OCR (B) Chemistry A-level

Storyline 1: Elements of Life

Detailed Notes

Formulae, Equations and Amount of Substance

Introduction

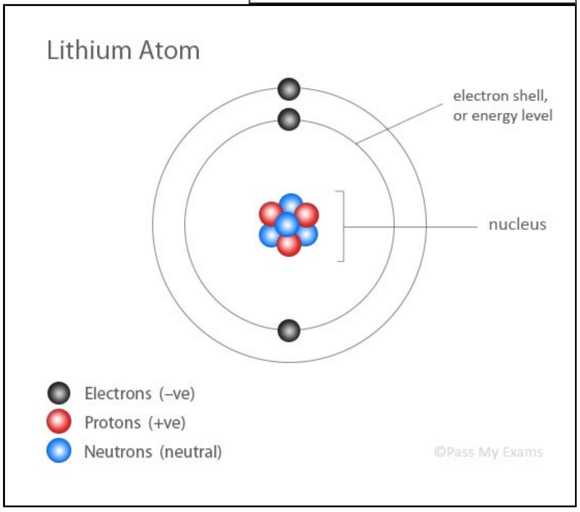
Fundamental Particles

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

The current, accepted model of 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.

Image courtesy of passmyexam.co.uk



Particle	Proton	Neutron	Electron
Relative Charge	+1	0	-1
Relative Mass	1	1	1/1840

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 $\mathbf{2n^2}$ where n is the number of the shell.
Example:

$$\textbf{Electrons in shell 2} = 2(2^2) = 8 \textbf{ electrons}$$

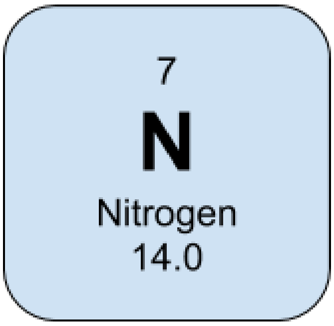
Each electron shell **must fill** before the next one can hold any electrons.

Atomic Number, Mass Number and Relative Mass

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, hence it can be referred to as proton number.

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

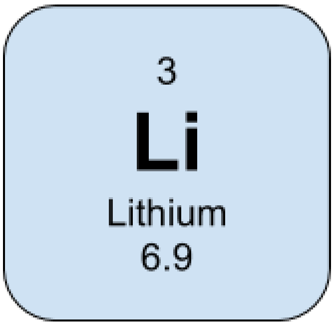


Atomic number = 7
Mass number = 14

Proton number = 7

Neutron number = 14 - 7
= 7

Ions are formed when an atom **loses or gains electrons.** This means that it is no longer neutral and will have an **overall charge**. In an ion, the number of electrons is equal to the number of protons minus the ionic charge.
Example:



Li = **3 electrons**

Li^+ = (3 - 1) electrons = **2 electrons**

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 numbers mean they have **different physical properties**.
Example:

Hydrogen	**= 1 proton and 1 neutron**
Deuterium	**= 1 proton and 2 neutrons**
Tritium	**= 1 proton and 3 neutrons**

Deuterium is used in heavy water (D_2O) to control nuclear processes.

Relative Mass

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

The weighted mean mass of an atom of an element, relative to 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.

$$Ar = \frac{\text{mean mass of an atom of an element}}{1/12 \times \text{mean mass of C-12 isotope}}$$

Relative isotopic mass is defined as:

The isotopic mass of an isotope relative to one twelfth of the mean mass of an atom of the carbon-12 isotope.

Relative molecular mass (*Mr*) is defined as:

The weighted mean mass of a molecule of a compound, relative to one twelfth of the mean mass of an atom of the carbon-12 isotope.

It can be calculated for a molecule by adding together the separate Ar values of the component elements.

Example:

$$\begin{aligned} \text{Mr of } H_2O &= 2 \times 1.0 \\ &\ \ 1 \times 16.0 \\ &= 18.0 \end{aligned}$$

Relative formula mass is similar to Mr but is used for compounds with giant structures.

The Mole

Amount of Substance defines the number of particles in a substance. It is measured in **moles**.

The mole is a **unit of measurement** for substances. It always contains the **same number of particles**.

$$N_A = 6.02 \times 10^{23} \text{ particles}$$

This number is the **Avogadro's Constant** (N_A) and is the number of particles per mole. It allows the number of particles present in a sample of a substance with known mass to be found:

$$\boxed{\text{Number of particles} = n \times N_A}$$

(n = moles) (N_A = Avogadro's constant)

The mole is a **very important unit of measurement** in many calculations:

$$\boxed{\text{Moles} = \frac{\text{mass}}{M_r} = \frac{\text{concentration} \times \text{volume}}{1000}}$$

(where concentration is in mol dm^{-3} and volume is in cm^3)

Molar mass is the mass per mole and has units g mol^{-1}.

Molar gas volume is the gas volume per mole and has units dm^3 mol^{-1}.

Definition of Formulae

Empirical formula is the simplest whole number ratio of atoms of each element present in a compound.

The empirical formula can be found by using the composition by mass or percentage composition by mass and the relative atomic masses of the elements present.

Molecular formula is the number and type of atoms of each element in a molecule. It is the true number of each atom in the molecule.

The molecular formula can be determined using the Mr of the empirical formula and the true Mr of the molecule. This gives a multiplier value which can be used to scale up the empirical formula.

$$\boxed{\frac{\text{Mr of molecule}}{\text{empirical Mr}} = \text{multiplier}}$$

Water of crystallisation is water that is part of the crystalline structure. The molecules are stoichiometrically chemically bonded into the crystal structure.

An **anhydrous** substance contains no water of crystallisation.

A **hydrated** substance contains water of crystallisation.

The formula of a hydrated salt can be calculated from experimental results or a given percentage or mass composition.

Calculations

Percentage Yield

$$\% \text{ yield} = \frac{\text{Experimental mass} \times 100}{\text{Theoretical mass}}$$

Experiments usually have a percentage yield less than 100%. This could be due to the reaction being incomplete, loss of products on equipment, or unwanted side reactions.

Percentage Composition

The percentage composition is the percentage of a compound made up by a single element.

$$\% \text{ composition} = \frac{\text{Mr of element}}{\text{Mr of compound}} \times 100$$

Example:

The percentage composition of carbon in ethanol, C_2H_5OH is:
Mr of carbon = (12 x 2) = 24
Total Mr = (12 x 2) + (1 x 6) + (16 x 1) = 46
% composition = 24/46 x 100 = 52%

Concentrations

The concentration of a solution can be measured in **mol dm^{-3}** or **g dm^{-3}** which can be calculated using the following equations:

$$\textbf{Concentration (mol dm}^{-3}\textbf{)} = \frac{\text{Number of moles (mol)}}{\text{Volume (dm}^3\text{)}}$$

$$\textbf{Concentration (g dm}^{-3}\textbf{)} = \frac{\text{Mass (g)}}{\text{Volume (dm}^3\text{)}}$$

Equations

Full or ionic chemical equations must be **balanced** before they can be used in calculations. This is because the **reacting ratios** must be correct. For a chemical equation to be balanced, it must have the **same number and type** of each atom present on both sides of the equation.

It can be useful to also include **state symbols** so it is clear what might be observed during the reaction, for example, **bubbles** of gas, a **precipitate** forming, or a **colour change** that may infer a **displacement reaction.**
There are four state symbols:

- (s) - solid
- (l) - liquid
- (g) - gas
- (aq) - aqueous (dissolved in water)

These balanced equations can then be used to calculate **reacting masses, percentage yield** and **atom economy**.

Ionic equations

Ionic equations show just the **reacting particles** that undergo a change during the reaction and not the **spectator species**. As with normal chemical equations, it must be balanced. The reacting species are shown as **dissociated ions.**

Acid-Base Titrations

A titration is a practical method where a **standard solution** of known concentration is reacted with a solution of **unknown concentration** in order to determine the property of this solution. For this, there is a standard method to make up the standard solution and carry out the titration.

Volumetric Solution - simple method

1. Weigh the sample bottle containing the solid on a (2 d.p.) balance.
2. Transfer solid to beaker and reweigh sample bottle.
3. Record the difference in mass.
4. Add distilled water and stir with a glass rod until all the solid has dissolved.
5. Transfer to a volumetric flask with washings.
6. Make up to the 250cm^3 mark with distilled water.
7. Shake flask.

Titration - simple method

1. Fill the burette with the standard solution of known concentration, ensuring the jet space in the burette is filled and doesn't contain air bubbles.
2. Use a pipette filler and pipette to transfer 25cm^3 of the solution with unknown concentration into a conical flask.

3. Add two to three drops of indicator.
4. Record the initial burette reading.
5. Titrate the contents of the conical flask by adding solution to it from the burette until the indicator undergoes a definite, permanent colour change.
6. Record the final burette reading and calculate the titre volume.
7. Repeat until at least two concordant results are obtained (within 0.1cm^3 of each other).

Experimental Techniques

Use a balance to measure mass. It is important to use a balance with a suitable **resolution** for your experiment.

Use a measuring cylinder to measure the volume of a solution. If you are making up a standard solution, you should use a volumetric flask of the required volume.

Use a gas syringe to measure the volume of gas produced in an experiment. Alternatively, measure the mass lost on a balance and calculate the moles of gas produced from this.

Atomic Structure

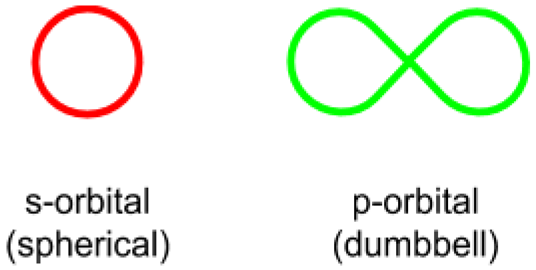
Shells

Electrons orbit the nucleus at different energy levels, which increase with distance from the nucleus- these are called **shells**. A shell is a group of atomic orbitals which have the same value of the principal quantum number, n. They can be split up into separate sub-shells, labelled s, p, d, and f.

The maximum numbers of electrons that can fill the first four shells are: 2, 8, 18, and 32. Given the atomic number of an element, you can deduce its electron configuration.

Electron Orbitals

Electrons are held in **clouds of negative charge** called **orbitals**. An atomic orbital is a region around the nucleus that can hold up to two electrons with opposite spins. There are different types of orbitals; ***s, p, d, and f.*** Each one has a different shape:



Each subshell has a different number of orbitals and therefore can hold a different number of electrons before the next one is filled:

s-subshell = 2 electrons
p-subshell = 6 electrons
d-subshell = 10 electrons

These orbitals correspond with **blocks** on the Periodic Table. Each element in the block has **outer electrons in that orbital**.

When atoms lose/gain electrons to form ions, for s-block and p-block elements, electrons are added to the next available, empty orbital and are removed from the most recent orbital to have been filled.

Electronic Configuration

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

It has 3 energy levels and 4 orbitals holding the 11 electrons.

There are two main **exceptions** to electron configuration. A completely full or half full d sublevel is more stable than a partially filled d sublevel, so an electron from the 4s orbital is excited to the 3d orbital.

Chromium: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^1$
Copper: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^1$

Fusion Reactions

In a fusion reaction **two lighter nuclei** join to give a **single heavier nucleus**, this process releases energy but requires some extreme conditions of high temperature and pressure. This is how some elements are formed.

Lots of different nuclear fusion reactions are occuring in the sun. One of these reactions is the combination of four hydrogen nuclei becoming one helium nuclei.

$$4\,{}^{1}_{1}H \rightarrow {}^{4}_{2}He + 2e^{+} + 2\nu_{e} + 2\gamma$$

The mass of four hydrogen nuclei is 6.693×10^{-27} kg whereas the mass of one helium nucleus is 6.645×10^{-27} kg. This means there is a mass of 0.048×10^{-27} kg that is leftover, this is converted to and released as energy.

Bonding and Structure

Ionic Bonding

Ionic bonding is an **electrostatic attraction** between positive and negative ions.

It occurs between a **metal and a non-metal**. Electrons are **transferred** from the metal to the non-metal to achieve full outer shells.

Ionic substances only **conduct electricity** when molten or aqueous as when they are solid the ions cannot move to carry a charge.

When the electrons are transferred, it creates **charged particles** called **ions**. Oppositely charged ions **attract through electrostatic forces** to form a **giant ionic lattice**.
Example:

Sodium Chloride is an ionic compound formed from Na$^+$ and Cl$^-$ ions. Sodium loses an electron and Chlorine gains an electron to produce ions with a full outer electron shell. These then attract into an ionic lattice:

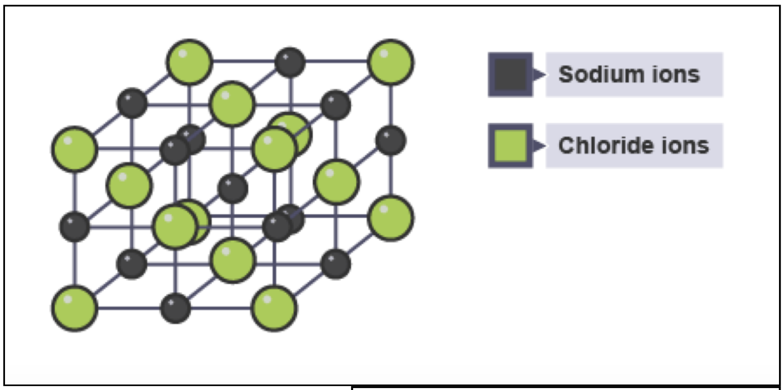


Image courtesy of Blogspot IGCSE Chemistry

Dots and Cross Diagrams

Cations (+ve) and **anions** (-ve) can be represented using **dot and cross diagrams** - and so can ionic bonding. The electrons being transferred from the cation can be displayed on the outer shell of the anion.

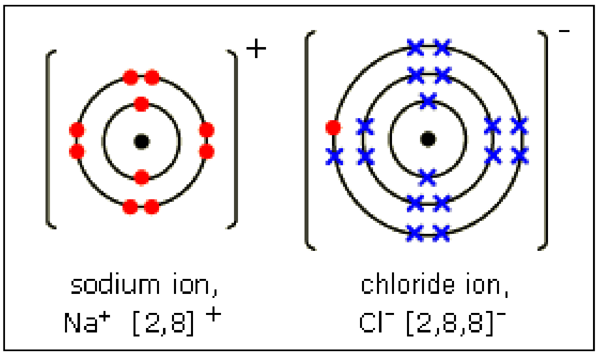


Image courtesy of BBC Bitesize

The red dot clearly shows the transferred electron from sodium to chloride to produce two ions with full outer electron shells.

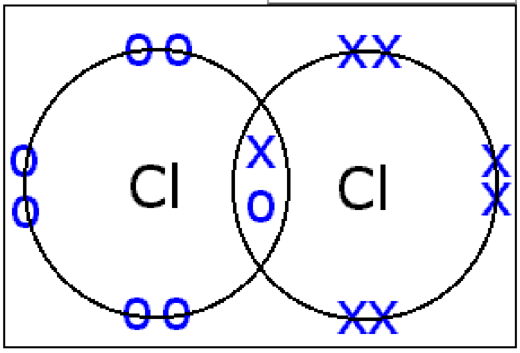
Covalent Bonding

A covalent bond is the strong **electrostatic attraction** between a **shared pair of electrons** and the **nuclei** of the bonded atoms.

Covalent bonds form between **two non-metals**. Electrons are **shared** between the two outer shells in order to achieve **full outer shells**. **Multiple electron pairs** can be shared to form **multiple covalent bonds**.

The shared electron pairs can be represented using **dot and cross diagrams** and a covalent bond shown with a straight line.
Example:

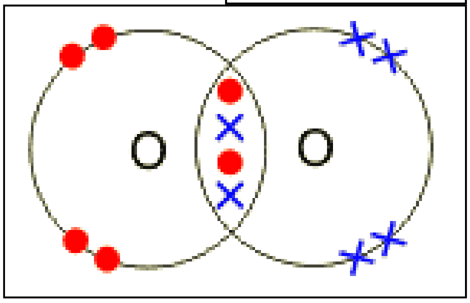
Image courtesy of IB Chem



Cl—Cl

Double and triple bonds can also be shown on dot and cross diagrams with the multiple electron pairs being displayed in the shared segment between the two atoms.
Example:

Image courtesy of BBC Bitesize



O═O

Dative Covalent Bonds

Dative or **coordinate** bonds form when both of the **electrons in the shared pair** are supplied from a **single atom**. It is indicated using an **arrow** from the lone electron pair.

Example:

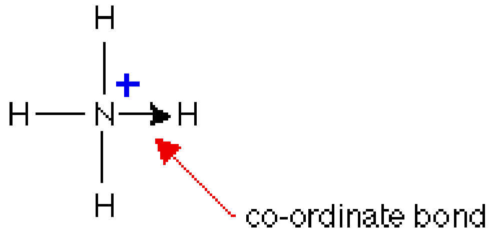


Image courtesy of Chemguide

Ammonia (NH_3) has a lone electron pair that can form a dative bond with a H^+ ion to produce an ammonium ion (NH_4^+).

Once a dative bond has formed, it is treated as a **standard covalent bond** because it **reacts in exactly the same way** and has the same properties regarding length and strength.

Since both electrons come from the **same atom** in a dative covalent bond, in dot and cross diagrams both electrons in that bond will have the **same shape**.
In other words, they will both be dots or both be crosses.

Simple Covalent

Substances with a simple molecular structure consist of **covalently bonded molecules** held together with **intermolecular forces.**

The shape of a simple molecule or ion is determined by the number of **electron pairs around the central atom** and the repulsion between them. Each electron pair **naturally repels** each other so that the **largest bond angle possible** exists between the covalent bonds.

Lone Pair Repulsion

Any lone pairs present around the central atom provide **additional repulsive forces**, which changes the bond angle. For every lone pair present, the bond angle between covalent bonds is **reduced by 2.5°**.

Molecule Shapes

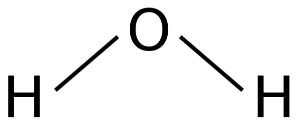
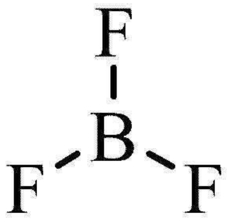
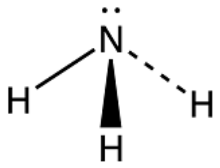
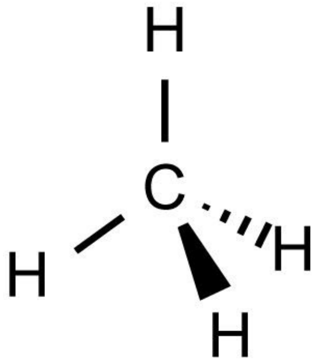
The shape of a molecule can be determined by considering the **type and quantity of electron pairs**:

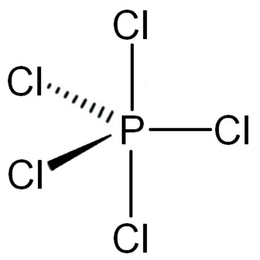
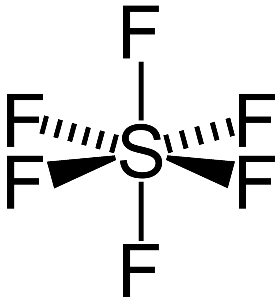
1. Find the number of electron pairs.
2. Determine how many of the pairs are bonding pairs and how many are lone pairs.
3. Bonding pairs indicate the basic shape and lone pairs indicate any additional repulsion.

Molecules may also be described in terms of their bond lengths and bond angles.

- **Bond length** - the average distance between two nuclei in a covalent bond.
- **Bond angle** - the angle between two covalent bonds from the same atom.

This table shows some common molecule shapes:

Name	**Bonding e^- Pairs**	**Lone e^- Pairs**	**Bond Angle (°)**	**Example**
Linear	2	0	180	Cl - Be - Cl O=C=O
V - Shaped	2	2	104.5	
Trigonal Planar	3	0	120	
Triangular Pyramid	3	1	107	
Tetrahedral	4	0	109.5	CH_4, NH_4^+ 

Trigonal Bipyramidal	5	0	180 and 120	
Octahedral	6	0	90	

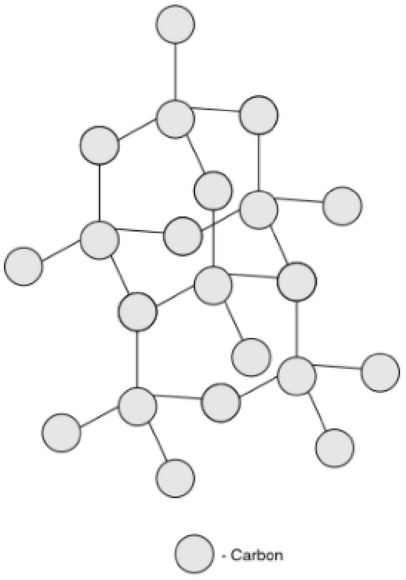
Images courtesy of World of Chemicals, Socratic, Quora, and Alchetron

Giant Covalent Structures

Macromolecular covalent substances are **covalently bonded** into a **giant lattice** structure. Each atom has **multiple covalent bonds** which are very strong, giving the substance a **very high melting point**.

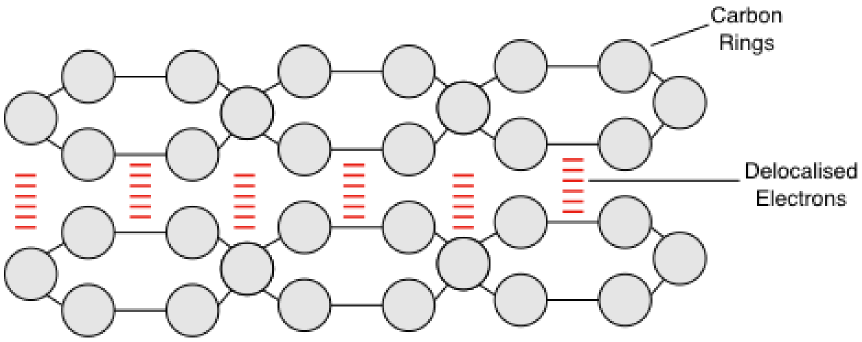
Diamond is a **macromolecular structure** made up of carbon atoms each bonded to four further carbon atoms. This forms a **rigid tetrahedral structure**, making diamond one of the **hardest, strongest** materials known - which is why it is often used on the tips of drills.

Example: Structure of diamond



Graphite is another macromolecular structure made up of carbon atoms. However, in graphite, each carbon atom is bonded to three others in **flat hexagonal sheets**. This means there is one **delocalised electron** per carbon atom. These electrons can move freely, allowing graphite to **conduct electricity**. Graphite can therefore be used in an electrode. The **intermolecular forces** between layers of graphite are **weak** and can easily slide over each other, meaning graphite can be used as a **lubricant**.

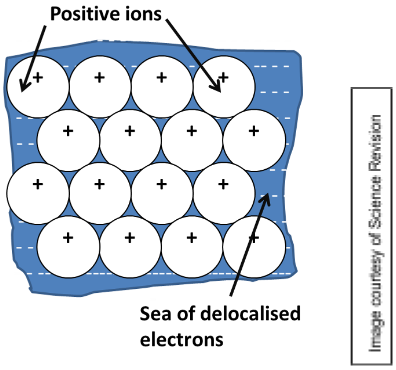
Example: Structure of graphite



Metallic Bonding

Metallic bonding consists of a **giant lattice of positively charged ions** surrounded by a **'sea' of delocalised electrons**. There are very strong **electrostatic forces of attraction** between the opposite charged particles.

Example:



The **greater the charge** on the positive ion, the **stronger the attractive force** since more electrons are released into the 'sea'.

Ions that are **larger in size**, such as barium, produce a **weaker attraction** due to their **greater atomic radius**.

Metallic Structure (eg. Aluminium)

Substances with metallic structure are often **good conductors**. The 'sea' of delocalised electrons is able to move and **carry a flow of charge**.

Metals are also **malleable** because the uniform layers of positive ions are able to slide over one another. The delocalised electrons prevent fragmentation as they can move around the lattice.

Example:

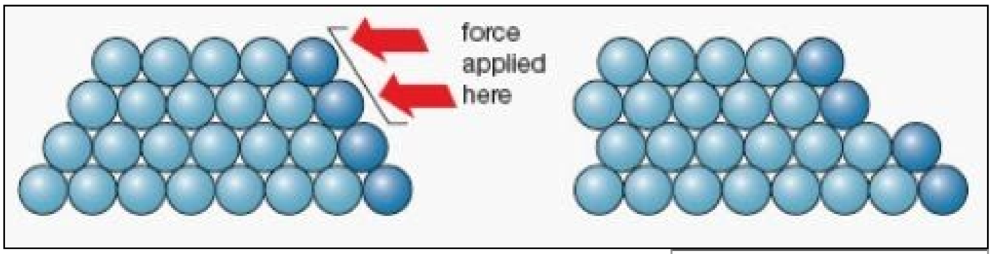


Image courtesy of Pintrest Teachers

The **electrostatic forces of attraction** between the positive ions and delocalised electrons are very strong and therefore require a lot of energy to overcome. This means metallic substances have **high melting points** and are nearly always **solid at room temperature**. Mercury is the only metal which is liquid at room temperature.

Inorganic Chemistry and the Periodic Table

The Periodic Table arranges the known elements in order of **increasing proton number**. All the elements along a **period** (row) have the same number of **electron shells**. All the elements down a **group** (column) have the same number of **outer electrons** which is indicated by the group number. Elements in the same group have similar chemical properties.

Elements are classified into **blocks** within the Periodic Table, and elements in the same block have their outer electrons in the same type of **orbital**.

s-block = Groups 1 and 2
p-block = Groups 3 to 0
d-block = Transition metals
f-block = Lanthanides & actinides

Different electron configurations are often **linked to other trends** within the Periodic Table. Periodicity is the study of these trends.

The **energy** of the orbitals **increases from s to f,** meaning the orbitals are **filled in this order**. Each orbital is filled before the next one is used to hold electrons. For Period 2, first the s orbitals are filled, followed by the p orbitals. The same applies to Period 3.

Example:

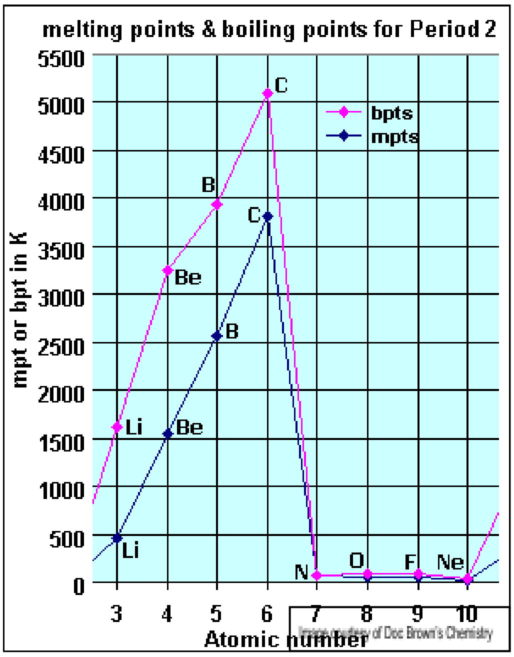
Nitrogen has the atomic number 7 so has 7 electrons and has the configuration: **$1s^2 2s^2 2p^3$**

Variation in Melting Points across Periods 2 and 3

The melting points of the Period 2 elements peaks towards the middle of the period due to the different **bond strength and structures**:

- Lithium and beryllium have **metallic bonding**. Their melting points increase due to a greater **positive charge of the ions** (Li = +1, Be = +2). There are **more electrons released** as free electrons in the beryllium lattice so the attractive electrostatic forces are greater than for lithium.

- **Boron** and **carbon** form giant covalent lattices with **very strong covalent bonds.** Covalent bonds require a lot of energy to break, giving them very high melting points.



- Nitrogen, oxygen, fluorine and neon are all **small**, **simple covalent molecules** with weak **van der Waals** intermolecular forces. These intermolecular forces don't require much energy to overcome so these molecules have relatively low, similar melting points.

The melting points of the Period 3 elements are also linked to the **bond strength and structure**:

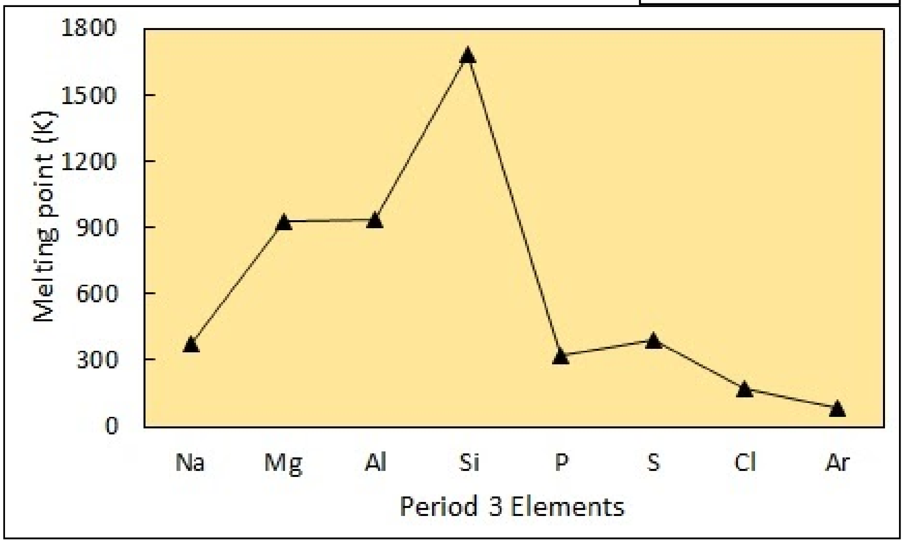
- Sodium, magnesium and aluminium are all metals with **metallic bonding**. Their melting points increase due to greater **positive charged ions** (Na = +1, Mg = +2, Al = +3). This also means **more electrons are released** as free electrons so the attractive electrostatic forces increase from Na to Al.

- Silicon is macromolecular meaning that it has a **very strong covalent structure**. These covalent bonds require a lot of energy to break, giving it a very high melting point.

- Phosphorus, sulfur and chlorine are all **simple covalent molecules** with weak **Van der Waals** forces. These intermolecular forces don't require much energy to overcome so these molecules have relatively low, similar melting points.

- Argon is a noble gas that exists as **individual atoms** with a **full outer shell of electrons**. This makes the atom **very stable** and the Van der Waals forces between them very weak. As a result, the melting point of argon is very low and it exists as a gas at room temperature.

Image courtesy of CapeChemistry



Ions

The Group an element is in in the periodic table represents how many electrons it will have to lose or gain to have a complete outer shell of electrons. For example: Group 1 = 1+ (loss of 1 electron), Group 7 = 1- (gain of 1 electron). The transition metals do not follow this rule.

The table below shows the ions you will be expected to know:

Name of ion:	Formula of ion
Nitrate	NO_3^-
Sulfate	SO_4^{2-}
Carbonate	CO_3^{2-}
Hydroxide	OH^-
Ammonium	NH_4^+
Bicarbonate	HCO_3^-
Copper	Cu^{2+}
Zinc	Zn^{2+}
Lead	Pb^{2+}
Iron	Fe^{2+}
Iron	Fe^{3+}

Reactions of Group 2 Compounds

Reactions with Water

The Group 2 metals react with water in a redox reaction to produce a **metal hydroxide and hydrogen**. The metal hydroxide forms as an **alkaline solution**, hence why the Group 2 metals are known as the alkaline earth metals.

Example:

$$\boxed{Mg + 2H_2O \longrightarrow Mg(OH)_2 + H_2}$$

The Magnesium is oxidised from an oxidation state of 0 to +2.
(Oxidation is loss of e^-***)***

Magnesium reacts very slowly in this way with liquid water, however, the reaction can be much **faster with steam** as it provides the reaction with **extra energy**. When steam is used, the magnesium burns with a **bright white flame** to form hydrogen and magnesium oxide, a **white powder**.

Example:

$$\boxed{Mg + H_2O \longrightarrow MgO + H_2}$$

Down the group, the **reactivity** of the Group 2 metals with water **increases**. Calcium, strontium, and barium all react with cold water with **increasingly vigorous** reactions. These reactions all form the metal hydroxide and hydrogen gas.

The **metal oxides** of the Group 2 elements react with water to form basic metal hydroxides. The alkalinity of these increases down the group as the solubility of the metal hydroxides increases.

Reactions with Oxygen

Group 2 metals react with oxygen to form **oxides**. Once the reaction has been initiated it is **vigorous**. **Strontium** and **barium** can react with excess oxygen and heat energy to form **metal peroxides**.

The general equation of Group 2 metals with oxygen is:

$$2M + O_2 \rightarrow 2MO$$

Strontium or barium may react with oxygen and form the peroxide:

$$M + O_2 \rightarrow MO_2$$

Thermal Decomposition of Group 2 Carbonates

All Group 2 carbonates undergo **thermal decomposition** to produce a **metal oxide** and **carbon dioxide**. The carbonates are **heated more strongly** as you go down the group.
The general equation for this reaction (where X is the Group 2 metal) is:

$$XCO_3 \rightarrow XO + CO_2$$

Observations: The carbonate and the oxide are both **white solids**. Carbon dioxide is a **colourless gas**.

Group 2 carbonates become **more stable to heat** as you go down the group. This means as you go down the group, the carbonates have to be **heated more strongly** for thermal decomposition to occur.

The smaller 2+ ion has a higher **charge density** than a larger 2+ ion. An increasing charge density means the ion will have more of a **distorting effect** on neighbouring negative ions. The positive ion attracts the delocalised electrons on an oxygen atom in the carbonate ion towards itself. The carbonate ion becomes **polarised**. This polarisation weakens the C-O bond, meaning with some heat this easily breaks to release CO_2.

This explains why as you move down the group more heat is required to thermally decompose the group 2 carbonates, as the ions increase in size and decrease in charge density and are therefore less polarising.

Solubility of Group 2 Carbonates

The **solubility** of Group 2 carbonates tends to decrease down the group, however none of them are more than sparingly soluble.

Solubility of Group 2 Hydroxides

The **solubility** of Group 2 hydroxides varies, allowing the compounds to have different uses. Solubility **increases down the group** meaning magnesium hydroxide, $Mg(OH)_2$, is the least soluble and barium hydroxide, $Ba(OH)_2$, is the most soluble.

As a result, **magnesium hydroxide** is used in medicine as an **antacid** to treat indigestion as it is alkaline and can neutralise acids. **Calcium carbonate** can also be used as an **antacid**. **Calcium hydroxide** is also used in **agriculture** to neutralise acidic soils.

Ionisation Energy

First 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}.

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

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 as they are influenced by proton-electron forces of attraction and electron shielding.

- **Along a Period** - first ionisation energy **increases** due to a **decreasing atomic radius** (from the increasing nuclear charge) and greater electrostatic **forces of attraction**.

- **Down a Group** - first ionisation energy **decreases** due to an **increasing atomic radius** and **electron shielding** which reduces the effect of the electrostatic forces of attraction.

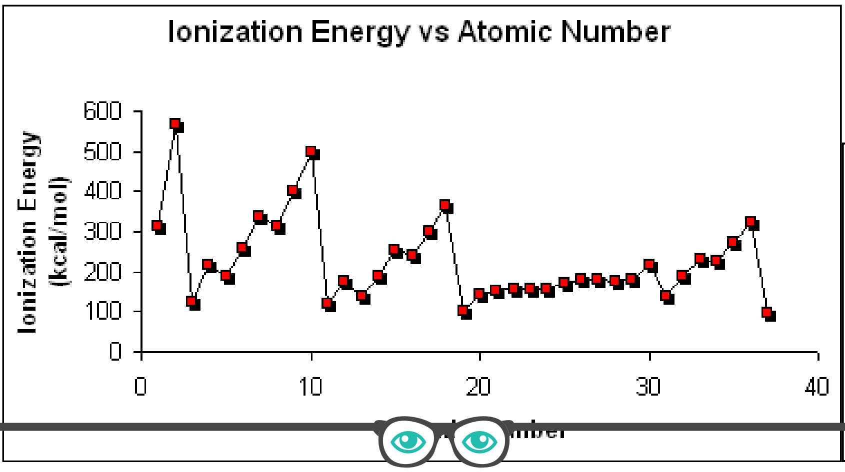


Image courtesy of Science with Mrs Welch

Successive ionisation energies involve removing one mole of electrons from **one mole of gaseous ions**. For example, the third ionisation energy of potassium would involve removing one electron from $K^{2+}(g)$ to form $K^{3+}(g)$.
Successive ionisation energies increase because atomic radius decreases and there is greater attraction between outer shell electrons and the nucleus.

A large **jump** between successive ionisation energies indicates which **group** an element is in. The successive ionisation energies for an element are shown below:

1st	2nd	3rd	4th	5th
801	2427	3660	25026	32827

The **large jump between the third and fourth ionisation energy** shows there are 3 electrons that are relatively easy to remove then a fourth one which requires a lot more **energy to remove**. This shows that there are 3 electrons in an outer shell. This means the element is in **Group 3**. There are 5 ionisation energies for this element so it has **5 electrons**. An element with 5 electrons in Group 3 is boron.

Period 2

First ionisation energies follow a general increasing trend along Period 2. This is due to the decreasing atomic radius and increasing nuclear charge which means that outer electrons are **held more strongly**.

Boron and oxygen are **exceptions** to this trend. **Boron** has a **lower first ionisation energy** than expected by the general trend as a result of the energy difference between the 2s and 2p sub-shells. The electron is being removed from a **higher energy level** that is further from the nucleus, so the electron is held less strongly.

Oxygen has a lower first ionisation energy than would be otherwise expected due to **repulsion** within the 2p orbital when two electrons with opposite spins are placed in the same orbital. This repulsion is **destabilising** in comparison to the configuration of nitrogen and allows the electron to be removed from oxygen more easily.

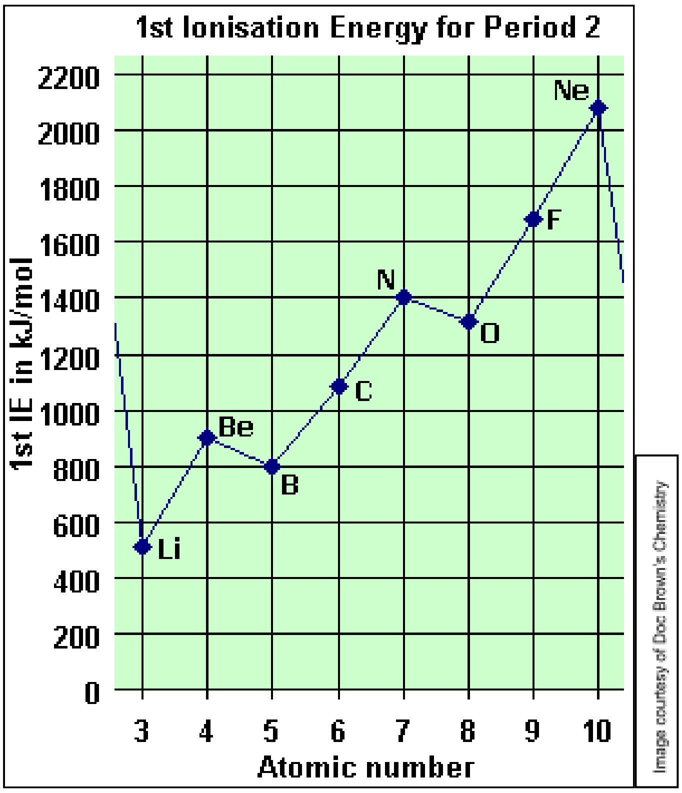


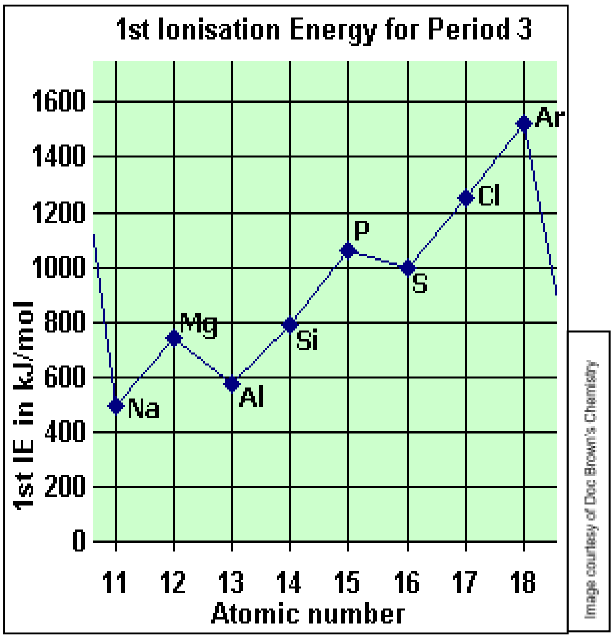
Image courtesy of Doc Brown's Chemistry

Period 3

First ionisation energies follow a **general increasing trend** along Period 3. This is due to the decreasing atomic radius and increasing nuclear charge meaning outer electrons are **held more strongly**.

Aluminium and sulfur are **exceptions** to this trend. **Aluminium** has a **lower first ionisation energy** than expected by the general trend as a result of the energy difference between the 3s and 3p sub-shells. The electron is being removed from a **higher energy level** that is further from the nucleus, so it is held less strongly.

Sulfur has a lower first ionisation energy than would be otherwise expected due to **repulsion** within the 3p orbital when two electrons with opposite spins are placed in the same orbital. This repulsion is **destabilising** in comparison to the configuration of phosphorus and allows the electron to be removed from sulfur more easily.



Equilibria (Acid–Base)

Acid-base equilibria involve the **transfer of protons** between substances. Therefore, substances can be classified as acids or bases depending on their interaction with protons.

A Brønsted-Lowry **acid** is a **proton donor**. For example, ammonium ions (NH_4^+).
A Brønsted-Lowry **base** is a **proton acceptor**. For example, hydroxide ions (OH^-). (An **alkali** is a base which is soluble in water).

An example of some acids and bases are as follows:
Acids- Hydrochloric acid(HCl), Sulfuric acid (H_2SO_4)
Base-Sodium hydroxide(NaOH)

A reaction between an acid and a base to form water and a salt is a **neutralisation reaction**. The ionic equation for neutralisation is:

$$H^+_{(aq)} + OH^-_{(aq)} \rightarrow H_2O_{(l)}$$

Basicity of Group 2 Oxides and Hydroxides

The oxides of group 2 metals become increasingly more basic as you move down the Group.

BeO and $Be(OH)_2$ are both **amphoteric** which means they react with acids and bases. MgO is basic and $Mg(OH)_2$ is weakly basic. The oxides of calcium, strontium, and barium are basic whilst the hydroxides are all strongly basic.

Reactions of Group 2 Hydroxides with Dilute Acids

Group 2 hydroxides react with dilute acid to form **a salt** and **water.** This is a type of **neutralisation** reaction as group 2 hydroxides are basic. The salt formed depends on the acid used:

- **Hydrochloric** acid forms **chloride** salts.
- **Sulfuric** acid forms **sulfate** salts.
- **Nitric** acid forms **nitrate** salts.

Example: Calcium hydroxide with hydrochloric acid

$$\boxed{Ca(OH)_2 + 2HCl \rightarrow CaCl_2 + 2H_2O}$$

Energy and Matter

The Electromagnetic Spectrum

The relationship between the energy **absorbed** or **emitted** and the **frequency** of the line produced in the spectra is as follows:

$$\Delta E = h\nu$$

E = energy of the light
h = planck's constant
ν = *frequency of light*

The relationship between the **wavelength** and **frequency** of a particular colour of light and the **speed of light** is as follows:

$$c = \lambda\nu$$

c = speed of light
λ = wavelength
ν = *frequency of light*

Visible Light

The visible light region of the electromagnetic spectrum in the order of decreasing wavelength and increasing frequency and energy are as follows: **infrared**, **visible**, **ultraviolet**.

Absorption and Emission Atomic Spectra

Each element has a unique **electronic configuration** that means that each element has its own specific set of energy levels. This arrangement of energy levels act as the atom's **fingerprint**.

Emission

Atoms can absorb **electromagnetic radiation** of the correct energy and **promote** electrons to a higher energy level. As the electrons 'fall' back down to their ground state they release electromagnetic radiation. The light emitted has different wavelengths, this is called the **emission spectrum**, in this spectrum only certain wavelengths (of certain colours) of light are seen. These colours are produced by the atom releasing a photon as the electrons return to ground state, this photon's energy is equal to the energy difference between the two energy levels (ΔE).

Absorption

If a photon with an energy the same as the gap between two energy levels hits an atom, then the electron in the lower energy level can absorb the energy and be **promoted** to the higher energy level. The photon will not be absorbed if its energy does not correspond to the difference between two energy levels.

To obtain an **absorption spectra** white light is shined on the material that is being investigated. White light is used as it contains all the wavelengths of visible light. The gaps found in the absorption spectra correspond to energies for which there is a difference in **energy levels** for the particular element; they appear as gaps as this is where the wavelengths have been absorbed.

The absorption spectrum is the exact *inverse* of the emission spectrum.

The table below shows some of the similarities and differences between absorption and emission spectra:

Similarities	Differences
Both are line spectra	Emission spectrum consists of bright/coloured lines on a black background
The lines are in same position for a given element	Absorption spectra consist of black lines on coloured/bright background.
The lines become closer at higher frequencies	
They are both a series of lines representing transitions to or from a particular energy level	

Flame Tests

The basis of flame tests is that different metal ions produce different **flame colours** when they are heated strongly. The process of a flame test:

1) A nichrome wire loop is cleaned using concentrated hydrochloric acid until it produces no colour when placed in a blue bunsen burner flame.
2) The wire is dipped into a solid sample of the compound being tested
3) The loop is inserted into the **blue** flame on a bunsen burner
4) The colour flame produced will be observe and recorded

Metal Ion	**Colour of Flame**
Li^+	Red
Na^+	Yellow
K^+	Lilac
Ca^{2+}	Orange-red
Ba^{2+}	Green
Cu^{2+}	Blue-green

Mass Spectrometry

Mass spectrometry is an **analytical technique** used to identify different molecules and find the overall relative molecular mass.

Time of Flight (TOF) Mass Spectrometry

TOF mass spectrometry records the time it takes for ions to reach a detector. Using this, **spectra** can be produced showing **each isotope present along with their relative abundances**.

1. **Ionisation** - A sample is **vaporised** and injected into the mass spectrometer where a **high voltage** is passed over the chamber. This causes electrons to be removed from the atoms 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 the path is dependent on the charge and mass of the ion.

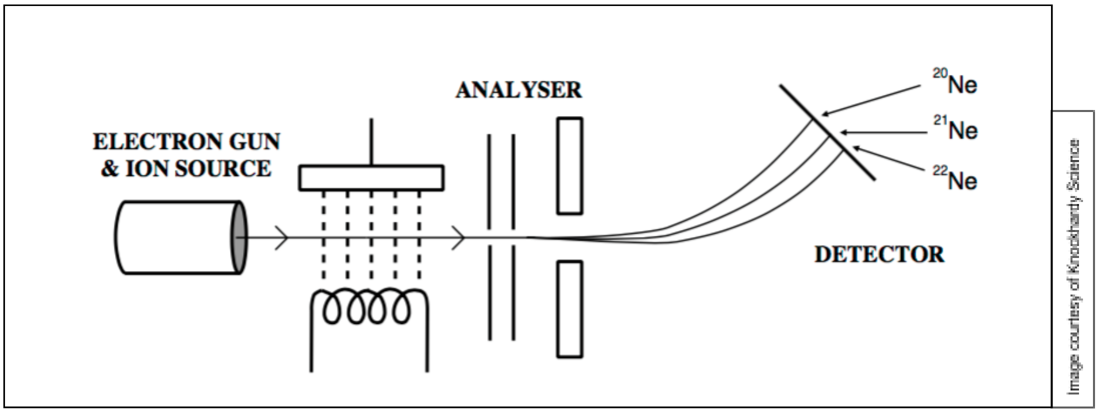
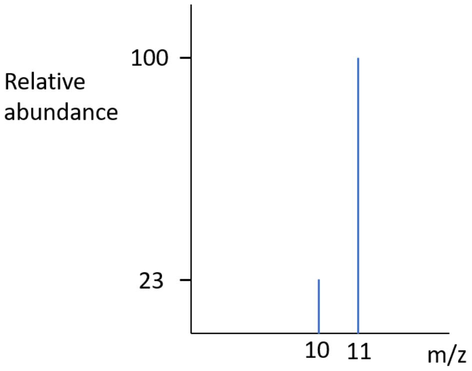


Image courtesy of Knockhardy Science

4. **Detection** - When the positive ions hit the negatively charged detection plate, they **gain an electron,** producing a **flow of charge**. The greater the current produced, the greater the abundance of that particular ion.

5. **Analysis** - The 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.

A graph is produced with the **mass to charge ratio (m/z)** on the x axis and **relative abundance** on the y axis:



Relative Abundance of Isotopes

This graph can be used to calculate the isotopic abundance of ^{10}B:

$$23 \div (100 + 23) = 0.187$$

To calculate the relative atomic mass of an atom of boron:

$$(10 \times 23) + (11 \times 100) = 1330$$

$$1330 \div (23 + 100) = 10.8$$

Molecular Mass

The molecular ion peak (**M^+**) is the peak with the **greatest mass to charge ratio**. The molecular mass of a compound is equal to the m/z value of this peak. This is the peak that is furthest to the right on the spectrum.

M^{+1} peak

The M^{+1} peak is a tiny peak which is 1 unit to the right of the molecular ion peak. This is **caused by the presence of the ^{13}C isotope** (the relative abundance of ^{13}C is 1.11%). ^{13}C has one more neutron than ^{12}C meaning that the relative formula mass is increased by 1.

The relative heights of the M^+ and M^{+1} peaks can be used to predict the number of carbon atoms (n) in a molecule:

$$n = \frac{100}{1.1} \times \frac{\text{abundance of } M^{+1} \text{ ion}}{\text{abundance of } M^{+} \text{ ion}}$$