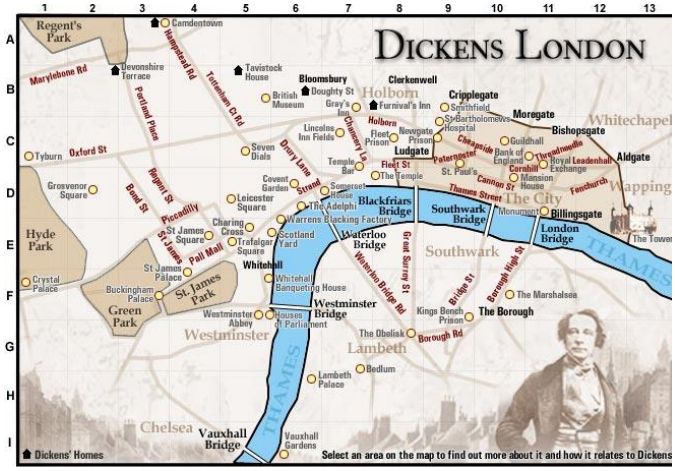
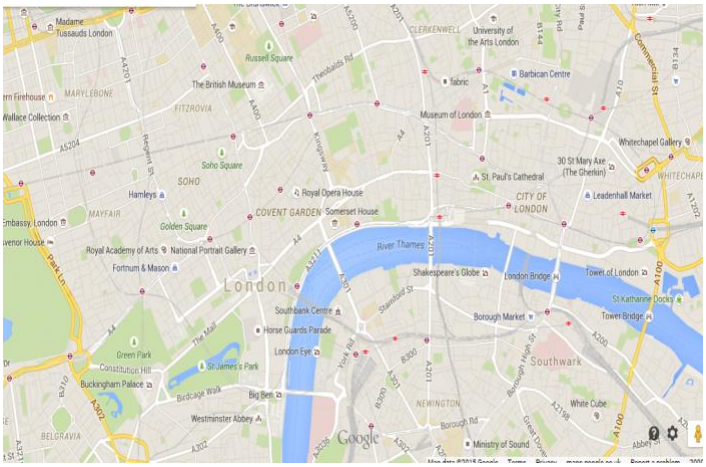
1.1 Atomic structure

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.

Joseph J Thompson (1906) ‘Plum – Pudding’ model of an atom.

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

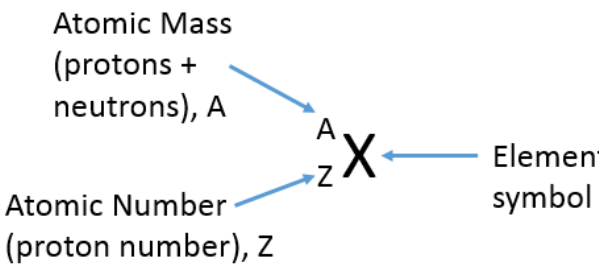
Louis De Broglie (1923) Wave particle duality

Erwin Shrodinger (1926) Atomic orbitals

James Chadwick (1932) Discovery of the neutron

Atomic structure

Protons, electrons and neutrons



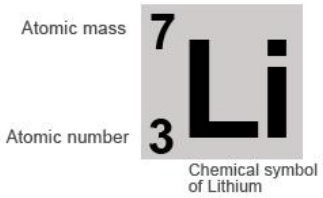
Particle	Mass	Charge	Working out
Proton	1	+1	bottom
Electron	1/1890	-1	bottom
Neutron	1	0	top - bottom

- Different atoms have different numbers of protons and neutrons (and electrons).
- This means that atoms of different elements atoms **must** have different masses.

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

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

Examples:-



- **Mass number -** the total number of **protons and neutrons = 7**
- **Atomic number - the number of protons = 3**
- **Atoms are neutral - 3 protons and 3 electrons**.
- **Number of neutrons - 7 - 3 = 4 neutrons**.

A quick method is:

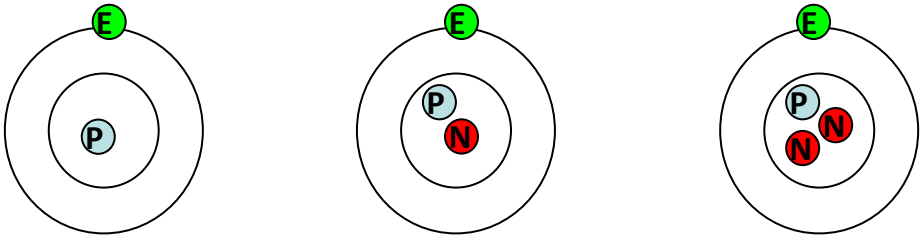
Protons	bottom number	3
Electron	bottom number	3
Neutrons	top – bottom number	7 - 3 = 4

Isotopes

> ***Isotopes - atoms of the same element that has the same number of protons and electrons but a different number of neutrons.***

- Isotopes have the same chemical properties as they have the **same number of electrons in the outer shell**
- All elements have the **same number of protons**

Hydrogen can be used as an example:-



Hydrogen – 0 Neutrons	Hydrogen – 1 Neutron (deuterium)	Hydrogen – 2 Neutrons (tritium)
^{1}H	^{2}H	^{3}H

Chemical symbols:

$^{23}_{11}Na$: P = 11
e = 11
N = (23 - 11) = 12

$^{23}_{11}Na^{+}$: P = 11
e = (11- 1) = 10
N = (23 - 11) = 12
(+)ve ions lose electrons

$^{16}_{8}O^{2-}$: P = 8
e = (8 - 2) = 6
N = (16 – 8) = 8
(-)ve ions gain electrons

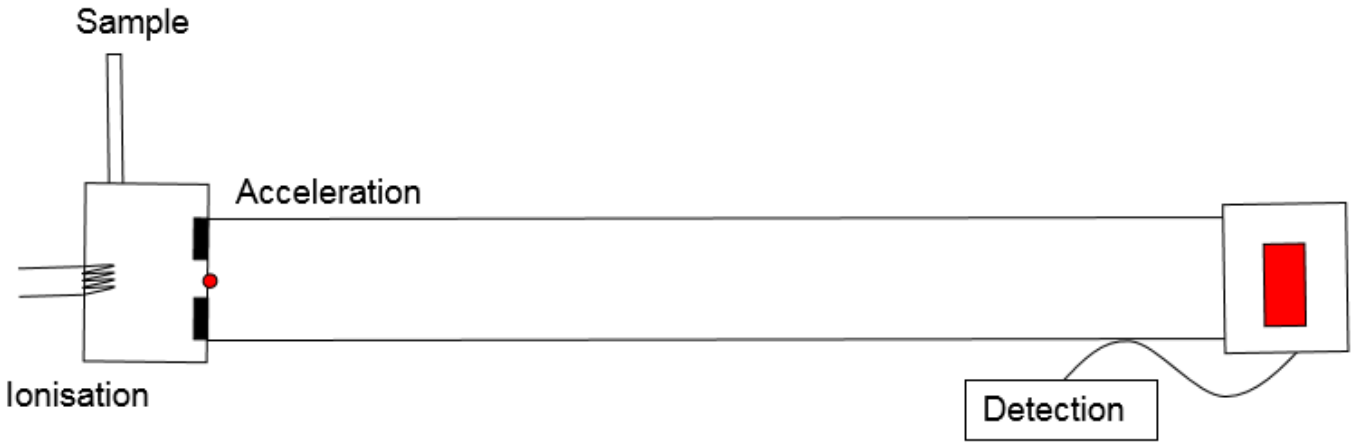
$^{37}_{17}Cl$: P = 17
e = 17
N = (37 - 17) = 20

$^{35}_{17}Cl$: P = 17
e = 17
N = (35 - 17) = 18

Questions:

Symbol	Atomic number	Mass number	Number of protons	Number of electrons	Number of neutrons
Mg atom					
F atom					
Ca^{2+} ion					
S^{2-} ion					
Al^{3+} ion					
^{54}Fe					
^{56}Fe					

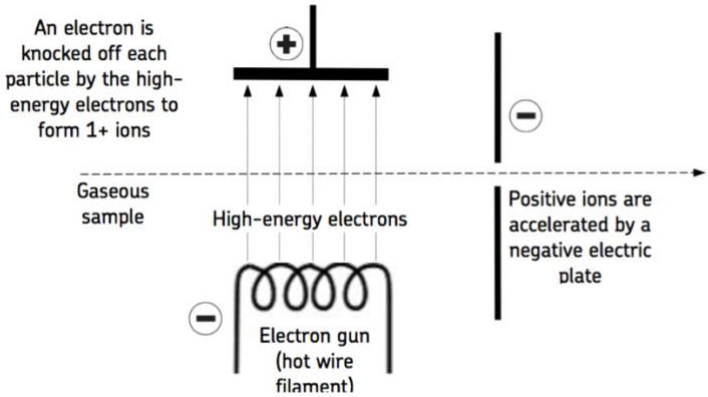
The mass spectrometer:



How a mass spectrometer works:

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:

$$M_{(g)} + e^- \rightarrow M^+_{(g)} + 2e^-$$

Or simplified:

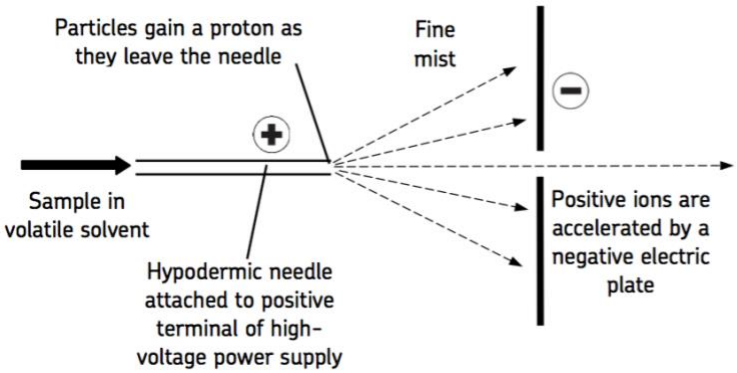
$$M_{(g)} \rightarrow M^+_{(g)} + e^-$$

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

$$CH_{4(g)} \rightarrow CH_4{}^+_{(g)} + e^-$$

- 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 = 1/2mv²**
- 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 = kinetic energy of particle (J)

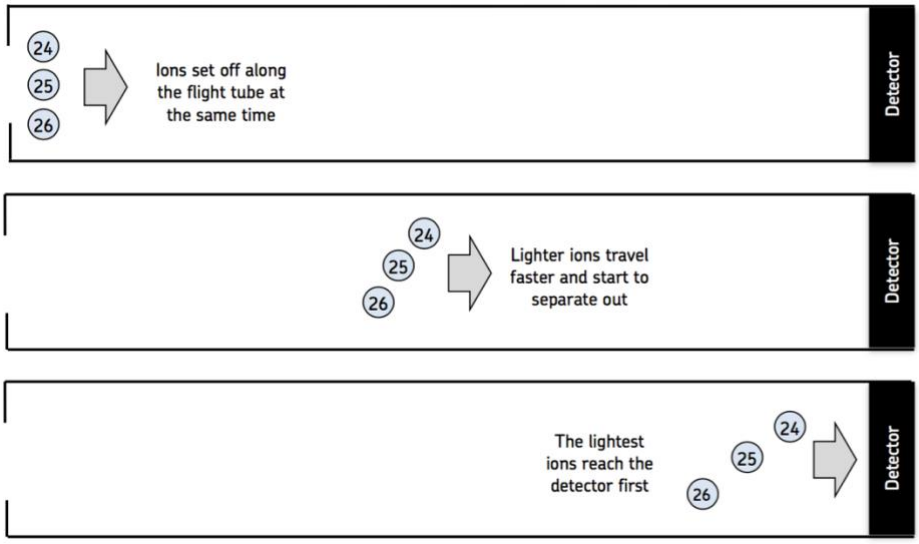
m = mass of the particle (kg)

v = 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:

$$t = \frac{d}{v}$$

$$t = d\sqrt{\frac{m}{2KE}}$$

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

t = time of flight (s)

d = length of flight tube (m)

v = velocity of the particle (m s^{-1})

m = mass of the particle (kg)

KE = 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

$$M^+_{(g)} + e^- \rightarrow M_{(g)}$$

$$^{16}O^+_{(g)} + e^- \rightarrow {}^{16}O_{(g)}$$

- 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 of air**
- The sample **must be ionised** in order to be **accelerated and detected.**

Calculations in TOF Mass Spectrometry

Formula: **$KE = \frac{1}{2}mv^2$** **$v = d/t$** **$L = 6.022 \times 10^{23}$**

Where:

KE:	**J**	**d:**	**m**
m:	**kg**	**t:**	**s**
v:	**ms^{-1}**		

Calculating the mass of an ion (in kg)

- **Avogadro's constant, L**, is the number of ions present in a sample with a mass equal to its relative isotopic mass in g - **Avogadro's constant, L = 6.022×10^{23}**

Example:

24g of $^{24}Mg^+$ ions contains 6.022×10^{23} ions

24×10^{-3} kg of $^{24}Mg^+$ ions contains 6.022×10^{23} ions

This means the mass of one $^{24}Mg^+$ ions in kg $= \frac{24 \times 10^{-3}}{6.022 \times 10^{23}} = 3.985 \times 10^{-26}$ kg

A mathematical representation:

$$\textit{Mass of one ion (kg)} = \frac{\textit{relative isotopic mass} \times 10^{-3}}{6.022 \times 10^{23}}$$

Calculate the mass, in kg of the following ions:

1) $^{40}K^+$

2) $^{19}F^+$

3) $^{35}Cl^+$

4) $^{40}Ar^+$

Calculating kinetic energy (KE) or velocity of an ion:

- **KE = ½mv^2**
- **Mass must be in kg**
- **v = d/t**

Example:

1) A $^{40}Ca^+$ ion is accelerated to a velocity of 5.643 x 10^4 ms^{-1} n a mass spectrometer. What is its kinetic energy:

$$\text{Mass} = \frac{\text{relative isotopic mass} \times 10^{-3}}{6.022 \times 10^{23}}$$

$$\text{Mass} = \frac{40 \times 10^{-3}}{6.022 \times 10^{23}} = 6.642 \times 20^{-26} \text{ kg}$$

$$\text{KE} = ½mv^2$$

$$\text{KE} = 0.5 \times 6.642 \times 10^{-26} \times (5.643 \times 10^4)^2$$

$$\text{KE} = 1.058 \times 10^{-16} \text{ J}$$

2) A $^{100}Ru^+$ ion travels through the flight tube with an energy of 5.77 x 10^{-16} J. Calculate the velocity of the ion:

$$\text{Mass} = \frac{\text{relative isotopic mass} \times 10^{-3}}{6.022 \times 10^{23}}$$

$$\text{Mass} = \frac{100 \times 10^{-3}}{6.022 \times 10^{23}} = 1.661 \times 20^{-25} \text{ kg}$$

$$\text{KE} = ½mv^2$$

$$v = \sqrt{\frac{2KE}{m}}$$

$$v = (2 \times 5.77 \times 10^{-16} \ / \ 1.661 \times 10^{-25})^{1/2}$$

$$v = 83363 \text{ or } 83400 \text{ ms}^{-1} \text{ (3sf)}$$

Other calculations:

- There are of course other calculations you'll be required to carry out:
  - Distance of flight tube, d
  - Time of flight, TOF, t
- You'll be required to use the following and be able to re arrange them

Mass = $\frac{\text{relative isotopic mass} \times 10^{-3}}{6.022 \times 10^{23}}$ KE = ½mv^2 v = d/t L = 6.022 x 10^{23}

Questions:

1) A sample of ^{14}N were placed in a mass spectrometer.
   a. Calculate the mass of one ion of nitrogen

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

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

(1.135 x 10^{-13} 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 2.0×10^{-6} s. Calculate its kinetic energy.

(1.68 x 10^{-14} J)

3) A sample of Aluminium atoms were placed through a mass spectrometer. The $^{27}Al^{+}$ travelled down a 5m flight tube. Its Kinetic energy is 1.45×10^{-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

(1.965995×10^{-6} J)

4) A $^{79}Se^{+}$ ion travels through the flight tube with an energy of 6.27×10^{-16} J. Calculate the velocity of the ion:

($97765\ ms^{-1}$)

5) A sample of Sodium atoms were placed through a mass spectrometer. The $^{23}Na^{+}$ travelled down a 3m flight tube. Its Kinetic energy is 1.63×10^{-14} J.
Calculate its time of flight. Give your answer to 3 significant figures

(3.247×10^{-6} J)

6) A $^{86}Sr^{+}$ ion travels through the TOF of a mass spectrometer with an energy of 1.921×10^{-15} J.
The ion takes 1.09×10^{-5} s to reach the detector. Calculate the length of the flight tube in metres.
Give your answer to 3 significant figures.

(1.79 m)

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***:

$$KE_a = KE_b$$

$$\frac{m_a \times V_a^2}{2} = \frac{m_b \times V_b^2}{2}$$ Cancel the 2's

$$m_a \times V_a^2 = m_b \times V_b^2$$

For Velocity calculation:

$$V_a^2 = \frac{m_b \times V_b^2}{m_a}$$

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

For Time of flight calculation:

$$m_a \times V_a^2 = m_b \times V_b^2$$

$$\frac{m_a \times d^2}{t_a^2} = \frac{m_b \times d^2}{t_b^2}$$ 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:

$$m_a V_a^2 = m_b V_b^2 \qquad \frac{m_a}{t_a^2} = \frac{m_b}{t_b^2}$$

Questions:

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

(1.16×10^{6} ms^{-1})

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

(1.26×10^{-6} s)

3) A sample of copper atoms were placed through a mass spectrometer. Copper atoms contain 2 isotopes: ^{63}Cu and one other.

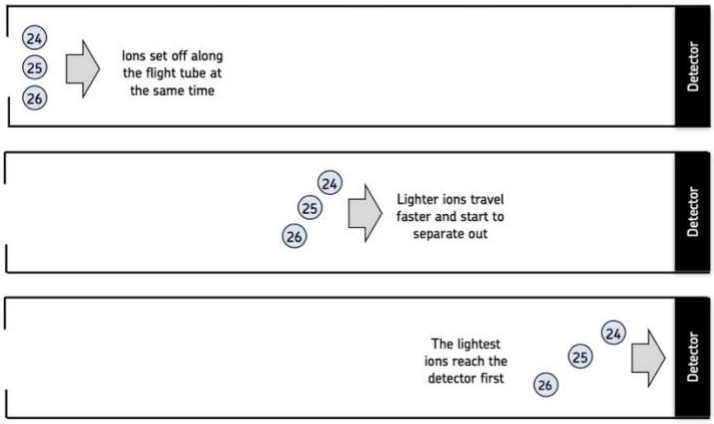
a. Calculate the velocity of the ^{63}Cu if it travels down a 5m flight tube in 4.200×10^{-6} s

b. The other isotope takes 4.266×10^{-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:

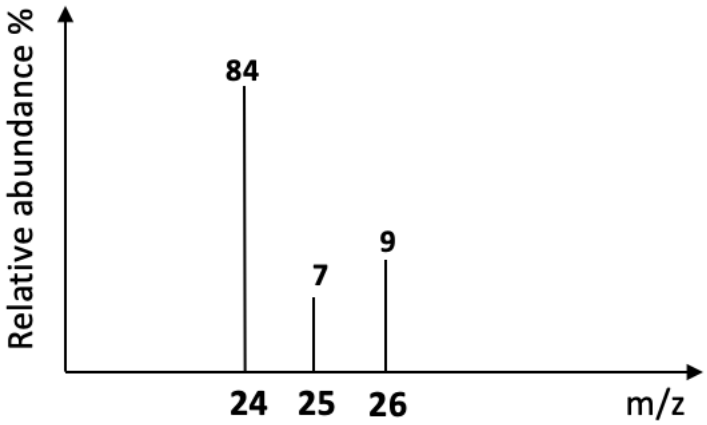
c. Use the Periodic table to calculate the relative abundances of these 2 isotopes

Analysis of Mass Spectra of elements:

- The data is displayed as a plot of relative abundance against mass / charge ratio (m/z) in a 'mass spectrum'.
- If you recall the example using a sample of Mg:



- This would be shown as:



- 3 peaks = 3 isotopes of Mg
- ^{24}Mg is the most abundant. It generates the biggest current at the detector.
- The relative atomic mass of Mg is however 24.3 (from the Periodic table).
- This is the weighted mean mass of all of the isotopes.

Relative masses:

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

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

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

$^{24.3}$Mg:

Is the weighted mean mass of the ^{24}Mg, ^{25}Mg and ^{26}Mg taking into account their abundancies.

Calculating Relative Atomic Mass (RAM) from abundance)

Use the formula:

$$\text{RAM} = \frac{\sum \text{(Abundance x m/z)}}{\text{Total Abundance}}$$

$$\text{RAM} = \frac{\text{(Abundance x m/z) + (Abundance x m/z) + ...}}{\text{(Abundance + Abundance + ...)}}$$

Worked example for Mg:

$$\text{RAM} = \frac{(84 \times 24) + (7 \times 25) + (9 \times 26)}{100}$$

$$\text{RAM} = 24.3$$

The information mav be tabulated:

RAM of Neon isotopes	Abundance %
20	90.9
21	0.2
22	8.9

Calculation

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

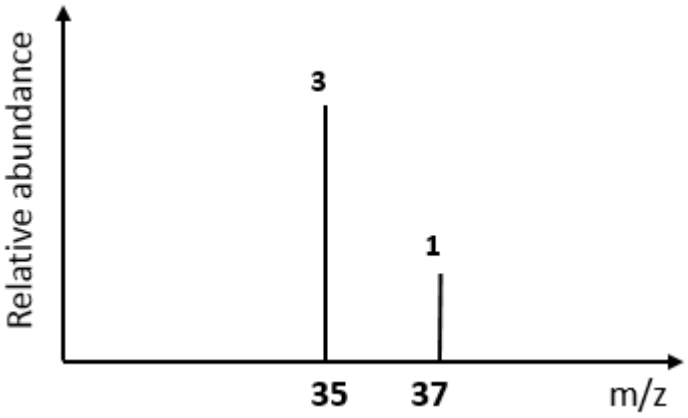
RAM = 20.18

Practise Questions:

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

RAM of silicon isotopes	% Abundance
28	**92.2**
29	**4.7**
30	**3.1**

2) Calculate the RAM from the spectra given below:



Tip: it doesn't matter how the abundances are given: They could be %, g, relative abundance or number of atoms

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

4) Chlorine exists as 2 naturally occurring isotopes ^{37}Cl and ^{35}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}Xe, is missing.

Isotope	**^{129}Xe**	**^{131}Xe**	**^{132}Xe**	**^{m}Xe**
% abundance	28.0	25.0	27.0	To be calculated

Use the data to calculate the abundance of isotope ^{m}Xe and calculate m, the mass number of ^{m}Xe. Show your working.

Mass spectrometry and molecular elements

- Bromine has two isotopes, ^{79}Br and ^{81}Br, in the ration 1:1.
- In a mass spectrometer bromine forms ions with formula $[Br_2]^+$ but also Br^+ ions
- This will give multiple peaks in the mass spectrum

There are 5 possibilities that exist:

Ions of atoms:

Ion:	$^{79}B^+$		^{81}Br
m/z =	79		81
Ratio	1	:	1

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

Ions of molecules:

Ion:	$[^{79}Br – ^{79}Br]^+$		$[^{79}Br – ^{81}Br]^+$		$[^{81}Br – ^{79}Br]^+$		$[^{81}Br – ^{81}Br]^+$
m/z =	158		160		160		162
Calc:	(1 x 1)		(1 x 1)		(1 x 1)		(1 x 1)
Ratio:	1	:	1	:	1	:	1
Ratio:	1	:			2	:	1

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:

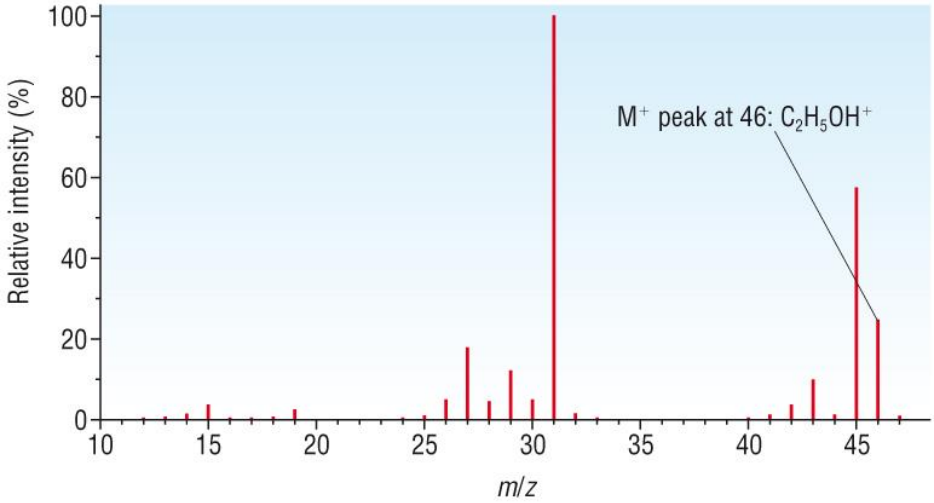
Question

- Chlorine has two isotopes, ^{35}Cl and ^{37}Cl, in a 3: 1 ratio.
- In a mass spectrometer chlorine forms ions with formula $[Cl_2]^+$
  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:

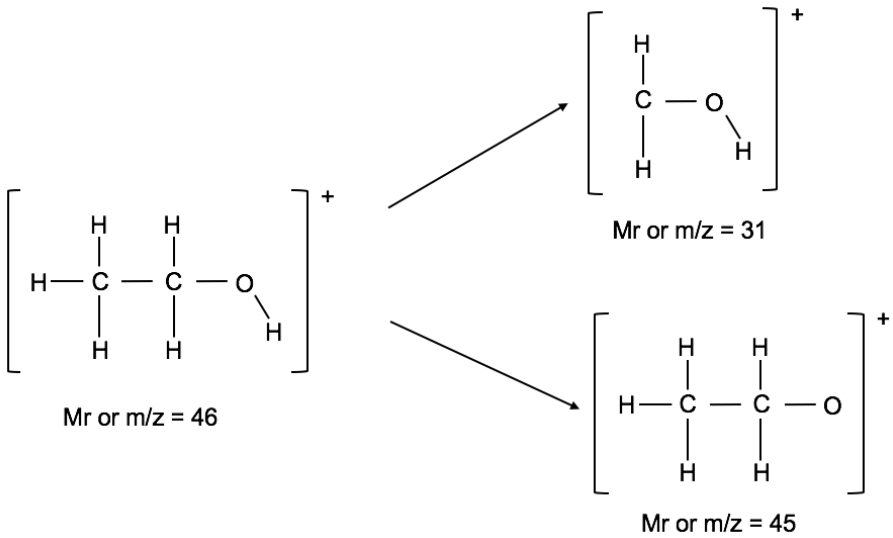


Mr of C_2H_5OH = 46

- Highest **m/z = Mr** of the molecule. This is called the **molecular ion peak, M^+**

$$C_2H_5OH \rightarrow C_2H_5OH^+ + e^-$$

- The fragments are caused by the molecule breaking apart under the conditions in the ionisation chamber in the spectrometer.

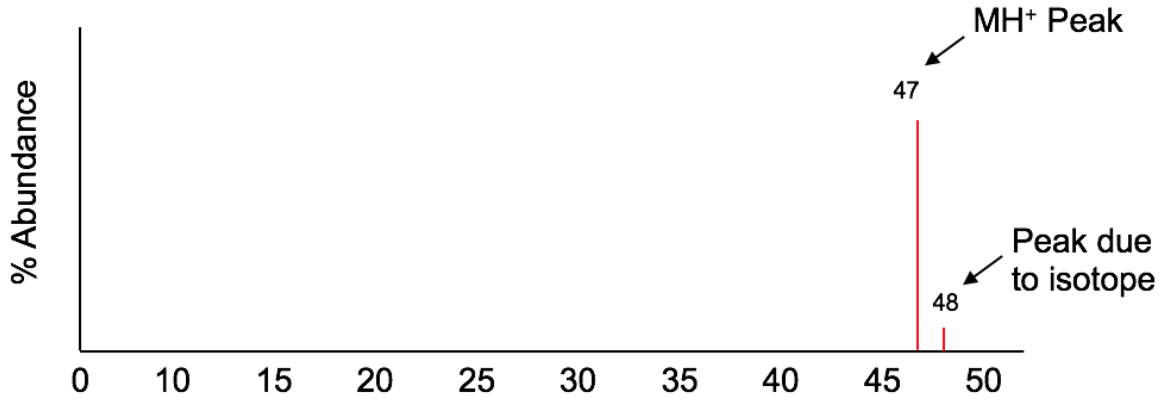


b) Using electrospray ionisation:

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

$$\mathbf{M + H^+ \rightarrow MH^+}$$

$$C_2H_5OH + H^+ \rightarrow C_2H_5OH_2^+$$

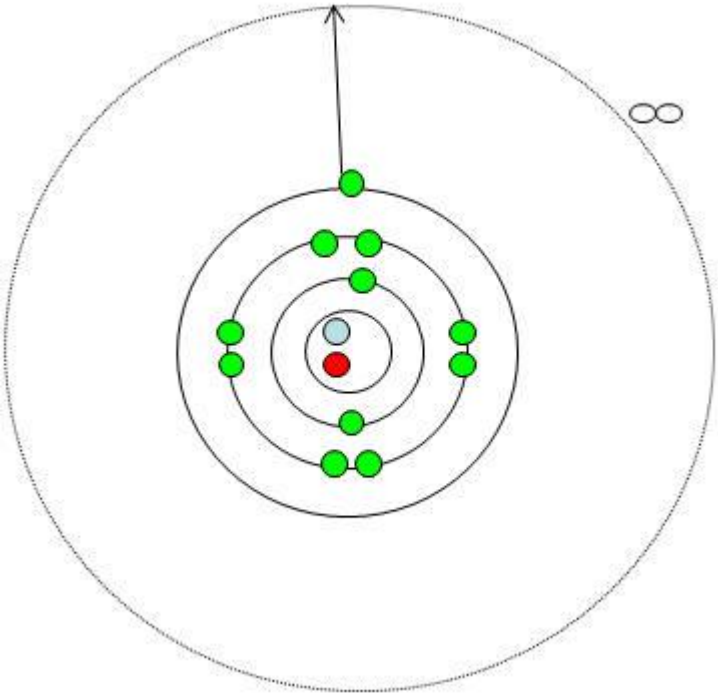


- No fragments are made during this process
- Highest **m/z = Mr + 1** of the molecule. This is called the **MH^+** peak.
- To get the Mr, you need to take 1 away from the **MH^+** peak.

	Electron impact	**Electrospray ionisation**
Ion	M^+ = Mr	MH^+ Mr = MH^+ - 1
Used for	Atoms / small molecules	Large molecules
Fragmentation	Yes	No

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=∞.
- At n=∞ the electron has sufficient energy to escape the attraction from the nucleus.

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

1st ionisation energy:

$Ca_{(g)} \rightarrow Ca^{+}_{(g)} + e^{-}$ **1st IE = +590 KjMol^{-1}**

2nd ionisation energy:

$Ca^{+}_{(g)} \rightarrow Ca^{2+}_{(g)} + e^{-}$ **2nd IE = +1150 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 from the positive nucleus.
    - Distance always outweighs any other changes

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) 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.

- Always finish the explanation by referring to Attraction & Energy

S: Shells – More / Same / Less (this is distance)

S: Shielding – More / Similar / Less

P: Protons – More / Same / Less

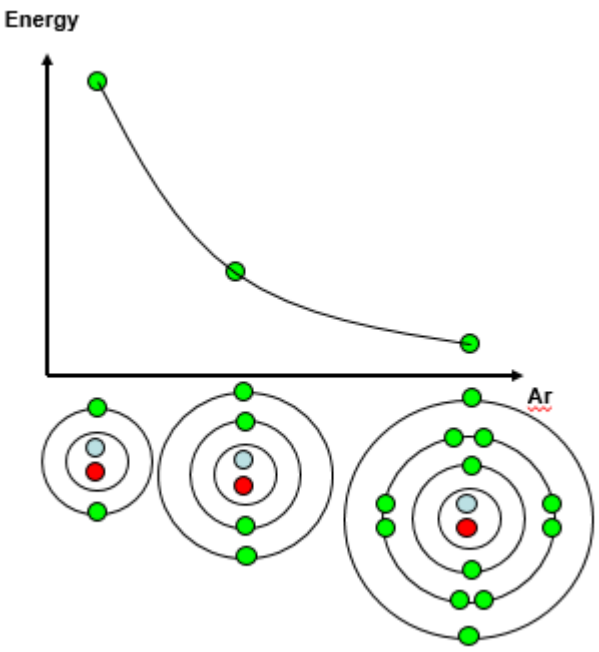
A: Attraction – More / Less – ***Between*** *positive protons in the nucleus & outer negative electron*

E: Energy – More / Less

*Shielding is never the same as shells move in / out slightly due to the removal / addition of electrons.

Trends in Ionisation energies:

1) Ionisation energies down a Group



As you go down a group:

S: More Shells

S: More shielding

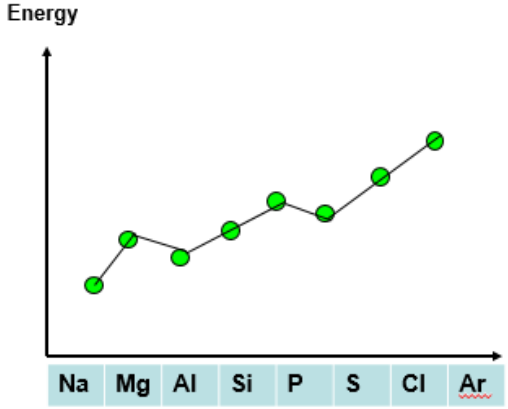
P: More protons so an Increase in nuclear charge (outweighed by above)

A: Less attraction *between* positive protons in the nucleus & outer negative electron

E: Less energy required

2) Ionisation energies across a period

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



S: Same Shells

S: Similar shielding

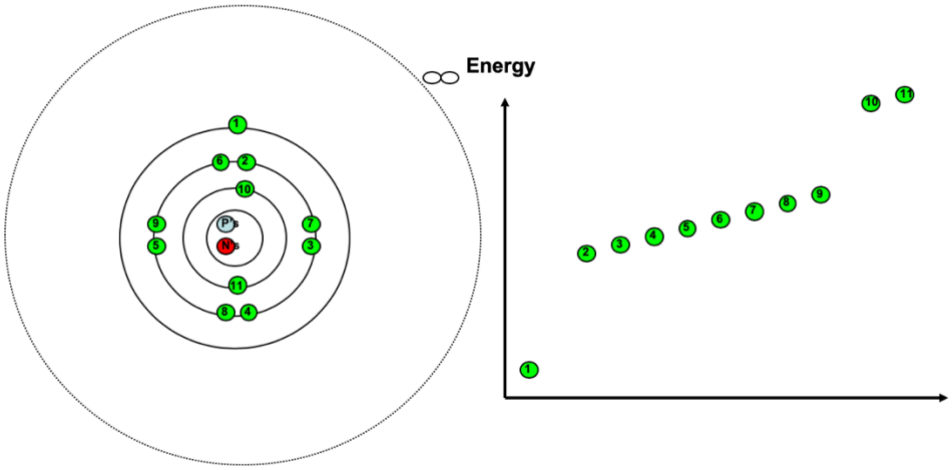
P: More protons

A: More attraction *between* positive protons in the nucleus & outer negative electron

E: More energy required

- However it is not a straight / linear line.
- There are dips showing the model must be more complex (later)

3) Successive ionisation energies – removed from the same atom



$Na_{(g)}$	→	$Na^{+}_{(g)}$	+	e	Removed from 3rd shell - lowest
$Na^{+}_{(g)}$	→	$Na^{2+}_{(g)}$	+	e	Removed from 2nd shell – big jump
$Na^{2+}_{(g)}$	→	$Na^{3+}_{(g)}$	+	e	Removed from 2nd shell – small increase
$Na^{3+}_{(g)}$	→	$Na^{4+}_{(g)}$	+	e	Removed from 2nd shell – small increase

- Large jumps indicate movement to another **electron shell closer to the nucleus**
- Large jump between 1st & 2nd indicates that element has 1 electron in its outer shell.
- This means it must be in Group 1
- These patterns are often given in a table:

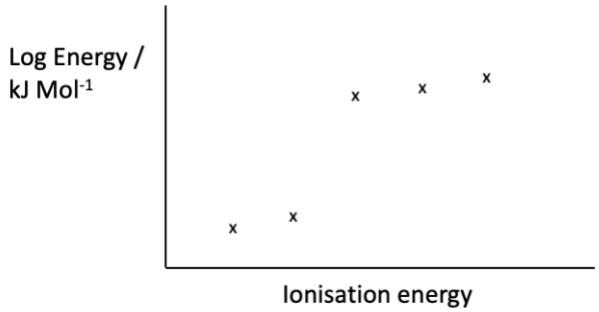
	1st	2nd	3rd	4th	5th	6th	7th	8th	9th	10th	11th
Ionisation energy / kJ mol^{-1}	324	1024	1134	1179	1243	1296	1316	1398	1476	17689	18768

Explanation:

Removing an electron in the same shell:	**Removing an electron from an inner shell:**
Explanation: Electrons are being removed from a more and more positive ion. **A: Attraction increases** **E: Energy required increases – Small amount**	**In addition:** **S: Less Shells** **S: Less shielding** **P: Same number of protons** **A: More attraction *between*** positive protons in the nucleus & outer negative electron **E: More energy required – Large amount**

Questions:

1) Using the successive ionisation energies below answer the following questions:



a) Circle the first electron to be removed from the atom in the chart above

b) **State and explain** which Group in the Periodic Table the element belongs

c) Explain why there isn't enough information to identify the element?

d) The Element is in Period 3 on the Periodic Table. Give the Chemical Symbol of the element

2) Use the information in the table below to answer the questions:

	1st	2nd	3rd	4th	5th	6th
Ionisation energy / kJ mol^{-1}	434	564	693	10176	10430	10965

a) **State and explain** which Group in the Periodic Table the element belongs

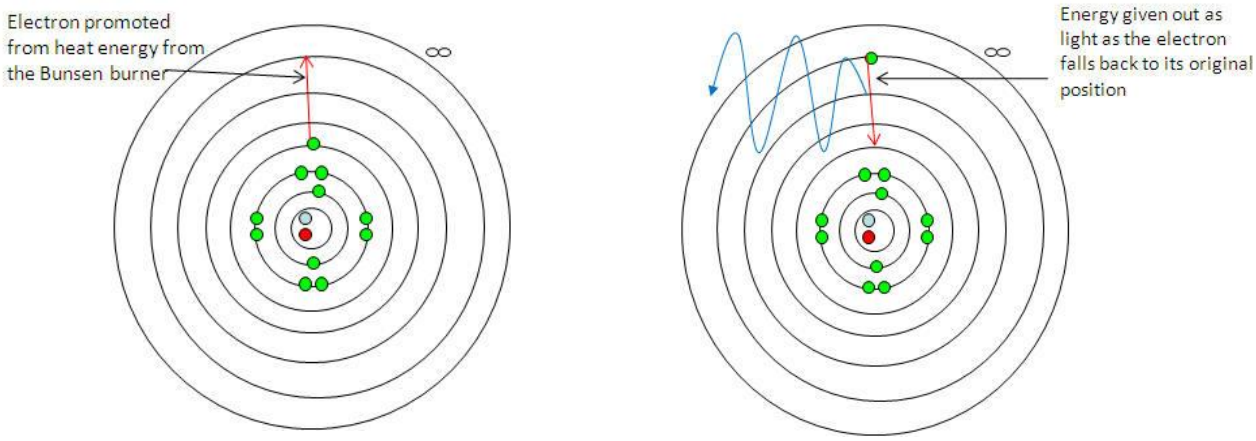
b) Explain why the fourth ionisation energy is very much larger than the third ionisation energy

c) Explain why the there is a gradual increase in ionisation energies from the first to the third

d) The Element is in Period 3 on the Periodic Table. Give the Chemical Symbol of the element

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 and ion.
   - We can promote electrons from a lower electron shell to a higher electron shell by providing heat energy.
   - When the electrons falls back to the lower shell a specific frequency of light is observed.



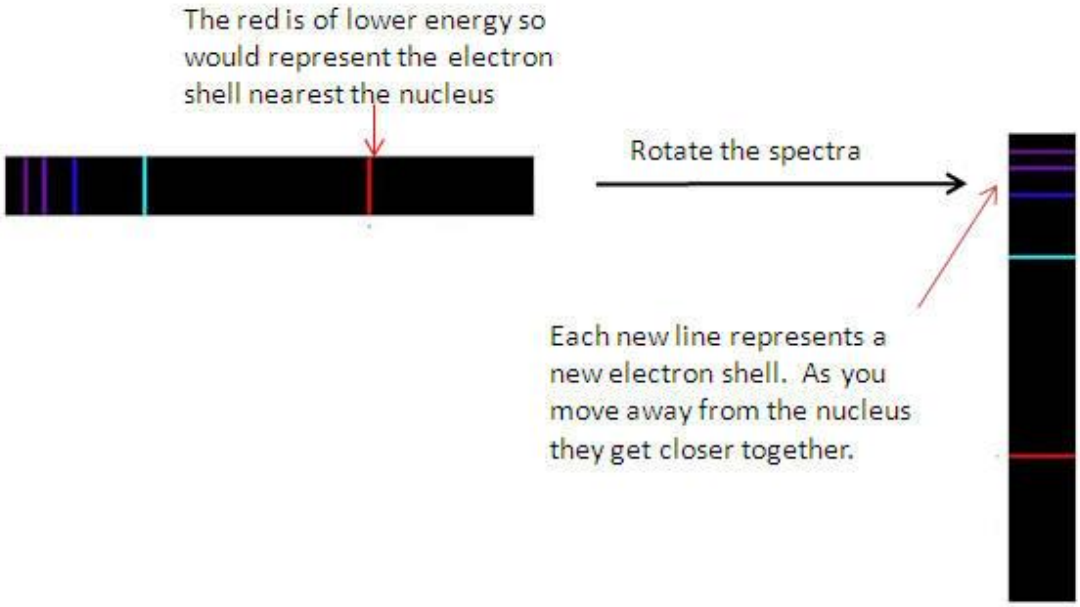
   - This gives us the series of lines as electrons move from higher to lower electron shells.
   - A spectroscope shows us the specific energies characteristic to that element.

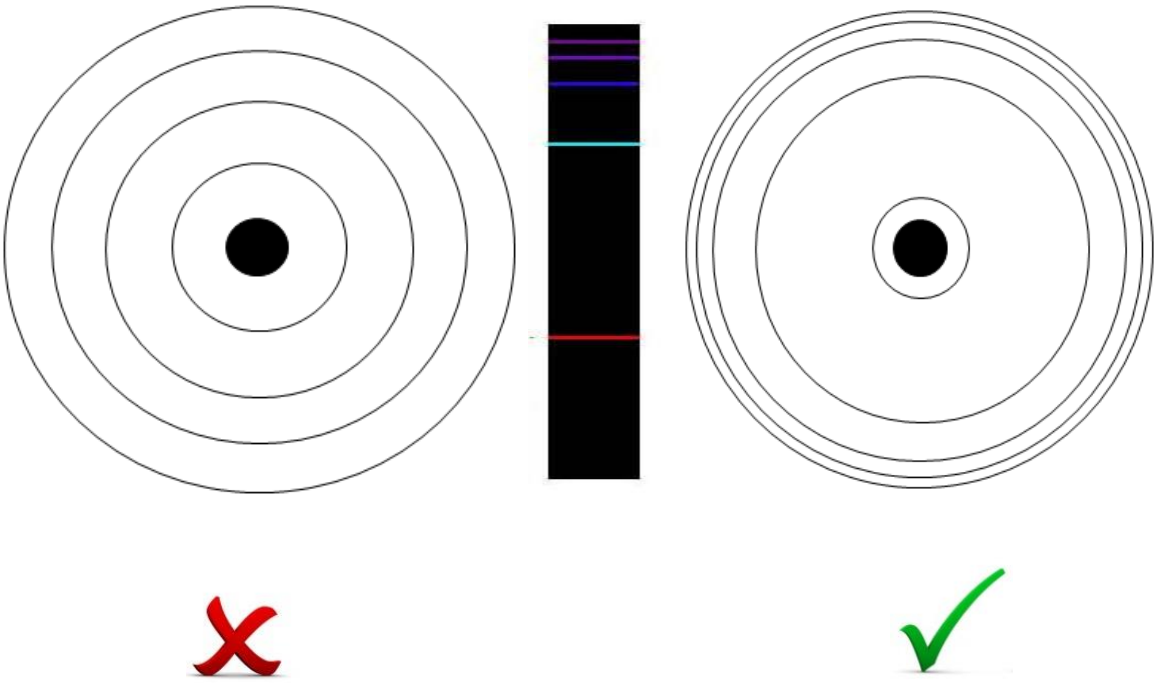
Looking at the line emission spectra 2 thing become apparent:

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

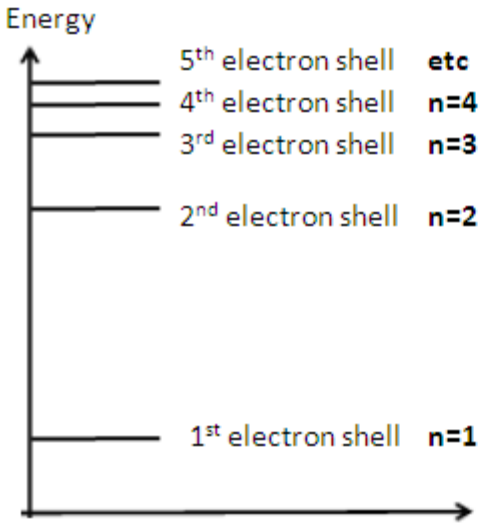
b) That as the move up in energy (towards the violet end) they get closer together (converge)

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





- That the electron shells can be converted into an energy level diagram showing the **Principle Quantum Number, n**



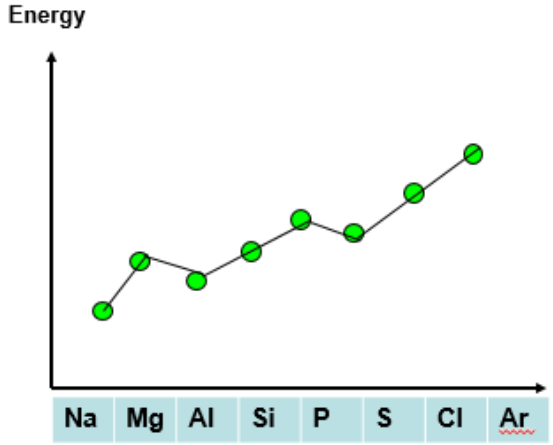
We call these diagrams energy level diagrams and each electron shell is now called '**The Principle Quantum Number, n**'

- 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 = $2n^2$**

Principle quantum number	Number of electrons
1	2
2	8
3	18
4	32

2) Ionisation energies across a period

- **Generally (recap):** There is an increase in ionisation energies across a period.



S: Same Shells

S: Similar shielding

P: More protons

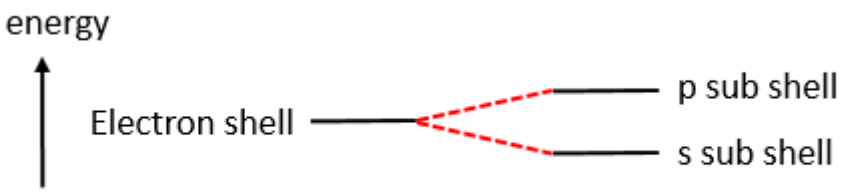
A: More attraction *between* positive protons in the nucleus & outer negative electron

E: More energy required

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

a) 3rd electron easier to remove than 2nd

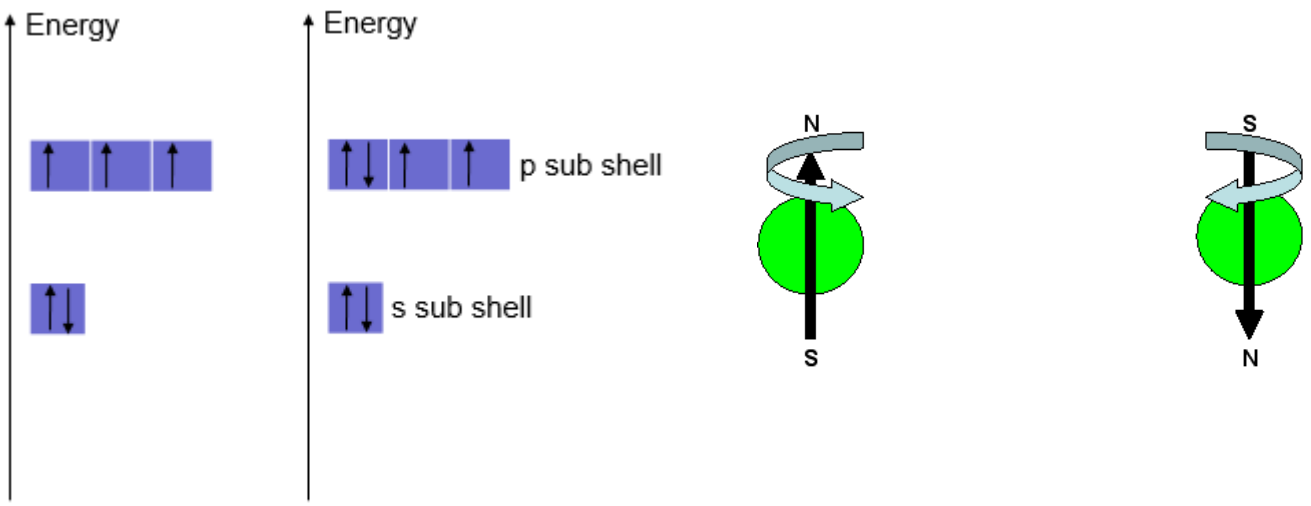
- The 1st 8 electrons are actually in 2 called **subshells** called **s** and **p** which are not at the same energy level. They have slightly different energy levels.



- 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).

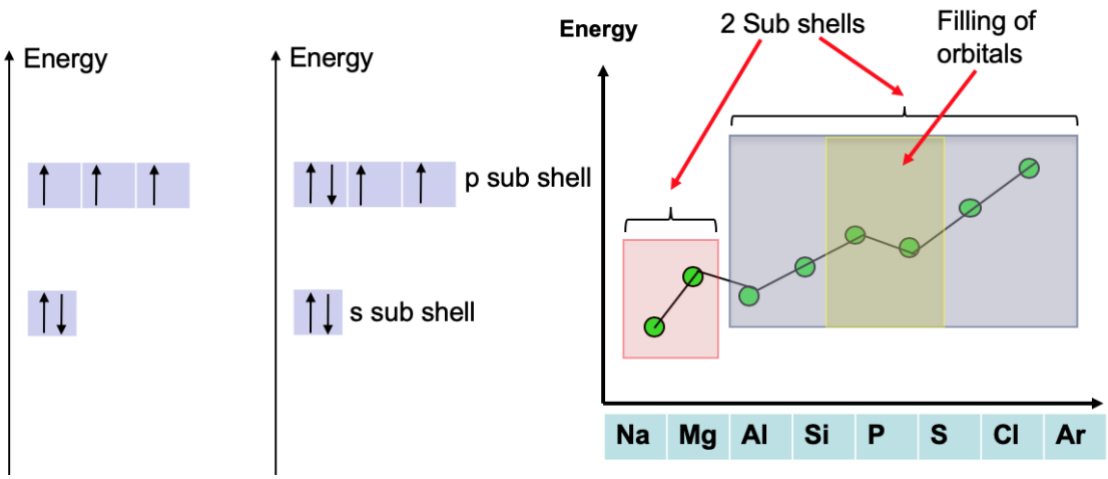
b) 6th electron easier to remove that the 5th

- 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.

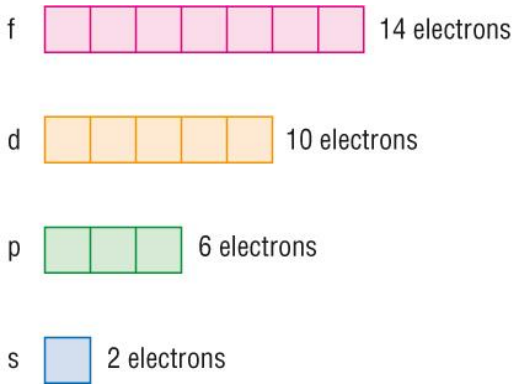


- If electrons are negative and repel each other how can they occupy the same orbital?
- Electrons spin on their axis. When anything with a charge spins a magnetic field is produced.
- One of the electrons in an orbital will spin one way and the other spins in the opposite direction.
- This gives opposing 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.

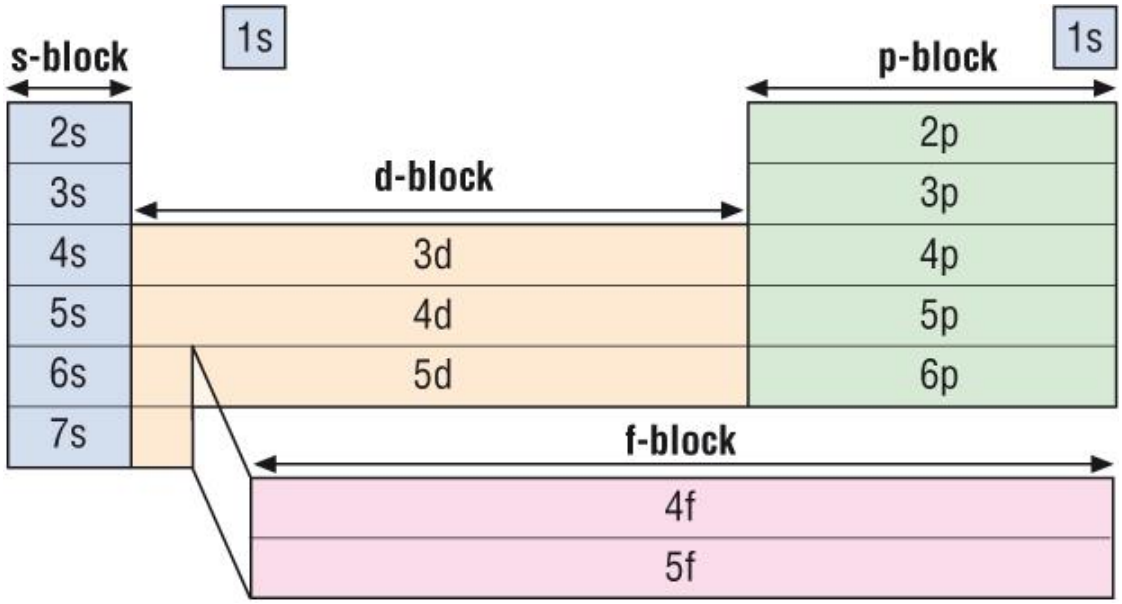


Arranged in 7 orbitals (boxes)

Arranged in 5 orbitals (boxes)

Arranged in 3 orbitals (boxes)

Arranged in 1 orbital (boxes)



A summary of sub shells and orbitals:

<u>n = 3 shell: maximum 18 electrons</u>

Sub - shell	**3s**	**3p**			**3d**				
Orbital									
Electrons	**2e**	**2e**	**2e**	**2e**	**2e**	**2e**	**2e**	**2e**	**2e**

<u>n = 2 shell: maximum 8 electrons</u>

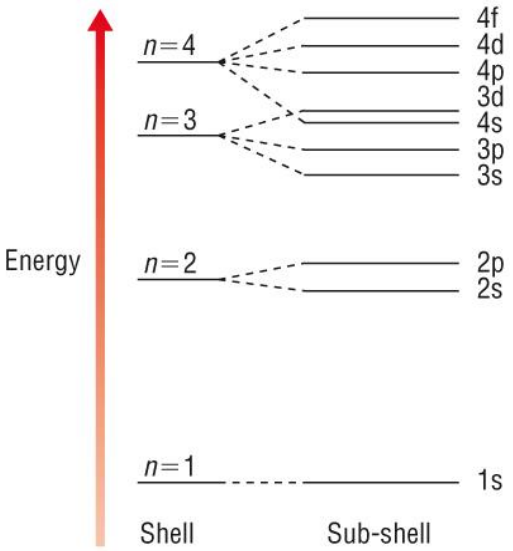
Sub - shell	**2s**	**2p**		
Orbital				
Electrons	**2e**	**2e**	**2e**	**2e**

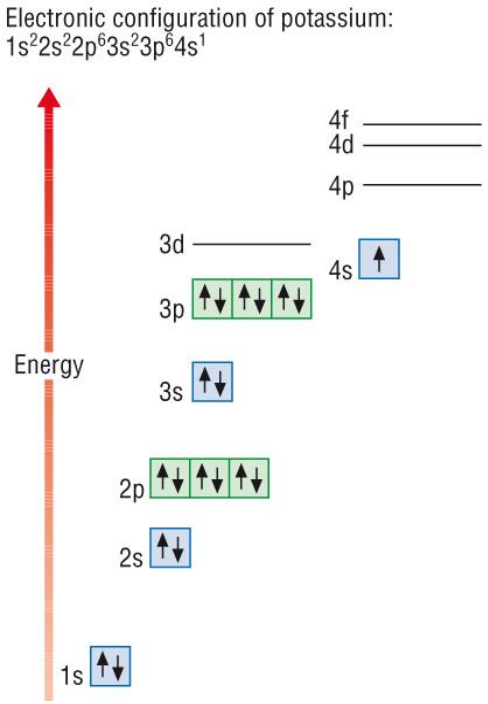
<u>n = 1 shell: maximum 2 electrons</u>

Sub - shell	**1s**
Orbital	
Electrons	**2e**

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**

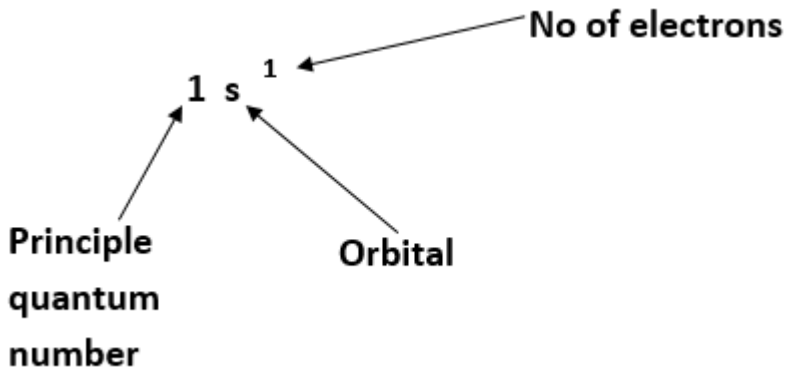




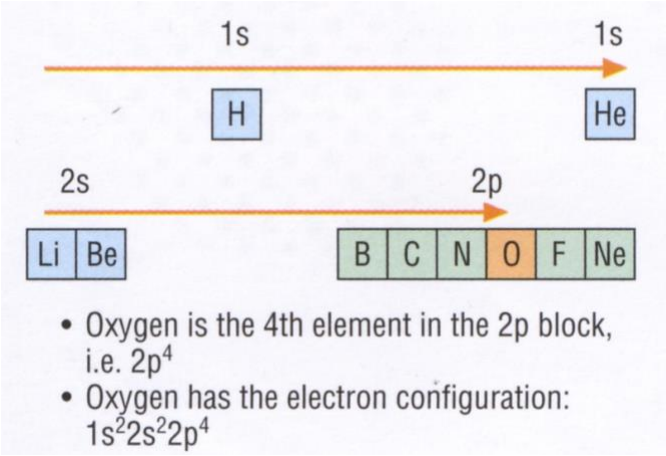
- After 3p it gets a bit complicated
- The 4s energy level is below the 3d energy level.
- This means that the 4s orbital fills before the 3d orbitals. (according to the Aufbau Principle)

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:



Electron configuration from the Periodic Table



Element	Electron configuration
B	**$1s^2 2s^2 2p^1$**
C	**$1s^2 2s^2 2p^2$**
N	**$1s^2 2s^2 2p^3$**
O	**$1s^2 2s^2 2p^4$**

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

Examples:

Na $1s^2\ 2s^2\ 2p^6\ 3s^1$

Sc $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^1\ 4s^2$ * 4s fills before 3d

Shortening an electron configuration

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

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:

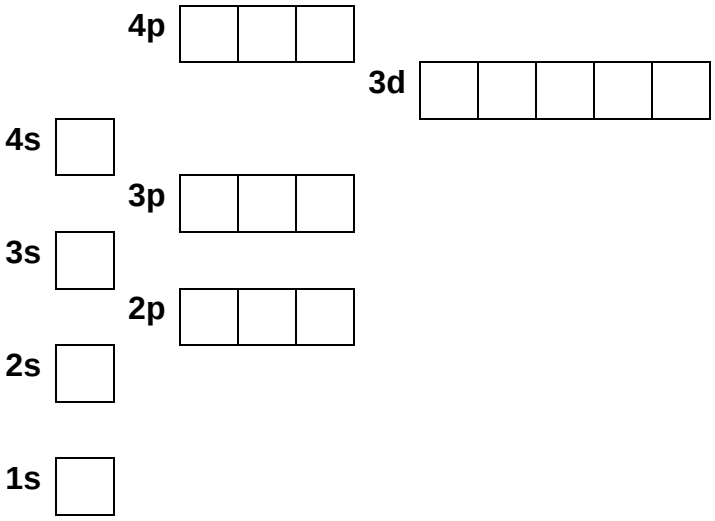
Sc $[1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6]$ $3d^1\ 4s^2$

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

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

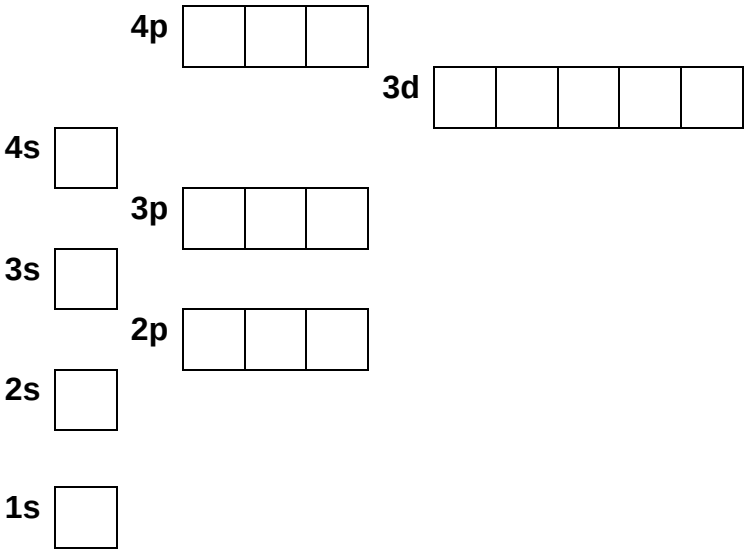
Complete the following FULL electron configurations:

Oxygen



$1s^2$ _____

Silicon



$1s^2$ _____

(i) Nitrogen

(ii) Potassium

(iii) Carbon

(iv) Titanium

Electronic configurations in ions

- Follow the same principle as for atoms but add electrons for negative ions
- Remove electrons for positive ions
- With Transition metals:

4s fills before 3d and also empties before 3d

Sodium ion Na^+

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

- To make a sodium ion 1 electron is removed

Chlorine ion Cl^-

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

- To make a chloride ion 1 electron is added

Iron ion Fe^{2+}

Fe atom = $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 4s^2$ Fe^{2+} ion = $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6$

- To make an iron 2+ ion 2 electrons are removed
- 4s empties before 3d

Questions:

Li atom Li^+ ion

Mg atom Mg^{2+} ion

Ti atom Ti^{2+} ion

F atom F^- ion

S atom S^{2-} ion

Give the full electronic structure of the following species:

	Full Electron Structure	"Short" version
Selenium atom		
Vanadium atom		
Cobalt atom		
O^{2-} ion		
Ca^{2+} ion		
Al^{3+} ion		

Transition Metals – an exception

- Chromium and Copper fills differently

  Cr: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^4 4s^2$ (expected) Cr: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^1$ (actual)

  Cu: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^9 4s^2$ (expected) Cu: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^1$ (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

Ions of Chromium and Copper:

Copper ion Cu^+

Cu atom = $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^1$ Cu^+ ion = $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10}$

Copper ion Cu^{2+}

Cu atom = $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^1$ Cu^{2+} ion = $1s^2 2s^2 2p^6 3s^2 3p^6 3d^9$

Chromium ion Cr^{2+}

Cr atom = $1s^2 2s^2 2p^6 3s^2 3p^6 3d^4 4s^2$ Cr^{2+} ion = $1s^2 2s^2 2p^6 3s^2 3p^6 3d^4$

Chromium ion Cr^{3+}

Cr atom = $1s^2 2s^2 2p^6 3s^2 3p^6 3d^4 4s^2$ Cr^{2+} ion = $1s^2 2s^2 2p^6 3s^2 3p^6 3d^3$