**Chemistry SAC Unit 4 Outcome 1: Data analysis task**

The whole of this SAC task relates to one molecule. You have to use the data provided to identify this molecule.

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

**Data**

A 1.424 g sample of an organic hydrocarbon molecule is found to contain 1.221 g of carbon.

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

|  |  |
| --- | --- |
| **Element** | **mass present (g)** |
| carbon |  |
| hydrogen |  |

1 mark

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

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

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

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

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

2 marks

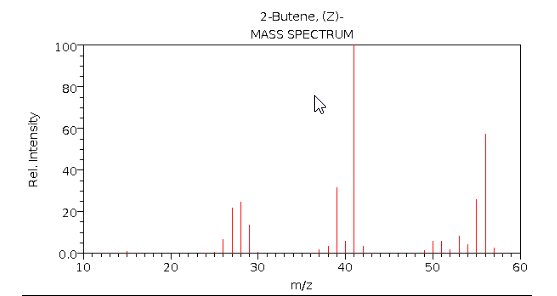
The mass spectrum of the molecule is shown below

**3. a. i**. What is the *m/e* ratio of the parent molecular ion?

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

**ii**. Suggest an explanation for the small peak with *m/e* ratio of 57.

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



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

with m/e ratio of 41? \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

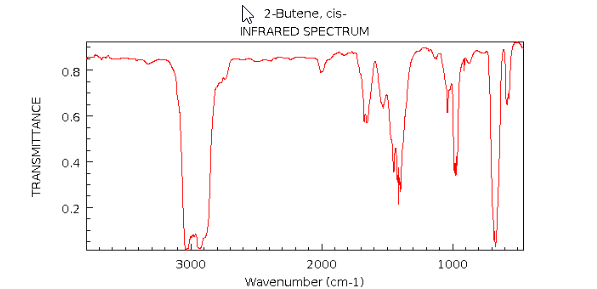
**ii**. What possible fragment might have caused the peak at 28? \_\_\_\_\_\_\_\_\_\_\_\_

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

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

2 + 2 + 1 = 5 marks

The infrared spectrum of the mystery molecule is shown below



**4**. **a**. How can the infrared spectrum be used to confirm the molecule is not an alkanol

molecule?

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

**b**. There is a significant absorption at 3000 cm-1. What type of bond might have caused

this?

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

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

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

**d.** There is an absorption around 1600 cm-1. What type of bond might have caused this?

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

1 + 1 + 1 + 1 = 4 marks

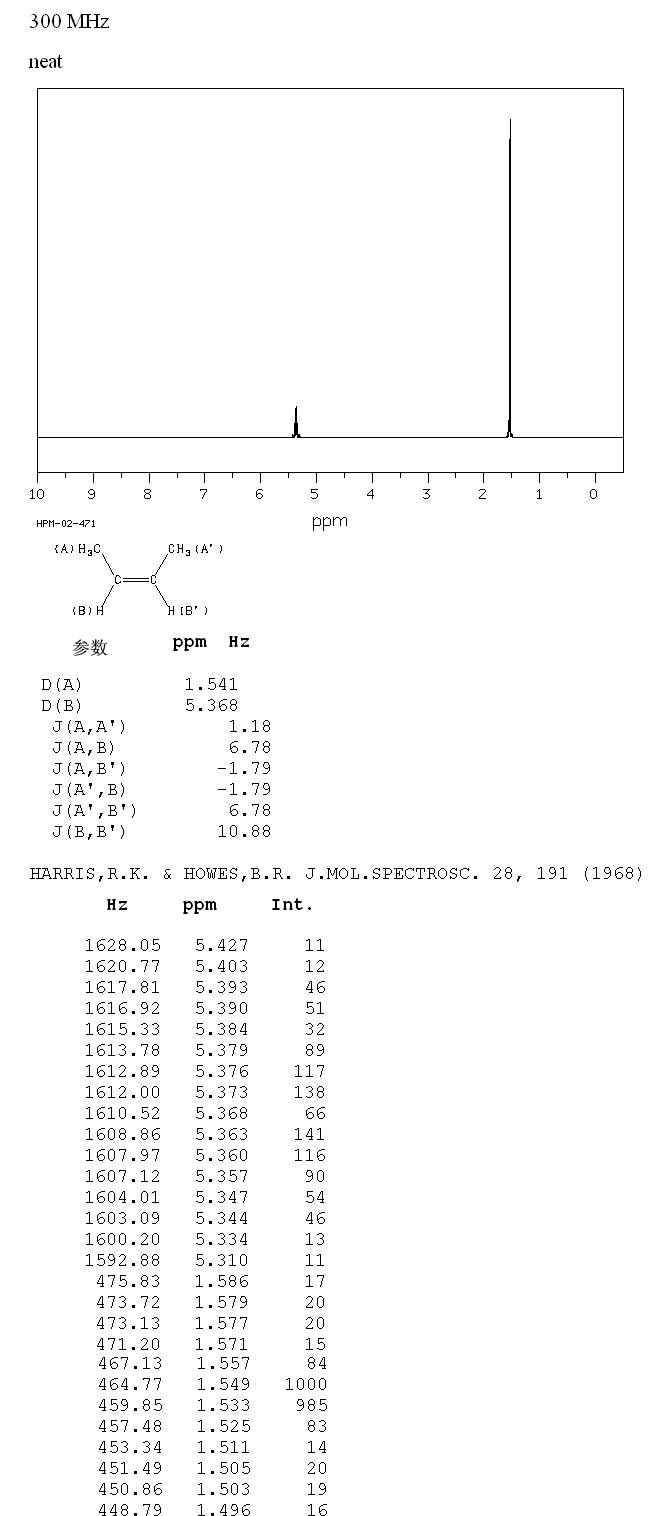
**5**. Draw and name two possible isomers with the molecular formula of this mystery

molecule.

Isomer 1: \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ Isomer 2: \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

2 marks

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



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

1. Given the shift values shown, and the molecular formula, what proton structure has produced the peak at shift

**i**. 1.6

**ii**. 5.4

1 + 2 = 3 marks

**7.** Use the NMR to explain carefully which isomer is the correct one.

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

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

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

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

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.

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

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

1 + 1 = 2 marks

**9**. This mystery molecule can be reacted with bromine solution.

**a**. Describe what change an observer will see.

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

**b**. Draw and name the product formed

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

1 + 1 = 2 marks

**10.** A polymer can be formed from the reaction of this molecule with itself.

Show a segment of the polymer chain that will form.

1 mark

**11**. A reaction occurs when the mystery molecule is heated with steam.

Draw and name all products formed in this reaction.

1 mark