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 in **orbitals**.

ORBITAL   *"A region in space where one is likely to find an electron each orbital can hold up to two electrons, with opposite spins".*

- 3-dimensional statistical maps showing the likeliest places to find electrons
- come in different shapes and sizes
- hold a **maximum of two electrons** each (as long as they have opposite spins)

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S ORBITAL   **P ORBITAL**
Spherical   **'Dumb-bell' shaped**

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ONE in each main shell   *THREE in each main shell*
(except the first)

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

Main shell	Sub-shells	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

FILLING ORDER

1s
2s 2p
3s 3p 3d
4s 4p 4d 4f
5s 5p 5d 5f
6s 6p 6d
7s
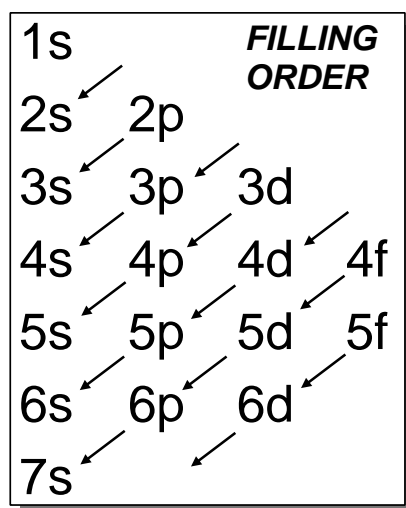
1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d ...

The diagram helps explain why the 4s orbitals are filled before the 3d orbitals
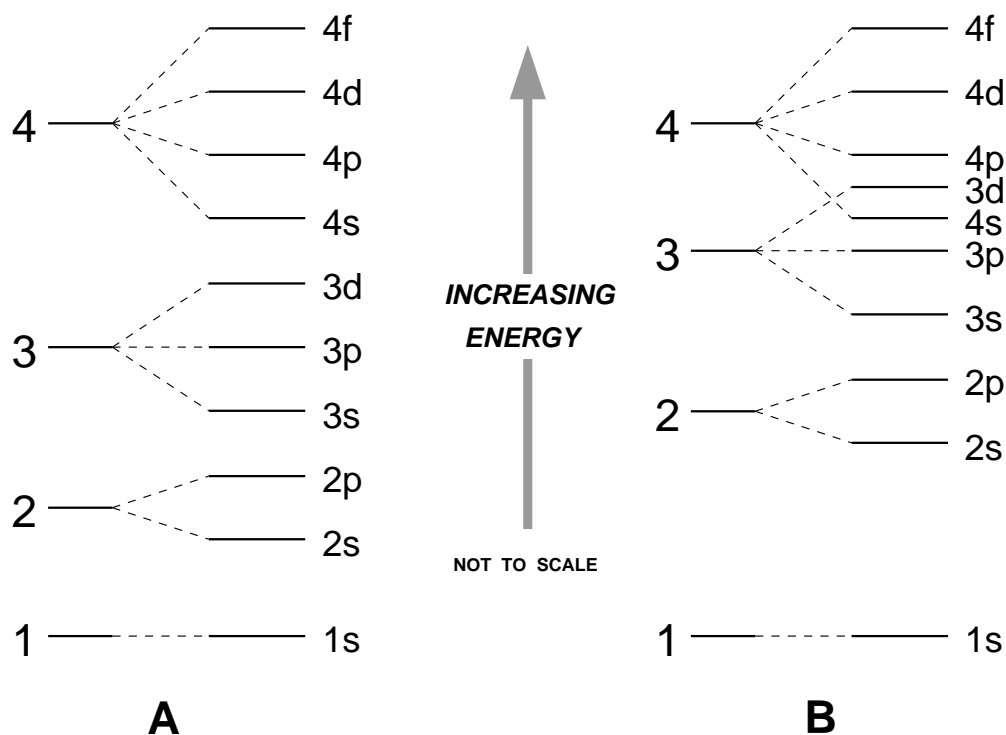
There is plenty of evidence to explain the filling order. This will be dealt with in sections on *Ionisation Energies and Periodicity.*

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.

1s

H - **1s^1**

He   **2s**

Li

Be   **2p**

B

C

N

O

F

Ne   **3s**

Na

Mg   **3p**

Al

Si

P

S

Cl

Ar   **4s**

K

Ca   **3d**

Sc

Ti

V

Cr

Mn

Fe

Co

Ni

Cu

Zn   **4p**

Ga

Ge

As

Se

Br

Kr

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 nuclear charge after passing through filled shells
- A simple way to compare effective nuclear charges is to knock off 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, the more energy needed to pull out the electron.

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.1   • *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**
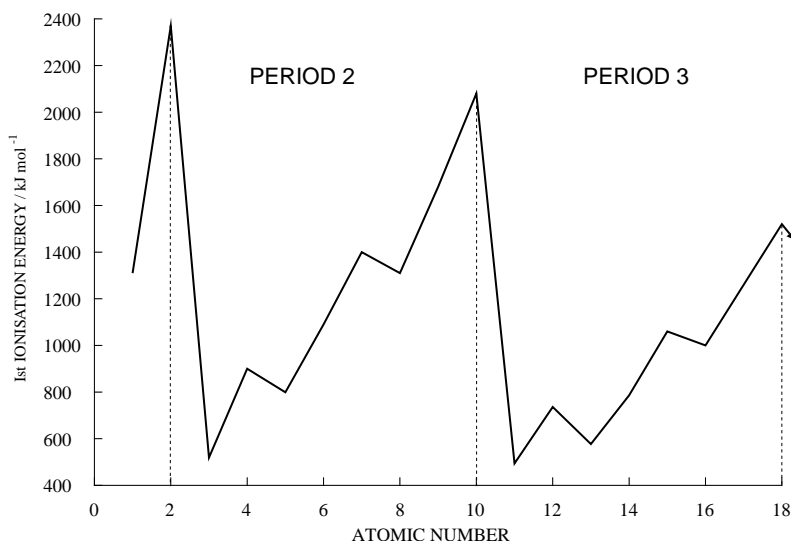
He > H   • **nuclear charge is greater** - one extra proton
             • extra electron has gone into the same energy level
             • increased attraction makes the electron harder to remove.

Li < He   • increased nuclear charge, but...
             • outer electron is held less strongly
             • it is **shielded** by full inner levels 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

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

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}

INCREASING ATOMIC NUMBER
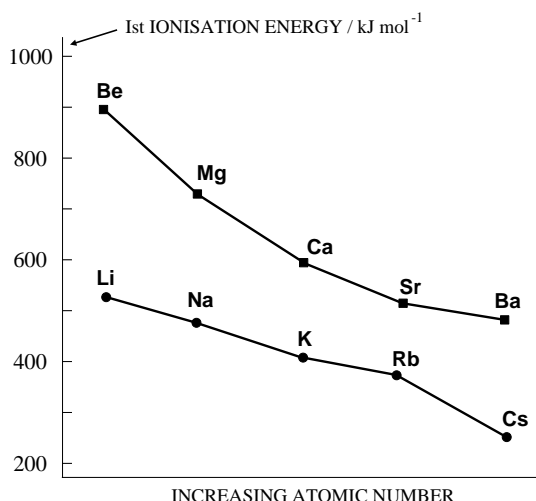
GROUP I   Value decreases down the Group

- 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

SUCCESSIVE IONISATION ENERGIES

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^-
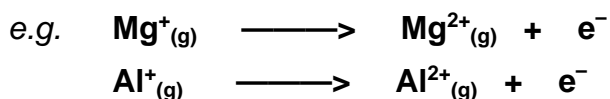
Successive I.E. values for calcium / kJ mol$^-$

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

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

Q.2   • *Plot a graph of* log_{10} *I.E. of calcium v. no. of electron removed.*