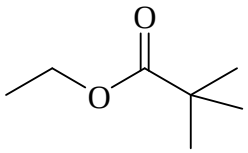
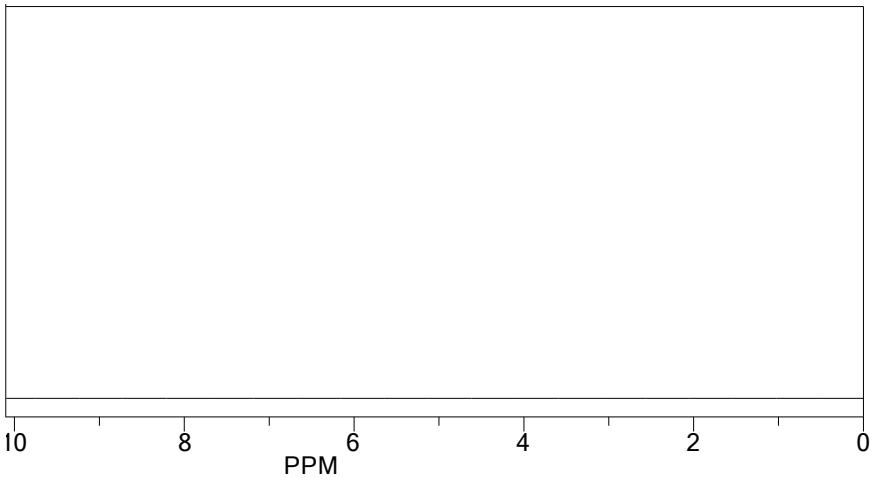
Marks 6

- Below is the structure of an ester.



Using the blank scale below, sketch the ^{1}H NMR spectrum that you would expect to see for this molecule. You will need to indicate the approximate chemical shift of each signal (by drawing it in the appropriate place on the blank spectrum and labelling the molecule to show which peak is which) as well as the integral associated with each peak and the splitting (multiplicity).



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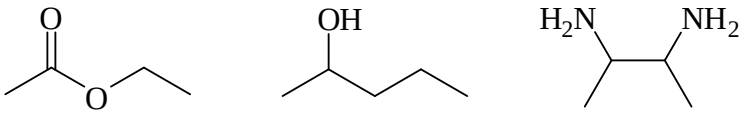
3

- Suppose a molecule has been isolated from a natural source. When a sample of the molecule is analysed by low resolution mass spectrometry, it shows a molecular ion peak that implies the molecule has a molecular weight of 88. You determine that the molecule might be one of the following three possibilities, all of which have a molecular weight of 88.



A **B** **C**

Further data are acquired for the compound as follows:

- Elemental analysis data: C, 68.13%; H, 13.72% (another element is also present)
- High resolution mass spectrum suggests the molecular weight is actually 88.0888.

Explain how ***either*** high resolution mass spectrometry ***or*** the elemental analysis data allows you to distinguish between these three possibilities and hence identify which of **A**, **B** or **C** is in the sample.

Information you may need:

Average atomic masses:	C: 12.0107,	H: 1.0079,	O: 15.9994,	N: 14.0067
Exact isotopic masses:	^{12}C: 12.0000,	^{1}H: 1.0078,	^{16}O: 15.9949,	^{14}N: 14.0031

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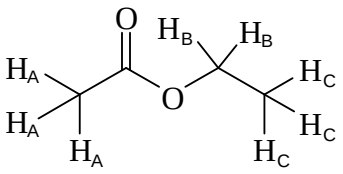
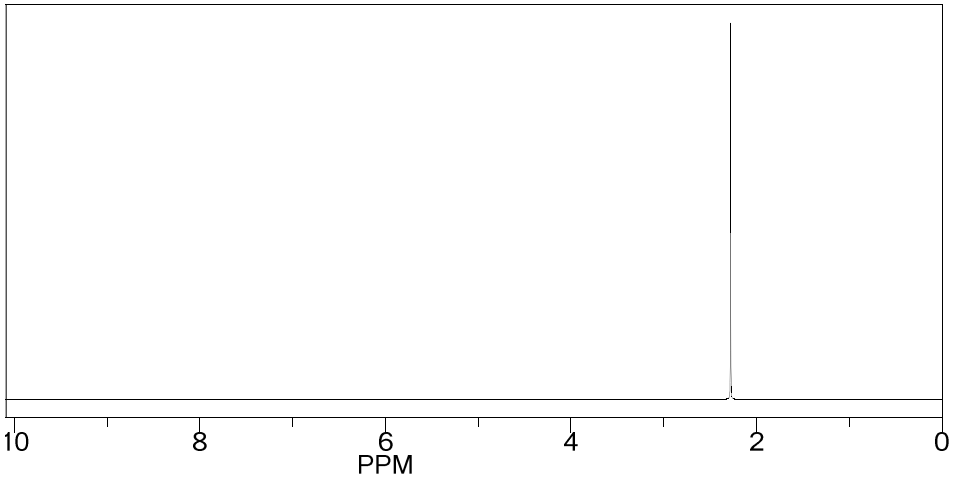
- Sketch the resonances you would expect to observe for protons H_B and H_C in the ^1H NMR spectrum of compound **X**. Ensure that the approximate chemical shifts, as well as peak splittings and signal integrations are incorporated in your answer. (The resonance for H_A is provided as a guide.)

X



H_A, singlet, Integration = 3



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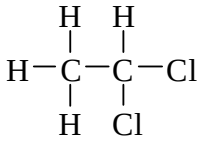
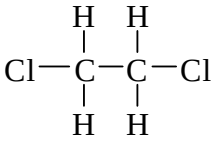
Marks 6

- Consider the isomers 1,1-dichloroethane and 1,2 dichloroethane, which can be readily identified by their ^{1}H NMR spectra.

  On the structures below, write the letters **a**, **b**, **c**, *etc*. as necessary to identify each **unique** hydrogen environment giving rise to a signal in the ^{1}H NMR spectra of these compounds.

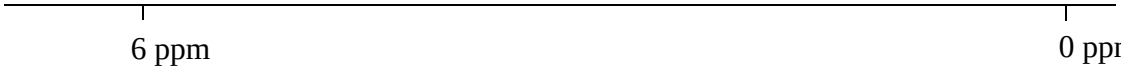




Sketch the ^{1}H NMR spectrum of each compound. Label each signal in the spectra with **a**, **b**, **c**, *etc.* to correspond with your assignments on the diagram above. Make sure you show the splitting pattern (number of fine lines) you expect to see for each signal. Also write the relative number of hydrogens you expect above each signal.

Spectrum of 1,1-dichloroethane

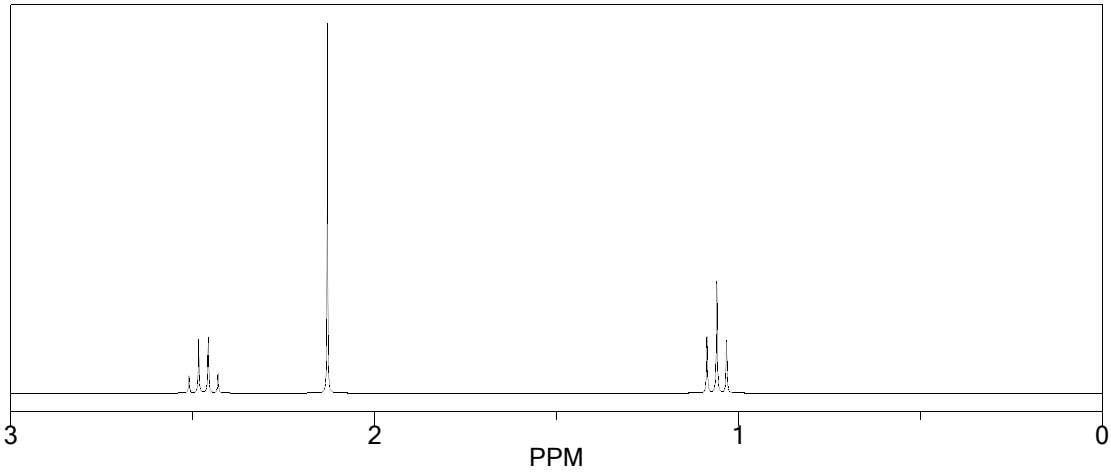
Spectrum of 1,2-dichloroethane



Marks
5

- An unknown compound **K** with the molecular formula C_4H_8O gives the following spectroscopic data.

  ^{1}H NMR: 1.06 ppm, triplet, integration = 3H
  2.13 ppm, singlet, integration = 3H
  2.47 ppm, quartet, integration = 2H

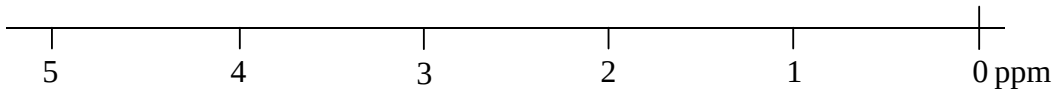


  IR spectroscopy: stretch at 1715 cm^{-1}.

  Use the information above to deduce the structure of compound **K**. Give reasoning for the structure chosen.

Marks 5

- Sketch the ^{1}H NMR spectrum of bromoethane, CH_3CH_2Br. The signals appear at 1.7 and 3.3 ppm. Clearly indicate the splitting patterns of both signals and show their relative intensities.



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