

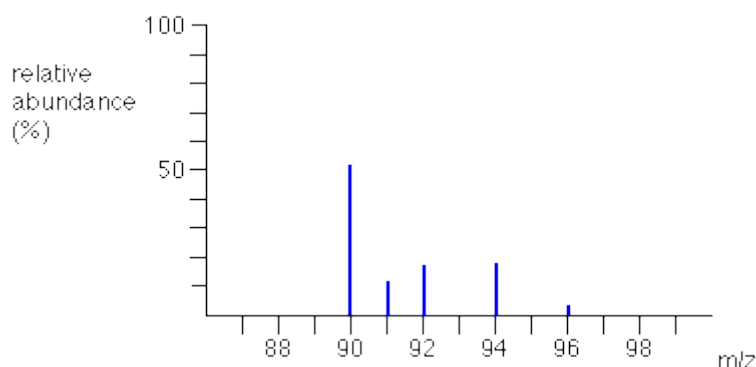
Topic 2a – Mass Spectrometry

Revision Notes

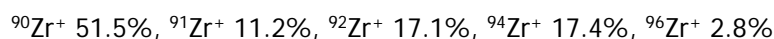
1) Mass Spectrometry

- The mass spectrum of an element gives the following information:
 - Number of peaks = number of isotopes
 - M/z of peak = mass number of isotope
 - Size of peak = relative abundance (i.e. percentage)

The mass spectrum for zirconium



- The 5 peaks in the mass spectrum shows that there are 5 isotopes of zirconium - with relative isotopic masses of 90, 91, 92, 94 and 96 on the ^{12}C scale.
- In this case, the five species detected (with their relative abundances) are:



a) **Operation**

- Four processes take place inside a mass spectrometer; ionisation, acceleration, deflection and detection
- The sample is vaporised and then ionised using high energy electrons from an electron gun. $\text{X}(\text{g}) + \text{e}^- \rightarrow \text{X}^+(\text{g}) + 2\text{e}^-$
- Ionisation is necessary to allow the remaining processes to take place. The energy of the electrons from the gun is controlled so that only one electron is knocked off each atom or molecule in the sample i.e. only $1+$ ions are formed
- The positive ions are accelerated by a negatively charged plates which also focus the ions into a beam
- The ions are deflected by a magnetic field. The amount of deflection depends on mass:charge ratio (m/z). As the ions have the same charge, deflection depends on mass with heavier ions deflected less and lighter ions deflected more. The strength of the magnetic field can be altered so that ions of different m/z are detected
- When an ion hits the detector a small current is produced which is recorded. The size of the current is proportional to relative abundance

b) Uses

- A mass spectrum can be used to calculate the relative atomic mass of an element (see below)
- Mass spectrometry can be used to identify elements from the mass numbers of the isotopes e.g. in space probes
- On another planet, such as Mars, the number of isotopes and their mass numbers will be the same as on Earth. However, the relative abundances may well be different so the relative atomic mass will be different as well.
- Mass spectrometry can also be used to determine the relative molecular mass of a covalent molecule (see Topic 16 – Analytical Techniques for more details)

2) Relative atomic mass

- Relative atomic mass is the weighted average mass of an atom of an element taking the mixture of isotopes into account. **However, learn the technical definition from definitions sheet**
- To calculate relative atomic mass, add together (mass number x abundance/total abundance) for each isotope
- Abundances can be given as percentages or may have to be worked out from the line heights on the spectrum

Example 1:

Calculate the relative atomic mass of Cl from the following information.

75% of Cl atoms have a mass number of 35

25% of Cl atoms have a mass number of 37

Total abundance = 100%

$$\begin{aligned}\text{Average mass of a Cl atom} &= (\text{mass no} \times \text{percent}/100) + (\text{mass no} \times \text{percent}/100) \\ &= (35 \times 75/100) + (37 \times 25/100) \\ &= 35.5\end{aligned}$$

Example 2:

Calculate the relative atomic mass of unknown metal Z from the following information.

M/z	Abundance
188	1.5
189	2.5
190	3.0
192	4.5

Total abundance = 11.5

$$\begin{aligned}\text{Average mass of a Z atom} &= (188 \times 1.5/11.5) + (189 \times 2.5/11.5) + \\ &\quad (190 \times 3.0/11.5) + (192 \times 4.5/11.5) \\ &= 24.52 + 41.09 + 49.57 + 75.13 \\ &= 190.3\end{aligned}$$

Example 3:

A mass spectrum of a sample of indium shows two peaks at $m/z = 113$ and $m/z = 115$. The relative atomic mass of indium is 114.5. Calculate the relative abundances of these two isotopes.

$$\begin{aligned} \text{Difference between mass numbers} &= 115 - 113 \\ &= 2 \end{aligned}$$

Relative atomic mass lies $1.5/2$ along this difference i.e. 75% of the way

Abundances are $m/z = 113$, 25%, $m/z = 115$, 75%

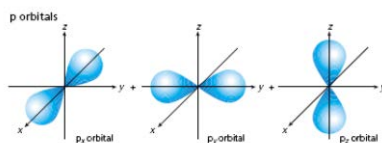
Topic 2b – Electronic Structure Revision Notes

1) Orbitals

- An orbital is the region in which an electron can be found
- Each orbital can hold up to two electrons of opposite spin
- Orbitals have different shapes called s, p, d, and f
- S orbitals are spherical in shape and come in sets of one



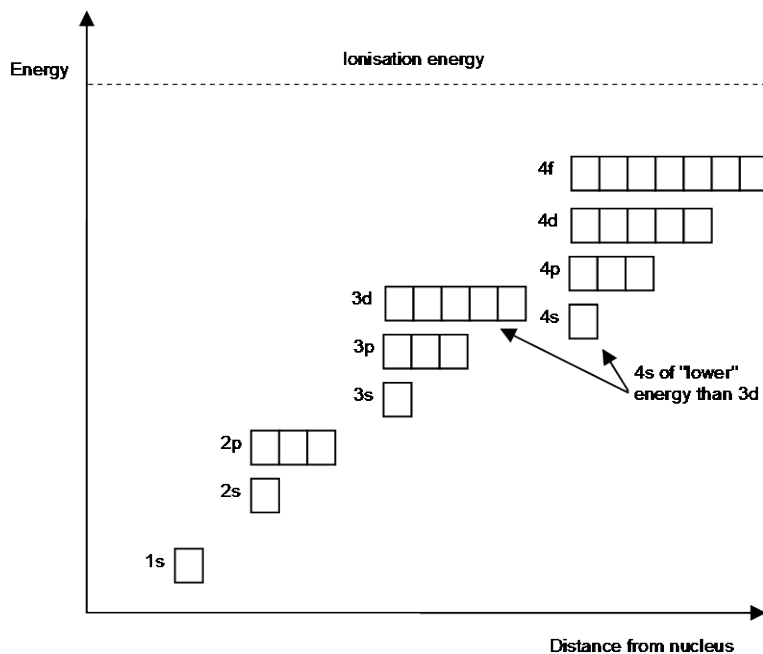
- P orbitals are hour-glass or egg-timer shaped and come in sets of three (which can hold up to 6 electrons)



- D orbitals come in sets of five and f orbitals come in sets of seven (which can hold up to 10 and 14 electrons, respectively)

2) Energy levels (or shells)

- The first energy level (or shell) only contains an s orbital, labelled 1s
- The second energy level contains an s orbital and three p orbitals, labelled 2s and 2p
- The third energy level contains an s orbital, three p orbitals and five d orbitals, labelled 3s, 3p and 3d
- The order in which the orbitals are filled is as follows: 1s 2s 2p 3s 3p 4s 3d 4p
- Note that the 4s fills before the 3d



Some examples of electronic structures are shown below.

Hydrogen	1 electron	$1s^1$	
Nitrogen	7 electrons	$1s^2 2s^2 2p^3$	
Sodium	11 electrons	$1s^2 2s^2 2p^6 3s^1$	
Sulphur	16 electrons	$1s^2 2s^2 2p^6 3s^2 3p^4$	
Calcium	20 electrons	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$	or [Ar] $4s^2$
Iron	26 electrons	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$	or [Ar] $4s^2 3d^6$

- There are 2 exceptions to the pattern: chromium and copper
- Cr is $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^5$ and Cu is $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^{10}$
- These electronic structures are more stable than the alternative structures that follow the pattern
- When transition metals, like iron and copper, form ions they lose their 4s electrons before their 3d electrons
- Fe^{2+} is $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6$ or $1s^2 2s^2 2p^6 3s^2 3p^6 4s^0 3d^6$
- There are various models to illustrate atomic structure. The model chosen depends on what we are trying to explain e.g. bonding can be explained by representing Na as 2.8.1 and Cl as 2.8.7 with both seeking to gain a full outer shell. Explaining why copper(II) sulphate is blue requires us to use the sub-shell model