THE BOHR MODEL OF THE ATOM

A small nucleus of protons and neutrons surrounded by electrons in shells each shell holding up to a maximum number of electrons and filled from the first shell outwards electrons in the first shell being the most strongly held and therefore at the lowest energy level.

<table>
<thead>
<tr>
<th>Shell</th>
<th>Maximum Electrons Per Shell</th>
</tr>
</thead>
<tbody>
<tr>
<td>1st</td>
<td>n = 1</td>
</tr>
<tr>
<td>2nd</td>
<td>n = 2</td>
</tr>
<tr>
<td>3rd</td>
<td>n = 3</td>
</tr>
<tr>
<td>4th</td>
<td>n = 4</td>
</tr>
</tbody>
</table>

The theory couldn't explain certain detailed aspects of the chemistry of the elements or their emission spectra.
The principal quantum numbers are listed below for the Bohr atom. Notice that as the electron jumps to a lower level, energy is lost. It takes energy to move an atom from a lower level to a higher level.
Isotopes of Hydrogen, Helium, Lithium and Sodium

Hydrogen–1
Helium–4
Lithium–6
Sodium–22

Neutron  Proton  Electron

©2001 How Stuff Works
A study of First Ionisation Energies across each period suggested that each ‘shell’ was in fact a group of ‘sub-shells’ at different but similar energy levels.

The electrons in different sub-shells have different energy levels.

Shell 1 contains only an s sub-shell
Shell 2 contains an s and p sub-shell
Shell 3 contains an s, p and d sub-shell
Shell 4 contains an s, p, d and f sub-shell

How are electrons arranged within these sub-shells?
RULES AND PRINCIPLES ARISING FROM QUANTUM MECHANICS

These four rules govern how electrons are arranged in atoms.

HEISENBERG’S UNCERTAINTY PRINCIPLE
“You cannot determine both the position and momentum of an electron at the same time.”

PAULI’S EXCLUSION PRINCIPLE
“No two electrons can have the same four quantum numbers.”

THE AFBAU (BUILDING UP) PRINCIPLE
“Electrons enter the lowest available energy level.”

HUND’S RULE OF MAXIMUM MULTIPLICITY
“When in orbitals of equal energy, electrons will try to remain unpaired.”
An orbital is a region in space where there is a 95% probability of finding the electron. (Heisenberg’s Uncertainty Principle)

Orbitals can hold one electron or two electrons as long as they have opposite spin. (Pauli Exclusion Principle)

Orbitals have different shapes depending on which sub-shell they are in.

DO NOT USE THE WORD ORBIT WHEN YOU MEAN AN ORBITAL
One s orbital makes the s sub-shell

spherical
SHAPES OF ORBITALS

Three p orbitals make the p sub-shell

dumb-bell shaped
SHAPES OF ORBITALS

Five d orbitals make the d sub-shell

Four are double dumb-bell shaped
The other a dumb-bell with a collar
SHAPES OF ORBITALS

Seven f orbitals make the f sub-shell
### ORDER OF FILLING ORBITALS

Orbitals are filled from the lowest energy level upwards.  
(The Aufbau Principle)

The quantum shells get closer together in space as you get further from the nucleus.

There is an overlap in the energy levels of the sub-shells of different shells.

The first example occurs when the 4s orbital is filled before the 3d orbitals because it is at a lower energy level.

The 4s orbital is still part of the forth shell and is physically further from the nucleus than the 3d sub-shell.

<table>
<thead>
<tr>
<th>Principal Quantum Number of Shell</th>
<th>Sub Shells</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>4f 4d 4p 3d 4s 3p 3s</td>
</tr>
<tr>
<td>3</td>
<td>2p 2s</td>
</tr>
<tr>
<td>2</td>
<td>1s</td>
</tr>
</tbody>
</table>

Increasing Energy / Distance from Nucleus
The 4s orbital is filled before the 3d orbitals.
The following sequence will show the ‘building up’ of the electronic structures of the first 36 elements in the periodic table.

Electrons are shown as half-headed arrows and can spin in one of two directions:

- s orbitals
- p orbitals
- d orbitals

The periodic table shows the energy level and increasing distance from the nucleus.
The electronic configurations of the first 36 elements

Hydrogen

$1s^1$

Hydrogen atoms have one electron.

This goes into a vacant orbital in the lowest available energy level.

The Aufbau Principle
Every orbital can contain 2 electrons, provided the electrons have opposite ‘spins’.

The two electrons in a helium atom can both go in the 1s orbital.

**Pauli’s Exclusion Principle**
The electronic configurations of the first 36 elements

Lithium

Orbitals hold a maximum of two electrons, so the third electron in a lithium atom must go into the next available orbital.

This is the 2s orbital. An s orbital is lower in energy than a p orbital in the same shell.
Beryllium atoms have four electrons, so the fourth electron pairs up in the 2s orbital.

The 2s sub-shell, which only contains the 2s orbital, is now full.
As the 2s sub-shell is now full, the fifth electron goes into one of the three p orbitals in the 2p sub-shell. The 2p orbitals are slightly higher in energy than the 2s orbital but each are at the same energy level, they are ‘degenerate’.
The next electron doesn't pair up with the other 2p electron as there is an empty orbital available of the same energy.

There is less repulsion between the electrons when in separate orbitals resulting in an arrangement of lower energy and more stability.
The electronic configurations of the first 36 elements

NITROGEN
1s² 2s² 2p³

The next electron goes into the vacant p orbital of the same energy.

All three electrons are now unpaired.

Less repulsion
Lower energy
More stability.

Hund's Rule of Maximum Multiplicity
**OXYGEN**

$1s^2 \ 2s^2 \ 2p^4$

With all three orbitals half-filled, the eighth electron in an oxygen atom must now pair up with one of the 2p electrons.

The repulsion between the two paired electrons raises their energy level.

This explains the drop in first ionisation energy from N to O.
The electronic configurations of the first 36 elements

**Fluorine**

$1s^2 2s^2 2p^5$

The electrons continue to pair up with those in the half-filled orbitals.
INCREASING ENERGY / DISTANCE FROM NUCLEUS

THE ELECTRONIC CONFIGURATIONS OF THE FIRST 36 ELEMENTS

NEON
1s\(^2\) 2s\(^2\) 2p\(^6\)

The electron pairs up with the one in the last half-filled p orbital.

The three 2p orbitals are now completely filled, filling the 2p sub-shell and the shell of principal quantum number 2.

The 'IG' electronic configuration would have been written as 2,8.
SODIUM - ARGON

With the second shell full, the next electron must go into the next available orbital with the lowest energy.

The third shell contains three sub-shells; s, p and d.

The one 3s and the three 3p orbitals are filled in exactly the same way as those in the 2s and 2p sub shells.
THE ELECTRONIC CONFIGURATIONS OF THE FIRST 36 ELEMENTS

SODIUM - ARGON

Na  $1s^2 \ 2s^2 \ 2p^6 \ 3s^1$
Mg  $1s^2 \ 2s^2 \ 2p^6 \ 3s^2$
Al  $1s^2 \ 2s^2 \ 2p^6 \ 3s^2 \ 3p^1$
Si  $1s^2 \ 2s^2 \ 2p^6 \ 3s^2 \ 3p^2$
P   $1s^2 \ 2s^2 \ 2p^6 \ 3s^2 \ 3p^3$
S   $1s^2 \ 2s^2 \ 2p^6 \ 3s^2 \ 3p^4$
Cl  $1s^2 \ 2s^2 \ 2p^6 \ 3s^2 \ 3p^5$
Ar  $1s^2 \ 2s^2 \ 2p^6 \ 3s^2 \ 3p^6$

Remember, Hund’s Rule is followed. Electrons remain unpaired if a vacant p orbital is available. This provides a lower energy level as the electrons repel less than when paired.
THE ELECTRONIC CONFIGURATIONS OF THE FIRST 36 ELEMENTS

The Aufbau Principle

POTASSIUM

1s² 2s² 2p⁶ 3s² 3p⁶ 4s¹

The 4s orbital is of a LOWER ENERGY than that of the 3d orbitals.
The 4s gets filled first!
INCREASING ENERGY / DISTANCE FROM NUCLEUS

THE ELECTRONIC CONFIGURATIONS OF THE FIRST 36 ELEMENTS

CALCIUM
1s\(^2\) 2s\(^2\) 2p\(^6\) 3s\(^2\) 3p\(^6\) 4s\(^2\)

The next electron pairs up and fills the 4s orbital.

All elements with an s\(^1\) electronic configuration are in Group 1.

All elements with an s\(^2\) electronic configuration are in Group 2.

Groups 1 and 2 are known together as the s block. The highest energy electron is in an s orbital.
There are five d orbitals. They are 'degenerate' i.e. are at the same energy level. So they are each filled with a single electron before any is filled with two 'spin paired' electrons.

Watch out for two special cases!

**Hund's Rule of Maximum Multiplicity**
These are the transition metals also known as the d block elements.

The highest energy electron enters a d orbital.
THE ELECTRONIC CONFIGURATIONS OF THE FIRST 36 ELEMENTS

The 3d orbitals are part of the 3\textsuperscript{rd} shell, which is an inner shell closer to the nucleus than the 4s orbital of the 4\textsuperscript{th} shell.

Therefore, the atomic size of d block elements remains relatively constant across a period.

Nuclear charge is increased by one proton but is shielded by one inner shell 3d electron.

So, the 4s electrons experience an approximately unchanged nuclear attraction across the d block.
The electronic configurations of the first 36 elements

Chromium

One would expect the electronic configuration of the chromium atom to be \([\text{Ar}]\) \(4s^2\ 3d^4\).

The 4s and 3d orbitals are close in energy.

The arrangement of six unpaired electrons has a lower energy than if two electrons are paired (repelling each other) in the 4s orbital.
The new electron goes into the 4s orbital to restore its filled state.
THE ELECTRONIC CONFIGURATIONS OF THE FIRST 36 ELEMENTS

INCREASING ENERGY / DISTANCE FROM NUCLEUS

IRON

1s² 2s² 2p⁶ 3s² 3p⁶ 4s² 3d⁶
The electronic configurations of the first 36 elements

**Cobalt**

\[ 1s^2 \, 2s^2 \, 2p^6 \, 3s^2 \, 3p^6 \, 4s^2 \, 3d^7 \]
THE ELECTRONIC CONFIGURATIONS OF THE FIRST 36 ELEMENTS

INCREASING ENERGY / DISTANCE FROM NUCLEUS

NICKEL

$1s^2 \ 2s^2 \ 2p^6 \ 3s^2 \ 3p^6 \ 4s^2 \ 3d^8$
THE ELECTRONIC CONFIGURATIONS OF THE FIRST 36 ELEMENTS

COPPER

\[ 1s^2 \ 2s^2 \ 2p^6 \ 3s^2 \ 3p^6 \ 4s^1 \ 3d^{10} \]

One would expect the configuration of chromium atoms to be...

\[ [\text{Ar}] \ 4s^2 \ 3d^9 \].

However, the actual arrangement...

\[ [\text{Ar}] \ 4s^1 \ 3d^9 \]

Is of lower energy and therefore the stable arrangement.

This can be rationalised by the symmetry of the full 3d sub-shell.
THE ELECTRONIC CONFIGURATIONS OF THE FIRST 36 ELEMENTS

ZINC

1s² 2s² 2p⁶ 3s² 3p⁶ 4s² 3d¹⁰

The electron goes into the 4s orbital to restore its filled state.

The inner 3rd shell is now complete. Zn is the last d block element in the 4th period.

The available orbitals of next highest energy are the 4p and these fill next.
The electronic configurations of the first 36 elements

GALLIUM - KRYPTON

The 4p orbitals are filled in exactly the same way as the 3p orbitals were.

These elements are in the p block.

The highest energy electron is in a p orbital.
THE ELECTRONIC CONFIGURATIONS OF THE FIRST 36 ELEMENTS

INCREASING ENERGY / DISTANCE FROM NUCLEUS

GALLIUM - KRYPTON

Ga
1s\(^2\)2s\(^2\)2p\(^6\)3s\(^2\)3p\(^6\)4s\(^2\)3d\(^{10}\)4p\(^1\)

Ge
1s\(^2\)2s\(^2\)2p\(^6\)3s\(^2\)3p\(^6\)4s\(^2\)3d\(^{10}\)4p\(^1\)

Or, in shortened form...

As
[Ar]4s\(^2\)3d\(^{10}\)4p\(^3\)

Se
[Ar]4s\(^2\)3d\(^{10}\)4p\(^4\)

Br
[Ar]4s\(^2\)3d\(^{10}\)4p\(^5\)

Kr
[Ar]4s\(^2\)3d\(^{10}\)4p\(^6\)
### Electronic Configurations of Elements 1-30

<table>
<thead>
<tr>
<th>Element</th>
<th>1s</th>
<th>2s</th>
<th>2p</th>
<th>3s</th>
<th>3p</th>
<th>4s</th>
<th>3d</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>1s</td>
<td></td>
<td>1s</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>He</td>
<td>1s</td>
<td>1s</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Li</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Be</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td></td>
</tr>
<tr>
<td>N</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
</tr>
<tr>
<td>O</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
</tr>
<tr>
<td>F</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
</tr>
<tr>
<td>Ne</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
</tr>
<tr>
<td>Na</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
</tr>
<tr>
<td>Mg</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
</tr>
<tr>
<td>Al</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
</tr>
<tr>
<td>Si</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
</tr>
<tr>
<td>P</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
</tr>
<tr>
<td>S</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
</tr>
<tr>
<td>Cl</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
</tr>
<tr>
<td>Ar</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
</tr>
<tr>
<td>K</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
</tr>
<tr>
<td>Ca</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
</tr>
<tr>
<td>Sc</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
</tr>
<tr>
<td>Ti</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
</tr>
<tr>
<td>V</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
</tr>
<tr>
<td>Cr</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
</tr>
<tr>
<td>Mn</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
</tr>
<tr>
<td>Fe</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
</tr>
<tr>
<td>Co</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
</tr>
<tr>
<td>Ni</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
</tr>
<tr>
<td>Cu</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
</tr>
<tr>
<td>Zn</td>
<td>1s</td>
<td>1s</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
<td>1p</td>
</tr>
</tbody>
</table>

**Examples:**
- Li: 1s$^2$, 2s$^1$
- Be: 1s$^2$, 2s$^2$
- 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$^4$
- F: 1s$^2$, 2s$^2$, 2p$^5$
- Ne: 1s$^2$, 2s$^2$, 2p$^6$
- Na: 1s$^2$, 2s$^2$, 2p$^6$, 3s$^1$
- Mg: 1s$^2$, 2s$^2$, 2p$^6$, 3s$^2$
- Al: 1s$^2$, 2s$^2$, 2p$^6$, 3s$^2$, 3p$^1$
- Si: 1s$^2$, 2s$^2$, 2p$^6$, 3s$^2$, 3p$^2$
- P: 1s$^2$, 2s$^2$, 2p$^6$, 3s$^2$, 3p$^3$
- S: 1s$^2$, 2s$^2$, 2p$^6$, 3s$^2$, 3p$^4$
- Cl: 1s$^2$, 2s$^2$, 2p$^6$, 3s$^2$, 3p$^5$
- Ar: 1s$^2$, 2s$^2$, 2p$^6$, 3s$^2$, 3p$^6$
ELECTRONIC CONFIGURATION OF IONS

Positive ions (cations) are formed by removing electrons from atoms. Negative ions (anions) are formed by adding electrons to atoms. Electrons are removed first from the occupied orbital of highest energy. Ions of s and p block elements are 'isoelectronic' with a noble gas but contain a different number of protons and are charged.

**SODIUM**

Na 1s\(^2\) 2s\(^2\) 2p\(^6\) 3s\(^1\)

Na\(^+\) 1s\(^2\) 2s\(^2\) 2p\(^6\) 1 electron removed from the 3s orbital

Ne 1s\(^2\) 2s\(^2\) 2p\(^6\)

**CHLORINE**

Cl 1s\(^2\) 2s\(^2\) 2p\(^6\) 3s\(^2\) 3p\(^5\)

Cl\(^-\) 1s\(^2\) 2s\(^2\) 2p\(^6\) 3s\(^2\) 3p\(^6\) 1 electron added to the 3p orbital

Ar 1s\(^2\) 2s\(^2\) 2p\(^6\) 3s\(^2\) 3p\(^6\)
FIRST ROW TRANSITION METALS

Despite being initially of lower energy and therefore having been filled first, the energy level of the 4s orbital becomes higher when the 3d orbitals contain electrons. Due to the repulsion between electrons in the 3d and 4s sub-shells, therefore, electrons in the 4s orbital are removed before any electrons in the 3d orbitals.

TITANIUM

<table>
<thead>
<tr>
<th>Charge</th>
<th>Electronic Configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ti</td>
<td>1s(^2) 2s(^2) 2p(^6) 3s(^2) 3p(^6) 4s(^2) 3d(^2)</td>
</tr>
<tr>
<td>Ti(^+)</td>
<td>1s(^2) 2s(^2) 2p(^6) 3s(^2) 3p(^6) 4s(^1) 3d(^2)</td>
</tr>
<tr>
<td>Ti(^{2+})</td>
<td>1s(^2) 2s(^2) 2p(^6) 3s(^2) 3p(^6) 3d(^2)</td>
</tr>
<tr>
<td>Ti(^{3+})</td>
<td>1s(^2) 2s(^2) 2p(^6) 3s(^2) 3p(^6) 3d(^1)</td>
</tr>
<tr>
<td>Ti(^{4+})</td>
<td>1s(^2) 2s(^2) 2p(^6) 3s(^2) 3p(^6)</td>
</tr>
</tbody>
</table>