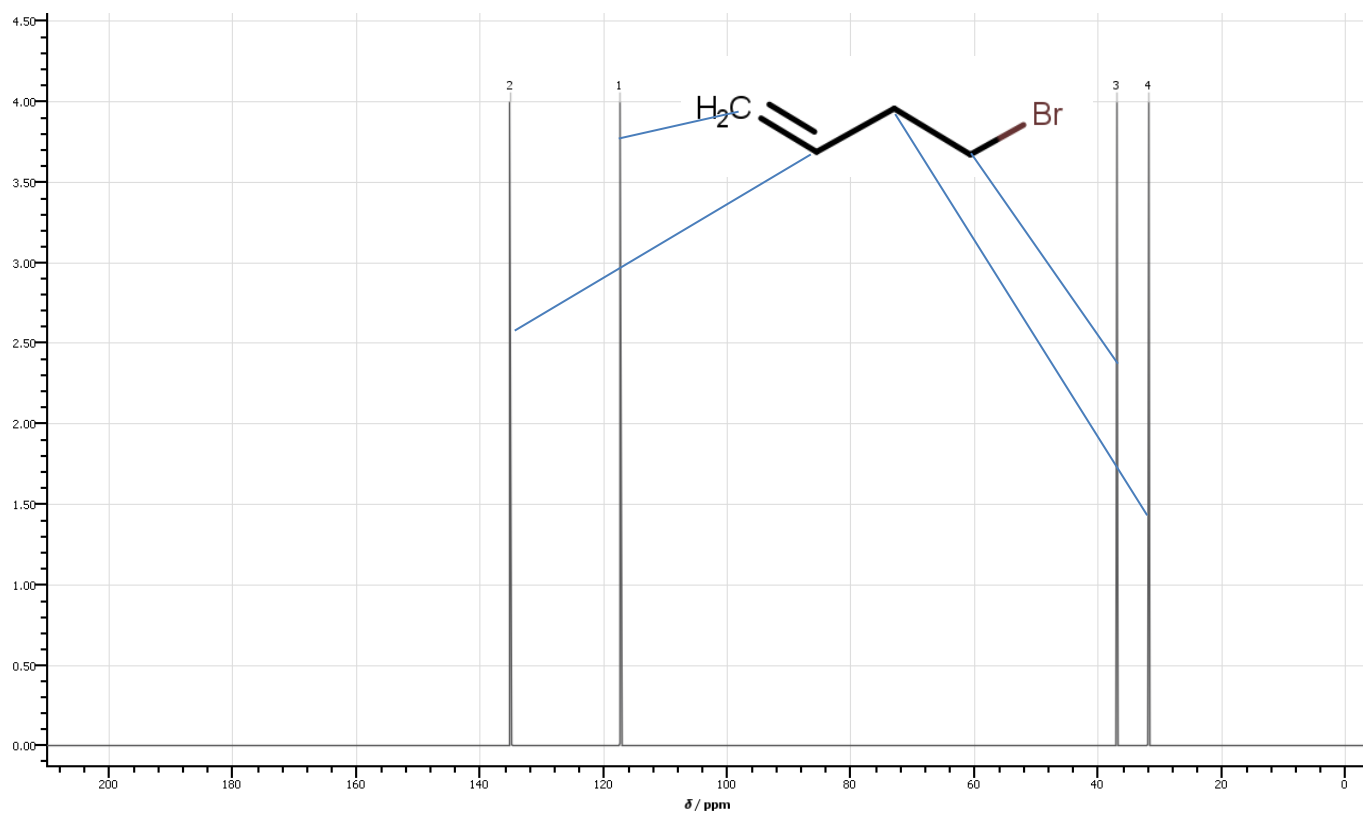
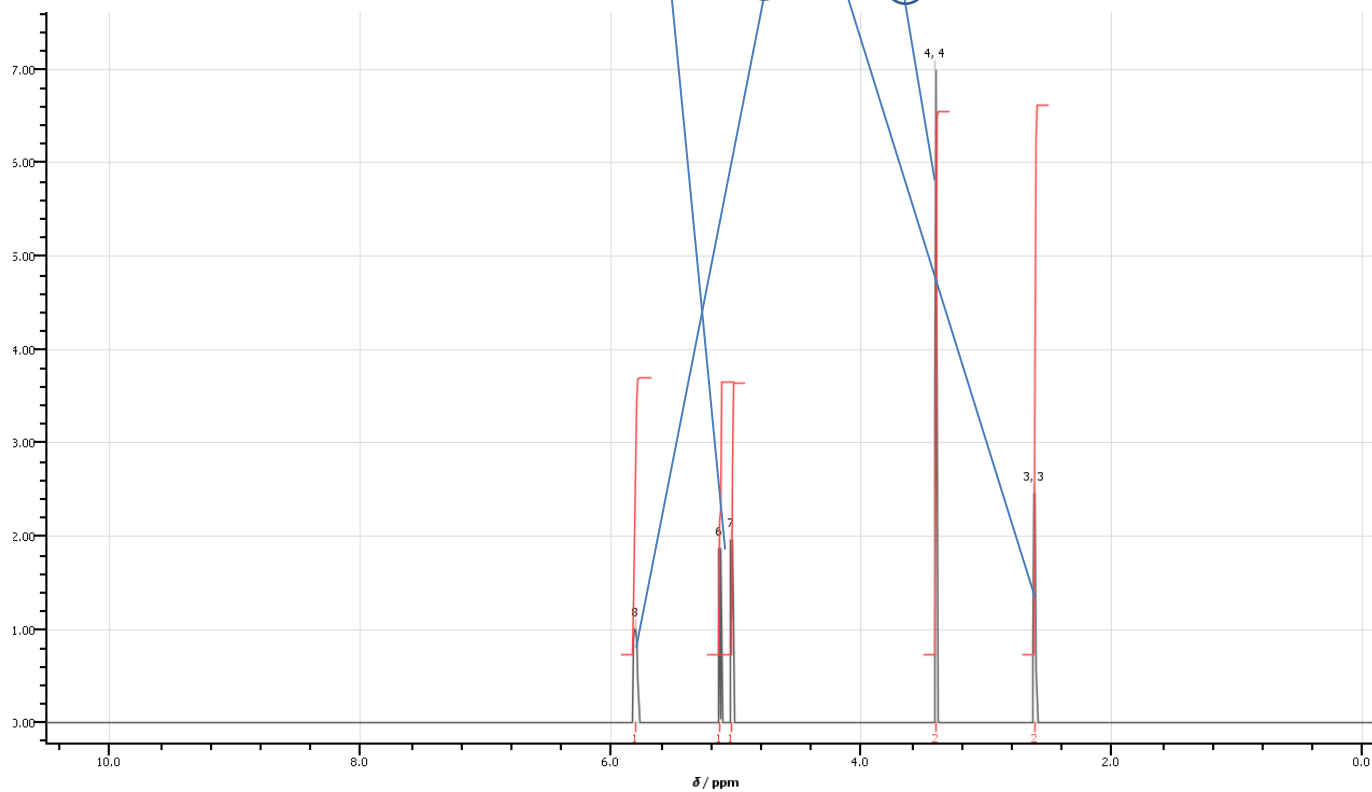
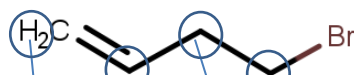
Compound produces a white precipitate when heated in a mixture of sodium hydroxide solution, ethanol and silver nitrate.

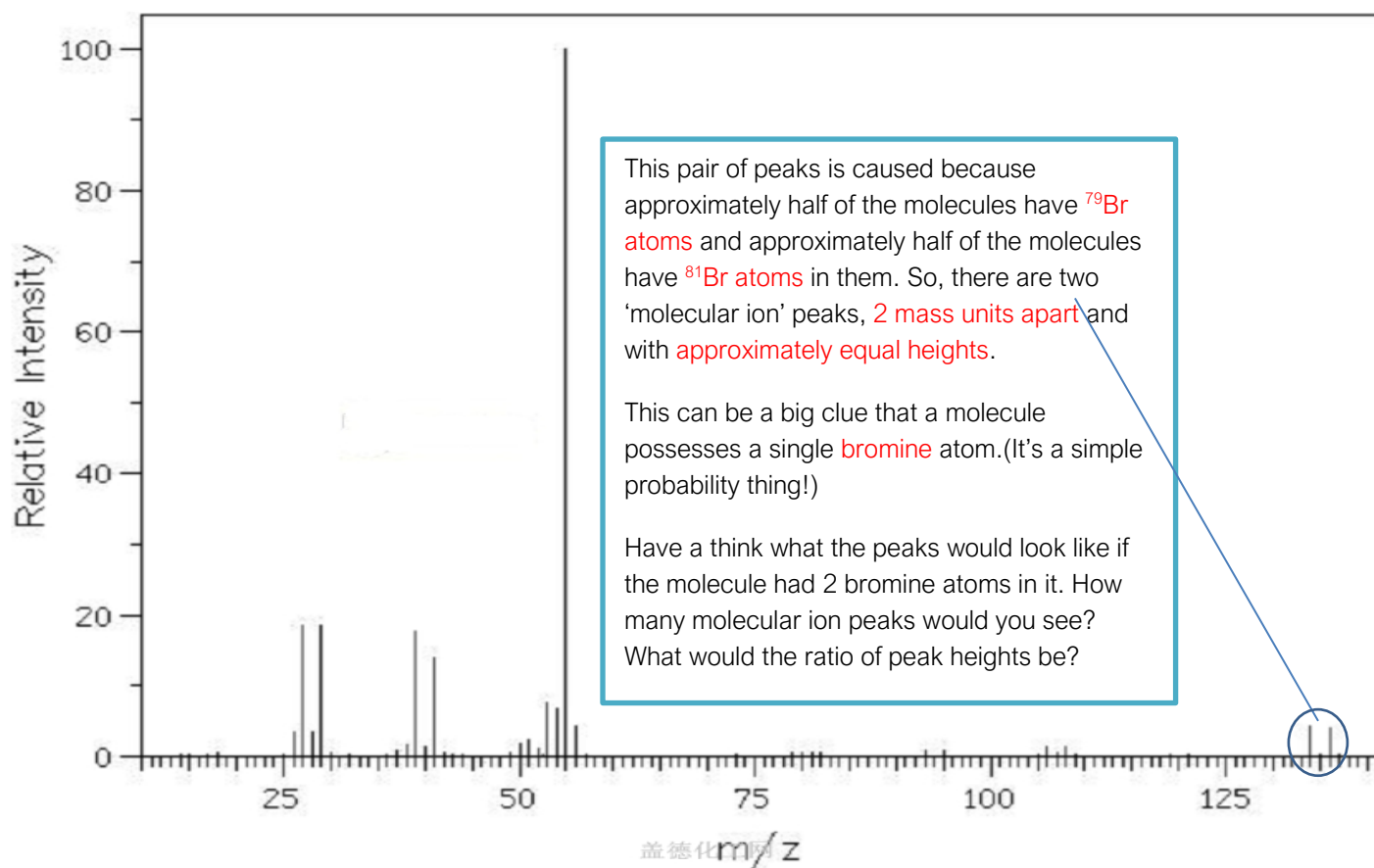
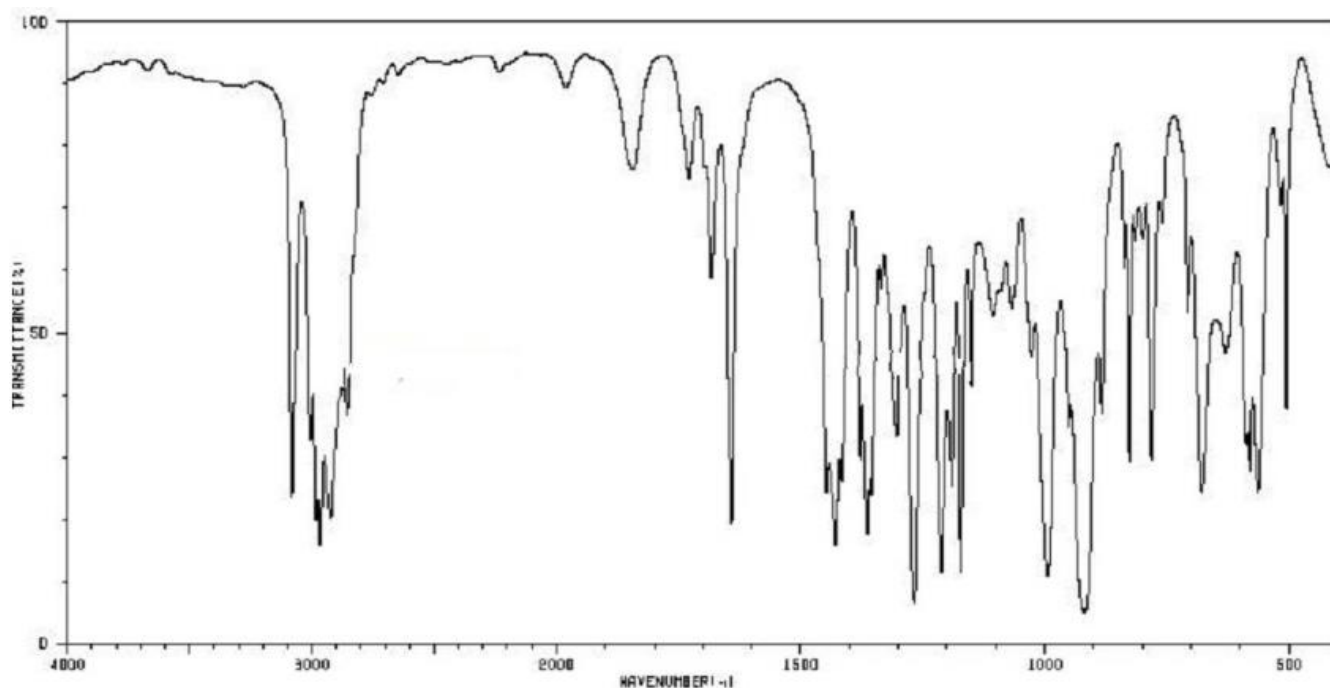
# Compound 10 ANSWERS

description: colourless volatile liquid

composition: C 35.59%; H 5.23%; Br 59.19%

molecular formula:  $C_4H_7Br$  4-bromobut-1-ene





#### Further Information:

Compound is immiscible (insoluble) in water.

Compound decolourises bromine water.