# THE STRUCTURE OF ATOMS

ATOMS   Atoms consist of a number of fundamental particles, the most important ones are ...

	Mass / kg	*Charge / C*	*Relative mass*	*Relative Charge*
PROTON				
NEUTRON				
ELECTRON				

MASS NUMBER & ATOMIC NUMBER

Atomic Number (Z)   Number of protons in the nucleus of an atom

Mass Number (A)   Sum of the protons and neutrons in the nucleus

$$^{23}_{11}Na$$

Mass number (protons + neutrons)

Atomic number (protons)
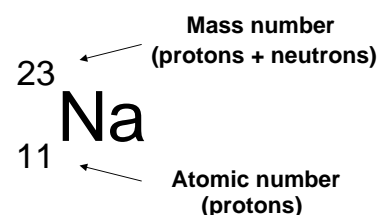
	Protons	*Neutrons*	*Electrons*	*Charge*	*Atomic No.*	*Mass No.*	*Symbol*
A	19	21	19				
B	20			Neutral		40	
C				+	11	23	
D	6	6		Neutral			
E	92			Neutral		235	
F	6		6			13	
G		18		2-	16		
H							$^{27}Al^{3+}$

Relative Atomic Mass (A_r)   The mass of an atom relative to that of the carbon 12 isotope having a value of 12.000 It can be calculated as follows...

$$A_r \quad = \quad \frac{\text{average mass per atom of an element} \times 12}{\text{mass of one atom of carbon-12}}$$

Relative Molecular Mass (M_r)   Similar to the above but uses the mass of a molecule / ion or any formula of a species

ISOTOPES

Definition   Atoms with ... the **same atomic number** but **different mass number**   or

the **same number of protons** but **different numbers of neutrons**.

Properties   Chemical properties of isotopes are identical

Theory   Relative atomic masses measured by chemical methods rarely produce whole numbers but they should do (allowing for the low relative mass of the electron). This was explained when the mass spectrograph revealed that **atoms of the same element could have different masses** due to the **variation in the number of neutrons** in the nucleus. The observed mass was a consequence of the abundance of each type of isotope.

	P	N
$^{1}_{1}H$	1	0
$^{2}_{1}H$	1	1
$^{3}_{1}H$	1	2

Example   *There are two common isotopes of chlorine - see table*

Calculate the average relative atomic mass of chlorine atoms

	P	N	%
$^{35}_{17}Cl$	17	18	75
$^{37}_{17}Cl$	17	20	25

Method 1   Three out of every four atoms will be chlorine-35

$$Average = \frac{35 + 35 + 35 + 37}{4} = 35.5$$

Method 2   Out of every 100 atoms   75 are ^{35}Cl
25 are ^{37}Cl

$$Average = \frac{(75 \times 35) + (25 \times 37)}{100} = 35.5$$

*Q.1   Calculate the average relative atomic mass of sulphur from the following isotopic percentages... ^{32}S 95% ^{33}S 1% ^{34}S 4%*

Q.2   Bromine has isotopes with mass numbers 79 and 81. If the average relative atomic mass is 79.908, calculate the percentage of each isotope present.
**Need help:- See example calculation on page 4 of these notes**

Mass Spectrometer

A mass spectrometer consists of ... an **ion source**, an **analyser** and a **detector**.
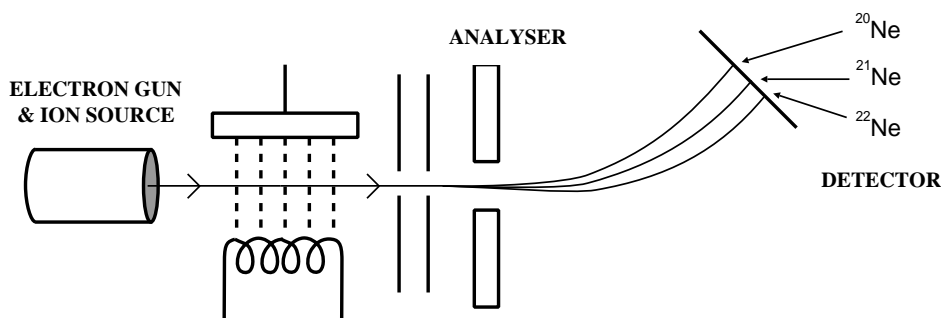
Ion source
- gaseous atoms are bombarded by electrons from an electron gun and are **IONISED**
- sufficient energy is given to form ions of 1+ charge
- resulting ions can be **ACCELERATED** out of the ion source by an electric field

Analyser
- charged particles will be **DEFLECTED** by a magnetic or electric field
- the radius of the path depends on the value of their mass/charge ratio (**m/z**)
- **ions of heavier isotopes have larger m/z values so follow a larger radius curve**
- as most ions are singly charged (1+), the amount of separation depends on their mass
- if an ion acquires a **2+ charge** it will be deflected more; its **m/z value is halved**


Changes when the ion is 2+

- **M/Z VALUE IS HALVED**

- **ABUNDANCE IS THE SAME**
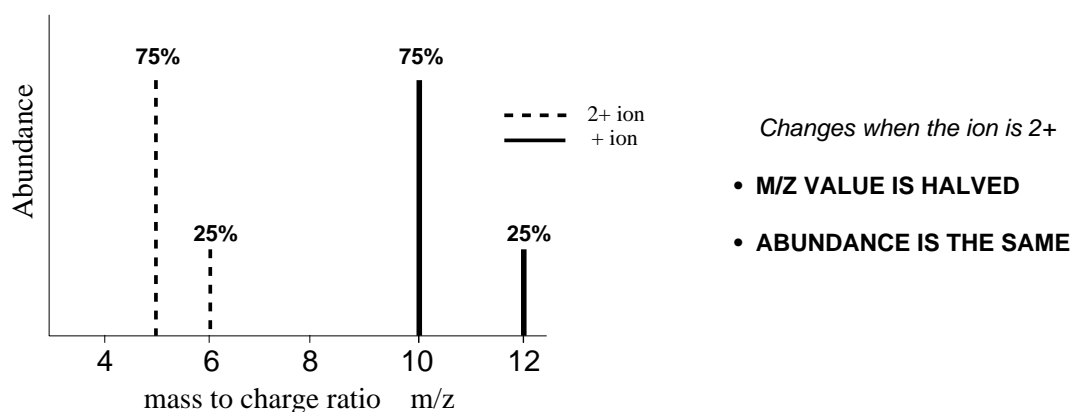
Detector
- by electric or photographic **DETECTION** methods
- mass spectra record the   **mass/charge** values   *and*
  relative abundance of each ion

Mass spectra

An early application was the demonstration by Aston, (Nobel Prize, 1922), that naturally occurring neon consisted of three isotopes ...

^{20}**Ne,** ^{21}**Ne and** ^{22}**Ne.**

- positions of the peaks gives atomic mass
- peak intensity gives the relative abundance
- highest abundance is scaled up to 100% and other values are adjusted accordingly.
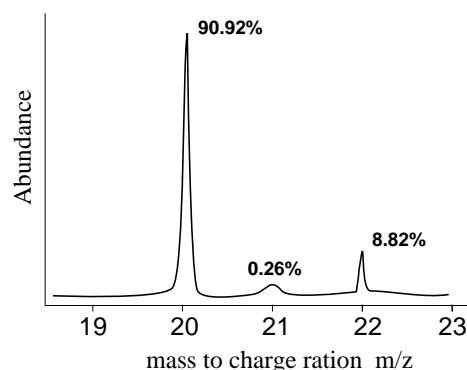
CALCULATIONS

Example 1   *Calculate the average relative atomic mass of neon using the above information.*

Out of every 100 atoms   *90.92 are ^{20}Ne,   0.26 are ^{21}Ne and   8.82 are ^{22}Ne*

Average = $\dfrac{(90.92 \times 20) + (0.26 \times 21) + (8.82 \times 22)}{100}$ *= 20.179*

Ans. =   *20.18*

Example 2   *Naturally occurring potassium consists of potassium-39 and potassium-41.*
               Calculate the percentage of each isotope present if the average is 39.1.

Assume that there are x nuclei of ^{39}K in every 100; there will then be (100-x) of ^{41}K.

so $\dfrac{39x + 41(100-x)}{100} = 39.1$ *therefore*   *39 x + 4100 - 41x = 3910*

thus   - 2x = - 190   so   x = 95   ANSWER   **95% ^{39}K and 5% ^{41}K**

Q.3   *Calculate the average relative atomic mass of an element producing the*
      following peaks in its mass spectrum...

m/z	*62*	*63*	*64*	*65*
Relative intensity	*20*	*25*	*100*	*5*

Mass spectra can also be used to find the relative molecular mass of compounds

ELECTRONIC CONFIGURATIONS

THEORY

Old
- electrons existed in definite energy levels or shells; the levels were concentric rings
- the further the energy level is from the nucleus, the higher its energy
- each level held a maximum number of electrons
- when a level was full up you moved to fill the next level

New   Instead of circulating in orbits around the nucleus, electrons were to be found in **orbitals**.

ORBITAL   ***"A region in space where one is likely to find an electron".***

- like 3-dimensional statistical maps showing the likeliest places to find electrons.
- come in different shapes and sizes but can only hold a maximum of two electrons each.

**ENERGY
LEVELS**   In the newer theory, the main energy levels are split into sub-levels. Each level has
orbitals and the electrons fill the orbitals. The orbitals in the first four main levels are ...

Main level	Sub-levels	Orbitals	Electrons	
n = 1	1	1s	2	= **2**
n = 2	2	2s	2	
		2p	6	= **8**
n = 3	3	3s	2	
		3p	6	
		3d	10	= **18**
n = 4	4	4s	2	
		4p	6	
		4d	10	
		4f	14	= **32**

RULES FOR FILLING ENERGY LEVELS

Aufbau Principle   *"Electrons enter the lowest energy orbital available."*

Energy levels are not entered until those below them are filled.

*Pauli's Exclusion
Principle*   *"No two electrons can have the same four quantum numbers."* or

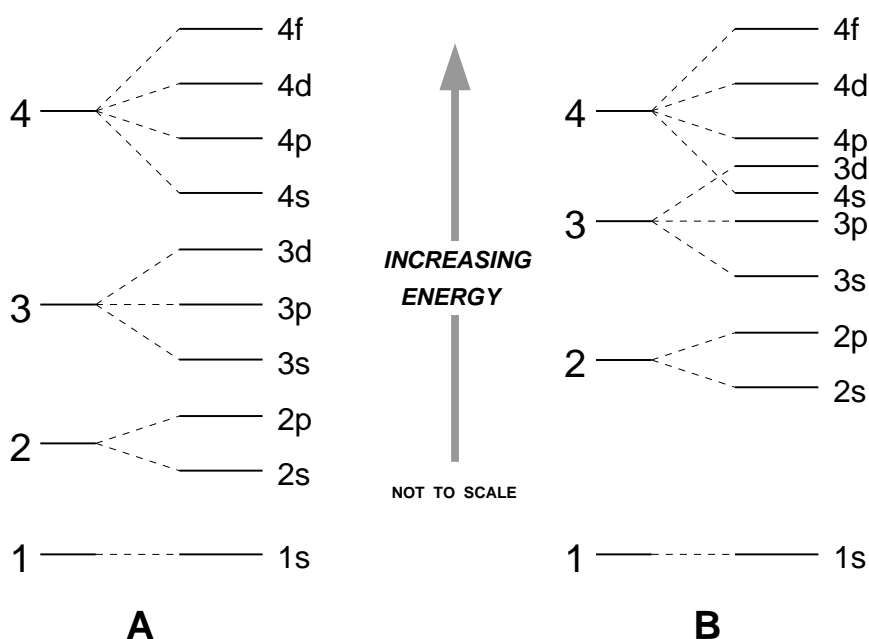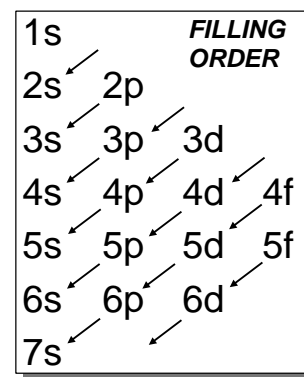Orbitals can hold a max. of 2 electrons provided they have opposite spin.

Hund's Rule   Orbitals of the same energy remain singly occupied before pairing up.
This is **due to the repulsion between electron pairs**.

**FILLING
ORDER**

- Orbitals are filled in order of increasing energy

- Orbitals are **not filled in numerical order ...**
  1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, etc.

  The 4s is filled before the 3d because it is lower in energy

- The effect can be explained by assuming the ...
  **principal energy levels get closer together as they
  get further from the nucleus**.

- As a result, the highest energy orbitals in one principal
  level may be above the lowest in the next level

```
1s                    FILLING
   ⟋                  ORDER
2s ⟋ 2p
3s ⟋ 3p ⟋ 3d
4s ⟋ 4p ⟋ 4d ⟋ 4f
5s ⟋ 5p ⟋ 5d ⟋ 5f
6s ⟋ 6p ⟋ 6d
7s
```


INCREASING
ENERGY

NOT TO SCALE

A   **B**

The diagram helps explain why the 4s orbitals are filled before the 3d orbitals

*There is plenty of evidence to explain the filling order. This will be dealt with when we look
a little later on at Ionisation Energies and Periodicity.*

| *Evidence* | Energy levels | Periodically there was a large drop in the energy to remove electrons caused by the electrons being further from the nucleus. |
| | Sub-levels | The energy required to remove electrons was sometimes less than expected due to shielding from filled sub-levels. |

Electronic configurations of the first 36 elements.

The filling proceeds according to the rules ... but watch out for **chromium** and **copper**.

Cr

Cu

IONISATION ENERGY

- A measure of the energy required to remove electrons from an atom.
- Value depends on the distance of the electron from the nucleus and the effective nuclear charge (not the nuclear charge) of the atom.
- There are as many ionisation energies as there are electrons in the atom.

Nuclear Charge (**NC**) The actual charge (relative) due to the protons in the nucleus

Effective nuclear Charge (**ENC**)
- The effectiveness of the nuclear charge after passing through filled inner shells
- A simple way to compare effective nuclear charges is to knock of a + for every electron in a filled inner level.

Species	Protons	Electron config.	NC	ENC
H	1	1	1+	1+
He	2	2	2+	2+
Li	3	2,1	3+	1+
Be	4	2,2	4+	2+
B	5	2,3	5+	3+
Ne	10	2,8	10+	8+
Na	11	2,8,1	11+	1+
K	19	2,8,8,1	19+	1+

1st I.E.   The energy required to remove one mole of electrons (to infinity) from one mole of isolated, gaseous atoms to form one mole of gaseous positive ions.

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

       $Mg_{(g)} \longrightarrow Mg^+_{(g)} + e^-$
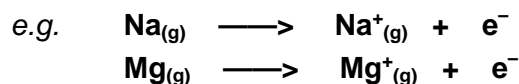
Its value gives an idea of how strongly the nucleus pulls on the electron being removed. The stronger the pull on the electron, the more energy one needs to pull it out of the atom.

First Ionisation Energies / kJ mol^{-1}

1	H	1310	15	P	1060	29	Cu	745	43	Tc	699
2	He	2370	16	S	1000	30	Zn	908	44	Ru	724
3	Li	519	17	Cl	1260	31	Ga	577	45	Rh	745
4	Be	900	18	Ar	1520	32	Ge	762	46	Pd	803
5	B	799	19	K	418	33	As	966	47	Ag	732
6	C	1090	20	Ca	590	34	Se	941	48	Cd	866
7	N	1400	21	Sc	632	35	Br	1140	49	In	556
8	O	1310	22	Ti	661	36	Kr	1350	50	Sn	707
9	F	1680	23	V	648	37	Rb	402	51	Sb	833
10	Ne	2080	24	Cr	653	38	Sr	548	52	Te	870
11	Na	494	25	Mn	716	39	Y	636	53	I	1010
12	Mg	736	26	Fe	762	40	Zr	669	54	Xe	1170
13	Al	577	27	Co	757	41	Nb	653	55	Cs	376
14	Si	786	28	Ni	736	42	Mo	694	56	Ba	502

Q.4 • *Plot a graph of 1st I.E. v. Atomic No. for the first 56 elements.*
      • *Plot graphs of 1st I.E. v. Atomic No. for the elements H to Na and for Ne to K*

Interpretation of Ionisation Energy graphs

**ACROSS
PERIODS**
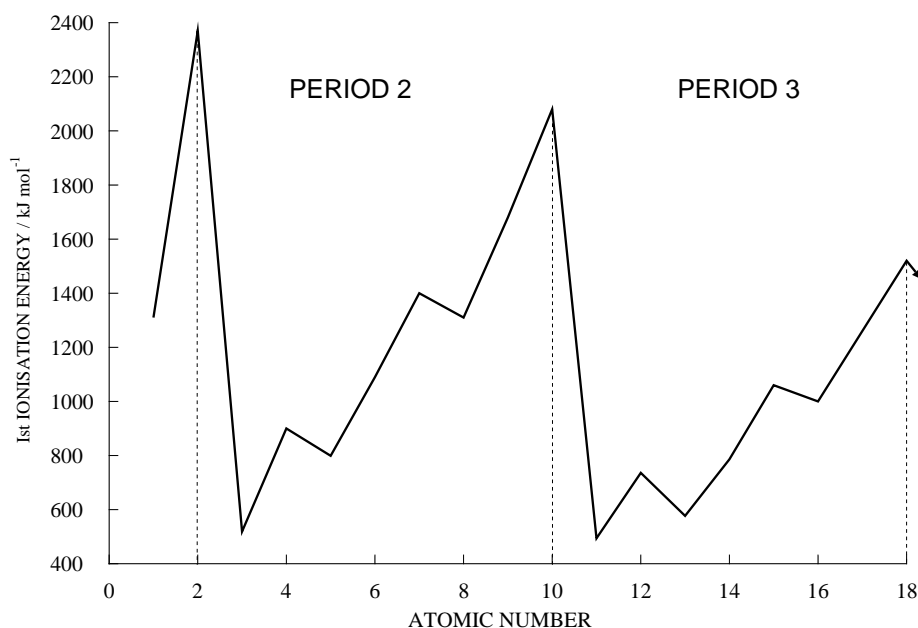
He > H • **nuclear charge is greater** - one extra proton
 • extra electron has gone into the same energy level
 • increased attraction makes the electron harder to remove.

Li < He • increased nuclear charge, but...
 • outer electron is held less strongly
 • it is **shielded** by full inner level of electrons and is **further away** - easier to remove

Be > Li • **increased nuclear charge**
Mg > Na • electrons in the same energy level

B < Be • despite the increased nuclear charge, the outer electron is held less strongly
Al < Mg • it is now shielded by the 2s energy sub-level and is also further away
 (LED TO EVIDENCE FOR SUB LEVELS)

O < N • despite the increased nuclear charge the electron is easier to remove
S < P • in N the three electrons in the 2p level are in separate orbitals whereas
 • in O two of the four electrons are in the same orbital
 • **repulsion between paired electrons** = less energy needed to remove of one of them

 **Values in Period 3 are always smaller than the equivalent Period 2 value because
 the electron removed is further from the nucleus and has more shielding** *e.g.*

Na < Li • despite the increased nuclear charge the electron is easier to remove
 • increased shielding and greater distance from the nucleus
 • outer electron in Na is held less strongly and easier to remove

**DOWN
GROUPS**

Ist IONISATION ENERGY / kJ mol^{-1}
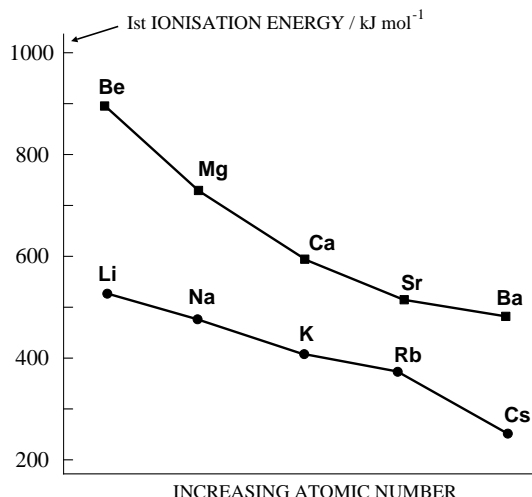
GROUP I 　　　Value decreases down the Group

- despite the increased nuclear charge the outer *s* electron is easier to remove
- this is due to **increased shielding** and **greater distance** from the nucleus
- outer electron is held less strongly and easier to remove

GROUP II 　　　Similar trend to Group I

- Group II values are greater than their Group I neighbours
- increased nuclear charge = stronger pull on electron
- more energy required to remove an *s* electron

2nd I.E. 　　　The energy required to remove one mole of electrons (to infinity) from one mole of gaseous unipositive ions to form one mole of gaseous dipositive ions.

　　　e.g. 　　$Mg^+_{(g)}$ 　⟶ 　$Mg^{2+}_{(g)}$ + e^-

　　　　　　$Al^+_{(g)}$ 　⟶ 　$Al^{2+}_{(g)}$ + e^-
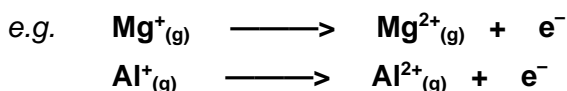
Trends 　　　• **Successive ionisation energies are always greater** than the previous one
　　　　　- the electron is being pulled away from a more positive species

　　　　　• **Large increases occur when there is a change of shell**
　　　　　- this can be used to predict the group of an unknown element

Successive I.E. values for calcium / kJ mol^{-1}

Q.5 　• *Plot a graph of* $\log_{10}$ *I.E. of calcium v. no. of electron removed.*

　　　• *Why plot* $\log_{10}$ *I.E. ?*

1	590	11	57048
2	1145	12	63333
3	4912	13	70052
4	6474	14	78792
5	8145	15	86367
6	10496	16	94000
7	12320	17	104900
8	14207	18	111600
9	18192	19	494790
10	20385	20	527759