Edexcel International AS Chemistry

Atomic Structure

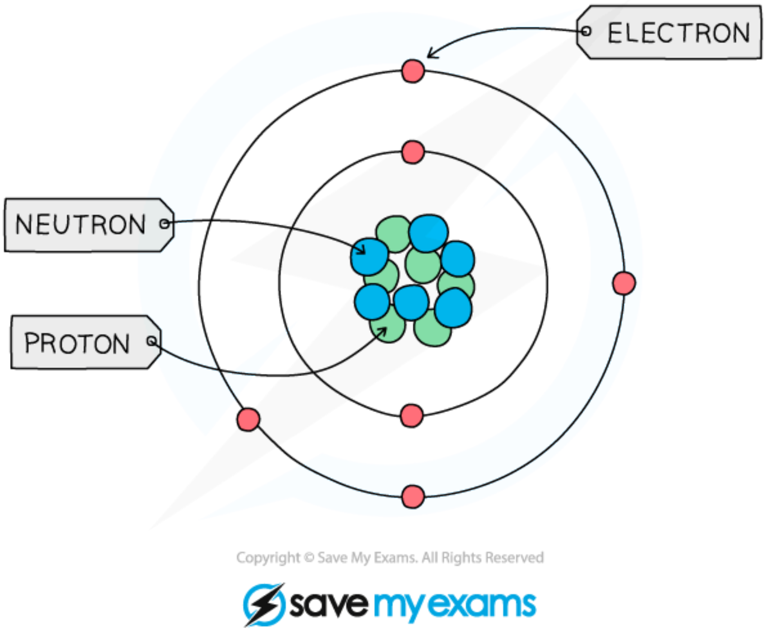
Your notes

Contents

Your notes

Sub-Atomic Particles

- All matter is composed of **atoms**, which are the smallest parts of an element that can take place in **chemical reactions**
- Atoms are mostly made up of **empty space** around a very small, dense **nucleus** that contains **protons** and **neutrons**
- The nucleus has an overall **positive charge**
  - The protons have a positive charge and the neutrons have a neutral charge
- **Negatively charged** electrons are found in orbitals in the empty space around the nucleus



The basic structure of an atom (not to scale)

- **Subatomic particles** are the particles an element is made up of and include **protons**, **neutrons** and **electrons**
- These subatomic particles are so small that it is not possible to measure their masses and charges using **conventional units** (such as grams and coulombs)
- Instead, their masses and charges are compared to each other using **'relative atomic masses'** and '**relative atomic charges**'
- These are not actual charges and masses but they are charges and masses of particles relative to each other

- Protons and neutrons have a very similar mass so each is assigned a relative mass of 1 whereas electrons are 1836 times smaller than a proton and neutron
- Protons are **positively** charged, electrons **negatively** charged and neutrons are **neutral**
- The relative mass and charge of the subatomic particles are:

Relative Mass & Charge of Subatomic Particles Table

Subatomic Particle	Relative Charge	Relative Mass
Proton	+1	1
Neutron	0	1
Electron	−1	$\frac{1}{1836}$

Examiner Tips and Tricks

The **relative mass** of an electron is **almost negligible.**

The **charge** of a single **electron** is -1.602 x 10^{-19} coulombs whereas the charge of a **proton** is +1.602 x 10^{-19} coulombs, however, relative to each other, their charges are -1 and +1 respectively.

Chemical Elements

- The **atomic number** (or **proton number**) is the number of protons in the nucleus of an atom and has **symbol *Z***
  - The atomic number is equal to the number of electrons present in a **neutral** atom of an element
  - E.g. the atomic number of lithium is 3 which indicates that the neutral lithium atom has 3 protons and 3 electrons
- The **mass number** (or **nucleon number**) is the total number of **protons** and **neutrons** in the nucleus of an atom and has **symbol *A***
- The number of **neutrons** can be calculated by:

Number of neutrons = mass number – atomic number

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- Protons and neutrons are also called **nucleons**

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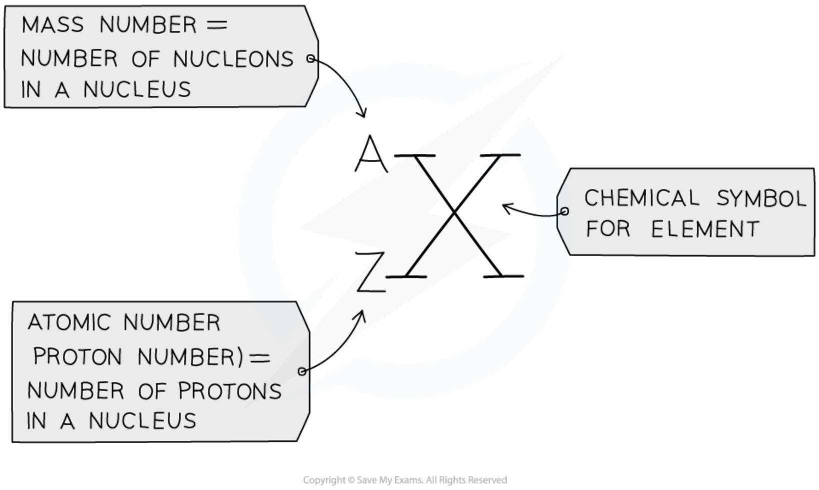
Examiner Tips and Tricks



The mass (nucleon) and atomic (proton) number are given for each element in the Periodic Table

- An atom is **neutral** and has no overall charge
- Ions on the other hand are formed when atoms either **gain** or **lose** electrons, causing them to become **charged**
- The number of **subatomic particles** in atoms and ions can be determined given their atomic (proton) number, mass (nucleon) number and charge

Protons

- The atomic number of an atom and ion determines which element it is
- Therefore, all atoms and ions of the **same element** have the same number of protons (atomic number) in the nucleus
  - E.g. lithium has an atomic number of 3 (three protons) whereas beryllium has atomic number of 4 (4 protons)
- The number of protons equals the **atomic (proton) number**
- The number of protons of an **unknown** element can be calculated by using its mass number and number of neutrons:

Mass number = number of protons + number of neutrons

Number of protons = mass number – number of neutrons

Electrons

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- An atom is **neutral** and therefore has the **same** number of **protons** and **electrons**
- Ions have a different number of electrons to their atomic number depending on their charge
  - A positively charged ion has **lost** electrons and therefore has **fewer** electrons than protons
  - A negatively charged ion has **gained** electrons and therefore has **more** electrons than protons

Neutrons

- The **mass** and **atomic numbers** can be used to find the number of **neutrons** in **ions** and **atoms:**

Number of neutrons = mass number (A) – number of protons (Z)

Worked Example

Determine the number of protons, electrons and neutrons for the following ions and atoms:

1. Mg^{2+} ion
2. Carbon atom
3. An unknown atom of element X with mass number 63 and 34 neutrons

Answer 1:

The atomic number of a magnesium atom is 12

- Therefore, the number of protons in a Mg^{2+} ion is also 12
  - However, the 2+ charge in Mg^{2+} ion suggests it has lost two electrons
    - Therefore, the Mg^{2+} ion only has 10 electrons left now

The atomic number of a magnesium atom is 12 and its mass number is 24

- Number of neutrons = mass number (A) - number of protons (Z)
  - Number of neutrons = 24 - 12 = 12
  - The Mg^{2+} ion has 12 neutrons in its nucleus

Answer 2:

The atomic number of a carbon atom is 6

- Therefore, the number of protons in a carbon atom is also 6

The atom has no overall charge so the number of protons = the number of electrons

- Therefore, the carbon atom has 6 electrons

The atomic number of a carbon atom is 6 and its mass number is 12

- Number of neutrons = mass number (A) - number of protons (Z)
  - Number of neutrons = 12 - 6 = 6
  - The carbon atom has 6 neutrons in its nucleus

Answer 3:

Use the formula to calculate the number of protons

- Number of protons = mass number - number of neutrons
  - Number of protons = 63 - 34
  - Number of protons = 29
  - (Element X is therefore copper)

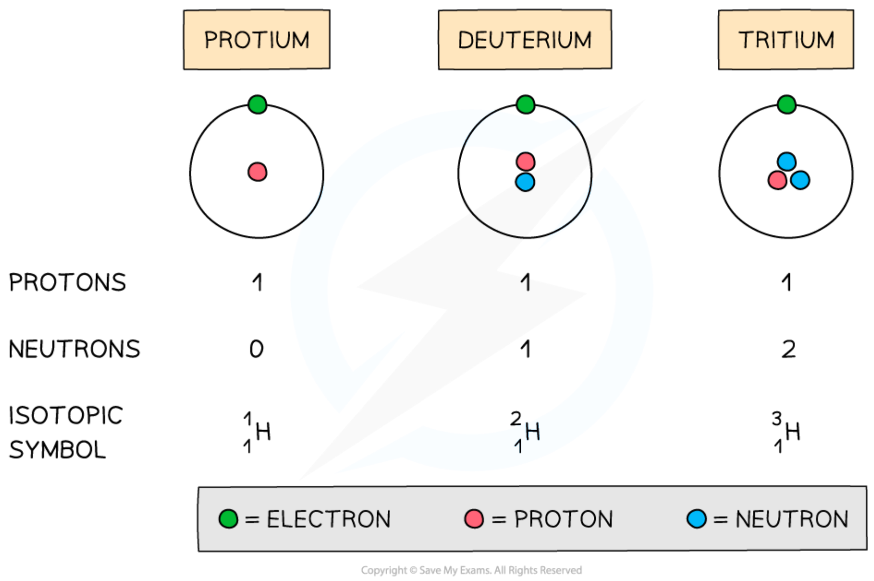
The atom is not charged so the number of protons = the number of electrons

- Therefore, the atom of element X has 29 electrons

The number of neutrons is 34 (given in the question)

Isotopes

- The symbol for an isotope is the **chemical symbol** (or **word**) followed by a **dash** and then the **mass number**
  - E.g. carbon-12 and carbon-14 are isotopes of carbon containing 6 and 8 neutrons respectively
- Isotopes are atoms of the **same element** that contain the same number of **protons** and electrons but a different number of **neutrons**



The atomic structure and symbols of the three isotopes of hydrogen

Properties of Isotopes

- Isotopes have **similar chemical properties** but **different physical properties**

Chemical properties

- Isotopes of the same element display the **same chemical characteristics**
- This is because they have the same number of electrons in their **outer shells**

- Electrons take part in **chemical reactions** and therefore determine the **chemistry** of an atom

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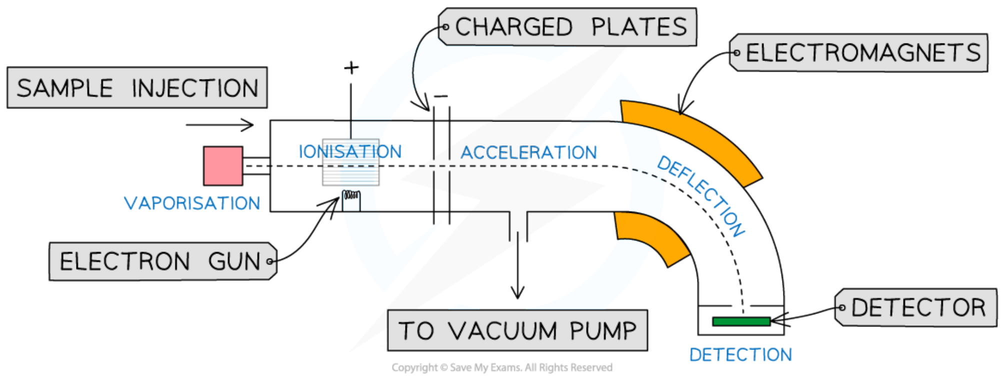
Physical properties

- The only difference between isotopes is the number of **neutrons**
- Since these are neutral subatomic particles, they only add **mass** to the atom
- As a result of this, isotopes have different **physical properties** such as small differences in their **mass**, **density**, **melting point** and **boiling point**

The Mass Spectrometer

- The mass spectrometer is an instrument used to determine the relative isotopic mass and the relative abundance of each isotope
- Relative isotopic mass is the mass of an individual isotope relative to the mass of carbon-12
- Apart from finding the masses of isotopes, mass spectrometry is a vey useful tool for detecting illegal drugs, forensic science, space exploration and carbon-14 dating



The components of a mass spectrometer

How the mass spectrometer works

- A sample is injected into the spectrometer where it is heated and vaporised
- The atoms or molecules are then bombarded by high energy electrons created by an electron gun
- The high energy electrons collide with the sample material and remove electrons creating positive ions
- The ions are then accelerated by attraction towards negatively charged plates
- Many ions strike the plate and are discharged, but a few will pass through a gap in the plates into a curved section of the spectrometer known as the flight tube
- The flight tube is encased in electromagnets which create a strong electromagnetic field that deflects the path of the ions in a curve
- The ions pass onto a charged detector plate where every strike is recorded as a small current which is then amplified
- By varying the electric and magnetic fields all the charged particles can be deflected to the detector which gives information about the mass/charge ratio and abundance of each ion

Isotopes & Mass Spectra

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- Isotopes are different atoms of the same element that contain the same number of protons and electrons but a different number of neutrons
  - These are atoms of the same elements but with different mass numbers
- Therefore, the mass of an element is given as relative atomic mass (A_r) by using the average mass of the isotopes
  - The relative atomic mass of an element can be calculated by using the relative abundance values

$$A_r = \frac{\left(relative\ abundance_{isotope\ 1} \times mass_{isotope\ 1}\right) + \left(relative\ abundance_{isotope\ 2} \times mass_{isotope\ 2}\right)\ etc}{100}$$

- The relative abundance of an isotope is either given or can be read off the mass spectrum

Worked Example

Calculating the relative atomic mass of oxygen

A sample of oxygen contains the following isotopes:

Isotope	Percentage abundance
^{16}O	99.76
^{17}O	0.04
^{18}O	0.20

What is the relative atomic mass, A_r, of oxygen in this sample, to 2dp?

Answer

- $A_r = \frac{(99.76 \times 16) + (0.04 \times 17) + (0.20 \times 18)}{100}$
  - $A_r = 16.0044$
  - $A_r = 16.00$

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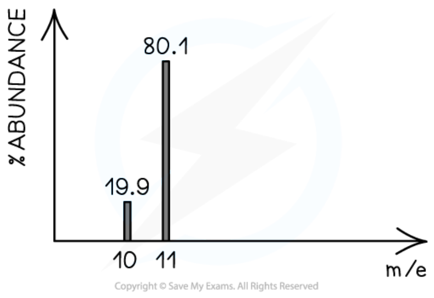
Worked Example

Calculating the relative atomic mass of boron

Calculate the relative atomic mass of boron using its mass spectrum, to 1dp:



Answer

- $A_r = \dfrac{(19.9 \times 10) + (80.1 \times 11)}{100} = 10.801 = 10.8$

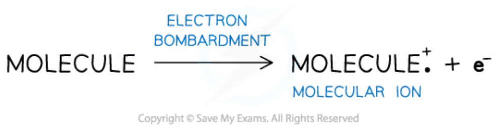
Examiner Tips and Tricks

You can be expected to work with tables or graphs of data to calculate relative atomic mass

You can also be expected to do these calculations backwards to determine the abundance of one isotope given sufficient information

Mass spectra of molecules

- When a compound is analysed in a mass spectrometer, vaporised molecules are bombarded with a beam of high-speed electrons
- These knock off an electron from some of the molecules, creating **molecular ions:**



- The relative abundances of the detected ions form a **mass spectrum**: a kind of molecular fingerprint that can be identified by computer using a spectral database
- The peak with the highest ***m/z*** value is the molecular ion (**M$^+$**) peak which gives information about the **molecular mass** of the compound
- This value of m/z is equal to the **relative molecular mass** of the compound

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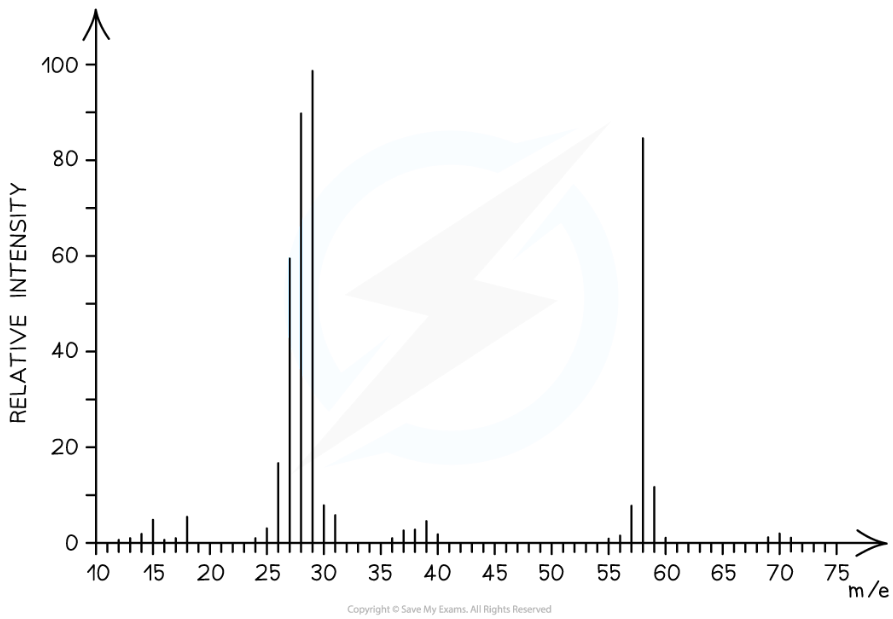
The M+1 peak

- The **[M+1]** peak is a smaller peak which is due to the natural abundance of the isotope **carbon-13**
- The height of the **[M+1]** peak for a particular ion depends on how many carbon atoms are present in that molecule; The more carbon atoms, the larger the **[M+1]** peak is
  - For example, the height of the **[M+1]** peak for an hexane (containing six carbon atoms) ion will be greater than the height of the **[M+1]** peak of an ethane (containing two carbon atoms) ion

Worked Example

Determine whether the following mass spectrum belongs to propanal or butanal



Answer:

- The mass spectrum corresponds to **propanal** as the molecular ion peak is at *m/z* = 58
  - Propanal arises from the $CH_3CH_2CHO^+$ ion which has a molecular mass of 58
  - Butanal arises from the $CH_3CH_2CH_2CHO^+$ ion which has a molecular mass of 72

Examiner Tips and Tricks

A mass spectrum can give lots of information about fragments of the overall compound being analysed

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Mass Spectra – Predictions

- You can also predict how a mass spectrum might appear for a given compound, e.g. ethanol, CH_3CH_2OH
  - The methyl, CH_3^+, fragment has a mass of 15.0
  - The ethyl, $CH_3CH_2^+$, fragment has a mass of 29.0
  - The base ion, CH_2OH^+, fragment has a mass of 31.0
  - The whole molecule has a mass of 46.0
- Predicting mass spectra becomes more complex with the inclusion of halogen isotopes such as chlorine and bromine

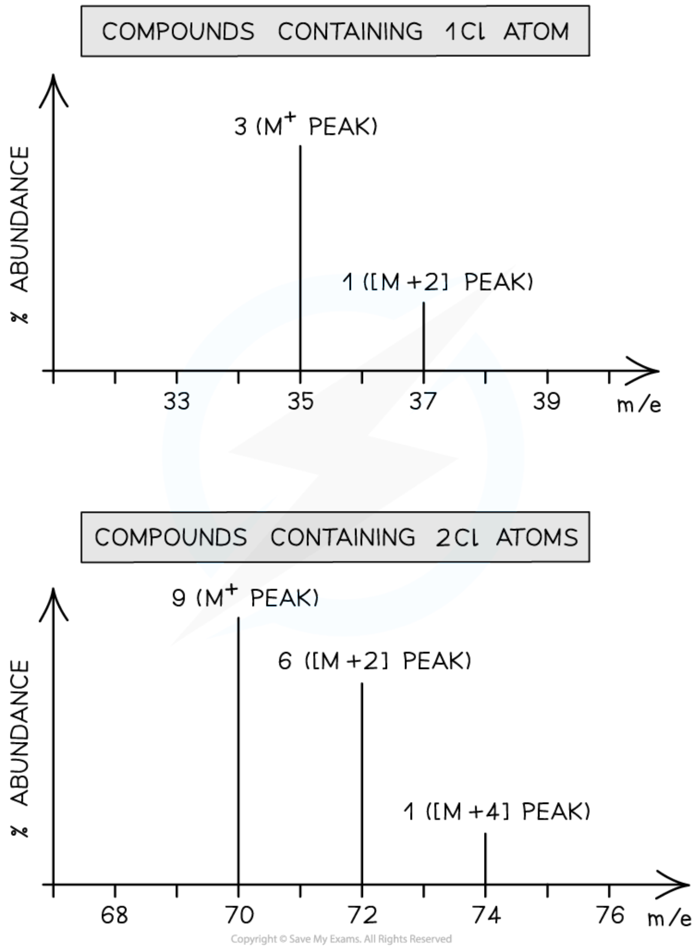
Chlorine

Chlorine exists as two isotopes, ^{35}Cl and ^{37}Cl

- A compound containing **one** chlorine atom will therefore have two molecular ion peaks due to the two different isotopes it can contain
  - ^{35}Cl = **M⁺** peak
  - ^{37}Cl = [**M+2]** peak
  - The ratio of the peak heights is 3:1 (as the relative abundance of ^{35}Cl is 3× greater than that of ^{37}Cl)
- A diatomic chlorine molecule or a compound containing **two** chlorine atoms will have three molecular ion peaks due to the different combinations of chlorine isotopes they can contain
  - $^{35}Cl + ^{35}Cl$ = **M⁺** peak
  - $^{35}Cl + ^{37}Cl$ = [**M+2]** peak
    - There is an alternative of $^{37}Cl + ^{35}Cl$ doubling the [**M+2]** peak
  - $^{37}Cl + ^{37}Cl$ = [**M+4]** peak
  - The ratio of the peak heights is **9:6:1**
    - This ratio can be deduced by using the probability of each chlorine atom being ^{35}Cl or ^{37}Cl
    - $^{35}Cl + ^{35}Cl = 3/4 \times 3/4 = 9/16$
    - $^{35}Cl + ^{37}Cl = 3/4 \times 1/4 = 3/16$ but this doubles for the $^{37}Cl + ^{35}Cl$ option, therefore, $6/16$

- $^{37}Cl + {}^{37}Cl = 1/4 \times 1/4 = 1/16$

- The presence of bromine or chlorine atoms in a compound gives rise to a **[M+2]** and possibly **[M+4]** peak



Mass spectrum of compounds containing one chlorine atom (1) and two chlorine atoms (2)

Bromine

- Bromine too exists as two isotopes, ^{79}Br and ^{81}Br
- A compound containing **one** bromine atom will have two molecular ion peaks
  - ^{79}Br = **M⁺** peak
  - ^{81}Br = **[M+2]** peak
  - The ratio of the peak heights is 1:1 (they are of **similar** heights as their relative abundance is the same!)
- A diatomic molecule of bromine or a compound containing **two** bromine atoms will have three molecular ion peaks
  - $^{79}Br + {}^{79}Br$ = **M⁺** peak

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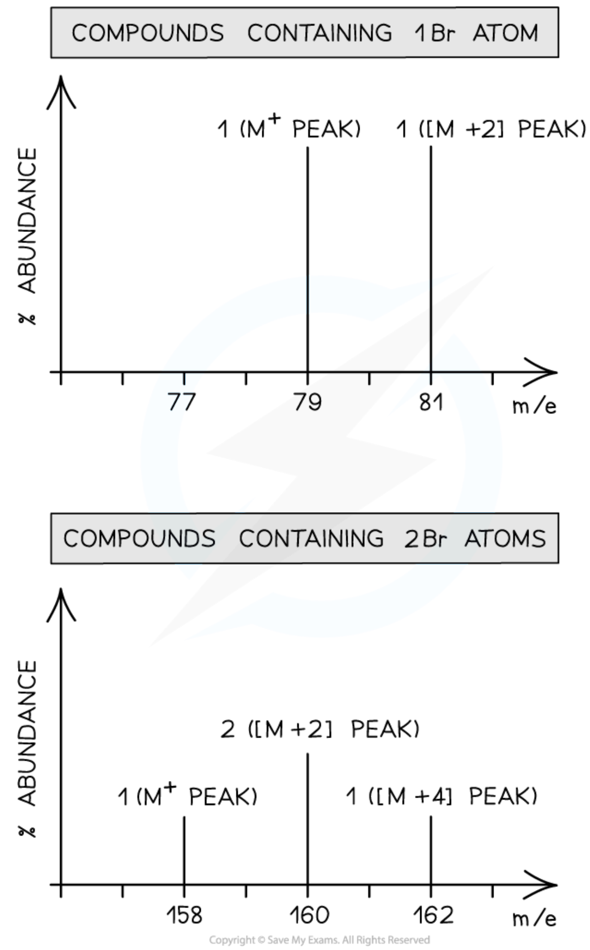
- $^{79}Br + ^{81}Br$ = **[M+2]** peak
- $^{81}Br + ^{81}Br$= **[M+4]** peak
- The ratio of the peak heights is **1:2:1**



Mass spectrum of compounds containing one bromine atom

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