Combinatorics with Isotopes

A Level

Chlorine consists of two isotopes, $^{35}\mathrm{Cl}$ and $^{37}\mathrm{Cl}$, in the abundance ratio 3:1. Phosphorus is mono-isotopic, $^{31}\mathrm{P}$.

Apart from the lines due to atomic ions, the mass spectrum of a chloride of phosphorus contains 9 lines arranged in 3 groups:

group	m/z values of lines
A	66, 68
B	101, 103, 105
C	136, 138, 140, 142

Part A Group A ion

Identify the ion responsible for group **A** (do not use isotope labels in your formula).

Part B Group B ion

Identify the ion responsible for group **B** (do not use isotope labels in your formula).

Part C Group C ion

Identify the ion responsible for group **C** (do not use isotope labels in your formula).

Part D Group A abundance ratio

Predict the abundance ratio of the different m/z values within group *A*. Your answer should be in the form $X_1 : X_2$ (no spaces), where X_1 and X_2 are the smallest possible integers, and the ordering is from lowest to highest m/z value.

Part E Group B abundance ratio

Predict the abundance ratio of the different m/z values within group *B*. Your answer should be in the form $X_1 : X_2 : X_3$ (no spaces), where X_1, X_2 and X_3 are the smallest possible integers, and the ordering is from lowest to highest m/z value.

Part F Group C abundance ratio

Predict the abundance ratio of the different m/z values within group *C*. Your answer should be in the form $X_1 : X_2 : X_3 : X_4$ (no spaces), where X_1, X_2, X_3 and X_4 are the smallest possible integers, and the ordering is from lowest to highest m/z value.

Adapted with permission from UCLES, A Level Chemistry, November 1995, Paper 1, Question 2

Mass spectrometry

A Level

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:

- $X^+(g) + e^- \longrightarrow X(g)$
- $X(g) + e^- \longrightarrow X^+(g) + 2e^-$
- $X(g) \longrightarrow X^-(g) + e^-$
- $X(g) + e^- \longrightarrow X^-(g)$

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:

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

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?

Created for isaacphysics.org by Andrea Chlebikova

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 $^{26}\mathrm{Mg}$.

Essential Pre-Uni Chemistry A2.5

A Level P P P

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?

Essential Pre-Uni Chemistry A2.4

A Level

P P P

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.

Physics. You work it out.

Lines in Mass Spectra

A Level

Part A Chlorine

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

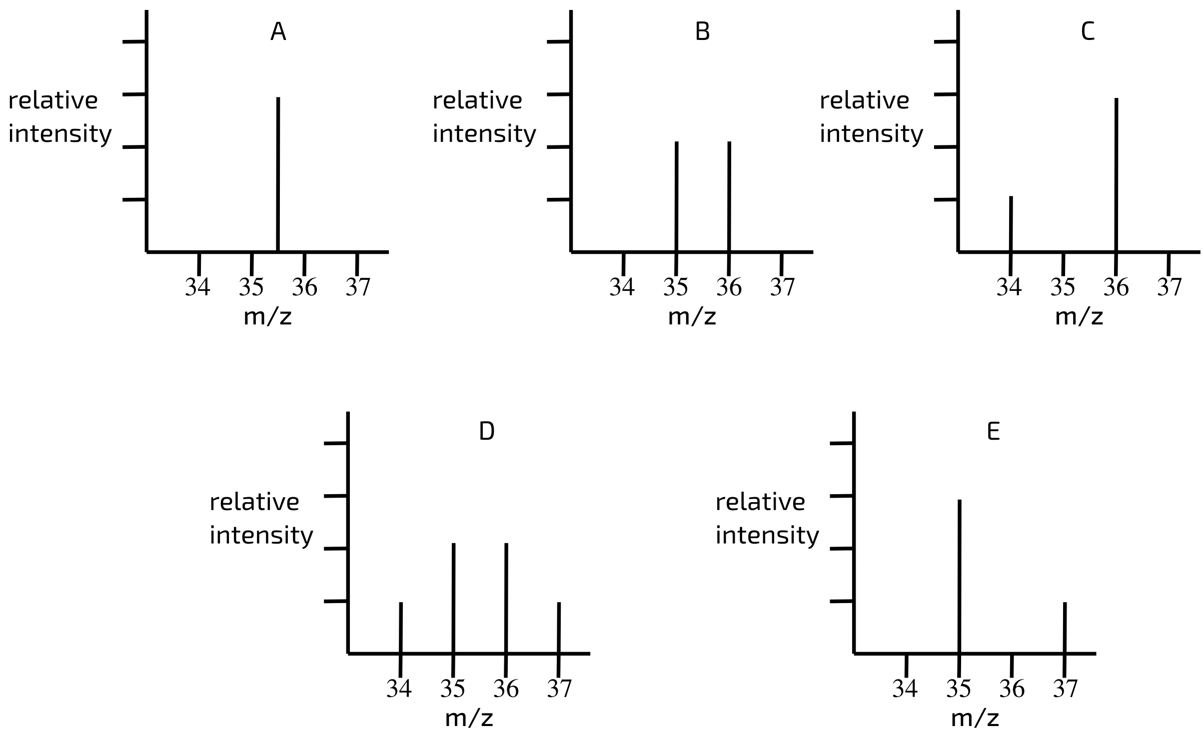

Figure 1: Mass Spectra

- A
- B
- C
- D
- E

Part B Bromine

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

The mass spectrum for $^{12}C_2\,^1H_4Br_2$ 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).

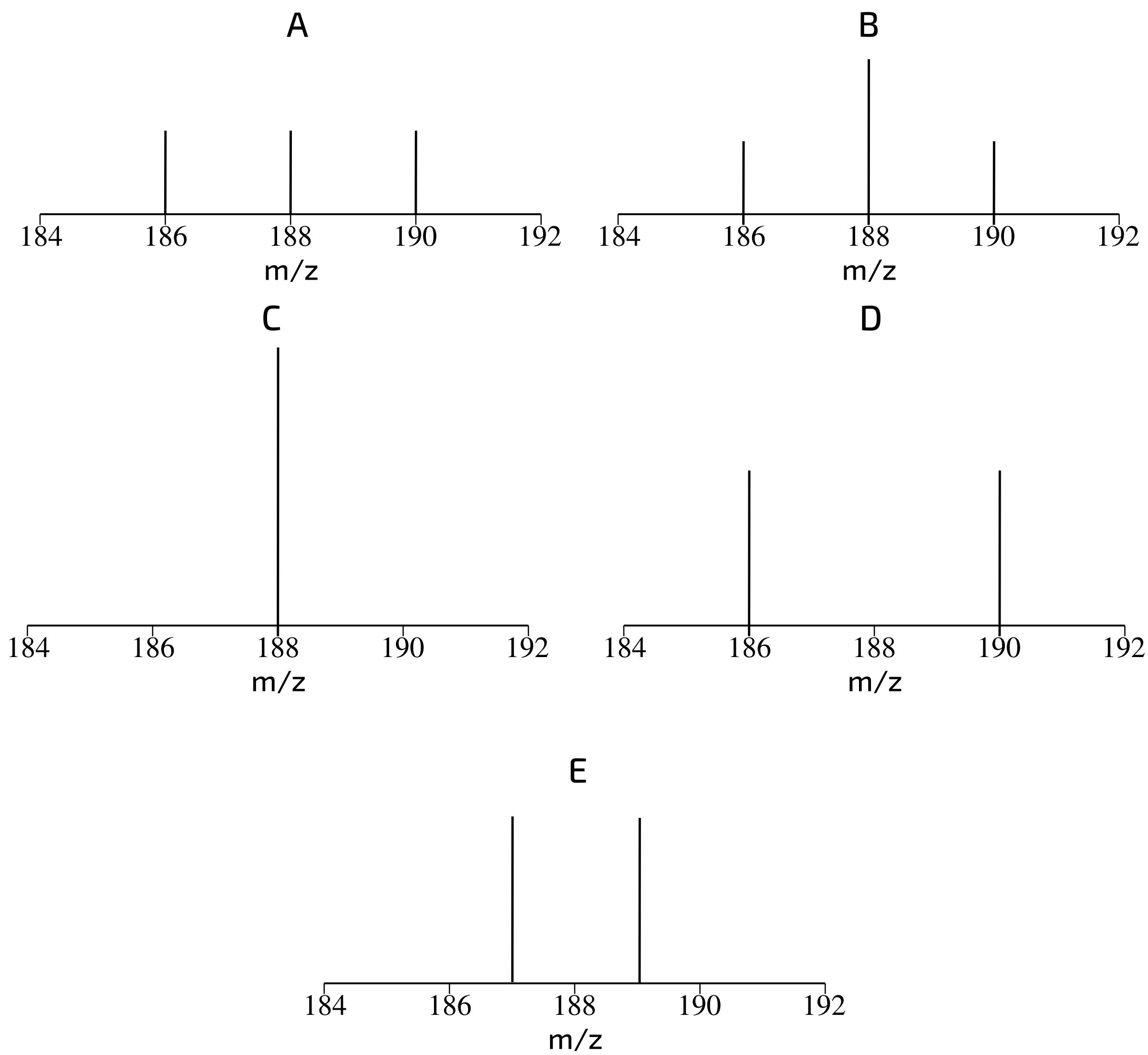

Figure 2: Mass spectra

- A
- B
- C
- D
- E

Part C Unknown

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

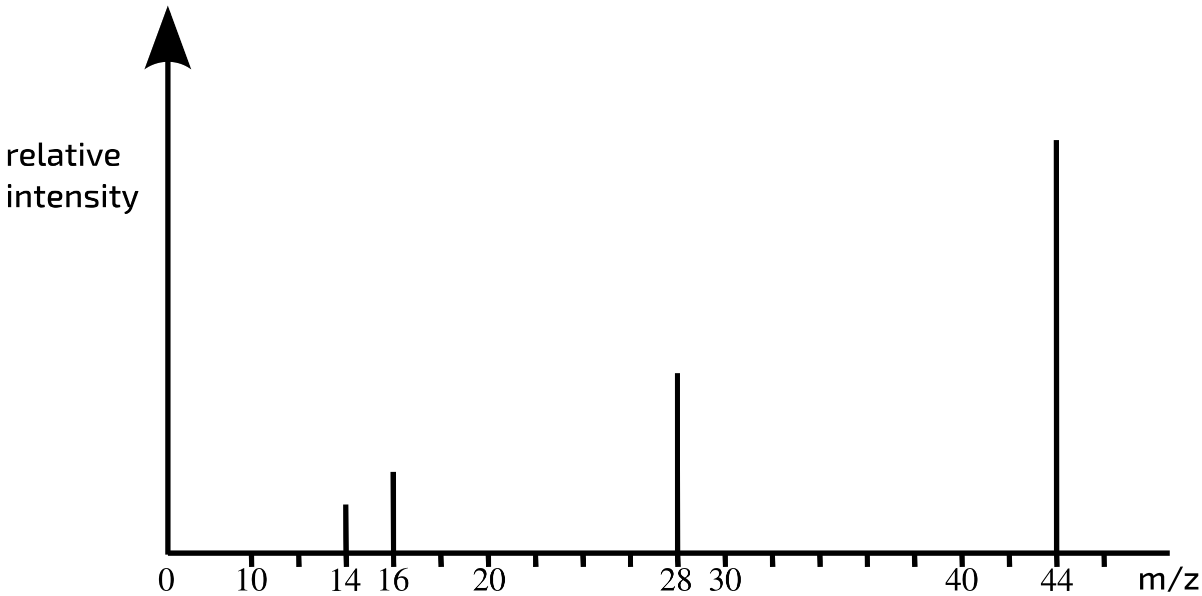

Figure 3: Mass spectrum

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

Physics. You work it out.

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Essential Pre-Uni Physics L1.8

A Level

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

Essential Pre-Uni Chemistry A2.2

A Level P P P

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

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

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