

Student guide: Time of flight mass spectrometry – example questions and answers

01.1 One of the methods of ionising samples in time of flight mass spectrometry is by electron impact. How is this ionisation done?

[4 marks]

01.2 A second method of ionising samples in time of flight mass spectrometry is by electrospray ionisation. How is this ionisation done?

[4 marks]

01.3 Which method is most likely to lead to the break up of the ions into fragments? [1 mark]

01.4 Ionisation by electron impact causes removal of one electron from each particle. Write an equation for the ionisation of each of the following species by loss of one electron. [2 marks]

Ca _____

C₂H₆ _____

01.5 Electrospray ionisation creates an ion by protonation of a molecule. Write an equation for the formation of a positive ion by electrospray ionisation of lactic acid (C₃H₆O₂). [1 mark]

02 The 1+ ions are accelerated using a negatively charged electric plate.

02.1 Why is a negatively charged plate used? [2 marks]

02.2 Complete this sentence: The ions are accelerated by an electric field so that they each have the same _____ [1 mark]

03 The 1+ ions enter the flight tube through a hole in the negatively charged plate.

03.1 Explain why different ions take different times to travel through the flight tube. [2 marks]

03.2

Which of these ions will reach the detector first? Explain your answer in each case.

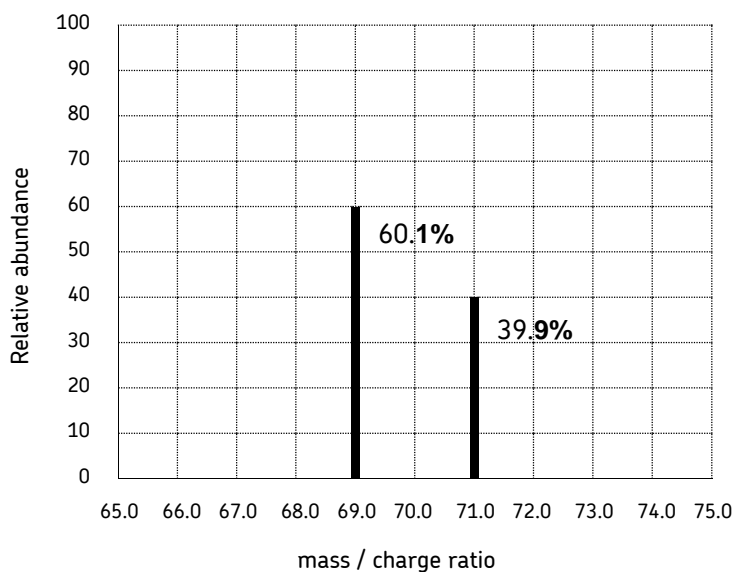
[2 marks]

$^{79}\text{Br}^+$ or $^{81}\text{Br}^+$ _____

$^{12}\text{C}^1\text{H}_4^+$ or $^{13}\text{C}^1\text{H}_4^+$ _____

04

The mass spectrum of a sample of gallium is shown.



04.1

What isotopes are present in this element?

[1 mark]

04.2

Calculate the relative atomic mass of this element.

Give your answer to the appropriate number of significant figures. Show your working.

[2 marks]

05

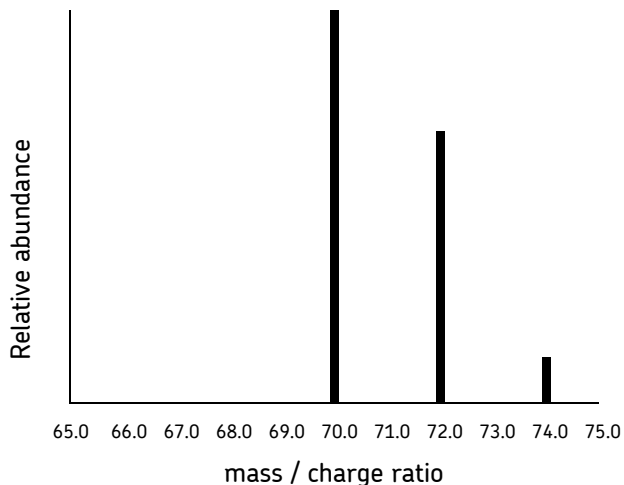
The mass spectrum of the element chlorine (Cl_2) is shown.

Identify the ion responsible for the peak at:

m/z 70 _____

m/z 72 _____

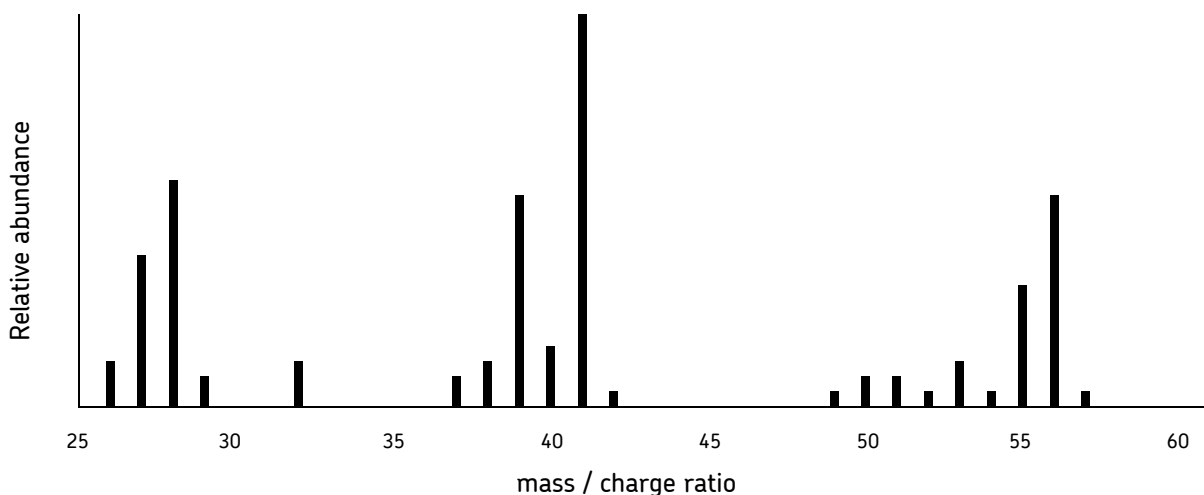
m/z 74 _____



[2 marks]

06

The mass spectrum shown is of a hydrocarbon that has been produced via electron impact ionisation.



06.1

What is the relative molecular mass of this compound?

[1 mark]

06.2

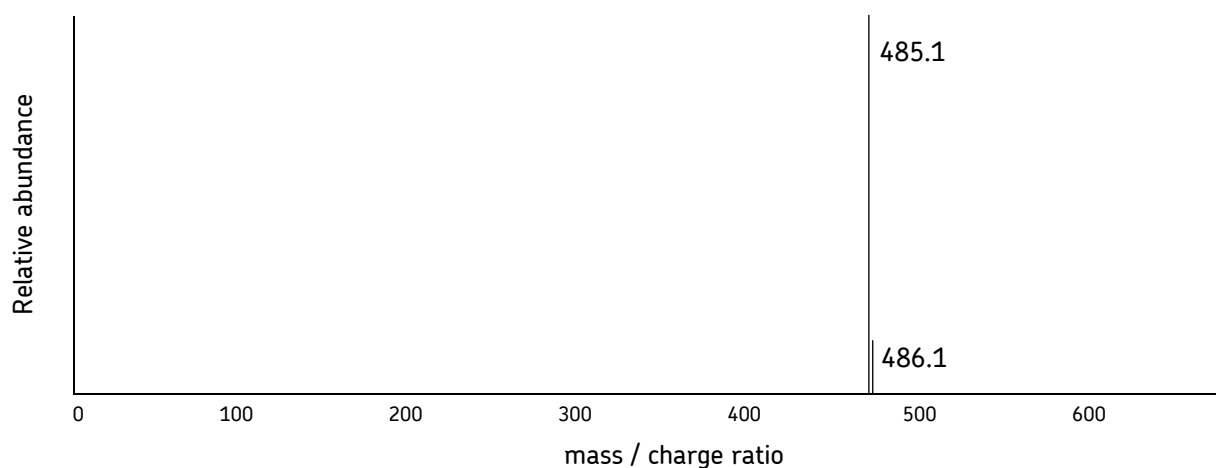
Why are there peaks with much lower m/z ratios?

[1 mark]

06.3 Why is there a peak / peaks with higher m/z ratios?

[1 mark]

07 The mass spectrum shown is of a protein that has been produced by electrospray ionisation.



What is the relative molecular mass of this protein?

[1 mark]

08 The kinetic energy of the ions in a TOF mass spectrometer is given as: $KE = \frac{1}{2}mv^2$

and the time to travel through the flight tube as: $t = \frac{d}{v}$

where:

- t = time of flight (s)
- KE = kinetic energy of particle (J)
- m = mass of the particle (kg)
- v = velocity of the particle (m s^{-1})
- d = length of flight tube (m)

08.1 Show how these expressions can be used to show the time of flight

as: $t = d\sqrt{\frac{m}{2KE}}$

[2 marks]

08.2 A sample of copper was analysed and found to contain two isotopes, 63-copper and 65-copper. All the ions were accelerated to have 1.000×10^{-16} J of kinetic energy and travelled through a flight tube that was 0.8000 m long. $^{63}\text{Cu}^+$ ions took 1.829×10^{-5} s.

How long would $^{65}\text{Cu}^+$ ions of mass 1.079×10^{-25} kg take to travel along the same flight tube?

Give your answer to the appropriate number of significant figures.

Show your working.

[2 marks]

Example answers

- 01.1 ✓ high energy electrons
✓ from hot cathode / electron gun
✓ fired at sample
✓ knocks off one electron
- 01.2 ✓ sample dissolved in volatile solvent
✓ injected through a fine hypodermic needle giving a fine mist / aerosol
✓ tip of needle has high voltage
✓ each gains a proton as it leaves the needle
- 01.3 ✓ electron impact / electron ionisation
- 01.4 ✓ $\text{Ca(g)} \rightarrow \text{Ca}^+(\text{g}) + \text{e}^-$
✓ $\text{C}_2\text{H}_6(\text{g}) \rightarrow \text{C}_2\text{H}_6^+(\text{g}) + \text{e}^-$
- 01.5 ✓ $\text{C}_3\text{H}_6\text{O}_2 + \text{H}^+ \rightarrow \text{C}_3\text{H}_7\text{O}_2^+$
- 02.1 ✓ as the positively charged ions are attracted to the negative plate
- 02.2 ✓ same kinetic energy
- 03.1 ✓ time of flight depends on mass of ions
✓ lighter particles travel faster
- 03.2 ✓ $^{79}\text{Br}^+$ as it is lighter
✓ $^{12}\text{C}^1\text{H}_4^+$ as it is lighter
- 04.1 ✓ ^{69}Ga and ^{71}Ga
- 04.2 ✓
$$\frac{(69.0 \times 60.1) + (71.0 \times 39.9)}{60.1 + 39.9}$$

✓ = 69.8 (3sf)
- 05 $^{35}\text{Cl}_2^+$, $^{35}\text{Cl}^{37}\text{Cl}^+$, $^{37}\text{Cl}_2^+$
✓ for correct isotopes
✓ for + charge in each case
- 06.1 ✓ 56
- 06.2 ✓ due to fragmentation
- 06.3 ✓ due to some molecules containing ^2H or ^{13}C

07 ✓ 484.1

08.1 ✓ $v^2 = \frac{2KE}{m} \quad \therefore \quad v = \sqrt{\frac{2KE}{m}}$

✓ $t = \frac{d}{v} \quad \therefore \quad t = \frac{d}{\sqrt{\frac{2KE}{m}}} \quad \therefore \quad t = d\sqrt{\frac{m}{2KE}}$

08.2 ✓ $t = 0.8000 \sqrt{\frac{1.079 \times 10^{-24}}{2 \times 1.000 \times 10^{-16}}}$
✓ $1.858 \times 10^{-5} \text{ s (4sf)}$