Atoms and Isotopes

Mass Spectrometry

N Goalby
chemrevise.org

Details of Sub-atomic Particles

There are three fundamental sub-atomic particles

Particle	Position	Mass	Charge
Proton	Nucleus	1	+1
Neutron	Nucleus	1	0
Electron	Orbit	1/1800	-1

KEY

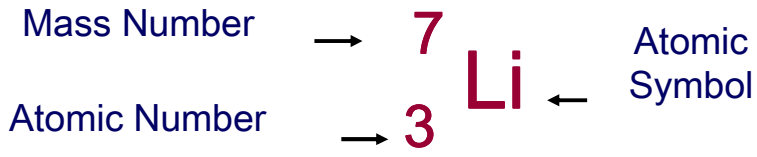
The Atomic Nucleus

The nucleus of an atom is tiny compared to the volume occupied by the electrons of the atom.

An electron has an incredibly small mass, which is about 1/2000 the mass of a neutron or a proton. Hence, the vast majority of the mass of an atom is found in the nucleus.

If an atom could be enlarged to the size of a football stadium, the nucleus of the atom would be about the size of a golf ball, somewhere above the centre spot.

An atom of Lithium (Li) can be represented as follows:



This shows that a Lithium (Li) atom has three protons, and four neutrons.

The **atomic number,** Z, is the number of protons in the nucleus.
The **mass number** ,A, is the total number of protons and neutrons in the atom.

Number of protons = Number of electrons = Z

Number of neutrons = A - Z

KEY

Exam Question

An atom of element **Q** contains the same number of neutrons as are found in an atom of ^{27}Al. An atom of **Q** also contains 14 protons.

(i) Give the number of protons in an atom of ^{27}Al.

(ii) Deduce the symbol, including mass number and atomic number, for this atom of element **Q**.

Isotopes

Isotopes are atoms with the same number of protons, but different numbers of neutrons.

Isotopes have similar chemical properties because they have the same electronic structure. They may have slightly varying physical properties because they have different masses.

$$ {}^{A}_{Z}X $$

Where:
X = symbol of element
Z = atomic number = p
A = Mass number = p + n

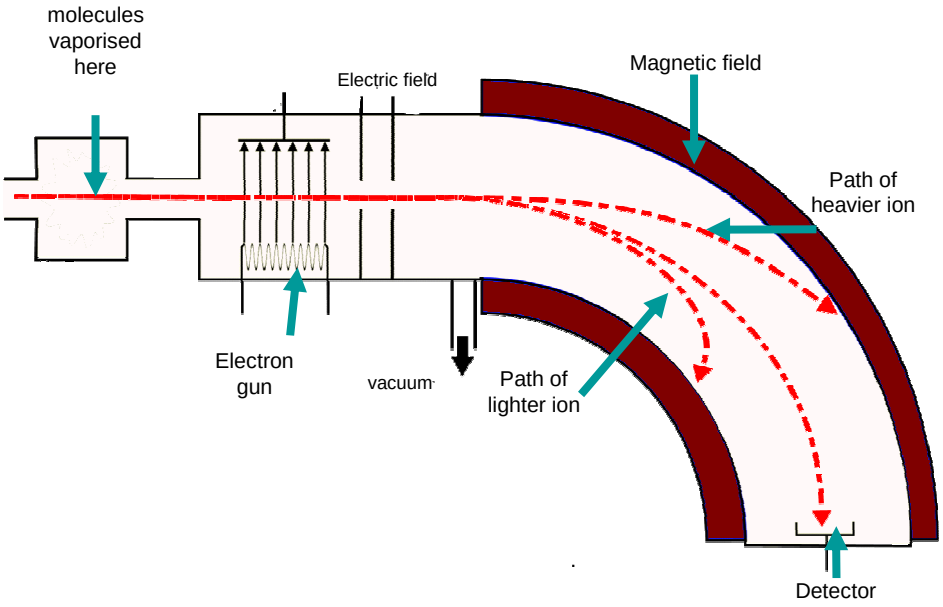
Isotopes of chlorine

$^{35}_{17}Cl$ Chlorine - 35

$^{37}_{17}Cl$ chlorine - 37

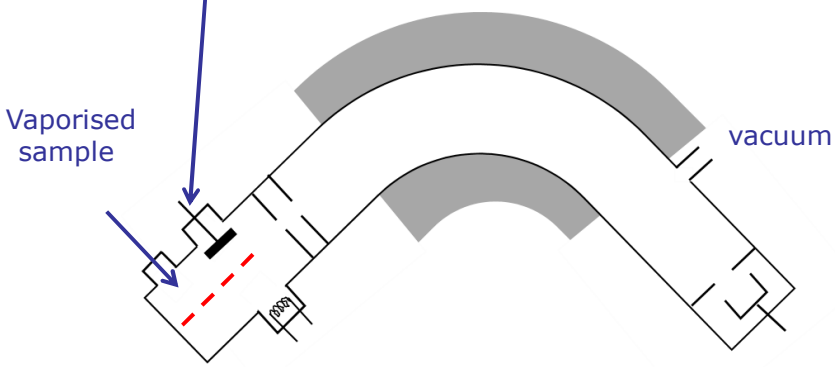
KEY

Mass Spectrometer



1. Ionisation

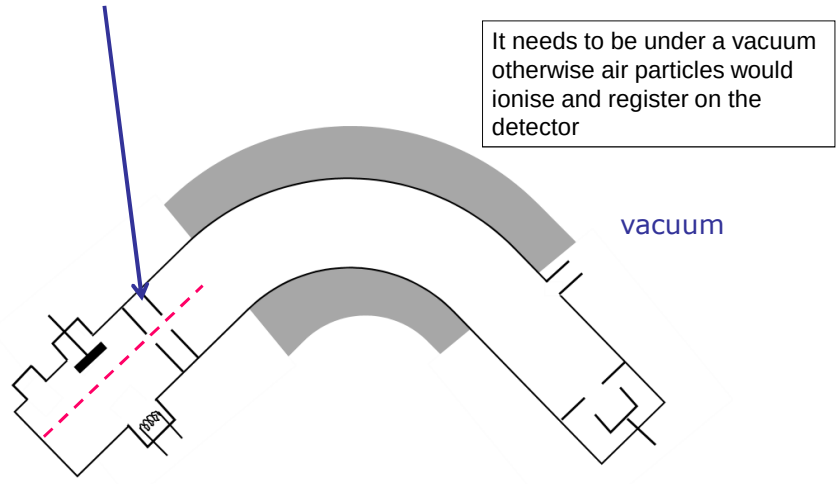
- A Vaporised sample is injected at low pressure
- An **electron gun fires** high energy electrons at the sample
- This Knocks out (outer) electron
- Forming positive ions with different charges
- Eg Ti → $Ti^+ + e^-$



KEY

2. Acceleration

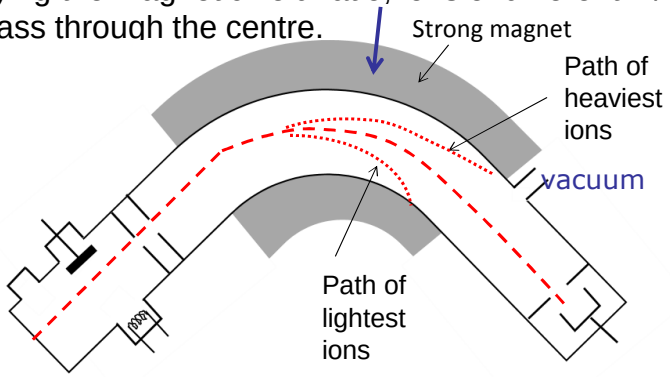
A negative electric field accelerates the positive ions and makes them into a beam



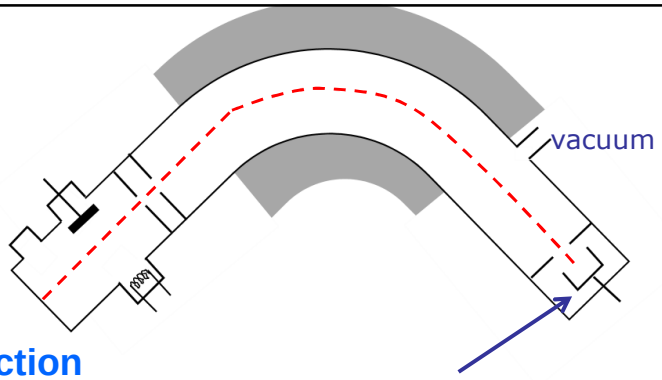
KEY

3. Deflection

- The beam of positive ions is deflected by a strong magnetic field.
- The degree of deflection depends on the mass-to-charge ratio, m/z.
- The smaller this ratio the larger the deflection.
- By varying the magnetic field ratio, ions of different m/z ratios pass through the centre.



KEY



4. Detection

The ions reaches the detector and generate a small current, which is fed to a computer for analysis

The size of the current is proportional to the abundance of the species

For each particle the mass spectrometer can measure a **m/z (mass/charge ratio)** and an **abundance**

Sometimes two electrons may be removed from a particle forming a 2+ ion. Mg^{24} with a 2+ charge would have a m/z of 12

KEY

Exam questions

(1) Parts (i) to (iv) below refer to the operation of a mass spectrometer.

(i) Name the device used to ionise atoms in a mass spectrometer.

(ii) Why is it necessary to ionise atoms before acceleration?

(iii) What deflects the ions?

(iv) What is adjusted in order to direct ions of different mass to charge ratio onto the detector?

(2) A gaseous sample of chromium can be analysed in a mass spectrometer. Before deflection, the chromium atoms are ionised and then accelerated.
(a) Describe briefly how positive ions are formed from gaseous chromium atoms in a mass spectrometer. (2)
(b) What is used in a mass spectrometer to accelerate the positive ions? (1)
(c) What is used in a mass spectrometer to deflect the positive ions? (1)

Relative Atomic Mass

The relative atomic mass is defined as the mass of one mole of atoms compared with one twelfth of the mass of a mole of carbon 12 atoms.

The mean mass of an atom relative to one twelfth of the mass of an atom of carbon 12

KEY

Exam Question

Some data obtained from the mass spectrum of a sample of carbon are given below.

Ion	$_{12}C^{+}$	$_{13}C^{+}$
Absolute mass of one ion/g	1.993×10^{-23}	2.158×10^{-23}
Relative abundance/%	98.9	1.1

Use these data to calculate a value for

a) the mass of one neutron,

b) the relative atomic mass of ^{13}C

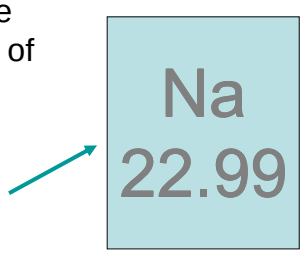
c) the relative atomic mass of carbon in the sample.
You may neglect the mass of an electron.

Relative Atomic Mass

The relative atomic mass quoted on the periodic table is a weighted average of all the isotopes

Average atom based on all the isotopes and their abundance %

Atomic mass is not a whole number

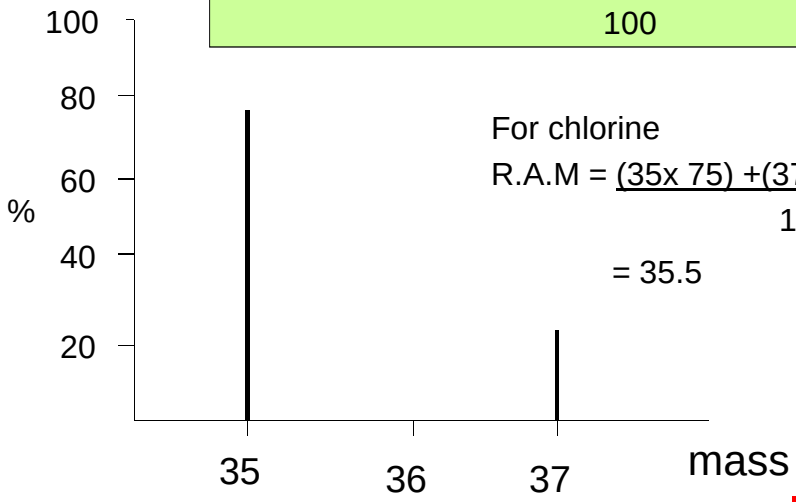


$$R.A.M = \frac{\Sigma \text{ (isotopic mass x \%abundance)}}{100}$$

KEY

A mass spectrum for chlorine

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



For chlorine

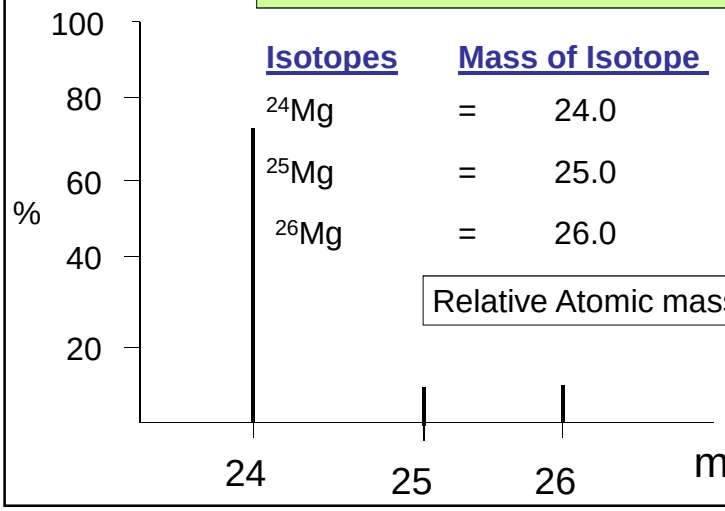
$$R.A.M = \frac{(35x\ 75) + (37x25)}{100}$$

$$= 35.5$$

KEY

A mass spectrum for magnesium

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



Isotopes	Mass of Isotope		Abundance
^{24}Mg	=	24.0	78.70%
^{25}Mg	=	25.0	10.13%
^{26}Mg	=	26.0	11.17%

Relative Atomic mass Mg = 24.3

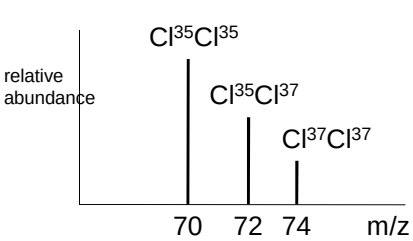
KEY

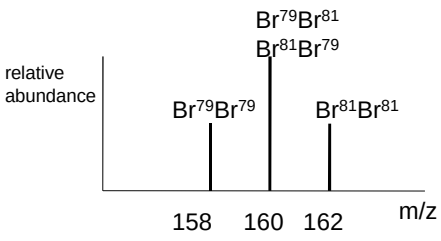
Mass spectra for Cl_2 and Br_2

Cl has two isotopes Cl^{35} (75%) and Cl^{37}(25%)

Br has two isotopes Br^{79} (50%) and Br^{81}(50%)

These lead to the following spectra caused by the diatomic molecules

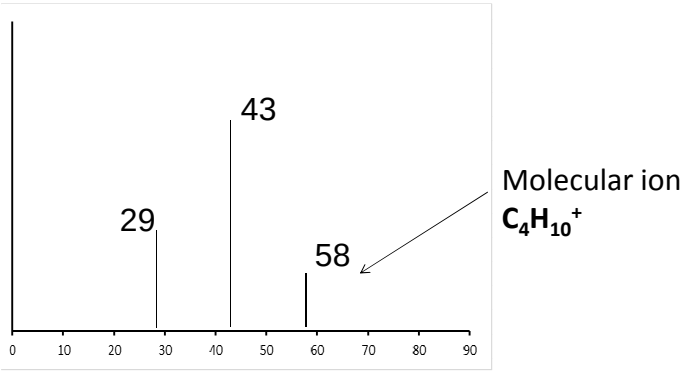




Measuring the M_r of a molecule

If a molecule is put through a mass spectrometer it will often break up and give a series of peaks caused by the fragments. The peak with the largest m/z, however, will be due to the complete molecule and will be equal to the M_r of the molecule. This peak is called the parent ion or **molecular ion**

Spectra for C_4H_{10}



Question

1. In a sample of gallium, there is 60.2% of gallium-69 (68.9 amu) atoms and 39.8% of gallium-71 (70.9 amu) atoms. What is the atomic mass of gallium?

Atomic mass Ga = 69.7 amu

2. A sample of boron contains 20% by mass of ^{10}B and 80% by mass of ^{11}B.
Calculate the relative atomic mass of boron in this sample.

Exam Questions

1.

Isotope	^{46}Ti	^{47}Ti	^{48}Ti	^{49}Ti	^{50}Ti
% abundance	8.02	7.31	73.81	5.54	5.32

Calculate the relative atomic mass, Ar, of titanium

2. The mass spectrum of a sample of chromium shows four peaks. Use the data below to calculate the relative atomic mass of chromium in the sample. Give your answer to two decimal places.

m/z	50	52	53	54
Relative abundance / %	4.3	83.8	9.5	2.4

Exam Question

Bromine gas contains the isotopes ^{79}Br and ^{81}Br in almost equal proportions. Part of the spectrum of bromine gas, showing one of the peaks for the molecular ion Br_2^+, is given below.

(i) Complete the **Figure** below to show the full spectrum of the molecular ion peaks of Br_2^+.

(ii) Explain the number of peaks present in your diagram. (1)

(iii) Explain the ratio of the heights of the peaks shown in your diagram. (1)