1.1 Atomic structure

History of the atom

- The model of the atom has changed as our observations of its behavior and properties have increased.
- A model is used to explain observations. The model changes to explain any new observations.
- A map gives you an overview of a town/city. As technology has improved our maps have become more accurate and detailed. This is the same for scientific models.

Democritus (5th century) The Greek 'atom' - indivisible

John Dalton (1800’s) Atoms of the same element are the same

George Johnstone Stoney (1891) Electrolysis. The charge of an electron.

Joseph J Thompson (1897) The cathode ray tube and e/m deflection. The mass / charge of an electron.


Robert Milikan (1909) Oil drop experiment. The mass / charge of an electron.

Rutherford (and Marsden) (1909) Alpha particle deflection. The nuclear model.

Henry Moseley (1913) Atomic number

Neils Bohr (1913) Planetary model of the atom

Louis De Broglie (1923) Wave particle duality

Erwin Shrodinger (1926) Atomic orbitals

James Chadwick (1932) Discovery of the neutron
Atomic structure

Protons, electrons and neutrons

<table>
<thead>
<tr>
<th>Particle</th>
<th>Mass</th>
<th>Charge</th>
<th>Working out</th>
</tr>
</thead>
<tbody>
<tr>
<td>Proton</td>
<td>1</td>
<td>+1</td>
<td>bottom</td>
</tr>
<tr>
<td>Electron</td>
<td>1/1890</td>
<td>-1</td>
<td>bottom</td>
</tr>
<tr>
<td>Neutron</td>
<td>1</td>
<td>0</td>
<td>top - bottom</td>
</tr>
</tbody>
</table>

- Since different elements are made from different atoms.
- These atoms have different numbers of protons and neutrons (and electrons).
- This means that different elements atoms **must** have different masses.
- So an atom of one element **must** have a different mass from another element, we call this the **Mass Number**, $A$.
- The number of protons determines which element an atom is and the bottom number tell us this, we call this the **Atomic number**, $Z$.

**Examples:**

- The top number is the **Mass number**. This means that the total number of **protons and neutrons are 7**.
- The bottom number is the **Atomic number**. This is the **number of protons**.
- Because an **atom is neutral**, this means that this is also the number of electrons. This atom has 3 **protons and 3 electrons**.
- If we take the **Atomic number ($Z$) from the Mass number ($A$)** we get the number of neutrons. $7 - 3 = 4$ **neutrons**.

**Atomic number:** The number of protons in the nucleus of an atom

**Mass Number:** The number of protons and neutrons in the nucleus of an atom

A quick method is:

- **Protons**
- **Electron**
- **Neutrons**

<table>
<thead>
<tr>
<th>Particle</th>
<th>bottom number</th>
<th>Working out</th>
</tr>
</thead>
<tbody>
<tr>
<td>Protons</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>Electron</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>Neutrons</td>
<td>top – bottom number</td>
<td>7 - 3 = 4</td>
</tr>
</tbody>
</table>
Isotopes

An atom of the same element that has the same number of protons and electrons but a different number of neutrons.

- As the atom has the same number of protons and electrons it will have the same chemical properties.
- They are all hydrogen atoms because they all have the same number of protons.
- Hydrogen can be used as an example:

\[
\begin{align*}
\text{Hydrogen – 0 Neutrons} & \quad \text{H} \\
\text{Hydrogen – 1 Neutron (deuterium)} & \quad \text{D} \\
\text{Hydrogen – 2 Neutrons (tritium)} & \quad \text{T}
\end{align*}
\]

Example:

\[
\begin{align*}
^{23}_{11}\text{Na}: & \quad P = 11 \quad e = 11 \quad N = (23 - 11) = 12 \\
^{23}_{11}\text{Na}^+: & \quad P = 11 \quad e = (11 - 1) = 10 \quad N = (23 - 11) = 12 \\
^{16}_{8}\text{O}^2-: & \quad P = 8 \quad e = (8 - 2) = 6 \quad N = (16 - 8) = 8
\end{align*}
\]

\[
\begin{align*}
^{37}_{17}\text{Cl}: & \quad P = 17 \quad e = 17 \quad N = (37 - 17) = 20 \\
^{35}_{17}\text{Cl}: & \quad P = 17 \quad e = 17 \quad N = (35 - 17) = 18
\end{align*}
\]

Questions:

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Atomic number</th>
<th>Mass number</th>
<th>Number of protons</th>
<th>Number of electrons</th>
<th>Number of neutrons</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mg atom</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>F atom</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ca(^{2+}) ion</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>S(^{2-}) ion</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Al(^{3+}) ion</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(^{54}\text{Fe})</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(^{56}\text{Fe})</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
The mass spectrometer:

1) **Ionisation**
- Carried out in a vacuum to avoid collisions with air.
- Ions are made in one of 2 ways

    a. **Electron impact:**

    - Sample is vaporised and bombarded with electrons from an *electron gun*.
    - This knocks an additional electron off the sample:

        \[
        \text{M}^{(g)} + e^- \rightarrow \text{M}^+(g) + 2e^-
        \]

    Or simplified:

        \[
        \text{M}^{(g)} \rightarrow \text{M}^+(g) + e^-
        \]

        \[
        \text{Na}^{(g)} \rightarrow \text{Na}^+(g) + e^-
        \]

        \[
        \text{CH}_4^{(g)} \rightarrow \text{CH}_4^+(g) + e^-
        \]

    - Used for elements and low Mr molecules.
    - Mr / Ar = M* Often referred to as m/z (mass / charge)
    - Produces fragments - later
b. Electrospray ionisation:

- The sample is vaporised by dissolving in a volatile solvent.
- Volatile solvent is used to ensure it evaporates leaving a positive ion
- Fed through a fine needle attached to a high voltage.
- This produces droplets that gain a proton, \( H^+ \)
- As the solvent evaporates, the sample has gained a proton, \( H^+ \)

\[
M_{(g)} + H^+ \rightarrow MH^+_{(g)}
\]

\[
C_6H_{14}O_{(g)} + H^+ \rightarrow C_6H_{15}O^+_{(g)}
\]

- Used for high Mr molecules.
- \( Mr + 1 = MH^+ \) Often referred to as m/z + 1 (mass / charge)
- Soft ionisation therefore no fragments.

Note:
Mr of the ion depends upon the type of ionisation:
- Electron impact: Mass of ion = mass of element or compound
- Electrospray ionisation: Mass of ion = mass of element or compound + 1

2) Acceleration
- The ions are accelerated towards a highly negatively charged plate with a hole in.
- They are all given the same kinetic energy, \( KE = \frac{1}{2}mv^2 \)
- The velocity at which the ion will travel will depend upon the mass of the ion.

\[
KE = \frac{1}{2}mv^2
\]

(students would be given this equation if expected to use it in an exam)

\[
KE = \text{kinetic energy of particle (J)}
\]

\[
m = \text{mass of the particle (kg)}
\]

\[
v = \text{velocity of the particle (m s}^{-1})
\]

Therefore, the velocity of each particle is given by: 

\[
v = \sqrt{\frac{2KE}{m}}
\]
3) Separation: Time of flight, TOF - ion drift down the flight tube

- Ions with a small mass travel faster → have a shorter TOF
- Ions with a large mass travel slower → have a longer TOF

The time of flight along the flight tube is given by the following expression:

\[
t = \frac{d}{v}
\]

\[
t = \frac{d \sqrt{\frac{m}{2KE}}}{v}
\]

(students would be given this equation if expected to use it in an exam)

\( t = \text{time of flight (s)} \)
\( d = \text{length of flight tube (m)} \)
\( v = \text{velocity of the particle (m s}^{-1}) \)
\( m = \text{mass of the particle (kg)} \)
\( KE = \text{kinetic energy of particle (J)} \)

4) Detection

- The ion picks up an electron from the detector to complete the circuit.
- The bigger the current → Greater the abundance

\[
\text{M}^+_{(g)} + e^- \rightarrow \text{M}_{(g)}
\]
\[
^{16}\text{O}^+_{(g)} + e^- \rightarrow ^{16}\text{O}_{(g)}
\]

- The most abundant element will generate the largest current at the detector

Summary

A short time of flight = small mass / charge \( m/z \)

A long time of flight = large mass / charge \( m/z \)

- Whole process is carried out in a **vacuum** to avoid collisions with molecules in air
Questions:

<table>
<thead>
<tr>
<th>Formula</th>
<th>KE = ( \frac{1}{2}mv^2 )</th>
<th>( v = \frac{d}{t} )</th>
<th>( N_A = 6.022 \times 10^{23} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>KE:</td>
<td>J</td>
<td>d: m</td>
<td></td>
</tr>
<tr>
<td>m:</td>
<td>Kg</td>
<td>t: s</td>
<td></td>
</tr>
<tr>
<td>v:</td>
<td>ms(^{-1})</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

1) A sample of Nitrogen atoms were placed through a mass spectrometer. Only one peak was observed in its mass spectrum.
   a. Calculate the mass of one atom of nitrogen

   b. Calculate the velocity of its 1+ ion traveling down a 5m flight tube in \( 1.6 \times 10^{-6}s \)

   c. Calculate its kinetic energy. Give your answer to 3 significant figures

\( (1.135 \times 10^{-13} \text{ J}) \)

2) A sample of Beryllium atoms were placed through a mass spectrometer. Only one peak was observed in its mass spectrum. The 1+ ion travelled down a 3m flight tube in \( 2.0 \times 10^{-8} \text{s} \). Calculate its kinetic energy.

\( (1.68 \times 10^{-14} \text{ J}) \)
3) A sample of Aluminium atoms were placed through a mass spectrometer. The $^{27}\text{Al}^+$ travelled down a 5m flight tube. Its Kinetic energy is $1.45 \times 10^{-13}$ J.

a) Calculate the mass of one ion of Aluminium:

b) Calculate the velocity of its 1+ ion travelling down the flight tube

c) Calculate its time of flight. Give your answer to 3 significant figures

(1.965995 x 10^{-6} J)

4) A sample of Sodium atoms were placed through a mass spectrometer. The $^{23}\text{Na}^+$ travelled down a 3m flight tube. Its Kinetic energy is $1.63 \times 10^{-14}$ J.

Calculate its time of flight. Give your answer to 3 significant figures

(3.247 x 10^{-6} J)
Comparing 2 or more isotopes during Mass Spectroscopy:

- Remember, when the 1+ isotopes are accelerated, all isotopes are given the **same kinetic energy**.
- This allows us to simplify the formula during calculations, we’ll call one of the isotopes **a** and the other **b**:

\[
KE_a = KE_b \\
\frac{m_a \times V_a^2}{2} = \frac{m_b \times V_b^2}{2} \quad \text{Cancel the 2's} \\
\frac{m_a \times V_a^2}{2} = m_b \times V_b^2
\]

For Velocity calculation:

\[
V_a = \sqrt{\frac{m_b \times V_b^2}{m_a}}
\]

For Time of flight calculation:

\[
\frac{m_a \times V_a^2}{t_a^2} = \frac{m_b \times V_b^2}{t_b^2} \quad \text{d's are the same so cancel the d's} \\
\frac{m_a}{t_a^2} = \frac{m_b}{t_b^2} \\
\frac{m_a}{t_a^2} = \frac{m_b}{t_b^2} \\
\frac{m_a}{t_a^2} = \frac{m_b}{t_b^2} \\
t_a = \sqrt{\frac{t_b^2 \times m_a}{m_b}}
\]

Mass calculations:

- You would not need to convert the masses into Kg by dividing by 1000
- You would not need to divide by \(N_A\) either. (you’ll understand this later)
- This would be done to both masses and therefore cancel out:

**Summary:**

\[
m_a V_a^2 = m_b V_b^2 \quad \frac{m_a}{t_a^2} = \frac{m_b}{t_b^2}
\]
Questions:

1) A sample of chlorine atoms were placed through a mass spectrometer. Two peaks were observed in its mass spectrum at m/z = 35 and m/z = 37. The velocity of $^{35}\text{Cl}^+$ ion traveling down the flight tube is $1.19 \times 10^6$ ms$^{-1}$. Assuming all Cl$^+$ ions are given the same kinetic energy, calculate the velocity of the $^{37}\text{Cl}^+$ ion.

$\text{Velocity} = (1.16 \times 10^6 \text{ ms}^{-1})$

2) A sample of Boron atoms were placed through a mass spectrometer. Two peaks were observed in its mass spectrum: m/z = 10 and m/z = 11. The $^{10}\text{B}^+$ travelled down a flight tube in $1.20 \times 10^{-6}$ s. Calculate the time of flight of the other isotopic ion.

$\text{Time} = (1.26 \times 10^{-6} \text{ s})$
3) A sample of copper atoms were placed through a mass spectrometer. Copper atoms contain 2 isotopes: $^{63}\text{Cu}$ and one other.
   a. Calculate the velocity of the $^{63}\text{Cu}$ if it travels down a 5m flight tube in $4.200 \times 10^{-6}$ s
   
   b. The other isotope takes $4.266 \times 10^{-6}$ s to travel down the flight tube. Calculate the atomic mass of the other isotope. Give your answer to the nearest whole number and identify the other isotope:

   c. Use the Periodic table to calculate the relative abundances of these 2 isotopes
Relative masses:

**RAM, Relative Atomic Mass:** the weighted mean mass of an atom compared with 1/12th of the mass of carbon -12

**Relative isotopic mass:** the mass of an isotope compared with 1/12th of the mass of carbon -12

- Where 1/12th of Carbon 12 is essentially the mass of a proton / neutron

**Mass Spectrometer of elements:**

**Calculating Relative Atomic Mass (RAM) from abundance**

Use the formula:

\[
\text{RAM} = \sum \left( \frac{\text{Abundance} \times \text{m/z}}{\text{Total Abundance}} \right)
\]

**Worked example:**

<table>
<thead>
<tr>
<th>RAM of Neon isotopes</th>
<th>Abundance %</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>90.9</td>
</tr>
<tr>
<td>21</td>
<td>0.2</td>
</tr>
<tr>
<td>22</td>
<td>8.9</td>
</tr>
</tbody>
</table>

**Calculation**

\[
\text{RAM} = \frac{(90.9 \times 20) + (0.2 \times 21) + (8.9 \times 22)}{(90.9 + 0.2 + 8.9)}
\]

\[
\text{RAM} = 20.18
\]
Practise Questions:

1) Calculate the RAM from the information given in the table below:

<table>
<thead>
<tr>
<th>RAM of silicon isotopes</th>
<th>% Abundance</th>
</tr>
</thead>
<tbody>
<tr>
<td>28</td>
<td>92.2</td>
</tr>
<tr>
<td>29</td>
<td>4.7</td>
</tr>
<tr>
<td>30</td>
<td>3.1</td>
</tr>
</tbody>
</table>

2) Calculate the RAM from the spectra given below:

![Relative abundance graph](image)

3) A sample of rubidium contains the isotopes $^{85}\text{Rb}$ and $^{87}\text{Rb}$ only. The isotope $^{85}\text{Rb}$ has an abundance 2.5 times greater than that of $^{87}\text{Rb}$. Calculate the relative atomic mass of rubidium in this sample. Give your answer to one decimal place.

*Tip: it doesn’t matter how the abundances are given: They could be %, g, relative abundance or number of atoms*
4) Chlorine exists as 2 naturally occurring isotopes $^{37}\text{Cl}$ and $^{35}\text{Cl}$. Calculate the % abundance of each isotope given the Ar of chlorine is 35.5

5) A sample of xenon has $A_r = 131.31$. The sample consists of four isotopes. The abundances of three of the isotopes are shown in the table below. The data for one of the isotopes, $^m\text{Xe}$, is missing.

<table>
<thead>
<tr>
<th>Isotope</th>
<th>$^{129}\text{Xe}$</th>
<th>$^{131}\text{Xe}$</th>
<th>$^{132}\text{Xe}$</th>
<th>$^m\text{Xe}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>% abundance</td>
<td>28.0</td>
<td>25.0</td>
<td>27.0</td>
<td>To be calculated</td>
</tr>
</tbody>
</table>

Use the data to calculate the abundance of isotope $^m\text{Xe}$ and calculate $m$, the mass number of $^m\text{Xe}$. Show your working.
Mass spectrometry and molecular elements

- Bromine has two isotopes, $^{79}\text{Br}$ and $^{81}\text{Br}$, in the ratio 1:1.
- In a mass spectrometer bromine forms ions with formula $[\text{Br}_2]^+$ but also $\text{Br}^+$ ions
- This will give multiple peaks in the mass spectrum

There are 5 possibilities that exist:

**Ions of atoms:**

<table>
<thead>
<tr>
<th>Ion:</th>
<th>$^{79}\text{B}^+$</th>
<th>$^{81}\text{Br}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>m/z =</td>
<td>79</td>
<td>81</td>
</tr>
<tr>
<td>Ratio</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

These will give peaks at m/z = 79 and 81 in a 1:1 ratio

**Ions of molecules:**

<table>
<thead>
<tr>
<th>Ion:</th>
<th>$[^{79}\text{Br} - ^{79}\text{Br}]^+$</th>
<th>$[^{79}\text{Br} - ^{81}\text{Br}]^+$</th>
<th>$[^{81}\text{Br} - ^{79}\text{Br}]^+$</th>
<th>$[^{81}\text{Br} - ^{81}\text{Br}]^+$</th>
</tr>
</thead>
<tbody>
<tr>
<td>m/z =</td>
<td>158</td>
<td>160</td>
<td>160</td>
<td>162</td>
</tr>
<tr>
<td>Calc:</td>
<td>(1 x 1)</td>
<td>(1 x 1)</td>
<td>(1 x 1)</td>
<td>(1 x 1)</td>
</tr>
<tr>
<td>Ratio:</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Ratio:</td>
<td>1</td>
<td>2</td>
<td>:</td>
<td>1</td>
</tr>
</tbody>
</table>

These will give additional peaks at m/z = 158, 160 and 162 in a 1:2:1 ratio

*Transfer the information to the blank spectra below:*
Question

- Chlorine has two isotopes, $^{35}\text{Cl}$ and $^{37}\text{Cl}$, in a 3:1 ratio.
- In a mass spectrometer chlorine forms ions with formula $[\text{Cl}_2]^+$

Sketch the pattern of peaks you would expect to see in the mass spectrum of a sample of chlorine.
Mass Spectrometry of compounds:

a) Using electron impact:

- Works in exactly the same way but you also get fragments of that molecule / compound:

\[
\begin{align*}
\text{Mr of } C_2H_5OH &= 46 \\
\text{Highest } m/z &= \text{Mr of the molecule. This is called the molecular ion peak, } M^+ \\
C_2H_5OH &\rightarrow C_2H_5OH^+ + e^-
\end{align*}
\]

- The fragments are caused by the molecule breaking apart under the conditions in the ionisation chamber in the spectrometer.
b) Using electrospray ionisation:

- Often referred to as soft ionisation
- Remember, the sample gains a proton during this process:

\[
\begin{align*}
M & \quad + \quad H^+ & \rightarrow & \quad MH^+ \\
C_2H_5OH & \quad + \quad H^+ & \rightarrow & \quad C_2H_5OH^+ \\
\end{align*}
\]

- No fragments are made during this process
- Highest \( m/z = Mr + 1 \) of the molecule. This is called the \( MH^+ \) peak.
- To get the Mr, you need to take 1 away from the \( MH^+ \) peak.

<table>
<thead>
<tr>
<th></th>
<th>Electron impact</th>
<th>Electrospray ionisation</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Ion</strong></td>
<td>( M^+ = Mr )</td>
<td>( MH^+ )</td>
</tr>
<tr>
<td><strong>Used for</strong></td>
<td>Atoms / small molecules</td>
<td>Large molecules</td>
</tr>
<tr>
<td><strong>Fragmentation</strong></td>
<td>Yes</td>
<td>No</td>
</tr>
</tbody>
</table>
Electron Configuration

Ionisation energies:

- To form positive ions, electrons must be completely removed i.e. ionisation.
- To do this the electron must completely escape the attraction of the atom. i.e. reach \( n = \infty \).
- At \( n = \infty \) the electron has sufficient energy to escape the attraction from the nucleus.

\[ \text{1st ionisation energy of an element: The energy required to remove 1 mole of electrons from 1 mole of gaseous atoms to form 1 mole of gaseous 1+ ions} \]

1\textsuperscript{st} ionisation energy:

\[ \text{Ca}(g) \rightarrow \text{Ca}^+(g) + e^- \quad \text{1st IE} = +590 \text{ KJmol}^{-1} \]

2\textsuperscript{nd} ionisation energy:

\[ \text{Ca}^+(g) \rightarrow \text{Ca}^{2+}(g) + e^- \quad \text{2nd IE} = +1150 \text{ KJmol}^{-1} \]

Factors affecting ionisation energy

1) Number of electron shells: The distance of the electron from the nucleus
   - The further an electron is from the nucleus, the lower the force of attraction:
   - This means that the electron will be easier to remove which means the ionisation energy will be lower.

2) Shielding: effect by full inner shells
   - A full inner shell of electrons will repel electrons in outer shells.
   - These ‘shields’ effect of the attraction from the nucleus on outer electrons.
   - The more inner shells the greater the shielding.

3) Size of the positive nuclear charge
   - The more protons in the nucleus, the higher the nuclear charge, the harder it is to remove an electron, the higher the ionisation energy.
Evidence for a change in atomic structure:

1) Flame colours and emission spectra: Energy levels or shells
   - We have already seen what happens when an electron is removed from an atom - the atom becomes a ion.
   - We can promote electrons from a lower electron shell to a higher electron shell by providing heat energy.
   - When the electrons fall back to the lower shell a specific frequency of light is observed.

   ![Diagram of electron promotion and energy levels](image)

   - This gives us the series of lines as electrons move from higher to lower electron shells.
   - A spectroscope shows us the specific energies characteristic to that element.

Looking at the line emission spectra 2 thing become apparent:

1) That the lines are specific colours representing specific energies / electron shells.

2) That as the move up in energy (towards the violet end) they get closer together (converge)

   - This tells us that the electron shells are not nicely spread out but get closer together as they get further away from the nucleus:

   ![Diagram of electron shells converging](image)
• That the electron shells can be converted into an energy level diagram showing the Principle Quantum Number, n

<table>
<thead>
<tr>
<th>Energy</th>
<th>1st electron shell</th>
<th>n=1</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>2nd electron shell</td>
<td>n=2</td>
</tr>
<tr>
<td></td>
<td>3rd electron shell</td>
<td>n=3</td>
</tr>
<tr>
<td></td>
<td>4th electron shell</td>
<td>n=4</td>
</tr>
<tr>
<td></td>
<td>5th electron shell</td>
<td>etc</td>
</tr>
</tbody>
</table>

We call these diagrams energy level diagrams and each electron shell is now called ‘The Principle Quantum Number, n’

• The number of electrons in each Principle Quantum Number, n can be calculated:
• To calculate the number of electrons in each shell: No e’s = 2n^2

<table>
<thead>
<tr>
<th>Principle quantum number</th>
<th>Number of electrons</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>8</td>
</tr>
<tr>
<td>3</td>
<td>18</td>
</tr>
<tr>
<td>4</td>
<td>32</td>
</tr>
</tbody>
</table>
2) Successive ionisation energies – removed from the same atom

- Large jumps indicate movement to another electron shell closer to the nucleus
- Ionisation energies are greater the closer to the nucleus
- The 8 electrons in the 2\textsuperscript{nd} shell still show a small increase due to fewer electron being attracted by the same number of protons

3) Ionisation energies down a Group – Group 2

As you go down a group:
- More Shells
- More shielding
- Increase in nuclear charge (outweighed by above)
- Less attraction = less energy required to remove electron
4) Ionisation energies across a period

Generally:
There is an increase in ionisation energies across a period.

As you go across a period:
- Same Shells
- Similar shielding
- Increase in nuclear charge
- Greater attraction = more energy required to remove electron

However it is not a straight / linear line. There are small peaks / troughs showing the model must be more complex:

a) 3rd electron easier to remove than 2nd
- The 1st 8 electrons are actually in 2 called subshells called s and p which are not at the same energy level. They have slightly different energy levels.

- The s subshell contains 2 electrons (Na and Mg, Group 1 & 2)
- The p subshell contains 6 electrons (Al – Ar, Groups 3-0)
- As the p subshell is higher in energy it is easier to remove the 1st electron from the p subshell (which is the 3rd electron).
b) 6th electron easier to remove that the 5th
- This tells us how the electrons fill in the shells and subshells.
- Within electron shells / sub shells there are *orbitals* (represented by a box)
- An orbital can hold 2 electrons.

- If electrons are negative and repel each other how can they occupy the same orbital?
- Electrons spin on their axis. When anything with a charge spins a magnetic field is produced.
- One of the electrons in an orbital will spin one way and the other spins in the opposite direction.
- This gives opposing magnetic fields which we represent with an arrow.
- This is the only way electrons can share an orbital as there is now some attraction between them.
- The 6th electron therefore is easier to remove as there is still repulsion between two negatively charged particles
A new model

- Each electron shell is made up of sub shells, s, p, d, f.
- We’ve already seen that **Group 1 & 2 are the s subshell** electrons and **Group 3-0 are the p subshell** electrons.
- **d sub shell are the elements between Group 2 and 3**
- **f sub shell are the elements in the lanthanides and actinides**
- Each sub shell contains orbitals.
- Each orbital can hold a maximum of 2 electrons with opposite spin.

<table>
<thead>
<tr>
<th>Subshell</th>
<th>Electrons</th>
<th>Arrangement</th>
</tr>
</thead>
<tbody>
<tr>
<td>f</td>
<td>14</td>
<td>7 orbitals</td>
</tr>
<tr>
<td>d</td>
<td>10</td>
<td>5 orbitals</td>
</tr>
<tr>
<td>p</td>
<td>6</td>
<td>3 orbitals</td>
</tr>
<tr>
<td>s</td>
<td>2</td>
<td>1 orbital</td>
</tr>
</tbody>
</table>
A summary of sub shells and orbitals:

### n = 3 shell: maximum 18 electrons

<table>
<thead>
<tr>
<th>Sub-shell</th>
<th>3s</th>
<th>3p</th>
<th>3d</th>
</tr>
</thead>
<tbody>
<tr>
<td>Orbital</td>
<td><img src="image" alt="3s orbital" /></td>
<td><img src="image" alt="3p orbitals" /></td>
<td><img src="image" alt="3d orbitals" /></td>
</tr>
<tr>
<td>Electrons</td>
<td>2e</td>
<td>2e</td>
<td>2e</td>
</tr>
</tbody>
</table>

### n = 2 shell: maximum 8 electrons

<table>
<thead>
<tr>
<th>Sub-shell</th>
<th>2s</th>
<th>2p</th>
</tr>
</thead>
<tbody>
<tr>
<td>Orbital</td>
<td><img src="image" alt="2s orbital" /></td>
<td><img src="image" alt="2p orbitals" /></td>
</tr>
<tr>
<td>Electrons</td>
<td>2e</td>
<td>2e</td>
</tr>
</tbody>
</table>

### n = 1 shell: maximum 2 electrons

<table>
<thead>
<tr>
<th>Sub-shell</th>
<th>1s</th>
</tr>
</thead>
<tbody>
<tr>
<td>Orbital</td>
<td><img src="image" alt="1s orbital" /></td>
</tr>
<tr>
<td>Electrons</td>
<td>2e</td>
</tr>
</tbody>
</table>
The Aufbau Principle - Filling shells and sub – shells

1. Electrons are added one at a time to 'build up' the atom.  
2. The lowest available energy level fills first.  
3. Each energy level must be full before the next, higher energy level can be filled.  
4. Each orbital in a sub-shell is filled by single electrons before pairing up.  
5. Each orbital can hold 2e of opposite spin.

- After 3p it gets a bit complicated
- The 4s energy level is below the 3d energy level.
- This means that the 4s orbital fills before the 3d orbitals. (according to the Aufbau Principle)

Electron configuration
- We use a shorthand to show how the electrons are arranged in an atom.
- Hydrogen is the simplest atom so we will use this to look at the shorthand:

No of electrons

1s 1

Principle quantum number

Orbital
Electron configuration from the Periodic Table

- The electron configuration can be worked out from the Periodic Table, filling from left to right then top to bottom

Fill in the following table:

<table>
<thead>
<tr>
<th>Element</th>
<th>No electrons</th>
<th>Electron configuration</th>
<th>What Period is this element in?</th>
<th>What is its highest Principle Quantum Number</th>
<th>What is the highest sub-shell</th>
<th>What Groups is the element in</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
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<tr>
<td>Al</td>
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</tbody>
</table>

Other examples:

1) Na $1s^22s^22p^63s^1$

2) Sc $1s^22s^22p^63s^23p^63d^14s^2$ (remember 4s fills before 3d)
Shortening an electron configuration

- For atoms with many electrons, the electron configuration can be long:

\[ \text{Sc } 1s^2 \, 2s^2 \, 2p^6 \, 3s^2 \, 3p^6 \, 3d^1 \, 4s^2 \]

- We can write a shorthand version by using the closest noble gas configuration for the inner shells:

\[ \text{Sc } [1s^2 \, 2s^2 \, 2p^6 \, 3s^2 \, 3p^6]3d^1 \, 4s^2 \]

Inner shells

[Ar] has the same electron configuration as the inner shells

[Ar] 3d$^1$ 4s$^2$ where [Ar] represents the electronic configuration of argon.

Electronic configurations in ions

- Follow the same principle as for atoms but add / remove electrons:

Eg Sodium ion Na$^+$

Na atom = 1s$^2$ 2s$^2$ 2p$^6$ 3s$^1$

To make a sodium ion 1 electron is removed

Na ion = 1s$^2$ 2s$^2$ 2p$^6$

Eg Chlorine ion Cl$^-$

Cl atom = 1s$^2$ 2s$^2$ 2p$^6$ 3s$^2$2p$^5$

To make a chlorine ion 1 electron is added

Cl$^-$ ion = 1s$^2$ 2s$^2$ 2p$^6$ 3s$^2$2p$^6$
Electronic configurations of the Transition Metals

- Chromium and Copper fill differently
  
  Cr: $1s^22s^22p^63s^23p^63d^44s^2$ (expected)  
  Cr: $1s^22s^22p^63s^23p^63d^54s^1$ (actual)
  
  Cu: $1s^22s^22p^63s^23p^63d^94s^2$ (expected)  
  Cu: $1s^22s^22p^63s^23p^63d^{10}4s^1$ (actual)

  A half-filled or full d-sub shell offers more stability than a full s-sub shell.

When forming ions:

4s-sub shell empties before 3d-sub shell

Example 1

Fe: $1s^22s^22p^63s^23p^63d^64s^2$

Fe$^{3+}$: $1s^22s^22p^63s^23p^63d^5$

Example 2

Cu: $1s^22s^22p^63s^23p^63d^{10}4s^1$

Cu$^{2+}$: $1s^22s^22p^63s^23p^63d^9$