

Video worksheet – Mass spectroscopy.

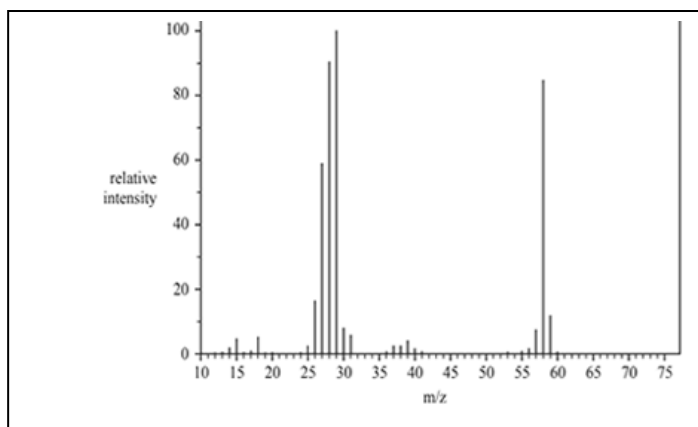
1. A sample of an unknown organic, white powder of mass 0.176 grams was analysed and found to have the following percentage composition, by mass, 54.5% carbon, 36.4% oxygen and 9.1% hydrogen. Below is its mass spectrum. This compound was also found to lower the pH of a 0.1M NaOH solution.

  - a. Find the compound's empirical formula.
  - b. Find the compound's molecular formula.
  - c. Identify the "**base peak**" in the mass spectrum. What is the significance of the base peak?
  - d. Account for the small signal at  $m/z$  89 and  $m/z$  15.
  - e. How can the signal at  $m/z$  73 be used to identify the compound?
2. The mass spectra of two substances A and B are shown below. Both substances have the same molecular formula. Both molecules A and B were formed via a condensation reaction between an organic acid and an alcohol. In the formation of compound A ethanol was used where as methanol was used in forming compound B.

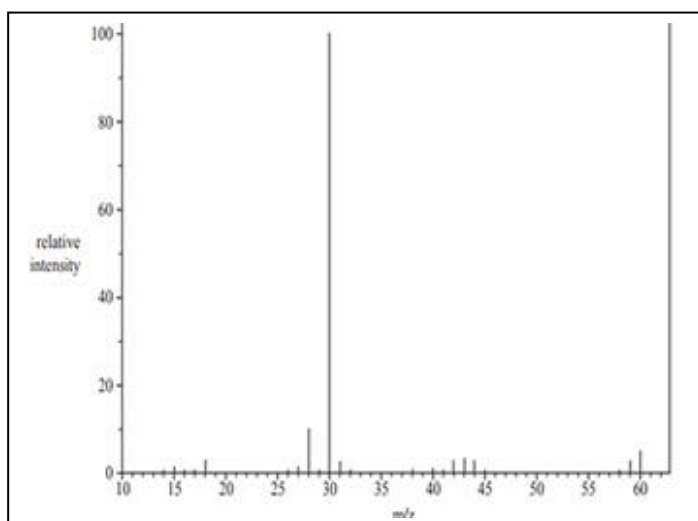
  - a. Name and draw possible molecular structures for A and B .
  - b. Using the mass spectrum of each compound identify molecules A and B and justify your choice.
  - c. The mass spectrum of molecule B shows a noticeable spike at  $m/z$  89. Give an explanation for the signal at  $m/z$  89 and suggest a reason as to why it is not present in the spectrum of compound A.
3. A sample of compound M is analysed in a mass spectrometer where it forms the molecular ion  $M^+$

  - a. Write an equation for the ionisation of M
  - b. Some of the molecular ions fragment as follows.  
 $M^+ \rightarrow A^+ + B$  and  
 $M^+ \rightarrow A + B^+$   
The mass spectrum would show peaks due to the species
    - A.  $M^+$ , A,  $A^+$ , B and  $B^+$  only.
    - B.  $M^+$ ,  $A^+$  and  $B^+$  only.
    - C.  $A^+$  and  $B^+$  only.
    - D. A and B only.

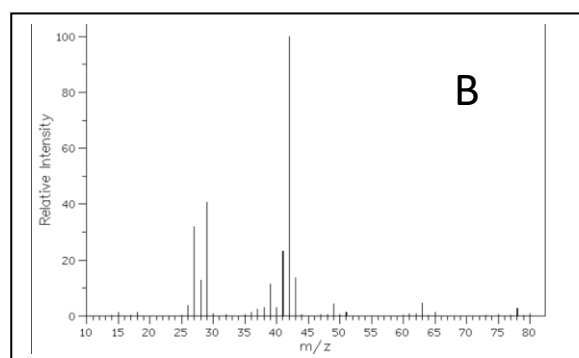
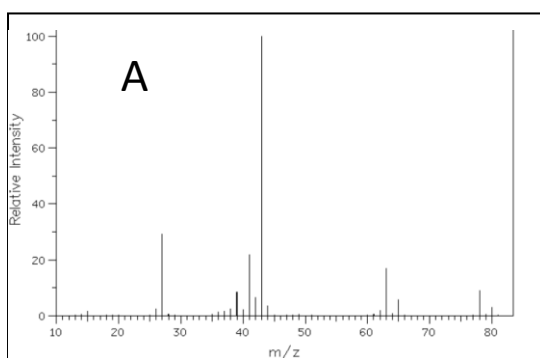
4. There are a number of structural isomers for the molecular formula  $C_3H_6O$ . Three of these are propanal, propanone and prop-2-en-1-ol. The mass spectrum below was produced by one of the three named isomers of  $C_3H_6O$ .
- Identify the fragment at 29  $m/z$
  - Name the isomer of  $C_3H_6O$  that produced this spectrum and justify your answer



5. A bottle containing an unknown organic compound was examined in a university laboratory. There was an incomplete label on the bottle that gave only the empirical formula for the contents:  $CH_4N$ . A chemist hypothesised that the unknown compound was 1,2-ethanediamine,  $NH_2CH_2CH_2NH_2$ . Mass spectrometry produced the following spectral data shown on the right.



- Identify the base peak.
  - At what  $m/z$  ratio is the principal peak that supports the chemist's hypothesis that the unknown compound has the formula  $NH_2CH_2CH_2NH_2$ ? Justify your answer
6. Two isomers of a chloroalkane are isolated. Their mass spectra are shown below.



- Looking at the spectra of both isomers what is the likely molecular formula for the compound?
- Account for the peak at  $m/z$  80
- Draw the structural formula for both isomers.
- Identify the ion fragment that formed the base peak in each spectra.
- Give the IUPAC name for compound A and B. Justify your choice with reference to the spectra.

