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Structure 1.2.3 — Mass Spectra

Higher Level only · Structure 1.2 The Nuclear Atom

Complete revision notes · Worked examples · Practice questions · Full mark scheme

What this topic asks of you

Syllabus statement (Structure 1.2.3, AHL): *Mass spectra are used to determine the relative atomic masses of elements from their isotopic composition.*

Guidance: Interpret mass spectra in terms of the **identity** and **relative abundance** of isotopes present. *The operational details of the mass spectrometer will not be assessed.*

Tools & links: Section 2 of the data booklet (relative atomic masses); Structure 1.2.2 (isotopes); Structure 3.1 (the periodic table); Structure 3.2.7 and Reactivity (mass spectrometry of organic compounds, HL).

1 Why chemists need mass spectra

Isotopes are atoms of the same element with the **same number of protons** but a **different number of neutrons**. Because they have identical electron configurations, isotopes are chemically *indistinguishable* — no chemical reaction can separate ^{35}Cl from ^{37}Cl .

They do, however, differ in **mass**. A **mass spectrometer** exploits exactly this: it separates particles by mass, not by chemistry. This gives chemists two things that nothing else can:

1. **Which isotopes** are present in a sample (from the *positions* of the peaks).
2. **How much** of each isotope is present (from the *heights* of the peaks).

Put those two pieces of information together and you can calculate the **relative atomic mass** of the element — the number printed in the periodic table.

The three masses you must not confuse

Mass number (A) — a *whole number*: the number of protons + neutrons in one particular atom. It is a count, so it is always an integer.

Relative isotopic mass — the mass of *one atom of a specific isotope* relative to $\frac{1}{12}$ the mass of one

atom of carbon-12. It is very close to the mass number (e.g. $^{35}\text{Cl} = 34.97$) and, at IB level, may be taken as equal to the mass number unless more precise data are given.

Relative atomic mass (A_r) — the **weighted mean** mass of the atoms in a *naturally occurring sample* of the element, relative to $\frac{1}{12}$ the mass of one atom of carbon-12. It is almost never a whole number, and it has **no units**.

Mass-to-charge ratio, m/z

The horizontal axis of a mass spectrum is the **mass-to-charge ratio**, m/z , where m is the relative mass of the ion and z is its charge. Because electron-impact ionisation produces **singly charged ions** ($z = 1+$) in the overwhelming majority of cases,

$$\frac{m}{z} = \frac{m}{1} = m \quad \Rightarrow \quad m/z \text{ reads directly as the relative isotopic mass.}$$

The vertical axis is **relative abundance** (sometimes called relative intensity, signal strength or % abundance).

2 Inside the instrument (background only — not assessed)

You will **not** be examined on the operational details, but understanding them makes every spectrum you meet obvious rather than mysterious. Five stages, easily remembered as **VIADD**:

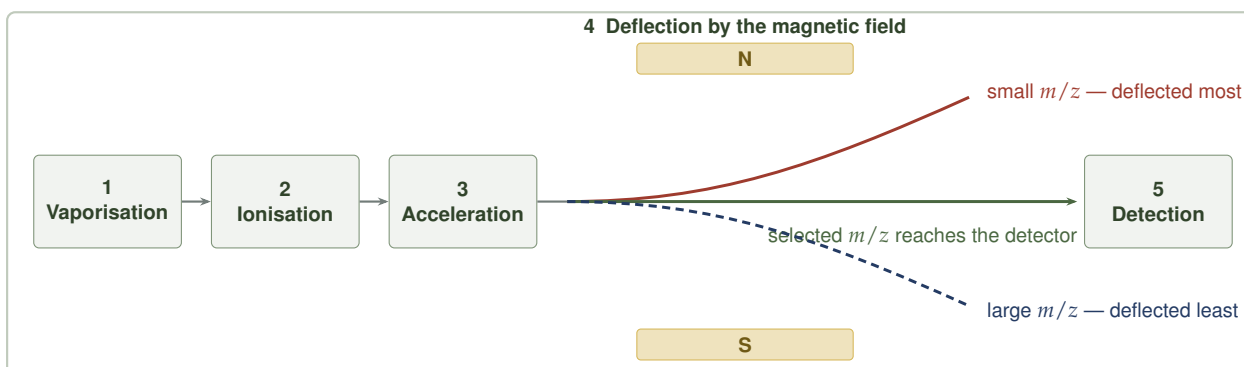
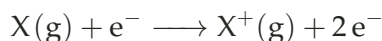


Figure 1. Schematic of a single-focusing magnetic-sector mass spectrometer. Only *positive* ions reach the detector; neutral atoms and negative ions are removed by the vacuum pumps and the electric field.

- Vaporisation** — the sample is turned into a gas so that individual particles are free.
- Ionisation** — a beam of high-energy electrons knocks an electron off each atom:



Ionisation is essential because **only charged particles can be accelerated and deflected** by electric and magnetic fields.

- Acceleration** — an electric field accelerates all the positive ions to the *same kinetic energy*. Since $E_k = \frac{1}{2}mv^2$, lighter ions end up moving faster.
- Deflection** — a magnetic field bends the ion beam into a circular arc. The radius of the path depends on m/z :

$$\text{deflection} \propto \frac{z}{m} = \frac{1}{(m/z)}$$

so **light ions are deflected most** and heavy ions least. Only ions with one particular m/z reach the detector for a given field strength; scanning the field sweeps the whole spectrum.

- Detection** — ions striking the detector generate a current. The **size of the current is proportional to the number of ions**, hence to the relative abundance of that isotope.

Read the syllabus carefully

The 2023 guide states that *operational details will not be assessed*. You will therefore not be asked to describe the five stages or to derive the deflection equation. You **will** be asked to **read, interpret and calculate from** a spectrum — so spend your revision time on Sections 4–7 of these notes, not on memorising instrument diagrams.

3 How to read a mass spectrum

Every atomic mass spectrum carries exactly three pieces of information. Learn to extract them in this order and you will never be stuck.

The three-step read

- Count the peaks** → tells you the **number of isotopes** in the sample.
- Read the m/z of each peak** → tells you the **relative isotopic mass** (and therefore the mass number, and therefore the number of neutrons).
- Read the height of each peak** → tells you the **relative abundance** of that isotope.

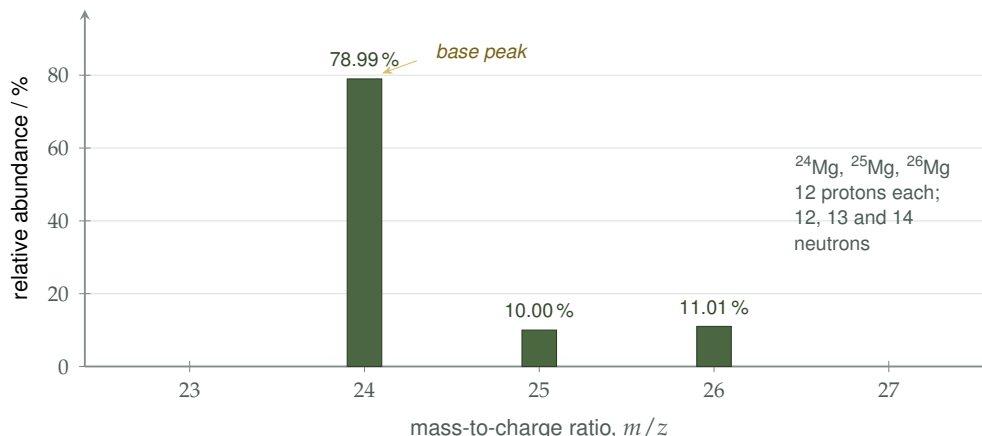


Figure 2. Annotated mass spectrum of naturally occurring magnesium. Three peaks $\Rightarrow$ three isotopes. The tallest peak is the **base peak**.

3.1 What the spectrum of magnesium tells you

- ▶ **Three peaks** $\Rightarrow$ magnesium exists naturally as three isotopes.
- ▶ Peaks at $m/z = 24, 25$ and $26 \Rightarrow$ mass numbers 24, 25 and 26, i.e. $^{24}\text{Mg}^+$, $^{25}\text{Mg}^+$ and $^{26}\text{Mg}^+$.
- ▶ All three have $Z = 12$ (12 protons, 12 electrons in the neutral atom); they differ only in neutron number: 12, 13 and 14 respectively.
- ▶ ^{24}Mg is by far the most abundant $\Rightarrow$ the A_r of magnesium must lie *close to 24*, and indeed it is 24.31.

4 Calculating relative atomic mass from a spectrum

This is the single most examined skill in Structure 1.2.3. It is a **weighted mean**.

$$A_r = \frac{\sum(\text{relative isotopic mass} \times \text{relative abundance})}{\sum \text{relative abundance}}$$

If the abundances are **percentages that add up to 100**, the denominator is simply 100. If the abundances are given as **relative peak heights** (e.g. the base peak set to 100), you **must** divide by the sum of the heights.

Solved example 1 — abundances given as percentages

Q. Use the data in Figure 2 to calculate the relative atomic mass of magnesium, giving your answer to two decimal places.

A. The percentages sum to $78.99 + 10.00 + 11.01 = 100$, so divide by 100:

$$\begin{aligned} A_r &= \frac{(24 \times 78.99) + (25 \times 10.00) + (26 \times 11.01)}{100} \\ &= \frac{1895.76 + 250.0 + 286.26}{100} = \frac{2432.02}{100} = \mathbf{24.32} \end{aligned}$$

Comment. The data booklet gives 24.31; the tiny difference arises because we used the whole-number mass numbers rather than the exact relative isotopic masses (23.985, 24.986, 25.983). Using those exact values returns 24.31.

Solved example 2 — abundances given as peak heights

Q. The mass spectrum of an element shows two peaks: at $m/z = 69$ with a relative height of 100, and at $m/z = 71$ with a relative height of 66.4. Calculate A_r and identify the element.

A. The heights do *not* sum to 100, so divide by their actual sum, $100 + 66.4 = 166.4$:

$$A_r = \frac{(69 \times 100) + (71 \times 66.4)}{166.4} = \frac{6900 + 4714.4}{166.4} = \frac{11\,614.4}{166.4} = \mathbf{69.8}$$

An A_r of 69.8 matches **gallium** ($A_r = 69.72$) in Section 7 of the data booklet.

Check: 69.8 lies between 69 and 71 and is nearer to 69 — consistent with ^{69}Ga being the more abundant isotope. *Always sanity-check that your answer lies between the lightest and heaviest isotope.*

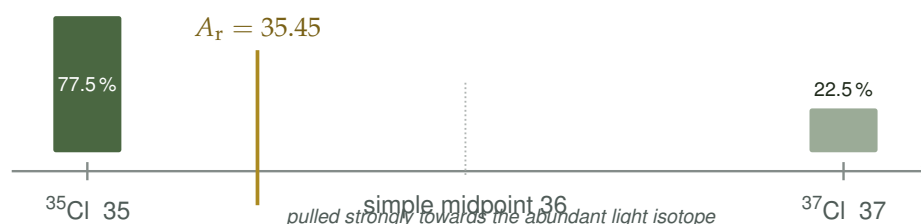


Figure 3. The weighted-mean idea. A_r is the balance point of the isotope masses, always pulled towards the *more abundant* isotope — never the simple midpoint unless the abundances happen to be equal.

5 Working backwards: finding abundances from A_r

The examiners' favourite reversal. You are given A_r and the two isotopic masses, and asked for the percentage abundances. Use **one unknown**, not two.

Let the abundance of the **lighter** isotope be $x\%$. The heavier one must then be $(100 - x)\%$, and

$$A_r = \frac{m_1x + m_2(100 - x)}{100} \implies \boxed{x = \frac{m_2 - A_r}{m_2 - m_1} \times 100}$$

Solved example 3 — reverse calculation

Q. Copper has two stable isotopes, ^{63}Cu (relative isotopic mass 62.93) and ^{65}Cu (relative isotopic mass 64.93). The relative atomic mass of copper is 63.55. Determine the percentage abundance of each isotope.

A. Let the abundance of ^{63}Cu be $x\%$; then ^{65}Cu is $(100 - x)\%$.

$$\begin{aligned} \frac{62.93x + 64.93(100 - x)}{100} &= 63.55 \\ 62.93x + 6493 - 64.93x &= 6355 \\ -2.00x &= -138 \\ x &= 69.0 \end{aligned}$$

$^{63}\text{Cu} = 69.0\%$ and $^{65}\text{Cu} = 31.0\%$

Check: 63.55 is much nearer 62.93 than 64.93, so the light isotope should dominate — and it does, at 69%. ✓

Three ways students throw marks away here

1. Setting up two unknowns and getting lost. Always use x and $(100 - x)$.
2. Forgetting to divide by 100 (or by the sum of the heights) — gives an answer in the thousands.
3. Quoting an abundance greater than 100% or a negative one and not noticing. If that happens, you have almost certainly swapped m_1 and m_2 .

6 Identifying an unknown element

If a question gives you a spectrum of “element X”, the route is always the same:

Step 1: Calculate A_r from the peak positions and heights.

Step 2: Look up that value in **Section 7 of the data booklet** (the periodic table).

Step 3: Name the element and, if asked, give its atomic number Z .

Step 4: Deduce neutron numbers as $A - Z$ for each isotope.

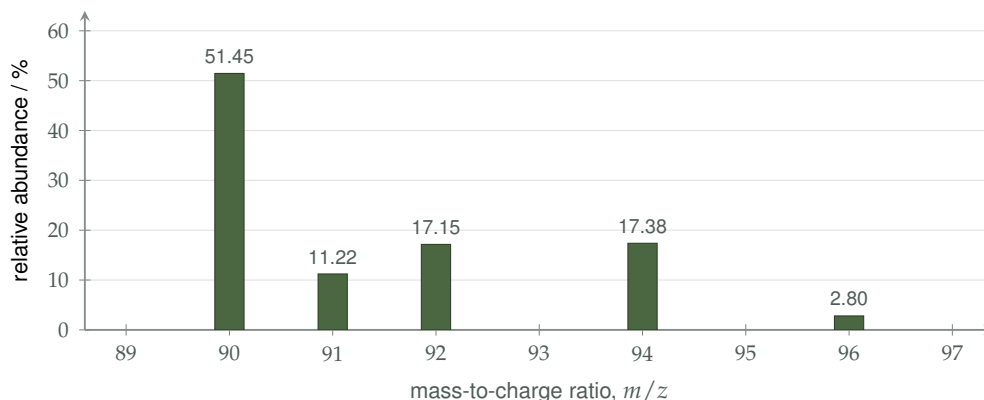


Figure 4. Mass spectrum of zirconium — an element with five natural isotopes. Note that the isotopes are *not* consecutive: there is no peak at $m/z = 93$ or 95 .

7 Subtleties that separate a 6 from a 7

7.1 Doubly charged ions

Occasionally a second electron is removed, giving X^{2+} . Since $z = 2$, such an ion appears at **half** its true mass:

$$^{24}\text{Mg}^{2+} : m/z = \frac{24}{2} = 12$$

So a small peak at $m/z = 12$ in a magnesium spectrum is $^{24}\text{Mg}^{2+}$, *not* carbon. Doubly charged peaks are always **much smaller** than the singly charged ones, because removing a second electron is far more difficult (see Structure 1.3.6, ionisation energies).

7.2 Relative abundance versus percentage abundance

Some spectra scale the tallest peak (the **base peak**) to 100 rather than expressing everything as a percentage of the whole. To convert:

$$\% \text{ abundance of isotope } i = \frac{h_i}{\sum h} \times 100$$

where h_i is the height of peak i . You do *not* need to convert before calculating A_r — the weighted-mean formula handles raw heights perfectly well, provided you divide by $\sum h$.

7.3 Why A_r values in the data booklet are not fixed constants

Relative atomic mass depends on the *isotopic composition of the sample*. For most elements this is essentially constant worldwide, but not always. Lead is the classic case: lead formed by the radioactive decay of uranium is enriched in ^{206}Pb , so lead ores of different geological origin have measurably different A_r values. Mass spectrometry is how geologists date rocks.

7.4 Mass spectra of diatomic elements

Chlorine and bromine exist as Cl_2 and Br_2 molecules, so their spectra show a **molecular ion cluster** as well as atomic peaks. If the two isotopes have fractional abundances p (light) and q (heavy), the three possible molecules occur in the ratio

$$p^2 : 2pq : q^2$$

The factor of 2 arises because the mixed molecule can form in two ways (light-heavy and heavy-light).

Solved example 4 — the chlorine molecular ion cluster

Q. Chlorine consists of 75 % ^{35}Cl and 25 % ^{37}Cl . Predict the m/z values and relative heights of the peaks in the molecular ion region of the mass spectrum of Cl_2 .

A. Take $p = 0.75$ and $q = 0.25$. Three molecular ions are possible:

Ion	m/z	Probability	Ratio
$^{35}\text{Cl}^{35}\text{Cl}^+$	70	$p^2 = 0.5625$	9
$^{35}\text{Cl}^{37}\text{Cl}^+$	72	$2pq = 0.3750$	6
$^{37}\text{Cl}^{37}\text{Cl}^+$	74	$q^2 = 0.0625$	1

Dividing through by the smallest gives **70 : 72 : 74 in the ratio 9 : 6 : 1**.

Note. Using the more precise abundances (75.77 % and 24.23 %) the ratio becomes 9.8 : 6.3 : 1; the 9 : 6 : 1 result is the standard IB answer.

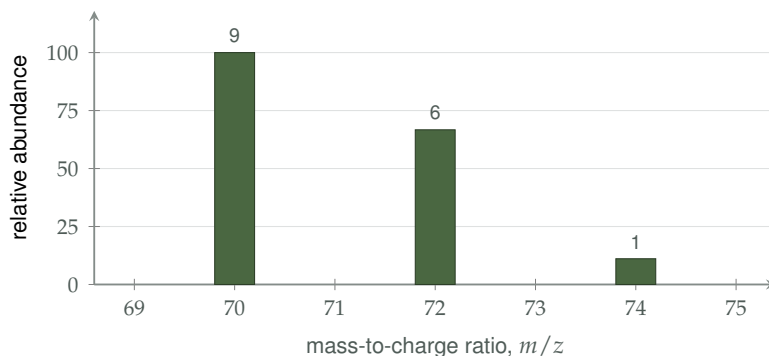


Figure 5. Molecular ion region of the mass spectrum of Cl_2 . Peaks two mass units apart in a 9:6:1 pattern are a fingerprint for two chlorine atoms.

For Br_2 the two isotopes ^{79}Br and ^{81}Br are almost equally abundant ($p \approx q \approx 0.5$), so the ratio $p^2 : 2pq : q^2$ becomes $0.25 : 0.50 : 0.25 = 1 : 2 : 1$, with peaks at $m/z = 158, 160$ and 162 .

8 Key points to memorise

Learn these ten statements word-perfect

- A_r is the **weighted mean** mass of the atoms of an element relative to $\frac{1}{12}$ the mass of a ^{12}C atom. It has **no units**.
- The x -axis of a mass spectrum is m/z ; because $z = 1+$ for almost all ions, m/z equals the relative isotopic mass.
- Number of peaks = number of isotopes** (in an atomic spectrum).
- Peak position = mass number; peak height = relative abundance.**
- $A_r = \frac{\sum(\text{mass} \times \text{abundance})}{\sum \text{abundance}}$ — divide by 100 *only* when the abundances are percentages

summing to 100.

6. Reverse problems: let the lighter isotope be $x\%$ and the heavier $(100 - x)\%$.
7. A_r always lies **between** the lightest and heaviest isotopic masses, and **closer to the more abundant** one.
8. Isotopes have **identical chemical properties** (same electron configuration) but **slightly different physical properties** (density, rate of diffusion, boiling point) because of their different masses.
9. A X^{2+} ion appears at **half** the m/z of X^+ .
10. For a diatomic element the molecular ion cluster follows $p^2 : 2pq : q^2$ ($Cl_2 \rightarrow 9:6:1$; $Br_2 \rightarrow 1:2:1$).

Command-term checklist

“Deduce” — give the answer with brief reasoning, no full working needed.

“Determine” / “Calculate” — show the substituted expression *and* the final answer. A bare number with no working typically scores 1 of 2 marks.

“State” — one short sentence or a number; do not waste time explaining.

Significant figures — match the data given. Isotopic abundances quoted to 4 s.f. deserve an A_r quoted to 4 s.f. Never round to fewer figures than the data booklet value.

Units — A_r and relative isotopic mass have **no units**. Writing “g” or “amu” after them loses the mark.

9 Solved examples

Work through these with a pen before reading the solution. The commentary explains not only *what* the answer is but *why the wrong options are tempting*.

9.1 A. Multiple choice — solved

Solved MCQ 1

The mass spectrum of element R shows two peaks: $m/z = 85$ (relative abundance 72.2%) and $m/z = 87$ (relative abundance 27.8%). What is the relative atomic mass of R?

A. 85.6 B. 86.0 C. 85.4 D. 86.4

Answer: A

$$A_r = \frac{(85 \times 72.2) + (87 \times 27.8)}{100} = \frac{6137 + 2418.6}{100} = 85.556 \approx 85.6$$

Why the distractors tempt you: B (86.0) is the *unweighted* mean of 85 and 87 — the classic error of ignoring abundance. D (86.4) weights the answer towards the *heavier* isotope, i.e. the abundances have been applied the wrong way round. C lies outside a sensible weighting. *Quick check:* 72% of the sample is mass 85, so the answer must be much closer to 85 than to 87 — only A qualifies.

Solved MCQ 2

Bromine consists of ^{79}Br (50.7 %) and ^{81}Br (49.3 %). How many peaks appear in the molecular ion region of the mass spectrum of Br_2 , and in what approximate ratio?

- A. 2 peaks, 1 : 1 B. 3 peaks, 1 : 2 : 1 C. 3 peaks, 1 : 1 : 1 D. 4 peaks, 1 : 3 : 3 : 1

Answer: B

Three distinct molecules are possible: $^{79}\text{Br}^{79}\text{Br}$ (m/z 158), $^{79}\text{Br}^{81}\text{Br}$ (m/z 160) and $^{81}\text{Br}^{81}\text{Br}$ (m/z 162). With $p \approx q \approx 0.5$:

$$p^2 : 2pq : q^2 = 0.25 : 0.50 : 0.25 = 1 : 2 : 1$$

Why B and not C: the mixed molecule can be assembled in *two* ways (^{79}Br first or ^{81}Br first), which doubles its statistical weight. Forgetting the factor of 2 gives the 1 : 1 : 1 trap in option C.

Solved MCQ 3

The mass spectrum of a pure sample of magnesium contains a small peak at $m/z = 12.0$. What causes it?

- A. $^{12}\text{C}^+$ B. $^{24}\text{Mg}^{2+}$ C. $^{24}\text{Mg}^+$ D. $^{12}\text{Mg}^+$

Answer: B

For $^{24}\text{Mg}^{2+}$, $m = 24$ and $z = 2$, so $m/z = 24/2 = 12.0$. A is excluded because the sample is stated to be *pure magnesium*. C would appear at $m/z = 24$. D is impossible: magnesium has 12 protons, so a mass number of 12 would require zero neutrons.

9.2 B. Short-answer — solved
Solved short question 1

Q. The mass spectrum of naturally occurring neon shows three peaks:

m/z	20	21	22
relative abundance / %	90.48	0.27	9.25

(a) Calculate the relative atomic mass of neon, giving your answer to two decimal places. [2]

(b) Deduce the number of protons, neutrons and electrons in a $^{22}\text{Ne}^+$ ion. [2]

(a) The abundances sum to 100, so

$$A_r = \frac{(20 \times 90.48) + (21 \times 0.27) + (22 \times 9.25)}{100} = \frac{1809.6 + 5.67 + 203.5}{100} = \frac{2018.77}{100}$$

$$A_r = 20.19$$

Mark 1: correct substituted expression. Mark 2: correct answer to 2 d.p. with no units.

(b) Neon has $Z = 10$, so every neon atom has **10 protons**. Neutrons = $A - Z = 22 - 10 = 12$. The ion carries a 1+ charge, so it has lost one electron: $10 - 1 = 9$ **electrons**.

The electron count is the discriminator here — roughly half of candidates give 10.

Solved short question 2

Q. Explain, in terms of isotopes, why the relative atomic mass of chlorine is quoted as 35.45 in the data booklet rather than as a whole number. [3]

Model answer:

Naturally occurring chlorine is a mixture of **two isotopes**, ^{35}Cl and ^{37}Cl , which have the same number of protons but different numbers of neutrons [1]. The relative atomic mass is the **weighted mean** of the relative isotopic masses, taking into account the **relative abundance** of each isotope [1]. Because the two isotopes are present in **unequal** proportions (approximately 77.5 % ^{35}Cl to 22.5 % ^{37}Cl), the mean lies between 35 and 37 but much nearer 35, and is therefore not an integer [1].

Not creditworthy: “because chlorine atoms have 18.5 neutrons on average” — no individual atom has a fractional number of neutrons, and examiners specifically penalise this phrasing.

9.3 C. Long structured — solved
Solved long question — neon, 11 marks

The mass spectrum of a sample of neon gives the data in Solved short question 1 above.

- (a) State what is meant by the term *relative atomic mass*. [2]
- (b) Explain why all three isotopes of neon have identical chemical properties. [2]
- (c) State one physical property that differs between ^{20}Ne and ^{22}Ne , and explain the difference. [2]
- (d) A researcher removes all the ^{21}Ne from the sample. Deduce, with reasoning, the effect on the relative atomic mass. [3]
- (e) Explain why a small peak is observed at $m/z = 10.0$. [2]

(a) The relative atomic mass is the **weighted mean mass of the atoms** in a naturally occurring sample of the element [1], measured relative to **one-twelfth of the mass of an atom of carbon-12** [1].

(b) Chemical properties are determined by the **electron configuration**, in particular the number of valence electrons [1]. All neon isotopes have 10 protons and therefore 10 electrons arranged as $1s^2 2s^2 2p^6$; the extra neutrons do not affect the electrons [1].

(c) **Density** (accept: rate of diffusion or effusion, boiling point) [1]. ^{22}Ne atoms have a greater mass but essentially the same size, so a given volume of ^{22}Ne is heavier; equivalently, at the same temperature the heavier atoms move more slowly and diffuse more slowly [1].

(d) A_r **decreases very slightly** [1]. Removing ^{21}Ne raises the proportion of both remaining isotopes, but ^{20}Ne is 90.48 % of the sample against only 9.25 % for ^{22}Ne , so far more “light” weighting is added than “heavy” [1]. Quantitatively:

$$A_r = \frac{(20 \times 90.48) + (22 \times 9.25)}{99.73} = \frac{2013.10}{99.73} = 20.19$$

which is 20.1855 against the original 20.1877 — a decrease of about 0.002 [1].

(e) The peak is caused by $^{20}\text{Ne}^{2+}$ [1], an ion formed when a second electron is removed; since $z = 2$, it appears at $m/z = 20/2 = 10.0$ [1].

10 Practice exercise

Instructions. Attempt all questions without notes. Allow **70 minutes** in total. A periodic table is permitted for Parts B and C but **not** for Part A. Total: **67 marks**. Full solutions begin on the following pages — do not look until you have finished.

10.1 Part A — Multiple choice (12 marks, 1 each)

- A1.** Which quantity is plotted on the horizontal axis of a mass spectrum?
- A. relative abundance B. mass number C. mass-to-charge ratio D. relative atomic mass
- A2.** The mass spectrum of element X shows peaks at $m/z = 63$ with a relative height of 100 and at $m/z = 65$ with a relative height of 44.6. What is the relative atomic mass of X?
- A. 63.4 B. 63.6 C. 64.0 D. 64.4
- A3.** An element has two isotopes of relative isotopic mass 10 and 11 and a relative atomic mass of 10.80. What percentage of the sample is the isotope of mass 11?
- A. 20 % B. 45 % C. 55 % D. 80 %
- A4.** Which statement about ^{63}Cu and ^{65}Cu is correct?
- A. They have different numbers of protons. B. They have different chemical properties.
 C. They have the same number of neutrons. D. They have the same electron configuration.
- A5.** Relative atomic mass is defined relative to which standard?
- A. the mass of one hydrogen atom B. one-twelfth the mass of a ^{12}C atom
 C. the mass of one proton D. the mass of one ^{12}C atom
- A6.** The mass spectrum of element Z shows peaks at $m/z = 24$ (79 %), 25 (10 %) and 26 (11 %). How many neutrons are present in the most abundant isotope?
- A. 11 B. 12 C. 13 D. 24
- A7.** Which best explains why the relative atomic mass of chlorine is 35.45?
- A. Chlorine atoms contain a fractional number of neutrons.
 B. It is the arithmetic mean of 35 and 37.
 C. It is the weighted mean of two isotopes present in unequal amounts.
 D. The mass of the electrons must be subtracted.
- A8.** In the mass spectrum of Cl_2 , peaks occur at $m/z = 70$, 72 and 74 in the ratio 9 : 6 : 1. Which ion is responsible for the peak at $m/z = 72$?



A9. Boron has a relative atomic mass of 10.81 and two isotopes of relative isotopic mass 10 and 11. Which statement about its mass spectrum is correct?

 A. The peak at $m/z = 10$ is taller.

 B. The peak at $m/z = 11$ is taller.

C. The two peaks are of equal height.

 D. Only one peak is observed, at $m/z = 10.81$.

A10. How many peaks appear in the molecular ion region of the mass spectrum of Br_2 , given that bromine has two natural isotopes?

A. 1

B. 2

C. 3

D. 4

A11. Which property would differ measurably between a sample of pure ^{20}Ne and a sample of pure ^{22}Ne at the same temperature and pressure?

A. first ionisation energy

B. density

C. electron configuration

D. reaction with fluorine

A12. An element has three isotopes. Its relative atomic mass is 63.6. Which statement must be **false**?

A. The lightest isotope has a relative isotopic mass below 63.6.

B. The heaviest isotope has a relative isotopic mass above 63.6.

C. The mass spectrum shows three peaks.

D. Every isotope has a relative isotopic mass greater than 63.6.

10.2 Part B — Short answer (23 marks)

B1. The mass spectrum of silicon gives the following data.

m/z	28	29	30
relative abundance / %	92.23	4.67	3.10

(a) State the number of isotopes present.

[1]

(b) Calculate the relative atomic mass of silicon to four significant figures.

[2]

(c) Explain why this value is not a whole number.

[1]

B2. (a) Define *relative atomic mass*.

[2]

(b) Explain what is meant by the term *mass-to-charge ratio* and why the horizontal axis of a mass spectrum can usually be read directly as relative isotopic mass.

[2]

B3. Element Q has two isotopes with relative isotopic masses of 107 and 109. Its relative atomic mass is 107.87.

(a) Calculate the percentage abundance of each isotope.

[3]

(b) Identify element Q.

[1]

B4. The mass spectrum of iron gives the following data.

m/z	54	56	57	58
relative abundance / %	5.85	91.75	2.12	0.28

- (a) Calculate the relative atomic mass of iron to two decimal places. [2]
 (b) Deduce the number of neutrons in an atom of ^{57}Fe . [1]
 (c) Explain why all four isotopes react identically with oxygen. [1]

B5. A mass spectrum of an unknown element shows the following relative peak heights.

m/z	84	86	87	88
relative height	0.56	9.86	7.00	82.58

- (a) Identify the base peak. [1]
 (b) Calculate the relative atomic mass to two decimal places. [2]
 (c) Identify the element. [1]
- B6.** (a) Explain why a small peak at $m/z = 30.0$ may be observed in the mass spectrum of a pure sample of ^{60}Ni . [2]
 (b) Suggest why this peak is very much smaller than the peak at $m/z = 60.0$. [1]

10.3 Part C — Long structured questions (32 marks)

C1. A sample of lead extracted from a galena ore gives the following mass spectrum.

m/z	204	206	207	208
relative abundance / %	1.40	24.10	22.10	52.40

- (a) State what is meant by the term *isotopes*. [2]
 (b) Calculate the relative atomic mass of this sample of lead, giving your answer to one decimal place. [3]
 (c) Deduce the number of protons, neutrons and electrons in one $^{207}\text{Pb}^{2+}$ ion. [3]
 (d) A second lead sample, extracted from an ore rich in uranium, is found to contain a much higher proportion of ^{206}Pb . Deduce, with reasoning, how the relative atomic mass of this second sample compares with your answer to (b). [2]
 (e) Explain why the isotopes of lead cannot be separated from one another by fractional crystallisation or any other chemical technique. [2]

C2. An unknown element X gives the mass spectrum below.

m/z	46	47	48	49	50
relative abundance / %	8.25	7.44	73.72	5.41	5.18

- (a) State the number of isotopes of X and identify the base peak. [2]
 (b) Calculate the relative atomic mass of X to two decimal places. [3]
 (c) Identify element X and state its atomic number. [2]

- (d) Deduce the number of neutrons in the most abundant isotope of X. [1]
- (e) The spectrum is re-plotted with the base peak scaled to a relative abundance of 100. State the new relative height of the peak at $m/z = 46$, and explain why the calculated relative atomic mass is unchanged. [3]

C3. Chlorine consists of ^{35}Cl (75.77 %) and ^{37}Cl (24.23 %).

- (a) Calculate the relative atomic mass of chlorine to four significant figures, using the mass numbers as the relative isotopic masses. [2]
- (b) The data booklet quotes 35.45. Suggest why your answer to (a) differs slightly. [1]
- (c) Predict the m/z values and the whole-number ratio of the peaks in the molecular ion region of the mass spectrum of Cl_2 , showing your reasoning. [4]
- (d) Predict the m/z values and approximate ratio of the peaks in the molecular ion region of the mass spectrum of HCl . Assume hydrogen is entirely ^1H . [2]



11 Mark scheme

How to mark yourself honestly. Award a mark only if your answer contains the underlined idea. In calculations, award the first mark for a correctly *substituted* expression even if the arithmetic then goes wrong, and carry your error forward — that is exactly what an IB examiner does. ECF means “error carried forward”.

11.1 Part A — Multiple choice

Q	Ans	Reasoning
A1	C	The axis is mass-to-charge ratio, m/z ; abundance is the vertical axis.
A2	B	$\frac{(63 \times 100) + (65 \times 44.6)}{144.6} = \frac{9199}{144.6} = 63.62 \approx 63.6$. The heights do not sum to 100, so you must divide by 144.6.
A3	D	$A_r = 10.80$ lies 0.80 of the way from 10 to 11, so the mass-11 isotope is 80 %. Option A is the abundance of the <i>lighter</i> isotope — read the question.
A4	D	Same $Z \Rightarrow$ same number of electrons $\Rightarrow$ same configuration $\Rightarrow$ identical chemistry. They differ only in neutron number.
A5	B	By definition, relative masses are referenced to $\frac{1}{12}$ the mass of a carbon-12 atom.
A6	B	$A_r \approx 24.3 \Rightarrow$ magnesium, $Z = 12$. Most abundant isotope is ^{24}Mg , so neutrons = $24 - 12 = 12$.
A7	C	A_r is a weighted mean over isotopes of unequal abundance. No atom has a fractional neutron count, so A is wrong; B would give exactly 36.
A8	A	$m/z = 72$ requires $35 + 37$, i.e. one atom of each isotope. ^{36}Cl is not a natural isotope.
A9	B	$A_r = 10.81$ lies closer to 11, so ^{11}B must be the more abundant isotope and gives the taller peak.
A10	C	Two isotopes give three distinct molecules: light–light, light–heavy, heavy–heavy.
A11	B	Identical electron configurations rule out A, C and D; only mass-dependent physical properties such as density (or rate of diffusion) differ.
A12	D	A_r is a mean, so at least one isotope <i>must</i> lie below it. D is therefore impossible; A, B and C are all consistent.

11.2 Part B — Short answer

B1 — Silicon [4]

(a) Three. [1]

(b) $A_r = \frac{(28 \times 92.23) + (29 \times 4.67) + (30 \times 3.10)}{100}$ correct substitution [1]

$$= \frac{2582.44 + 135.43 + 93.00}{100} = \frac{2810.87}{100} = 28.11$$

answer to 4 s.f., no units [1]

(c) It is a weighted mean of three isotopes of different mass present in different amounts, so it need not be an integer. [1]

B2 — Definitions [4]

(a) The weighted mean mass of the atoms in a naturally occurring sample of the element [1], relative to one-twelfth of the mass of a carbon-12 atom [1]. (Do not award if units are given — A_r is dimensionless.)

(b) m/z is the ratio of the relative mass of the ion to its charge [1]. Electron-impact ionisation produces almost exclusively $1+$ ions, so $z = 1$ and $m/z = m$ [1].

B3 — Element Q [4]

(a) Let the abundance of the mass-107 isotope be $x\%$:

$$\frac{107x + 109(100 - x)}{100} = 107.87$$

correct set-up [1]

$$107x + 10900 - 109x = 10787 \Rightarrow -2x = -113 \Rightarrow x = 56.5$$

rearrangement [1]

mass 107: 56.5 % and mass 109: 43.5 %

both values

[1]

(b) Silver (Ag).

[1]

B4 — Iron [4]

(a) $A_r = \frac{(54 \times 5.85) + (56 \times 91.75) + (57 \times 2.12) + (58 \times 0.28)}{100}$

[1]

$$= \frac{315.9 + 5138.0 + 120.84 + 16.24}{100} = \frac{5590.98}{100} = 55.91$$

[1]

(b) Iron has $Z = 26$, so neutrons = $57 - 26 = 31$.

[1]

(c) All isotopes have the same number of electrons in the same configuration, and chemical behaviour is determined by electrons, not neutrons.

[1]

B5 — Unknown element [4]

(a) The peak at $m/z = 88$ (the tallest peak).

[1]

(b) The heights sum to $0.56 + 9.86 + 7.00 + 82.58 = 100.00$, so

$$A_r = \frac{(84 \times 0.56) + (86 \times 9.86) + (87 \times 7.00) + (88 \times 82.58)}{100.00}$$

[1]

$$= \frac{47.04 + 847.96 + 609.00 + 7267.04}{100.00} = \frac{8771.04}{100.00} = 87.71$$

[1]

(c) Strontium (Sr, $A_r = 87.62$).

[1] Accept ECF from (b).

B6 — Doubly charged ions [3]

(a) The peak is due to $^{60}\text{Ni}^{2+}$ [1]; with $m = 60$ and $z = 2$, $m/z = 60/2 = 30.0$ [1].

(b) Removing a second electron requires much more energy (the second ionisation energy is far larger than the first), so only a small fraction of ions are doubly charged.

[1]

11.3 Part C — Long structured questions

C1 — Lead [12]

(a) Isotopes are atoms of the same element with the same number of protons [1] but different numbers of neutrons (hence different mass numbers) [1].

(b)

$$A_r = \frac{(204 \times 1.40) + (206 \times 24.10) + (207 \times 22.10) + (208 \times 52.40)}{100}$$

[1]

$$= \frac{285.6 + 4964.6 + 4574.7 + 10\,899.2}{100} = \frac{20\,724.1}{100}$$

correct numerator [1]

$$= 207.241 = \mathbf{207.2}$$

answer to 1 d.p. [1]

(c) ^{207}Pb has $Z = 82$.

► protons = **82** [1]

► neutrons = $207 - 82 = \mathbf{125}$ [1]

► electrons = $82 - 2 = \mathbf{80}$ (two lost to form the $2+$ ion) [1]

(d) The relative atomic mass would be lower than 207.2 [1], because a greater proportion of the lighter ^{206}Pb isotope shifts the weighted mean downwards [1].

(e) All lead isotopes have 82 protons and therefore 82 electrons in the same configuration [1]; chemical properties (and hence solubility, crystallisation behaviour and all reactions) depend on electrons, so the isotopes behave identically and cannot be separated chemically — only by a mass-dependent physical method such as mass spectrometry [1].

C2 — Unknown element X [11]

(a) **Five** isotopes [1]; base peak at $m/z = \mathbf{48}$ [1].

(b)

$$A_r = \frac{(46 \times 8.25) + (47 \times 7.44) + (48 \times 73.72) + (49 \times 5.41) + (50 \times 5.18)}{100}$$

[1]

$$= \frac{379.50 + 349.68 + 3538.56 + 265.09 + 259.00}{100} = \frac{4791.83}{100}$$

[1]

$$= \mathbf{47.92}$$

2 d.p., no units [1]

(c) **Titanium** [1], atomic number $Z = \mathbf{22}$ [1].

(d) Neutrons in $^{48}\text{Ti} = 48 - 22 = \mathbf{26}$. [1]

(e) Scaling factor = $100/73.72$, so the peak at $m/z = 46$ becomes

$$\frac{8.25}{73.72} \times 100 = \mathbf{11.19}$$

[1]

Every peak height is multiplied by the same constant factor [1], so that factor appears in both the numerator and the denominator of the weighted-mean expression and cancels — the relative atomic mass is therefore unchanged [1].

C3 — Chlorine [9]

$$\begin{aligned} \text{(a) } A_r &= \frac{(35 \times 75.77) + (37 \times 24.23)}{100} = \frac{2651.95 + 896.51}{100} \\ &= \frac{3548.46}{100} = \mathbf{35.48} \end{aligned}$$

4 s.f. [1]

(b) The calculation used whole-number mass numbers rather than the exact relative isotopic masses (34.97 and 36.97), which are slightly less than the mass numbers because of nuclear binding energy; using the exact values gives 35.45. [1]

(c) Three molecular ions are possible [1]:

Ion	$^{35}\text{Cl}^{35}\text{Cl}^+$	$^{35}\text{Cl}^{37}\text{Cl}^+$	$^{37}\text{Cl}^{37}\text{Cl}^+$
m/z	70	72	74
probability	p^2	$2pq$	q^2

correct m/z values 70, 72, 74

[1]

With $p = 0.75$ and $q = 0.25$: $p^2 = 0.5625$, $2pq = 0.3750$, $q^2 = 0.0625$

use of $p^2 : 2pq : q^2$

[1]

Dividing by 0.0625 gives the ratio **9 : 6 : 1** [1].

The factor of 2 for the mixed molecule must be shown or implied; a 9 : 3 : 1 answer scores the first two marks only.

(d) Only two molecular ions are possible, H^{35}Cl^+ at $m/z = \mathbf{36}$ and H^{37}Cl^+ at $m/z = \mathbf{38}$ [1], in the ratio of the chlorine abundances, $75.77 : 24.23 \approx \mathbf{3 : 1}$ [1].

Marking summary

Part A /12 Part B /23 Part C /32 **Total /67**

60–67 outstanding — grade 7 standard on this sub-topic. 50–59 secure; tighten significant figures and command-term phrasing. 38–49 the calculations are working but the definitions and explanations need learning word-perfect. **Below 38** re-read Sections 3–5 and redo every solved example with the solutions covered.



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