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 ____

C_2H_6 ____

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 ($C_3H_6O_2$).

[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]

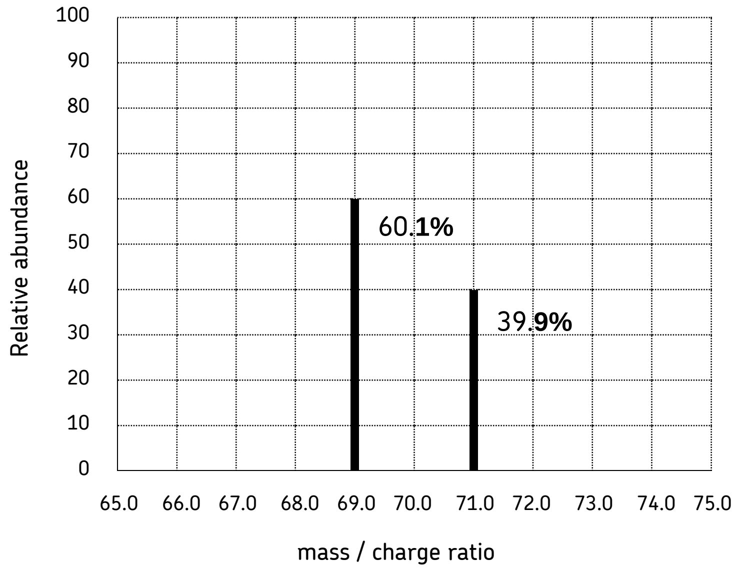
$^{79}Br^{+}$ or $^{81}Br^{+}$ ______________________________

____

$^{12}C^{1}H_4^{+}$ or $^{13}C^{1}H_4^{+}$ ______________________________

____

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]

____

____

____

____

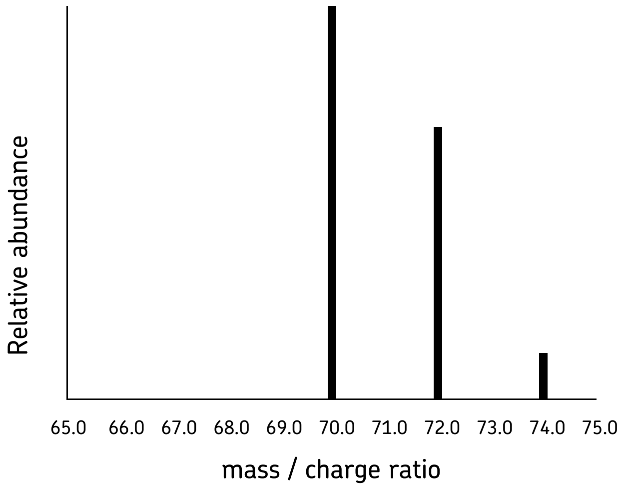
05 The mass spectrum of the element chlorine (Cl_2) is shown.

Identify the ion responsible for the peak at:

m/z 70 ______________

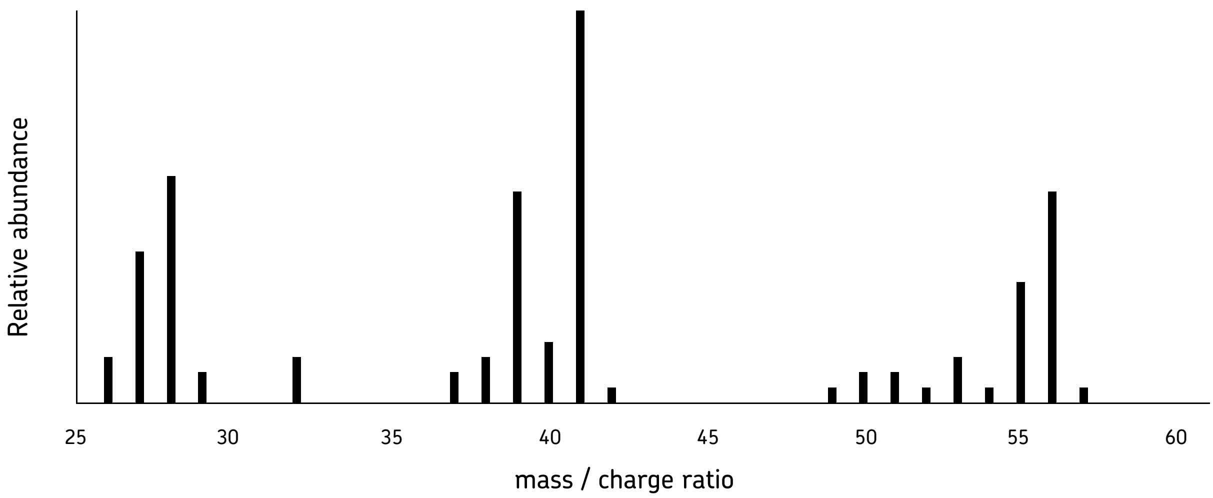
m/z 72 ______________

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]

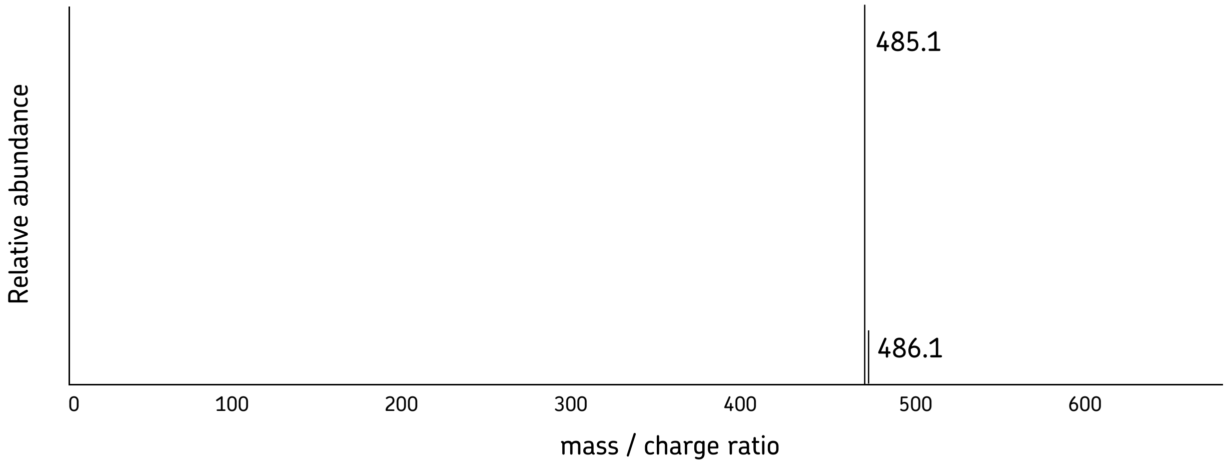
____

____

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: $\boldsymbol{KE = \frac{1}{2}mv^2}$

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

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

[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 x 10^{-16} J of kinetic energy and travelled through a flight tube that was 0.8000 m long. $^{63}Cu^{+}$ ions took 1.829 x 10^{-5} s.

How long would $^{65}Cu^{+}$ ions of mass 1.079 x 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 ✓ $Ca(g) \rightarrow Ca^{+}(g) + e^{-}$
✓ $C_2H_6(g) \rightarrow C_2H_6^{+}(g) + e^{-}$

01.5 ✓ $C_3H_6O_2 + H^{+} \rightarrow C_3H_7O_2^{+}$

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 ✓ $^{79}Br^{+}$ as it is lighter
✓ $^{12}C^{1}H_4^{+}$ 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 $^{35}Cl_2^{+}$, $^{35}Cl^{37}Cl^{+}$, $^{37}Cl_2^{+}$
✓ for correct isotopes
✓ for + charge in each case

06.1 ✓ 56

06.2 ✓ due to fragmentation

06.3 ✓ due to some molecules containing ^{2}H or ^{13}C

07 ✓ 484.1

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

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

08.2 ✓ $t = 0.8000\sqrt{\frac{1.079 \; x \; 10^{-24}}{2 \; x \; 1.000 \; x \; 10^{-16}}}$

✓ 1.858×10^{-5} s (4sf)