AQA Chemistry A-Level

3.1.1: Atomic Structure

Detailed Notes
3.1.1.1 - Fundamental Particles

The model for atomic structure has evolved over time as knowledge and scientific understanding changes.

**Plum Pudding Model**
It was initially thought that atoms consisted of a sphere of positive charge, with small negative charges distributed evenly within it.

**Electron Shell Model**
It is now known that the atom consists of a small, dense central nucleus surrounded by orbiting electrons in electron shells. This was discovered in the Rutherford scattering experiment in 1911.

The nucleus consists of protons and neutrons giving it an overall positive charge. It contains almost the entire mass of the atom.

In a neutral atom, the number of electrons is equal to the number of protons due to the relative charges.

<table>
<thead>
<tr>
<th>Particle</th>
<th>Proton</th>
<th>Neutron</th>
<th>Electron</th>
</tr>
</thead>
<tbody>
<tr>
<td>Relative Charge</td>
<td>+1</td>
<td>0</td>
<td>-1</td>
</tr>
<tr>
<td>Relative Mass</td>
<td>1</td>
<td>1</td>
<td>1/1840</td>
</tr>
</tbody>
</table>

The maximum number of orbiting electrons that can be held by any single shell, depends on the number of the shell. This can be calculated using $2n^2$ where $n$ is the number of the shell.

*Example:*

Electrons in shell 2 = $2(2^2) = 8$ electrons

Each electron shell must fill before the next one can hold any electrons.
3.1.1.2 - Mass Number and Isotopes

Mass number is represented using \( A \) and can be calculated as the sum of protons and neutrons in an atom.

Atomic number is represented using \( Z \) and is equal to the number of protons in an atom.

Using these, the quantity of each fundamental particle in an atom can be calculated.

Example:

\[
\begin{array}{c}
\text{Atomic number} = 7 \\
\text{Mass number} = 14 \\
\text{Proton number} = 7 \\
\text{Neutron number} = 14 - 7 \\
= 7
\end{array}
\]

Relative atomic mass (\( Ar \)) is defined as:

The mean mass of an atom of an element, divided by one twelfth of the mean mass of an atom of the carbon-12 isotope.

This takes the relative abundances of the different isotopes of an element into account.

\[
Mr = \text{mean mass of an atom of an element} \\
\quad \quad \quad 1/12 \times \text{mean mass of C-12 isotope}
\]

Isotopes

Isotopes are atoms of the same element with the same atomic number, but with a different number of neutrons, resulting in a different mass number.

Neutral atoms of isotopes will react chemically in the same way as their proton number and electron configuration is the same. The sharing and transfer of electrons is unaffected. However, the different mass number means they have different physical properties.
Example:

<table>
<thead>
<tr>
<th>Element</th>
<th>Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen</td>
<td>1 proton and 1 neutron</td>
</tr>
<tr>
<td>Deuterium</td>
<td>1 proton and 2 neutrons</td>
</tr>
<tr>
<td>Tritium</td>
<td>1 proton and 3 neutrons</td>
</tr>
</tbody>
</table>

**Ions**

Ions are formed when an atom **loses or gains electrons** meaning it is no longer neutral and will have an **overall charge**.

**Mass Spectrometry**

This is an **analytical technique** used to identify different isotopes and find the overall relative atomic mass of an element.

**Time of Flight (TOF) Mass Spectrometry**

This form of mass spectrometry records the time it takes for ions of each isotope to reach a detector. Using this, **spectra** can be produced showing each isotope present.

1. **Ionisation** - A sample of an element is **vapourised** and injected into the mass spectrometer where a **high voltage** is passed over the chamber. This causes electrons the be removed from the atoms (it is ionised) leaving **+1 charged ions** in the chamber.

2. **Acceleration** - These positively charged ions are then **accelerated** towards a negatively charged **detection plate**.

3. **Ion Drift** - The ions are then deflected by a **magnetic field** into a **curved path**. The radius of their path is dependant on the charge and mass of the ion.
4. **Detection** - When the positive ions hit the negatively charged detection plate, they **gain an electron** producing a **flow of charge**. The greater the abundance, the greater the current produced.

5. **Analysis** - These current values are then used in combination with the **flight times** to produce a **spectra print-out** with the relative abundance of each isotope displayed.

During the ionisation process, a **2+ charged ion** may be produced. This means it will be affected more by the magnetic field producing a curved path of **smaller radius**. As a result, its mass to charge ratio (m/z) is halved and this can be seen on spectra as a trace at **half the expected m/z value**.

*Example:*

![Graph showing mass to charge ratio (m/z) vs. abundance]

Using this spectra, the **Ar can be calculated**:

\[
\text{Ar} = \frac{m/z \times \text{abundance}}{\text{Total abundance}}
\]

*Example:*

\[
\text{Ar} = \frac{(10 \times 75) + (12 \times 25)}{75 + 25} = 10.5
\]
Chlorine Spectra
Spectra produced by the mass spectrometry of chlorine display a characteristic pattern in a 3:1 ratio for Cl\(^+\) ions and a 3:6:9 ratio for Cl\(_2^+\) ions. This is because one isotope is more common than the other and the chlorine molecule can form in different combinations. 

**Example:**

\[
\begin{align*}
70\text{Cl}_2^+ &= 35 + 35 \\
72\text{Cl}_2^+ &= 35 + 37 \text{ OR } = 37 + 35 \\
74\text{Cl}_2^+ &= 37 + 37
\end{align*}
\]

3.1.1.3 - Electron Configuration

**Electron Orbitals**
Electrons are held in clouds of negative charge called orbitals. There are different types of orbital; s, p, d and f. Each one has a different shape:

- s-orbital (spherical)
- p-orbital (dumbbell)
- d-orbital
These orbitals correspond with blocks on the Periodic Table. Each element in the block has outer electrons in that orbital.

Each orbital can hold a different number of electrons before the next one is filled:

- **s-orbital** = 2 electrons
- **p-orbital** = 6 electrons
- **d-orbital** = 10 electrons

The energy of the orbitals increases from **s** to **d** meaning the orbitals are filled in this order. Each orbital is filled before the next one is used to hold electrons.

**Example:**

Sodium has 11 electrons. These would be written in the following configuration:

\[
\text{Na} = 1s^22s^22p^63s^1
\]

It has 3 energy levels and 4 orbitals holding the 11 electrons.
Spin
Within an orbital, electrons pair up with opposite spin so that the atom is as stable as possible. Electrons in the same orbital must have opposite spin. Spin is represented by arrows.

Example:

![Image](Image courtesy of Socratic)

Overall there are three rules for writing out electron configurations:

1. The lowest energy orbital is filled first.
2. Electrons with the same spin fill up an orbital first before pairing begins.
3. No single orbital holds more than 2 electrons.

The following table (courtesy of Ellesmere Chemistry) shows the electron configuration and orbital diagrams for Period 2 elements:

<table>
<thead>
<tr>
<th>Element</th>
<th>Total Electrons</th>
<th>Orbital Diagram</th>
<th>Electron Configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li</td>
<td>3</td>
<td>![1s 2s 2p]</td>
<td>1s$^2$2s$^1$</td>
</tr>
<tr>
<td>Be</td>
<td>4</td>
<td>![1s 2s 2p]</td>
<td>1s$^2$2s$^2$</td>
</tr>
<tr>
<td>B</td>
<td>5</td>
<td>![1s 2s 2p]</td>
<td>1s$^2$2s$^2$2p$^1$</td>
</tr>
<tr>
<td>C</td>
<td>6</td>
<td>![1s 2s 2p]</td>
<td>1s$^2$2s$^2$2p$^2$</td>
</tr>
<tr>
<td>N</td>
<td>7</td>
<td>![1s 2s 2p]</td>
<td>1s$^2$2s$^2$2p$^3$</td>
</tr>
<tr>
<td>NE</td>
<td>10</td>
<td>![1s 2s 2p]</td>
<td>1s$^2$2s$^2$2p$^6$</td>
</tr>
<tr>
<td>Na</td>
<td>11</td>
<td>![1s 2s 2p]</td>
<td>1s$^2$2s$^2$2p$^6$3s$^1$</td>
</tr>
</tbody>
</table>
Exceptions to the Rules
If electron spins are unpaired and therefore unbalanced, it produces a natural repulsion between the electrons making the atom very unstable. If this is the case, the electrons may take on a different arrangement to improve stability.

Example:

The $3p^4$ orbital contains a single pair of electron with opposite spin making it unstable:

\[ \begin{array}{c}
\uparrow \\
\downarrow \\
\uparrow
\end{array} \]

Therefore the electron configuration changes to become $3p^34s^1$ which is a much more stable arrangement:

\[ \begin{array}{c}
\uparrow \\
\uparrow \\
\uparrow \\
\uparrow
\end{array} \]

Ionisation Energy
Ionisation energy is defined as:

the minimum energy required to remove one mole of electrons from one mole of atoms in a gaseous state. It is measured in kJmol$^{-1}$.

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

Successive ionisation energies occur when further electrons are removed. This usually requires more energy because as electrons are removed the electrostatic force of attraction between the positive nucleus and the negative outer electron increases. More energy is therefore needed to overcome this attraction so ionisation energy increases.

First ionisation energy follows trends within the Periodic Table.

Along a Period - first ionisation energy increases due to a decreasing atomic radius and greater electrostatic forces of attraction.

Down a Group - first ionisation energy decreases due to an increasing atomic radius and shielding which reduces the effect of the electrostatic forces of attraction.
When successive ionisation energies are plotted on a graph, a **sudden large increase** indicates a **change in energy level**. This is because the electron is being removed from an orbital **closer to the nucleus** so more energy is required to do so.

![Diagram of ionisation energy levels](image)

This large energy increase provides **supporting evidence for the atomic orbital theory**.

The first ionisation energy of **aluminium** is **lower than expected** due to a single pair of electrons with **opposite spin**. As a result there is a **natural repulsion** which reduced the amount of energy needed to be put in to remove the outer electron.