Magnesium Isotopes

A Level

Define the term *relative atomic mass* of an element.

The abundances of isotopes of magnesium isolated from an ore were determined by mass spectrometry.

$^{24}\mathrm{Mg} : 78.7\,\%$

$^{25}\mathrm{Mg} : 10.1\,\%$

$^{26}\mathrm{Mg} : 11.2\,\%$

Calculate the relative atomic mass of magnesium in the ore.

	protons	neutrons	electrons
$^{24}\mathrm{Mg}$	(A)	(B)	(C)
$^{25}\mathrm{Mg}$	(D)	(E)	(F)
$^{26}\mathrm{Mg}$	(G)	(H)	(I)

State the number of particles present in an atom of each isotope.

Part A Protons in $^{24}\mathrm{Mg}$

State the number of protons in an atom of $^{24}\mathrm{Mg}$.

Part B Neutrons in $^{24}\mathrm{Mg}$

State the number of neutrons in an atom of $^{24}\mathrm{Mg}$.

Part C Electrons in $^{24}\mathrm{Mg}$

State the number of electrons in an atom of $^{24}\mathrm{Mg}$.

Part D Protons in $^{25}\mathrm{Mg}$

State the number of protons in an atom of $^{25}\mathrm{Mg}$.

Part E Neutrons in $^{25}\mathrm{Mg}$

State the number of neutrons in an atom of $^{25}\mathrm{Mg}$.

Part F Electrons in $^{25}\mathrm{Mg}$

State the number of electrons in an atom of $^{25}\mathrm{Mg}$.

Part G Protons in $^{26}\mathrm{Mg}$

State the number of protons in an atom of $^{26}\mathrm{Mg}$.

Part H Neutrons in $^{26}\mathrm{Mg}$

State the number of neutrons in an atom of $^{26}\mathrm{Mg}$.

Part I Electrons in $^{26}\mathrm{Mg}$

State the number of electrons in an atom of $^{26}\mathrm{Mg}$.

Adapted with permission from UCLES, OCR AS Level Chemistry, June 1999, Paper 1, Question 2

Ar & Mr and Molecular Formula 2

A Level

P P P

Essential Pre-Uni Chemistry A2.2

Fluorine only occurs naturally in one isotope, $^{19}\mathrm{F}$, and has a relative atomic mass of 19.0.

Calculate the mass of a fluorine atom in kg. Give your answer to 3 significant figures.

Ar & Mr and Molecular Formula 4

A Level

P P P

Essential Pre-Uni Chemistry A2.4

Assume that the mass of an isotope in amu to 3 significant figures is equal to its mass number.

The relative atomic mass of boron is $10.8\,\mathrm{amu}$. Boron exists in two isotopes, $^{10}\mathrm{B}$ and $^{11}\mathrm{B}$.

Calculate the percentage abundance of $^{10}\mathrm{B}$. Give your answer to 2 significant figures.

Gameboard:

STEM SMART Chemistry Week 3

Ar & Mr and Molecular Formula 5

A Level

P P P

Essential Pre-Uni Chemistry A2.5

Assume that the mass of an isotope in amu to 3 s.f. is equal to its mass number.

Complete the table shown below.

Element	A_r	Isotope 1	Isotope 2	Isotope 3	Isotope 4
Bromine	**Part A**	$^{79}\mathrm{Br}\ 50.5\%$	$^{81}\mathrm{Br}\ 49.5\%$	n/a	n/a
Silver	107.9	**Part B** $^{107}\mathrm{Ag}$ **?** $\%$	**Part C** $^{109}\mathrm{Ag}$ **?** $\%$	n/a	n/a
Cerium	140.2	$^{136}\mathrm{Ce}\ 0.2\%$	$^{138}\mathrm{Ce}\ 0.2\%$	$^{140}\mathrm{Ce}\ 88.5\%$	**Part D** $^{?}\mathrm{Ce}\ 11.1\%$

Part A Br

Give the value of A_r for Br to 3 significant figures.

Part B $^{107}\mathrm{Ag}$

Give the percent abundance of $^{107}\mathrm{Ag}$ to 2 significant figures.

Part C $^{109}\mathrm{Ag}$

Give the percent abundance of $^{109}\mathrm{Ag}$ to 2 significant figures.

Part D Ce isotope 4

What is the mass number of isotope 4 of Ce?

Gameboard:

STEM SMART Chemistry Week 3

Mass Spectrometry

A Level

C C C

with focus on time-of-flight

Mass spectrometry is a technique for studying chemical substances. High resolution mass spectrometry allows us to determine relative atomic or molecular masses to a high degree of precision. Some forms of mass spectrometry can also provide structural information which is useful for structure determination.

Part A Electron ionisation

A mass spectrometer relies on the presence of ions, which it is able to separate by their mass to charge ratio. However, many samples we wish to study are neutral. The instrument therefore needs to use an ionisation technique to form these ions within the sample. We will first consider **electron ionisation (EI)**. This involves firing high energy electrons at the vaporised sample in order to remove electrons.

Which of the following equations is an accurate description of this electron ionisation process:

- $\mathrm{X\,(g) + e^- \longrightarrow X^-\,(g)}$
- $\mathrm{X\,(g) \longrightarrow X^-\,(g) + e^-}$
- $\mathrm{X\,(g) + e^- \longrightarrow X^+\,(g) + 2\,e^-}$
- $\mathrm{X^+\,(g) + e^- \longrightarrow X\,(g)}$

Part B Fragmentation

Electron ionisation is a hard ionisation technique, which means it often results in fragmentation of the molecular ion formed initially. As a consequence, when applied to large molecules, the mass spectrum often contains many features corresponding to these lighter ions. This can be helpful for structure determination: for a given molecular structure, we can predict likely ways in which the molecular ion might fragment (e.g. through particular bonds breaking) and check whether this is consistent with the spectrum. That said, some of the fragmentations are far more complex than simple bond breaking and involve rearrangements. This can make it difficult to account for the formation of certain ions even if we confidently know the molecular structure already.

A student was thinking about fragmentation in mass spectrometers and hypothesised that if they saw a fragment feature 15 mass units lighter than the molecular ion, they should also see a feature due to an ion with mass 15. However, consulting some real spectra, they found that it is in fact common not to see ion pairs that “complement” each other like this. By carefully considering a single, simple fragmentation process occurring on a molecular ion, suggest why this might be.

Part C Electrospray ionisation

A softer ionisation technique, resulting in far less fragmentation than electron ionisation, is **electrospray ionisation**. There are a number of variations of this, but in one type, the neutral atom or molecule bonds to a proton (hydrogen ion).

Select the correct equation describing this process for sodium:

- ○ $\mathrm{Na\,(g) + H^{-}\,(g) \longrightarrow [Na + H]^{-}\,(g)}$
- ○ $\mathrm{Na\,(g) + H^{+}\,(g) \longrightarrow [Na + H]^{+}\,(g)}$
- ○ $\mathrm{Na\,(g) + H^{-}\,(g) \longrightarrow Mg^{-}\,(g)}$
- ○ $\mathrm{Na\,(g) + H^{+}\,(g) \longrightarrow Ne^{+}\,(g)}$
- ○ $\mathrm{Na\,(g) + H^{+}\,(g) \longrightarrow Mg^{+}\,(g)}$
- ○ $\mathrm{Na\,(g) + H^{-}\,(g) \longrightarrow Ne^{-}\,(g)}$

Part D Time-of-flight expression

In a time-of-flight (TOF) mass spectrometer, the ions formed are accelerated through a potential so that all singly-charged ions have the same kinetic energy, E. These ions then travel along a flight tube of length d before reaching the detector. The delay is a function of the mass of a given ion, m.

Derive a formula for the time it takes an ion to travel along the flight tube (the time of flight) as a function of E, d and m. Assume that all quantities are provided in SI units, so your formula does not need to take into account any conversion factors.

The following symbols may be useful: `E`, `d`, `m`

Part E Calculating molecular mass

Based on the above formula, ions of different mass take different amounts of time to travel through the spectrometer. Calculate, in kg, the mass of an ion X^+ that takes $7.55 \times 10^{-6}\,\mathrm{s}$ to travel through the $2.00\,\mathrm{m}$ drift region, assuming it was previously accelerated to a kinetic energy of $5.83 \times 10^{-15}\,\mathrm{J}$.

Part F Converting to atomic mass units

Convert the above mass of X^+ in kg to atomic mass units (amu) in which you more typically express the mass of atoms, molecules and ions in chemistry.

Part G Electron mass

To obtain the mass of the neutral species, X, we would actually need to add on the mass of an electron. Why is this not a particularly meaningful calculation for the above quantities?

Mass Spectrometers 8

A Level

P P P

Essential Pre-Uni Physics L1.8

Give a practical application of mass spectrometry. Choose from the following.

1. Separating out different types of molecules.

2. Obtaining the relative molar mass of an unknown substance.

3. Separating isotopes of uranium to supply fuel rods to nuclear reactors.

4. Aiding with carbon dating.

5. Determining the accurate mass of a $^{12}\mathrm{C}$ atom.

6. Obtaining relative isotopic abundances in distant stars.

7. Obtaining the relative masses and abundances of isotopes in a sample.

- 1, 2, 4
- 1, 3, 5
- 2, 4, 6
- 2, 4, 7
- 3, 4, 6, 7
- 4, 6, 7

Lines in Mass Spectra

A Level P P P

Part A Chlorine

Which of the following could be an excerpt from the mass spectrum of chlorine?

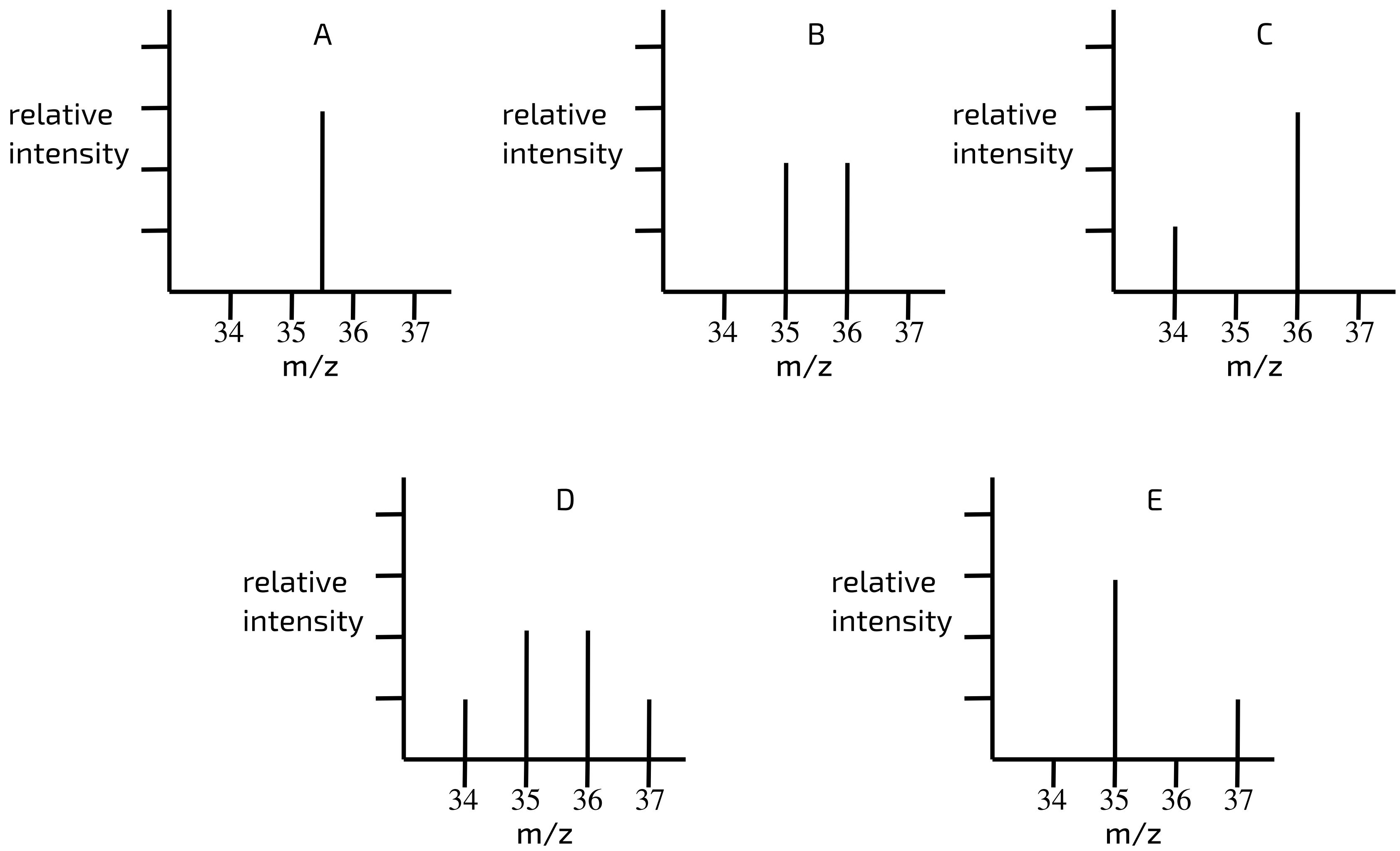

Figure 1: Mass Spectra

- A
- B
- C
- D
- E

Part B Bromine

Bromine occurs naturally as two isotopes, $^{79}\mathrm{Br}$ and $^{81}\mathrm{Br}$, in equal abundance.

The mass spectrum for $^{12}\mathrm{C}_2{}^{1}\mathrm{H}_4\mathrm{Br}_2$ is obtained. Select which of these resembles the mass spectrum for m/z values above 184 (the vertical axis should in each case be treated as relative intensity).

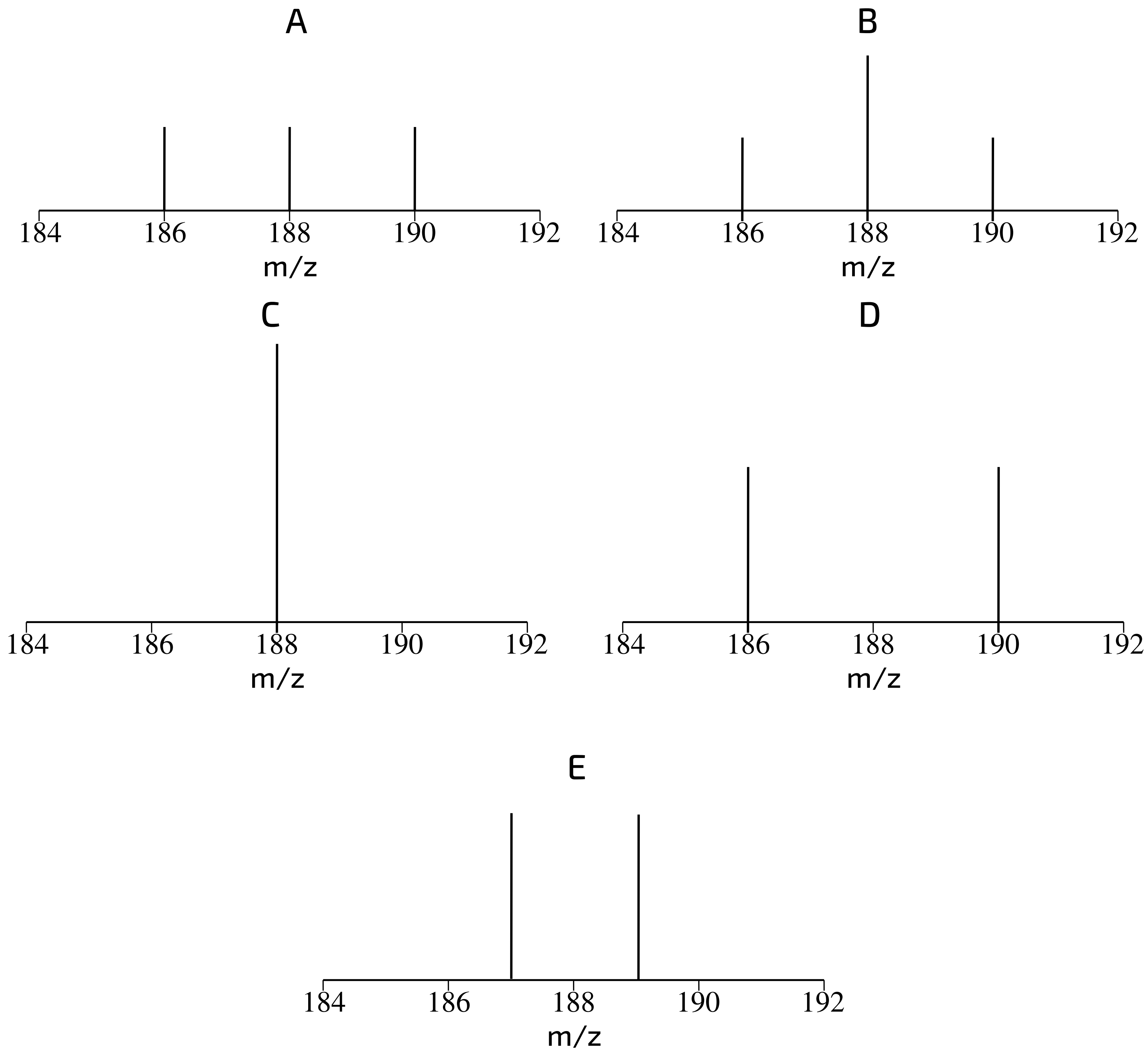

Figure 2: Mass spectra

- A
- B
- C
- D
- E

Part C   Unknown

Select which of the following gives the complete mass spectrum illustrated.

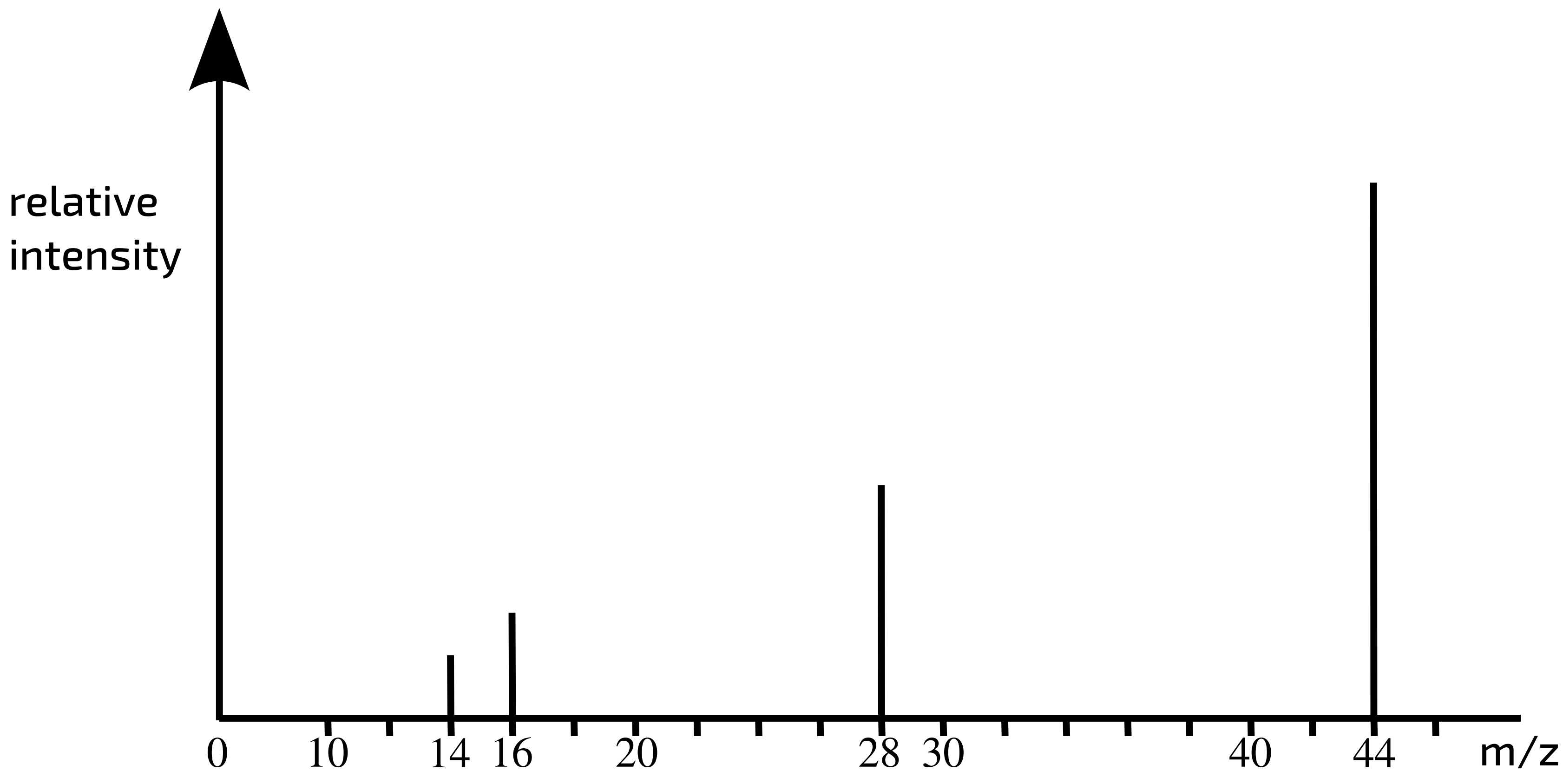

Figure 3: Mass spectrum

- CO_2
- C_3H_8
- N_2O
- a mixture of CH_4 and N_2

Adapted with permission from UCLES, A Level Chemistry, 1988, Paper 3, Question 3; November 1993, Paper 4, Question 5 and June 1994, Paper 4, Question 1

Gameboard:

STEM SMART Chemistry Week 3

Higher-charged Ions

A Level

C C C

(in mass spectrometry)

A small proportion of ions with higher charge can form during the ionisation process in a mass spectrometer. If a given potential accelerates a singly-charged ion to have a kinetic energy of E, a doubly-charged ion will instead acquire a kinetic energy of $2E$, a triply-charged ion a kinetic energy of $3E$, $\ldots$ and an ion with charge z a kinetic energy of zE. (If you are interested in the physics behind this, you may wish to read more about Electric fields and complete a physics question on accelerating charged particles.)

Part A Time of flight

Derive an expression for the time taken to travel through the drift region of length d by an ion with mass m and charge z, if it has a kinetic energy of zE.

The following symbols may be useful: `E, d, m, z`

Part B Isotopic clusters

Ions containing atoms with several stable isotopes form characteristic so-called "isotopic clusters". For example, the molecular ion $\mathrm{HCl^+}$ would be expected to give rise to two lines in the mass spectrum due to the two **isotopologues** $\mathrm{H^{35}Cl^+}$ and $\mathrm{H^{37}Cl^+}$. The lines would be expected to appear in a 3:1 ratio due to this being the ratio of abundances of the respective chlorine isotopes.

At what (integer) m/z value would you expect the lighter of the two ions above to appear?

At what (integer) m/z value would you expect the heavier of the two ions above to appear?

Part C Doubly positive

Now consider the two possible isotopologues for HCl^{2+} which has formed in the ionisation stage.

At what (integer) m/z value would you expect the lighter of the two ions above to appear?

At what (integer) m/z value would you expect the heavier of the two ions above to appear?

Part D More generally

If you know that a compound contains one chlorine atom, how can you identify the charge of the ion responsible for a particular ion cluster (assuming the ion contains the chlorine atom present in the original molecule)?

If you know that a compound contains chlorine, you can relatively easily identify the charge of the ion responsible for a particular isotopic cluster containing at least one chlorine atom. Give an expression for how many units apart individual, neighbouring lines in the isotopic cluster (corresponding to the different isotopologues) will appear on the mass spectrum, as a function of the charge on the ion, z.

The following symbols may be useful: z

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