CHEMISTRY ONLINE
TUITION

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CHEMISTRY

REVISION NOTES

ATOMIC STRUCTURE -1

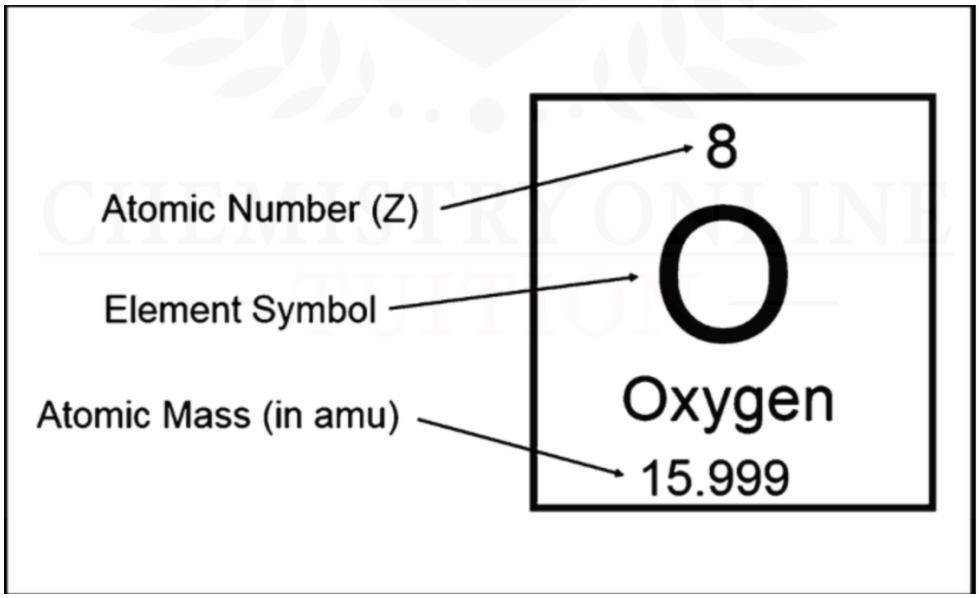
AQA Atomic Structure – 1.1

Three Sub-atomic (fundamental) Particles

Please learn the relative mass and charges.

Particle	Position	Relative Mass	Relative Charge
Proton	Nucleus	1	+1
Neutron	Nucleus	1	0
Electron	Orbitals	1/1840	-1

The Atomic symbol is used instead of mentioning the name of the element. An element of Oxygen is represented as follows;



The number of protons in an atom is known as the atomic number represented by Z.

- The atomic number is vital in identifying each element as it is unique to each one.
- Additionally, the periodic table is arranged based on the increasing atomic numbers of the elements

The atomic number of Calcium is 20, indicating it has 20 protons in its nucleus.

The nucleus of Calcium has 20 protons and 20 neutrons, giving it a mass number of 40, represented by A.

The number of Neutrons can be calculated by = Mass number (A) – Atomic number (Z) = 40-20 = 20 neutrons.

Exam point 1:

You should be able to calculate the number of protons, electrons, and neutrons.

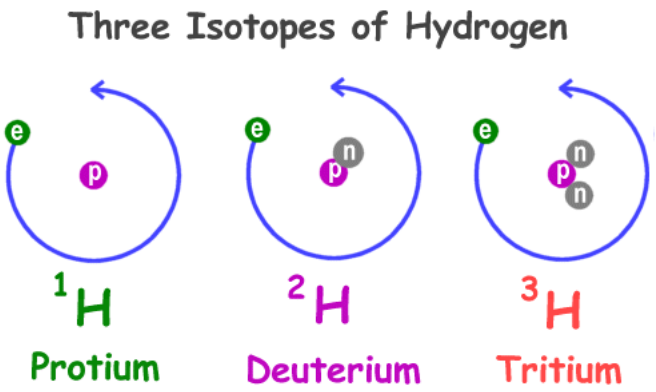
Please solve the following for practice:

COMPLETE THE TABLE

$^{2}_{4}He$	element_____ #protons_____ #neutron_____	$^{26}_{56}Fe$	element_____ #protons_____ #neutron_____	$^{13}_{27}Al$	element_____ #protons_____ #neutron_____
$^{20}_{40}Ca$	element_____ #protons_____ #neutron_____	$^{10}_{20}Ne$	element_____ #protons_____ #neutron_____	$^{2}_{4}C$	element_____ #protons_____ #neutron_____

Isotopes

Isotopes are atoms of the same element with different numbers of neutrons but the same number of protons. For instance, Hydrogen has three isotopes with mass numbers 1, 2, and 3.



Isotopes have the same chemical properties but different physical properties.

Exam point 2:

Chemical properties are the same because they have the same number of electrons, which means they have the same electronic configuration, e.g., the way isotopes react with other atoms.

Physical properties are different because of different numbers of neutrons, which results in different masses. This includes melting point, boiling point, etc.

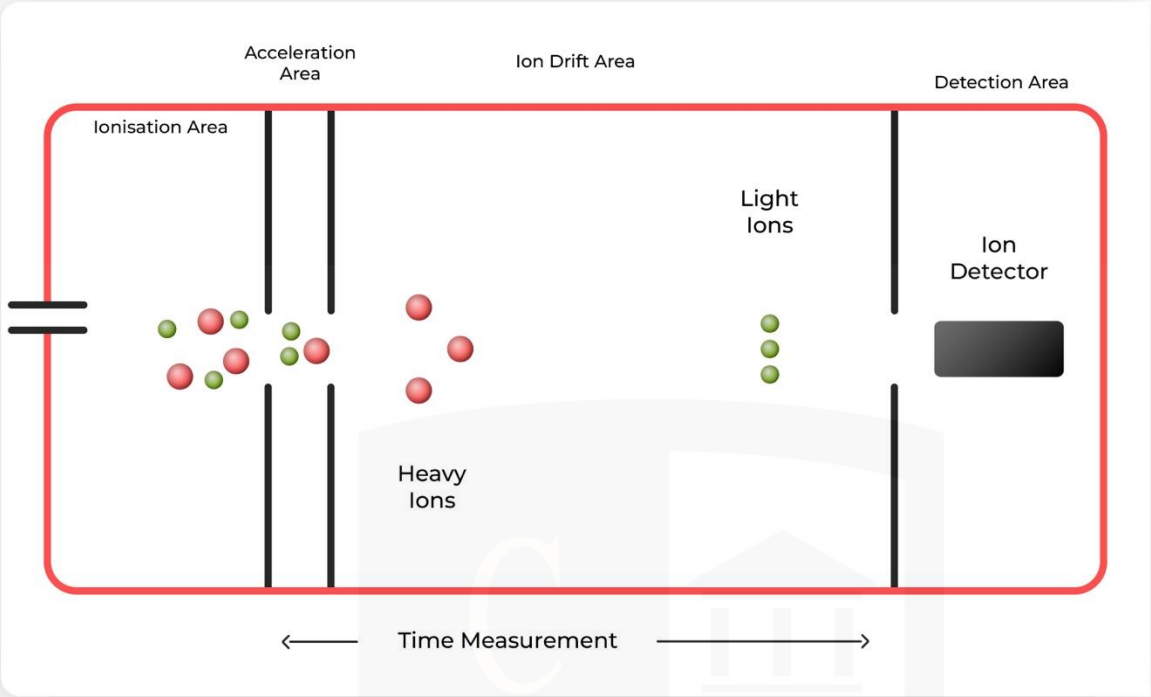
1.1.3 Time of Flight Mass Spectrometry

- Mass Spectrometry is an analytical technique:
  - It is the most helpful instrument for the accurate determination of the relative atomic mass of an element based on the abundance and mass of each of its isotopes.
  - It is also used to find the relative molecular mass of molecules.

A mass/charge ratio spectrum is produced against abundance as a sample passes through the mass spectrometer.

There are four critical stages in time of flight mass spectrometry:

- Ionization
- Acceleration
- Ion drift
- Detection



Stage 1: Ionization:

- Two key ways in which the sample could be ionized:
  - Electron Impact (or electron ionization)
  - Electrospray Ionization

Electron Impact Ionization

- The sample is vaporized and then bombarded with high-energy electrons.
- The electrons are 'fired' from an electron gun.
  - The electron gun is a hot wire filament that emits electrons as a current passes through it.
- As these electrons bombard the sample, an electron is knocked off each particle, forming a 1+ ion.

$$X\,(g) \rightarrow X^{+}\,(g) + e^{-}$$

- The 1+ ions are then attracted towards a negatively charged plate.

Note: The electron impact method is typically used for small molecules due to the slight danger of fragmentation. In contrast, electrospray ionization is used to ionize large molecules.

Electrospray Ionization

- Fragmentation is less likely to occur compared to electron impact ionization.
  - This is often called a soft ionization technique.
- For this method, the sample is dissolved in a volatile solvent.
- The solvent is injected into the mass spectrometer using a hypodermic needle.
  - This produces a fine mist or aerosol.
- The needle is attached to a high-voltage power supply, so as the sample is injected, the particles are ionized by gaining a proton from the solvent.
  - $X\,(g) + H^{+} \rightarrow XH^{+}\,(g)$
- The solvent evaporates, and the XH^{+} ions are attracted towards a negatively charged plate.

Stage 2: Acceleration:

- The 1+ ions formed from either ionization method are accelerated using an electric field.
- They are all accelerated to have the same kinetic energy.

K.E =1/2(mv^2)

  - ''This is important for you to remember when completing calculations.''
- Since all 1+ ions have the same kinetic energy, their velocity will depend on their mass.
  - When it comes to ions, the ones that have less weight will move at a faster pace, while the heavier ones will move at a slower pace.

Stage 3: Ion Drift (in the flight tube):

- The 1+ ions will pass through a hole in the negatively charged plate and move into a flight tube.
  - This is where the name 'Time of Flight' comes from.
  - The time of flight of each 1+ ion in this tube depends on their velocity.

Stage 4: Detection:

- Once they have passed through the mass spectrometer, the 1+ ions will hit a negatively charged 'detector' plate
- As they hit this electric plate, they gain an electron.
- This gaining of an electron discharges the ion and causes a current to be produced.
  - This size of the current is proportional to the abundance of those ions hitting the plate and gaining an electron
- The detector plate is connected to a computer, which produces the mass spectrum.

Exam Question 1:

In the TOF mass spectrometer, a germanium ion reaches the detector in 4.654×10^{-6} s. The kinetic energy of this ion is 2.438×10^{-15} J.

The length of the flight tube is 96.00 cm

The kinetic energy of an ion is given by the equation

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

where m = mass/kg

v = m s^{-1}

The Avogadro constant L = 6.022×10^{23} mol^{-1}

Use this information to calculate the mass, in g, of one mole of these germanium ions. Use your answer to state the mass number of this germanium ion

Step 1:

Highlight important information

Time ⇒ 4.654×10^{-6} s

K.E ⇒ 2.438×10^{-15}

Length of tube = 96cm

Convert in meters = 96/100 = 0.96m

Step 2:
Calculate velocity

$v \Rightarrow d/t = 0.96 / 4.654 \times 10^{-6} = 206274$ m/s

Step 3:
As we know K.E, we use the formula to calculate the mass of the single ion

2.438×10^{-15} s $= 1/2\ (M)\ (206274)^2$

$M = (2.438 \times 10^{-15}) \times 2 / (206272)^2$

Step 4:
Multiply by N_A

This is the mass of one ion in kg = 1.146×10^{-25} kg

mass of 1 mole ions = $1.146 \times 10^{-25} \times 6.022 \times 10^{23}$ = (0.06901 kg)

Convert in grams by multiplying by 1000 = 0.06901 x1000

Answer = 69 grams.

(Please note that if you're looking for more exam-style questions, you can visit the resources page on www.Chemistryonlinetuition.com)

Exam tip:

Students should be able to:

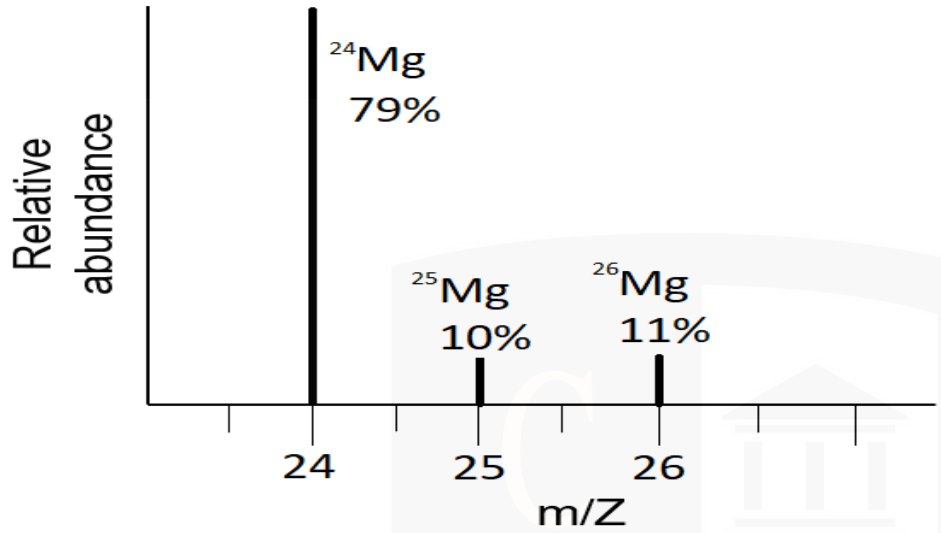
- interpret simple mass spectra of elements
- calculate relative atomic mass from isotopic abundance, limited to mononuclear ions.

Students should be able to use the formula to calculate Relative Atomic Mass

$$R.A.M = \frac{\Sigma\ (\text{isotopic mass} \times \%\ \text{abundance})}{100}$$

Exam-style Questions:

Please find below the R.A.M of Magnesium from the spectra below:



Important points;

1. The number of peaks represents the number of isotopes.

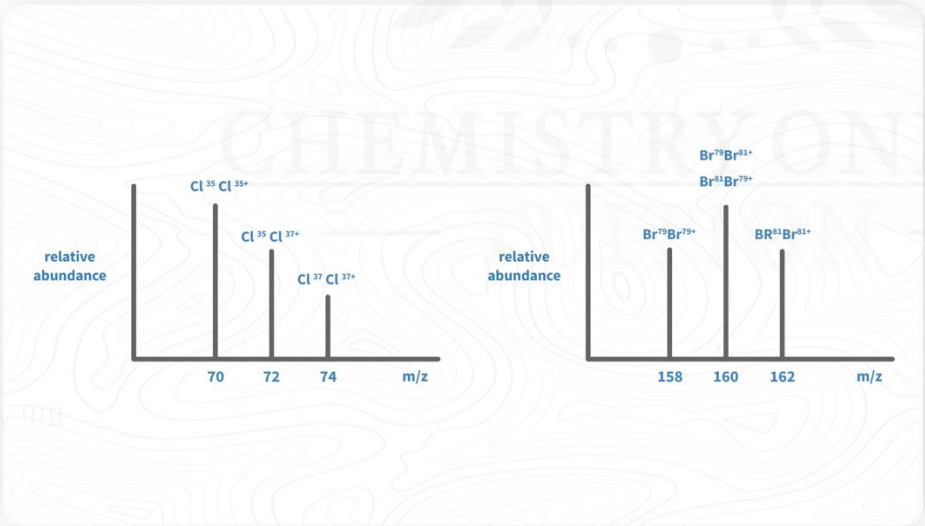
2. The height of each peak represents the relative abundance.

Below are the mass spectra of Chlorine and Bromine molecules as per the given specifications:

Cl has two isotopes: Cl-35 (75%) and Cl-37 (25%).

Br has two isotopes: Br-79 (50%) and Br-81 (50%).

These isotopes lead to distinct spectra in diatomic molecules.



Applications of Mass spectrometry:

Pharmaceutical analysis

- Drug analysis
- Screening of drugs
- Characterization of drugs

Environmental analysis

- Pesticides for foods
- Analysis for soil and groundwater content

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- Founder & CEO of Chemistry Online Tuition Ltd.
- Completed Medicine (M.B.B.S) in 2007
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