

1.01 Atomic structure and the mass spectrometer

OBJECTIVES

By the end of this section you should be able to:

- define the terms: atomic number, mass number, isotope
- determine the number of protons, neutrons, and electrons present in an atom or ion
- describe the steps in the mass spectroscopy experiment
- interpret a simple mass spectrum
- define relative atomic mass, relative molecular mass, and relative isotopic mass
- calculate relative atomic mass

Atomic number, mass number and isotopes

Atomic number (Z): The number of protons in the nucleus.

Mass number (A): The number of protons and neutrons in the nucleus.

Isotope: Atoms that have the same number of protons but different numbers of neutrons in their nucleus.

Atoms and sub-atomic particles

Atoms are made from sub-atomic or fundamental particles called **protons**, **neutrons**, and **electrons**. The masses and charges of these fundamental particles are very small so we look at them relative to the proton.

particle	relative mass	relative charge
proton	1	+1
neutron	1	0
electron	1/1836	-1

The mass of an electron is so small it is often considered to be negligible. Protons and neutrons are located in the nucleus of the atom while electrons orbit the nucleus.

Atomic number and mass number

Ensure that you can recall the definitions of atomic number and mass number.

- Atoms can be represented: ${}_Z^AX$
- Number of protons = atomic number (Z)
- Number of electrons = atomic number (Z) (ONLY for neutral atoms)
- Number of neutrons = mass number - atomic number ($A - Z$)

For ions (particles which have lost or gained electrons) the charge needs to be taken into account.

Beryllium atoms ${}_4^9\text{Be}$ protons = 4, electrons = 4,
neutrons = $9 - 4 = 5$

Fluoride ions ${}_9^{19}\text{F}^-$ protons = 9, electrons = $9 + 1 = 10$,
neutrons = $19 - 9 = 10$

Calcium ions ${}_{20}^{40}\text{Ca}^{2+}$ protons = 20, electrons = $20 - 2 = 18$,
neutrons = $40 - 20 = 20$

Isotopes

Make sure that you can remember the definition of an **isotope**.

- Isotopes contain differing numbers of neutrons but the same number of protons.
- As a result they are chemically identical.

There are two isotopes of chlorine

${}_{17}^{37}\text{Cl}$ protons = 17, electrons = 17, neutrons = 20

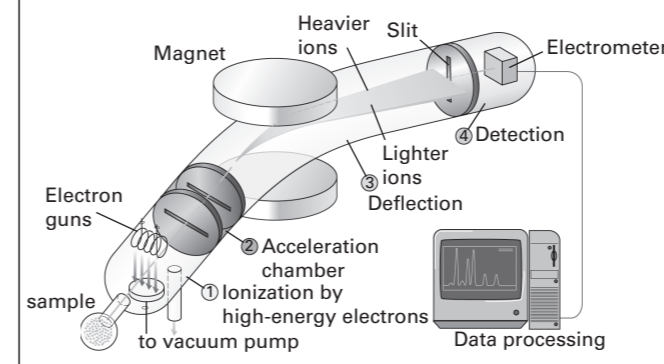
${}_{17}^{35}\text{Cl}$ protons = 17, electrons = 17, neutrons = 18

HSW: Early models of the atom

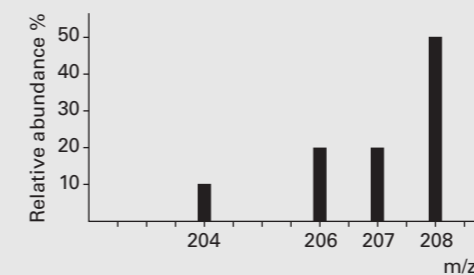
The model of the atom has been developed over many hundreds of years. Scientists are constantly working to improve this model.

Four elements exist 'Fire, Earth, Air, water' Aristotle 470-380 BCE	Discovered electrons. Proposed the plum pudding model of atoms. JJ Thomson 1600s	Linked atomic number to the number of protons in the nucleus. Moseley 1897
Leucippus and Democritus Early theory of the atom. All matter is made of atoms that are too small to see and cannot be cut up. 384-322 BCE	Dalton then Boyle Returned to and developed the original theory. Elements contain identical atoms. Atoms do not change in chemical reactions. 1911	Rutherford with Geiger and Marsden Proved that atoms had a nucleus containing protons. Electrons orbit the nucleus. 1913
		Chadwick Discovered neutrons. 1932

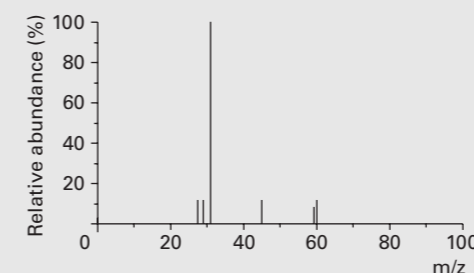
The mass spectrometer



The mass spectrum of lead



The mass spectrum of propanol



Definitions

Relative atomic mass

$$A_r = \frac{\text{mean mass of an atom of the element}}{\text{mass of one atom of } {}^{12}\text{C}} \times 12$$

Relative molecular mass

$$M_r = \frac{\text{mean mass of a molecule}}{\text{mass of one atom of } {}^{12}\text{C}} \times 12$$

Relative isotopic mass

$$= \frac{\text{mass of one atom of the isotope}}{\text{mass of one atom of } {}^{12}\text{C}} \times 12$$

Mass spectrometer

The mass spectrometer is a very sensitive machine used to analyse samples of elements in terms of the isotopes they contain and their relative amounts. The mass spectroscopy experiment is always carried out on gaseous samples under vacuum (so that no air is present). You must learn names and brief explanations for each step in the mass spectroscopy experiment.

- **Ionization** An electron gun is fired at the sample. This knocks off an outer shell electron forming a positive ion.
- **Acceleration** The positive ions are passed through an electric field (this also focuses the ions into a narrow beam).
- **Deflection** The fast moving positive ions are deflected by a strong magnetic field. Lighter ions are deflected more than heavier ions.
- **Detection** The positive ions are detected using an ion counter.

Relative atomic mass, A_r

The mass of all atoms is measured relative to the mass of a ${}^{12}\text{C}$ atom. Relative atomic mass can be calculated using the data from a mass spectrum. From the mass spectrum of lead opposite we obtain the following data:

m/z	204	206	207	208
relative abundance (%)	10	20	20	50

- m/z is the same as the mass of the ion if the charge is +1.
- relative abundance tells us the proportion of each isotope present in the sample.
- the A_r of lead can then be calculated as a weighted mean average.

$$A_r = \frac{(204 \times 10) + (206 \times 20) + (207 \times 20) + (208 \times 50)}{100} = 207$$

Determining relative molecular mass, M_r

Relative molecular mass is the mean mass of a molecule relative to the mass of a ${}^{12}\text{C}$ atom.

- If a molecule is placed in the mass spectrometer then the molecule will break up into smaller fragments or even its component elements.
- The complete molecule in the form of a molecular ion (the complete molecule minus an electron) will pass through the spectrometer.
- The peak for the molecular ion is the furthest peak to the right (i.e. the heaviest peak) on the mass spectrum. For the mass spectrum of propanol the peak at $m/z = 60$ is for the molecular ion.

Questions

- 1 Write down the numbers of protons, neutrons and electrons in the following:
 a ${}_{11}^{23}\text{Na}$ b ${}_{8}^{16}\text{O}^{2-}$ c ${}_{35}^{80}\text{Br}$ d ${}_{19}^{40}\text{K}^+$
- 2 Write out the steps in the mass spectroscopy experiment five times. Test yourself.
- 3 Use the spectra data to determine the relative atomic mass and identity of the atom.

m/z	20	21	22
relative abundance (%)	90.9	0.3	8.8