# FACTFILE:
# GCE CHEMISTRY
## 1.2 ATOMIC STRUCTURE

Rewarding Learning

## Atomic Structure

### Learning Outcomes

Students should be able to:

**1.2.1** describe the properties of electrons, protons and neutrons in terms of their location in the atom and their relative masses and charges;

**1.2.2** explain the terms atomic number and mass number and use them to deduce the numbers of protons, neutrons and electrons in an atom or ion;

**1.2.3** define the terms relative atomic mass and relative isotopic mass in terms of the carbon-12 standard;

**1.2.4** define and demonstrate understanding of the term isotopes;

**1.2.5** define the terms relative molecular mass (for molecules) and relative formula mass (for ionic compounds) in terms of the carbon-12 standard and calculate their values from relative atomic masses;

**1.2.6** interpret mass spectra of elements by calculating relative atomic mass from isotopic abundances and vice versa;

**1.2.7** predict the mass spectra of diatomic elements, for example chlorine;

**1.2.8** deduce the electronic configuration of atoms and ions up to krypton in terms of shells and sub-shells using the building up principle (s, p and d notation and electrons in boxes notation);

**1.2.9** demonstrate understanding that an orbital is a region within an atom that can hold up to two electrons with opposite spins and describe the shape of s and p-orbitals;

**1.2.10** classify an element as belonging to the s, p, d or f block according to its position in the Periodic Table;

**1.2.11** define and write equations for the first and successive ionisation energies of an element in terms of one mole of gaseous atoms and ions;

**1.2.12** demonstrate understanding that successive ionisation energies can be used to predict the group of an element, and that graphs of successive ionisation energies against number of electrons removed, for an element, give evidence for the existence of shells;

**1.2.13** explain the trend in the first ionisation energies of atoms down Groups, and across Periods in terms of nuclear charge, distance of outermost electron from the nucleus, shielding and stability of filled and half-filled sub-shells;

**1.2.14** demonstrate understanding that graphs of first ionisation energies of elements up to krypton provide evidence for the existence of shells and sub-shells

## Atomic Structure

All atoms consist of a number of fundamental, sub-atomic particles. There are three, the electron, the proton and the neutron. Different atoms (and therefore elements) have different numbers of these three fundamental particles.

| Particle | Relative Charge | Relative Mass | Position in Atom |
|---|---|---|---|
| protons | +1 | 1 | Nucleus |
| neutrons | 0 | 1 | Nucleus |
| electrons | -1 | 1/1840 | Shells |

The atomic number and mass number give us important information about an atom and are particularly useful in distinguishing one isotope of an element from another.

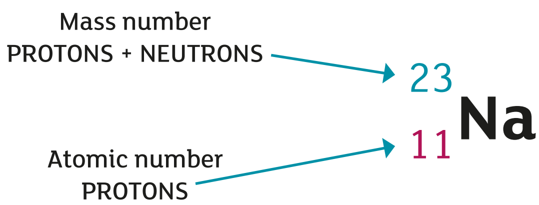
## Atomic number

**The atomic number is the number of protons (in the nucleus) of an atom.** For an atom (which is neutral), this number also corresponds to the number of electrons.

## Mass number

**The mass number is the total number of protons and neutrons (in the nucleus) of an atom.**

For example:




There are 11 protons, 11 electrons and 12 neutrons in a sodium atom.

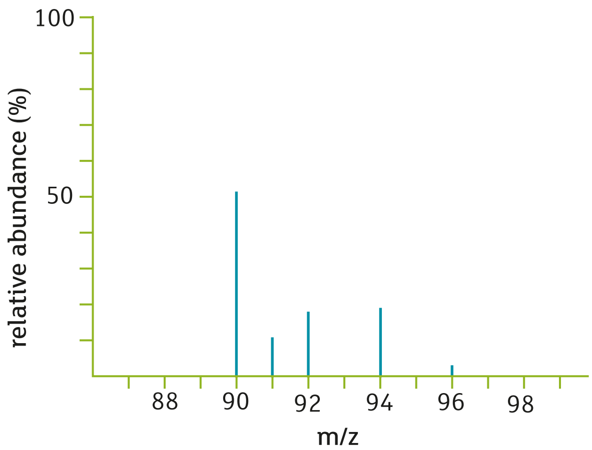
## Isotopes

**Isotopes are atoms which have the same atomic number but a different mass number (contain the same number of protons but a different number of neutrons).**

For example, $^{12}C$ contains 6 neutrons, whereas $^{13}C$ contains 7 neutrons. Both isotopes contain 6 protons and 6 electrons and have a different number of neutrons, and a different mass number.

A mass spectrometer, is used to obtain accurate atomic masses by measuring the masses and relative abundances of the isotopes of an atom. In a mass spectrometer, particles are turned into positive ions, accelerated and then deflected by an electromagnet. The resulting path of ions depends on their 'mass to charge' ratio (m/z). Whilst initially used to determine accurate relative atomic masses, mass spectrometry is now widely used to determine the relative formula masses of unknown compounds (e.g. in forensic science) in order to help identify them.

For example, consider the mass spectrum of zirconium.




The height of each peak is proportional to the amount of each isotope present (i.e. it's relative abundance). Most ions have a 1+ charge so that the m/z ratio is numerically equal to mass m of the ion. The five 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 C-12 scale. The relative sizes of the peaks gives you a direct measure of the relative abundances of the isotopes. In this case, the 5 isotopes (with their relative percentage abundances) are:

| | |
|---|---|
| zirconium-90 | 51.5 |
| zirconium-91 | 11.2 |
| zirconium-92 | 17.1 |
| zirconium-94 | 17.4 |
| zirconium-96 | 2.8 |

The relative atomic mass of zirconium is calculated by:

$$RAM = \frac{(90 \times 51.5)+(91 \times 11.2)+(92 \times 17.1)+(94 \times 17.4)+(96 \times 2.8)}{100}$$

$$= \frac{4635 + 1019.2 + 1573.2 + 1635.6 + 268.8}{100}$$

$$= \frac{9131.8}{100}$$

$$= 91.3$$

The relative atomic mass (RAM) is the average (weighted mean) mass of an atom of an element relative to one-twelfth of the mass of an atom of carbon-12.

The relative isotopic mass (RIM) is the mass of an atom of an isotope of an element relative to one-twelfth of the mass of an atom of carbon-12. RFM is for ionic compounds and for giant covalent compounds.

You should be able to predict the mass spectra of diatomic elements, for example chlorine. Chlorine has 5 peaks in the mass spectrum of $Cl_2$ one at 35, 37, 70, 72 and 74.

The relative formula mas (RFM) is the average (weighted mean) mass of a formula unit relative to one-twelfth of the mass of an atom of carbon-12.

The relative molecular mass (RMM) is the average (weighted mean) mass of a molecule relative to one-twelfth of the mass of an atom of carbon-12. RMM is used for molecular covalent substances.

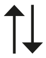
## Electronic configuration

Electrons are arranged in energy levels. The energy level n=1 is closet to the nucleus. Energy level are made of subshells which are made of orbitals.An orbital is a region within an atom that can hold up to two electrons with opposite spins. Examples include s orbitals which are spherical shaped and p orbitals which are dumbbell shaped:
An s subshell holds up to 2 electrons, a p up to 6 , a d up to 10 and an f up to 14.

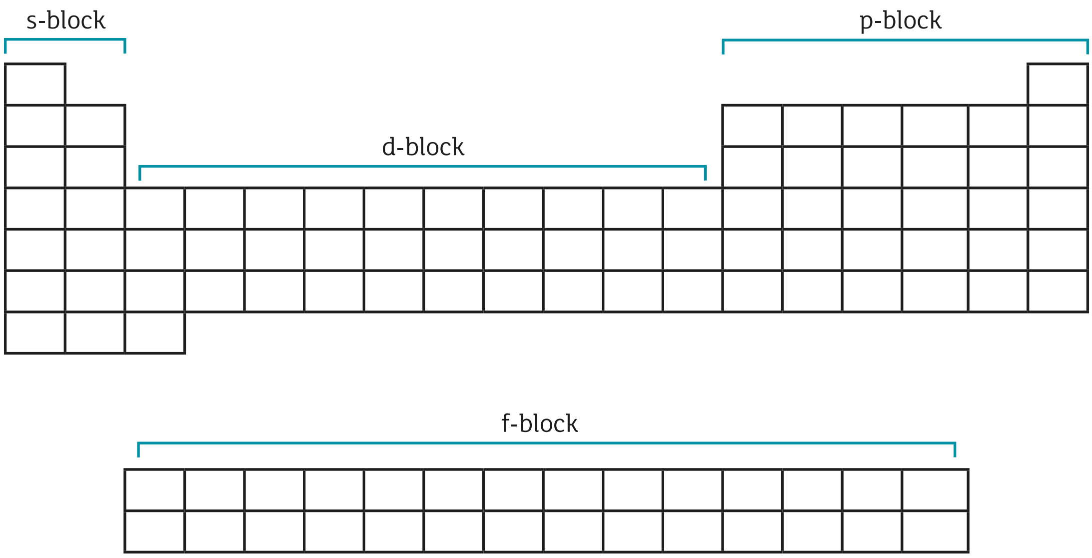
s orbital p orbital

| Quantum shell (Energy Level) | Sub-shells | Number of electrons | Number of orbitals |
|---|---|---|---|
| n = 1 | One sub-shell<br>1s | 2 | 1 |
| n = 2 | Two sub-shells<br>2s<br>2p | 2<br>6 } 8 | 1<br>3 |
| n =3 | Three sub-shells<br>3s<br>3p<br>3d | 2<br>6 } 18<br>10 | 1<br>3<br>5 |
| n=4 | Four sub-shells<br>4s<br>4p<br>4d<br>4f | 2<br>6 } 32<br>10<br>14 | 1<br>3<br>5<br>7 |

When writing electron configurations, electrons are placed in the first energy level (the energy level closest to the nucleus) and subsequent increasing energy levels. Electrons are not paired until a subshell is half filled. When two electrons are placed in the same orbital, they have opposite spin and are shown as vertical arrows in opposite directions.



| | | |
|---|---|---|
| Sodium (11 electrons) | Na | $1s^2\ 2s^2\ 2p^6\ 3s^1$ |
| Phosphorus (15 electrons) | P | $1s^2 2s^2 2p^6 3s^2 3p^3$ |




The Periodic Table of elements can be organised into different blocks based on the orbitals the outer electrons reside in:
**An s-block element is one which has an atom with highest energy/outer electron in an s-subshell (orbital).**

**A p-block element is one which has an atom with highest energy/outer electron in a p-subshell.**

When writing electronic configuration of *transition metal ions*, remember that the electrons are lost from the 4s subshell first. For example:

| | |
|---|---|
| Fe | $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^6\ 4s^2$ |
| Fe2+ | $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^6$ |

Copper and chromium have unusual electronic configuration:

Cr is not $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^4\ 4s^2$ but it is $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^5\ 4s^1$ due to the stability of half filled 3d.

Cu is not $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^9\ 4s^2$ but is $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^1$ due to the stability of the full 3d.

## Ionisation energy – the evidence for shells and sub-shells

Ionisation energy is a measure of the amount of energy needed to remove electrons from atoms. As electrons are negatively charged and protons in the nucleus are positively charged, there will be an attraction between them. The greater the pull of the nucleus, the harder it will be to pull an electron away from an atom.

**First ionisation energy is the energy required to convert one mole of gaseous atoms into gaseous ions with a single positive charge.** For example:

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

Note that state symbols should be given.

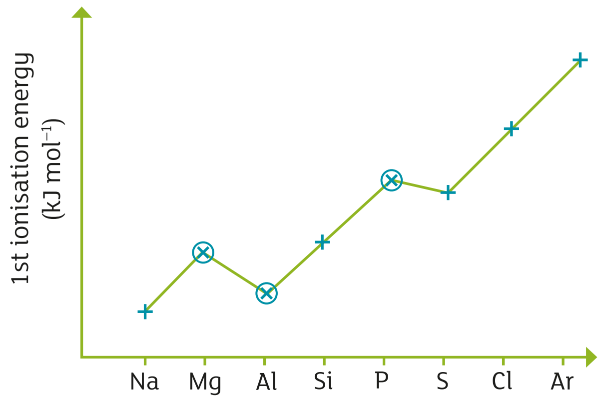
**Second ionisation energy is the energy required to convert one mole of gaseous ions with a single positive charge into gaseous ions with a double positive charge.**

$Na^{+}(g) \rightarrow Na^{2+}(g) + e^{-}$

**Third ionisation energy is the energy required to convert one mole of gaseous ions with a double positive charge into gaseous ions with a triple positive charge.**

$Na^{2+}(g) \rightarrow Na^{3+}(g) + e^{-}$

The trend in first ionisation energies across Periods of the Periodic Table provides evidence for shells and sub-shells, for example Period 3:




The dip at aluminium, for example, can be explained by considering its electronic configuration; aluminium's outer electron is in a 3p sub-shell which is further from the nucleus than the outer electron in magnesium which is in the 3s sub-shell. The dip at sulfur is explained by the outer electron configuration, $3p^4$, which compares with the outer configuration of $3p^3$ in phosphorus which is half filled and stable. The presence of one fully filled 3p orbital (compared to three half-filled 3p orbitals in phosphorus) increases repulsion between the paired electrons in the 3p orbital in sulfur which makes it easier for an electron to be removed.

Ionisation energy **increases across a period** due to
- Increasing nuclear charge
- Shielding is constant as the electron is being removed from the same shell

and so there is greater attraction between the nucleus and the outer electron.

Ionisation energy **decreases down a group** because
- Atomic radius increases
- Shielding increases due to increased number of shells

and so there is less attraction between the nucleus and the outer electron

Considering **successive ionisation energies** for individual elements allows an element's group to be identified. Consider the successive ionisation energies of aluminium, $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^1$:

The 1st ionisation energy is fairly low because the 3p electron is shielded from the nucleus by all the other electrons. The 2nd and 3rd ionisation energies are significantly higher than the 1st because the 3s electrons are being removed and are not as shielded as the 3p electron.

**1st: 578 kJ mol$^{-1}$, 2nd: 1817 kJ mol$^{-1}$, 3rd: 2745 kJ mol$^{-1}$**

There is a huge jump to the 4th ionisation energy, since a 2p electron is now being removed. The shielding has reduced as the 4th electron being removed is in a shell closer to the nucleus.

**4th: 11578 kJ mol$^{-1}$, 5th: 14831 kJ mol$^{-1}$, 6th: 18378 kJ mol$^{-1}$**

With three electrons being removed before a huge jump in the ionisation energy, this suggests the element is in Group III.

# Revision Questions

**1** Which one of the following represents the first five ionisation energies in kJ $mol^{-1}$ of an s-block element?

| | **1st** | **2nd** | **3rd** | **4th** | **5th** |
|---|---|---|---|---|---|
| **A** | 580 | 1800 | 2700 | 11600 | 14800 |
| **B** | 740 | 1500 | 7700 | 10500 | 13600 |
| **C** | 1000 | 2300 | 3400 | 4600 | 7000 |
| **D** | 14800 | 11600 | 2700 | 1800 | 580 |

**2** Neon has several isotopes.

a) Complete the table below.

| | **Number of protons** | **Number of electrons** | **Number of neutrons** |
|---|---|---|---|
| **Neon-20** | | | |
| **Neon-21** | | | |
| **Neon-22** | | | |

b) The table below gives the abundance of each isotope of neon.

Calculate the relative atomic mass of neon to two decimal places.

| **Isotope** | **% abundance** |
|---|---|
| Neon-20 | 90.92 |
| Neon-21 | 0.26 |
| Neon-22 | 8.82 |

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c) Name the isotope used as the standard to compare the relative atomic mass of atoms..

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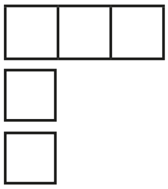
# ? Revision Questions

**2** d) Label the sub-shells below and draw the electronic sctucture of neon in the ground state.

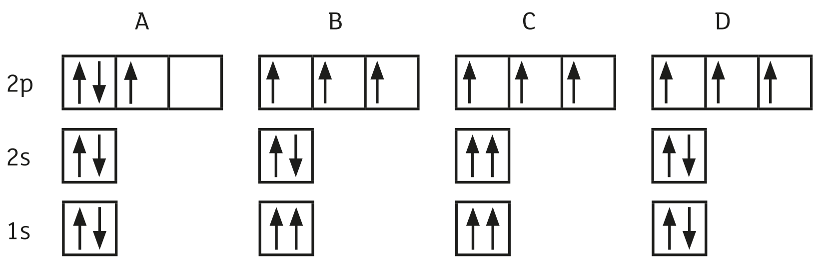


e) Draw the shape of an s and of a p orbital.

s orbital

p orbital

**3** Which one of the following represents the ground state electronic configuration of a nitrogen atom?



## Revision Questions

**4** Aluminium is the most abundant metal in the Earth's crust. It is used in electrical cables and is present in high strength alloys.

a) Atoms of aluminum have a mass number of 27.
How many neutrons are present in the nucleus of these atoms?

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b) (i) Write the equation, including state symbols, which represents the first ionisation energy of aluminium.

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(ii) Explain why the first ionisation energy of boron has a larger value than the first ionisation energy of aluminium.

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(iii) Explain why the first ionisation energy of magnesium has a larger value than the first ionisation energy of aluminium.

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(iv) Give the ground state electronic configuration of the $Al^{4+}$ ion.

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(v) Sketch a graph to show the successive ionisation energies of aluminium.