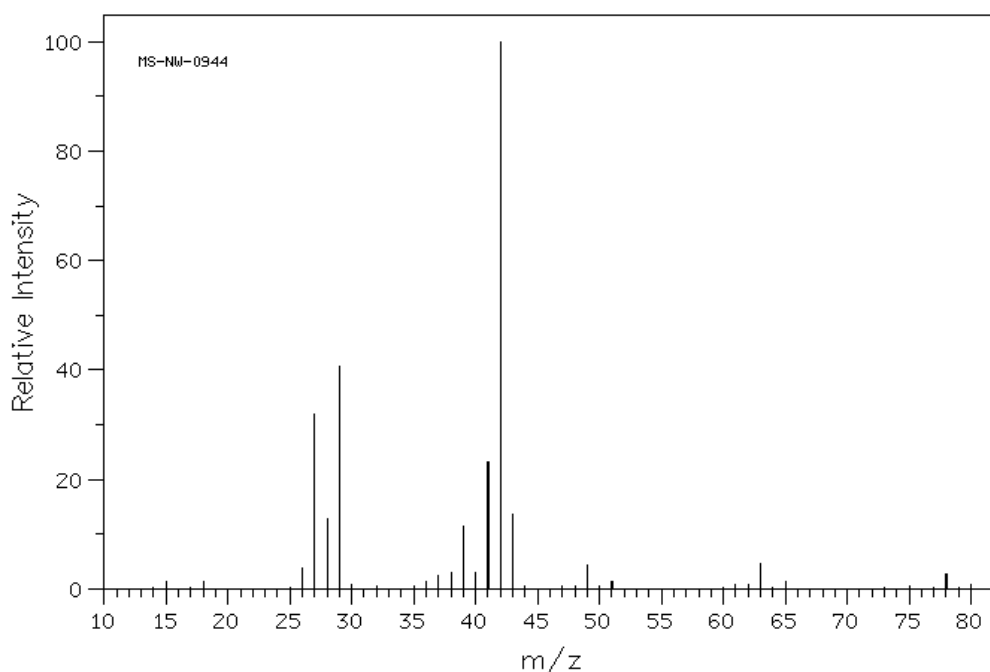# MASS SPECTROMETRY ANSWERS

EXERCISE 1

The following mass spectrum is for a compound determined to have an empirical formula of C_3H_7X.
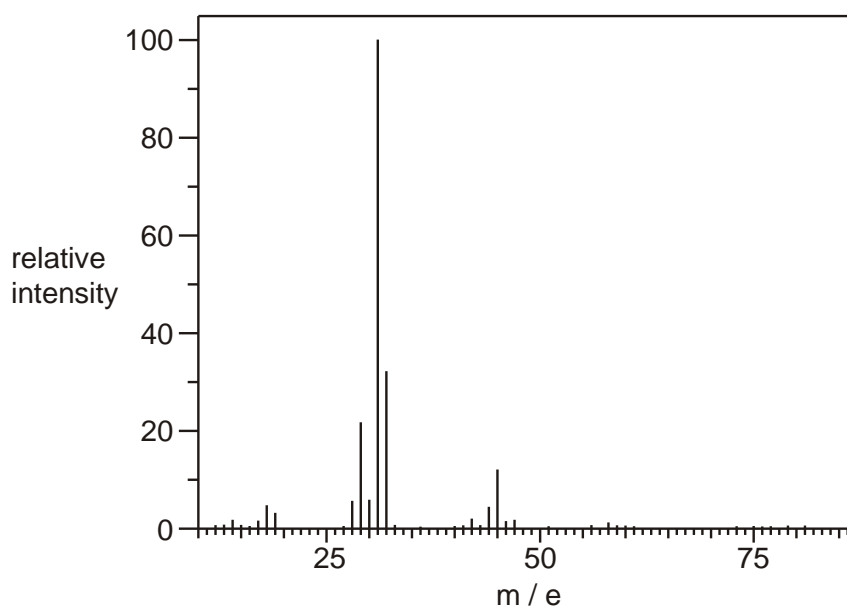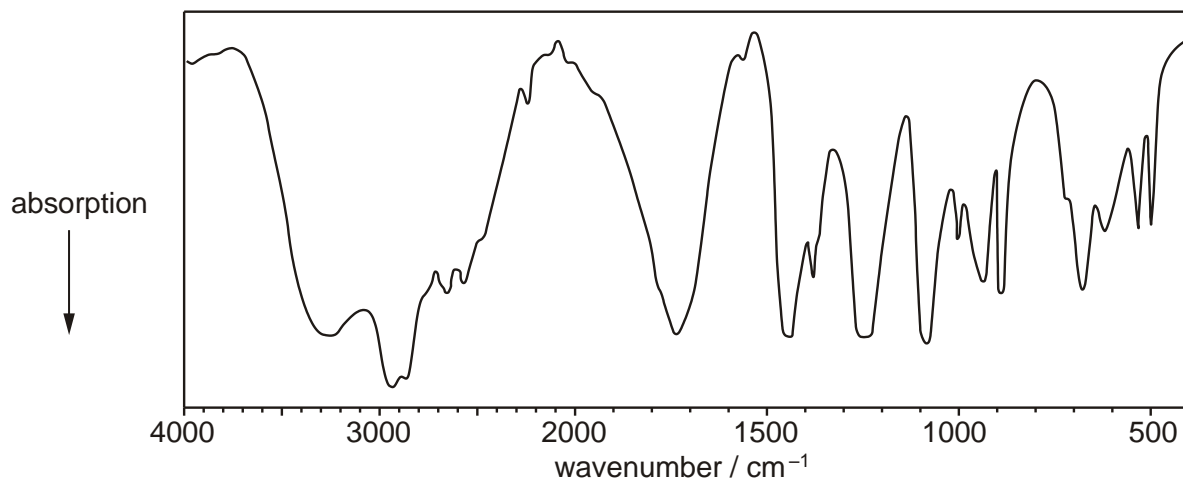

a) Work out the molecular mass (molar mass) of this compound and therefore the identity of the halogen. MOLAR MASS = 78 gmol^{-1}

b) Identify the peak with a m/z ratio of 43. $CH_3CH_2CH_2^+$
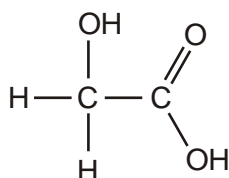
Exercise 2

Compound **G** can be extracted from sugar-cane and is commonly used in 'rejuvenating' skin creams because it helps to remove some of the dead cells from the skin surface.

The molecular formula of **G** is $C_2O_3H_4$ and the compound contains **two different** functional groups containing oxygen atoms.

The infra-red and mass spectra of **G** are shown below.

absorption

4000 3000 2000 1500 1000 500
wavenumber / cm^{-1}

relative intensity

100
80
60
40
20
0

25   50   75
m / e

The structure of compound **G** is shown below.

a) There is a peak missing from the mass spectra. What value would you expect it to have?

b) Explain how the infra-red and mass spectra confirm this structure. In your answer, you should suggest a possible structure for the ion that gives the base peak at m / e = 31 in the mass spectrum.

Answer:

a) 76 (the molar mass of the parent ion)
b) The mass spec gives the molecular fragments 31 and 45 which come from the ions formed when the C-C splits (CH_2OH is 31 and COOH is 45). The IR gives a broad –OH @ ~3000, a carbonyl C=O @ ~1700 and a C-O @~1200.