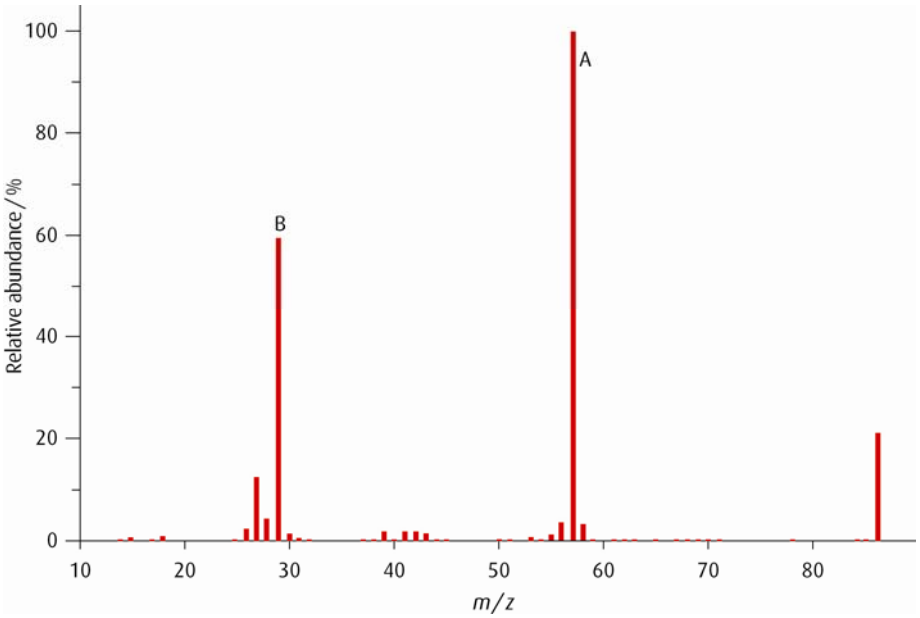
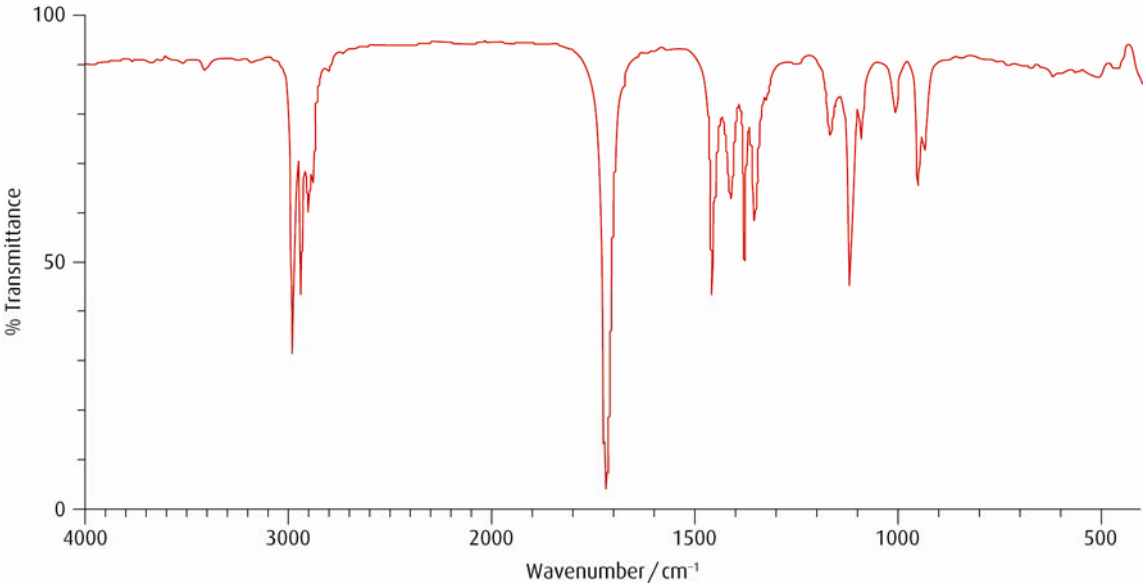
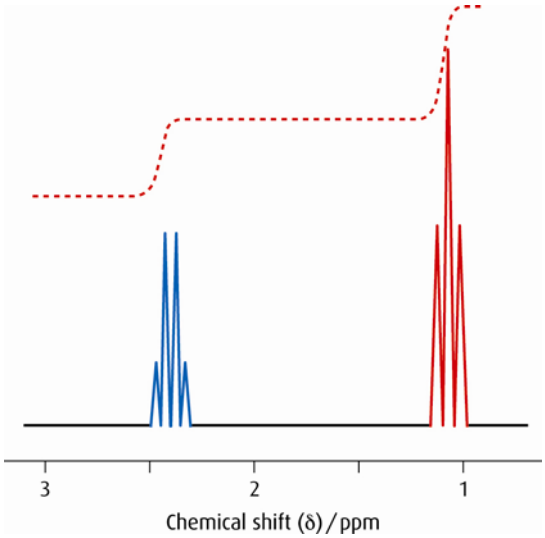
AHL Worksheet – Option A

1 The spectra below are for a molecule containing carbon and hydrogen atoms and one oxygen atom.







a Deduce the molecular formula of the compound. [1]

b Suggest the identities of the fragments labelled A and B in the mass spectrum. [2]

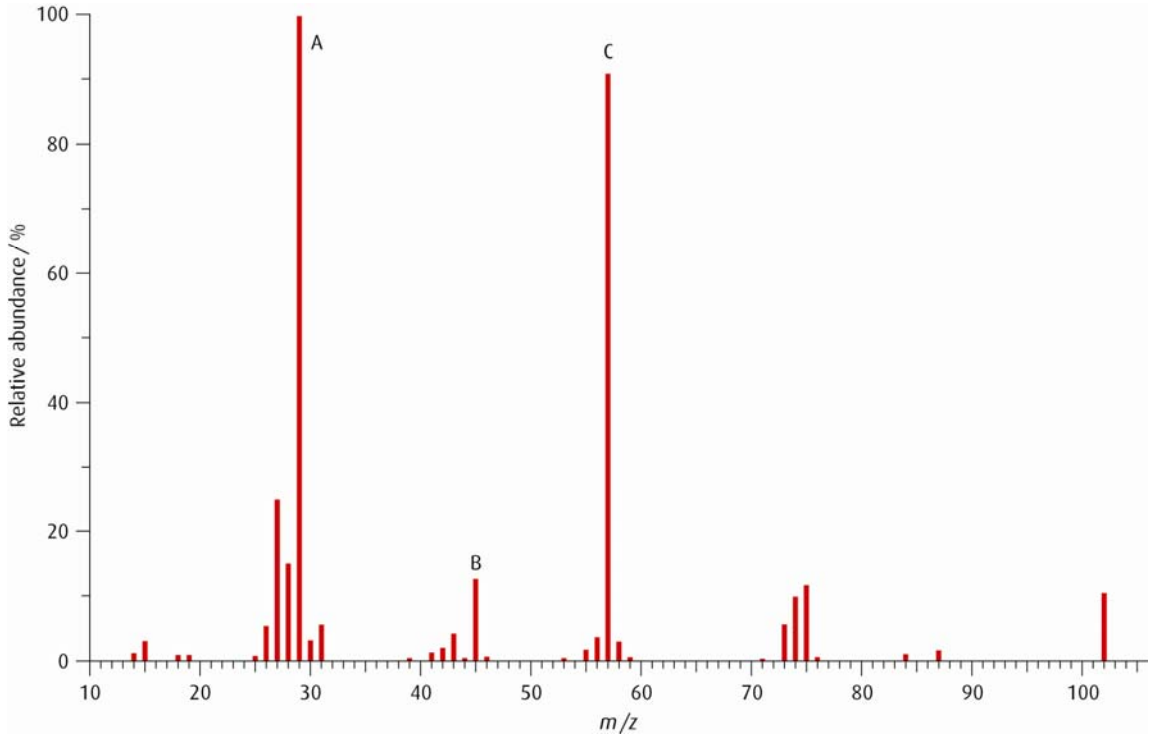
c Use the infrared spectrum to identify two possible functional groups in this molecule. [1]

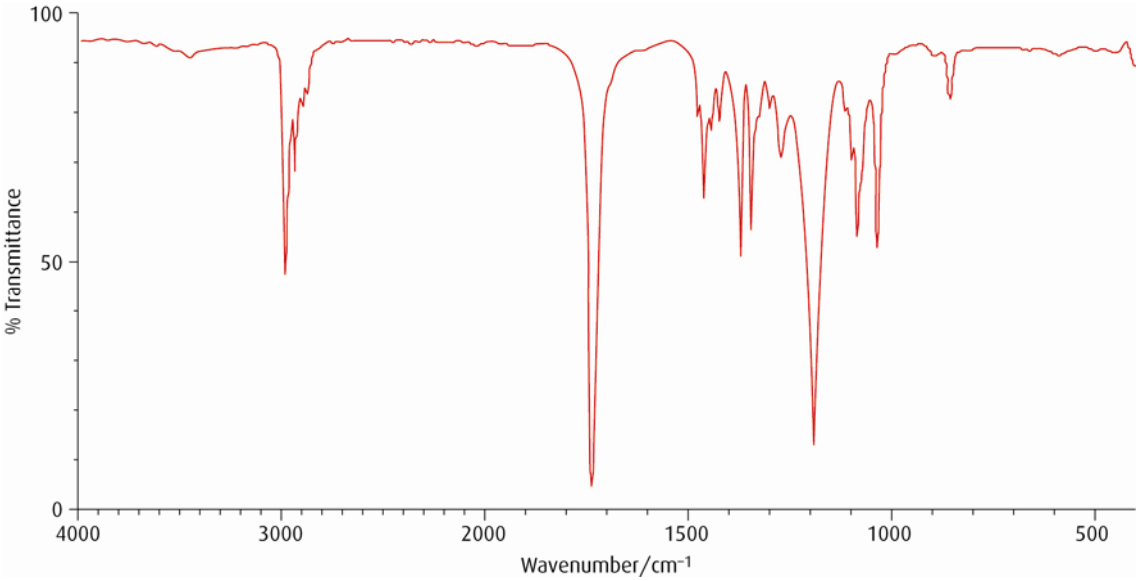
d Calculate the number of hydrogen atoms present in each environment from your answer to part **a** and the NMR spectrum. [2]

e What information can be obtained from the multiplicity of each peak in the NMR spectrum? [1]

f Deduce the structure of the molecule. [4]

2 The spectra and information below are for a molecule containing two oxygen atoms as well as carbon and hydrogen.





The NMR spectrum consists of:

- a triplet, integral 3, at 1.1 ppm
- a triplet, integral 3, at 1.3 ppm
- a quartet, integral 2, at 2.3 ppm
- a quartet, integral 2, at 4.1 ppm.

a What is the relative molecular mass of the molecule? [1]

b What is the molecular formula of the compound? [1]

c Identify the fragment ions responsible for the labelled peaks in the mass spectrum. [3]

d Deduce the structural formula of the molecule. [3]

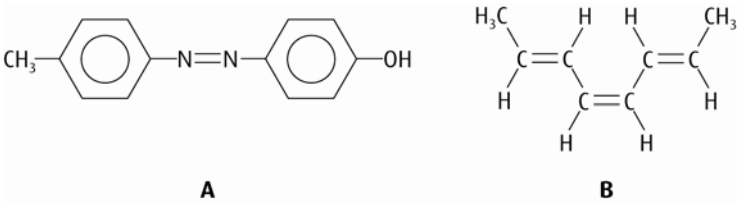
3 The following peaks occur in the NMR spectrum of compound X:

- triplet, integral 6, at 1.2 ppm
- singlet, integral 6, at 1.4 ppm
- quartet, integral 4, at 3.5 ppm.

The molecular formula of X is $C_7H_{16}O_2$ and the only peak in the IR spectrum in the region above 1500 cm^{-1} is at about 2950 cm^{-1}.

Use the information given above to deduce the structural formula of X. [6]

4 Consider the two molecules below:



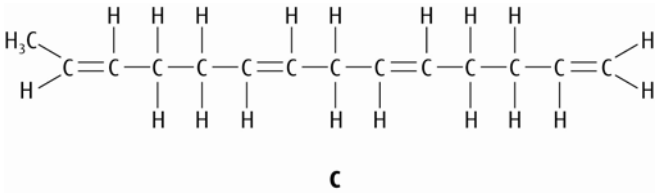
A B

One of the compounds is orange and the other is colourless.

a Identify which compound is coloured. [1]

b Explain, in terms of molecular structure and the absorption of light, why one of the compounds is colourless and the other is coloured although they both absorb electromagnetic radiation. [4]

c Would you expect the molecule C, shown below, to absorb radiation of shorter or longer wavelength than molecule B (above)? Explain your answer. [2]



C