**AOS 1 Unit 4 Chemistry SAC: Instrumentation**

**Aim**: To use the data provided to deduce the formula and structure of a molecule

**Data**

A 3.400 g sample of an organic molecule is found to contain 2.110 g of carbon and 0.352 g of hydrogen. The remainder is oxygen.

**1**. Complete the table provided to show the mass of each element present

|  |  |
| --- | --- |
| **element** | **mass present** |
| carbon |  |
| hydrogen |  |
| oxygen |  |

1 mark

**2**. Determine the empirical formula of the mystery molecule.

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 2 marks

The mass spectrum of the molecule is shown below





**3. a. i**. There are two distinct parent molecular ions. What are their masses?

 \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

 **ii**. How do their relative abundances compare?

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 **iii**. What is the likely difference between the two parent molecular ion peaks?

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1 + 1 + 1 = 3 marks

 **b**. **i**. What fragment has probably been broken from the molecule to produce a peak

 at 43? \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

**ii**. What fragment has caused the peak at 15? \_\_\_\_\_\_\_\_\_\_\_\_\_\_

  **iii**. What might the absence of a significant peak at mass 29 indicate?

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1 + 1 + 1 = 3 marks

 **c**. What is the molecular formula of the mystery molecule? \_\_\_\_\_\_\_\_\_\_

1 mark

The infrared spectrum of the mystery molecule is shown below



**4**. **a**. There is no significant peak over 3000 cm-1. What conclusion might this lead to?

  **\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_**

 **b**. There is a significant peak around 1700 cm-1. What conclusion might this lead to?

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 **c**. The infrared spectrum is a relatively plain one. What conclusion might this lead to?

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1 + 1 + 1 = 3 marks

The 1H NMR spectrum for the mystery molecule is drawn below



**5. a**. How many different hydrogen environments does this molecule have? \_\_\_\_\_\_\_\_

1. Why is there no evidence of peak splitting?

  **\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_**

1 + 1 = 2 marks

**6.** Time to put all of the evidence together.

 The molecular formula is \_\_\_\_\_\_

 The molecule cannot be an alkanol because

 \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

 The molecule cannot be an amine because

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 The molecule cannot be a carboxylic acid because ( 2 reasons wanted)

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 The number of different hydrogen environments is \_\_\_\_\_\_\_\_\_\_\_\_\_

 1 + 1 + 1 + 2 + 1 = 6 marks

**7**. Draw a structural diagram of the molecule. Name the molecule.

1 + 1 = 2 marks

**8. a**. How many different carbon environments does this molecule have? \_\_\_\_\_\_\_\_

 **b**. Would you expect this molecule to be polar or non polar. Explain your answer.

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1 + 2 = 3 marks

**9**. This molecule can be manufactured in a pathway that starts with propene. Outline the

 steps and reagents required in this synthesis.

 4 marks

Total out of 30 \_\_\_