AH Chemistry – Unit 1

Atomic Orbitals, Electronic Configurations and the Periodic Table

Principal Quantum Number

Bohr described each shell by a number,
the ***principal quantum number, n***

For the first shell, ***n = 1***

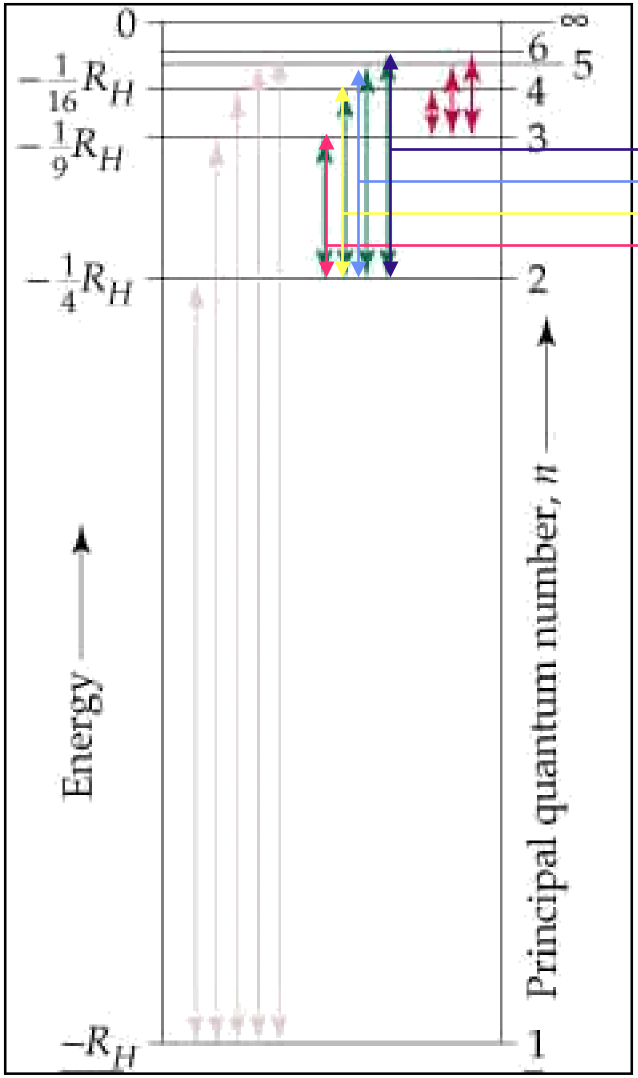
For the second shell, ***n = 2*** and so on.

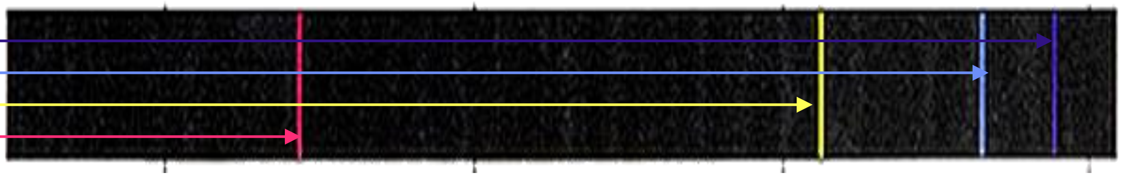
After lots of math, Bohr showed that

$$E_n = -R_H\left(\frac{1}{n^2}\right)$$

where n is the principal quantum number (i.e., ***n = 1, 2, 3,*** …),
and R_H is the Rydberg constant = 2.18×10^{-18} J.

Hydrogen Spectra

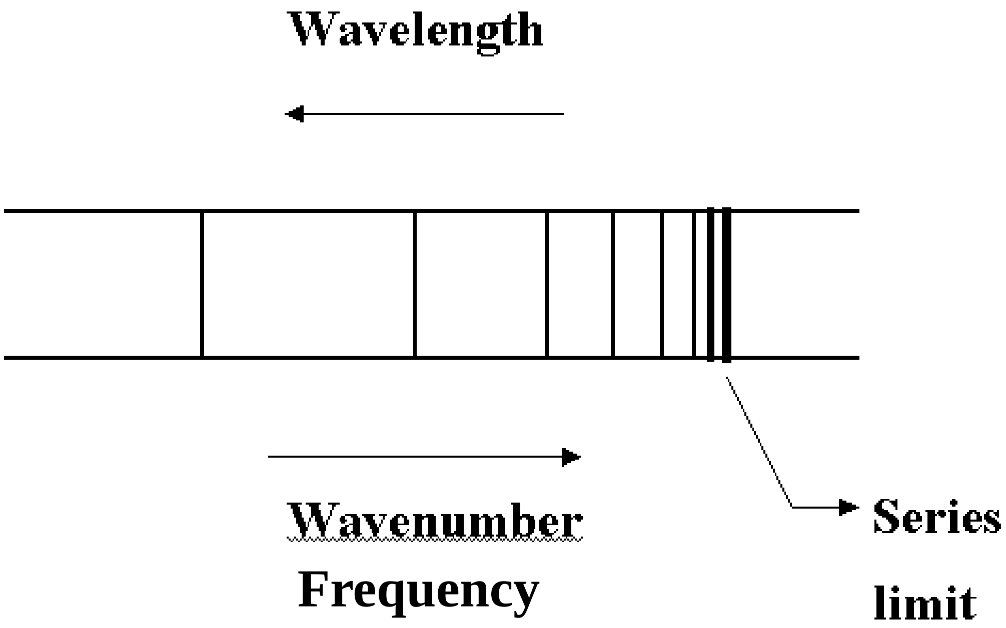




The lines detected in the visible spectrum were due to electrons returning to the ***n=2*** level and are called the ***Balmer Series***

Another series of lines called the ***Lyman Series*** are due to electrons returning to the ***n=1*** level. The ΔE values are higher and the lines appear in the ***ultra-violet*** region.

Ionisation Energy 1



When we examine spectra we notice that each series of lines ***converge***, i.e the gaps between the lines get smaller and smaller until the lines seem to merge.

The line of greatest energy (lowest wavelength, highest frequency), represents an electron returning from the outer limit of an atom to the ground state (***n=1*** in the case of Hydrogen).

With slightly more energy the electron would have removed from the atom completely, i.e. ***the Ionisation Energy***

Ionisation Energy 2

For example, the wavelength of the line at the convergence
Limit of the Lyman series in the Hydrogen spectrum is 91.2 nm.

91.2 nm = 91.2×10^{-9} m = 9.12×10^{-8} m.

For each ***photon*:**

$E = h \quad c \quad / \quad \lambda$

$= 6.63 \times 10^{-34} \times 3.00 \times 10^{8} / 9.12 \times 10^{-8}$

$= 2.18 \times 10^{-18}$ J

For ***1 mole of photons*:**

$E = 2.18 \times 10^{-18} \times 6.02 \times 10^{23}$ J

$= 1.31 \times 10^{6}$ J mol^{-1}

$= 1{,}310$ k J mol^{-1}

Data Book Value

1,311 kJ mol^{-1}

Subshells - Orbitals

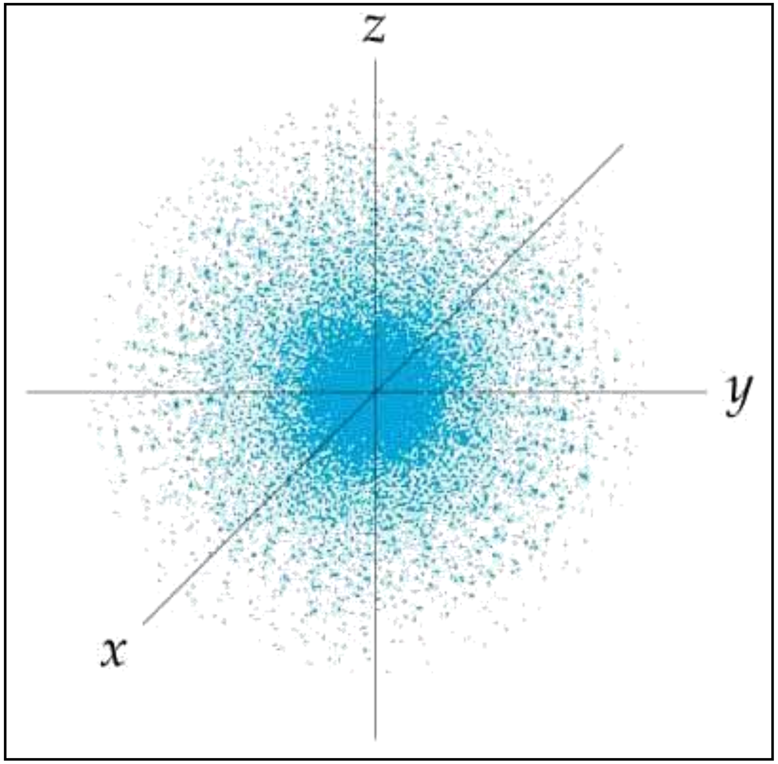
High resolution spectra of more complex atoms reveal that lines are often split into triplets, quintuplets etc.

This is evidence that Shells are further subdivided into ***Subshells***

These Subshells are called ***Orbitals***

Calculations using ***Quantum Mechanics*** have been able to determine the ***shapes*** of these Orbitals

s-orbitals



Quantum mechanics has shown that ***s orbitals*** are ***spherical*** in shape

An orbital is a ***region in space where there is a greater than 90% probability of finding an electron***.

Orbitals and Quantum Numbers

Angular Quantum Number, l. This quantum number describes the ***shape*** of an orbital. $l = 0, 1, 2,$ and 3 (4 shapes) but we use letters for l (*s*, *p*, *d* and *f*). Usually we refer to the ***s, p, d and f-orbitals***

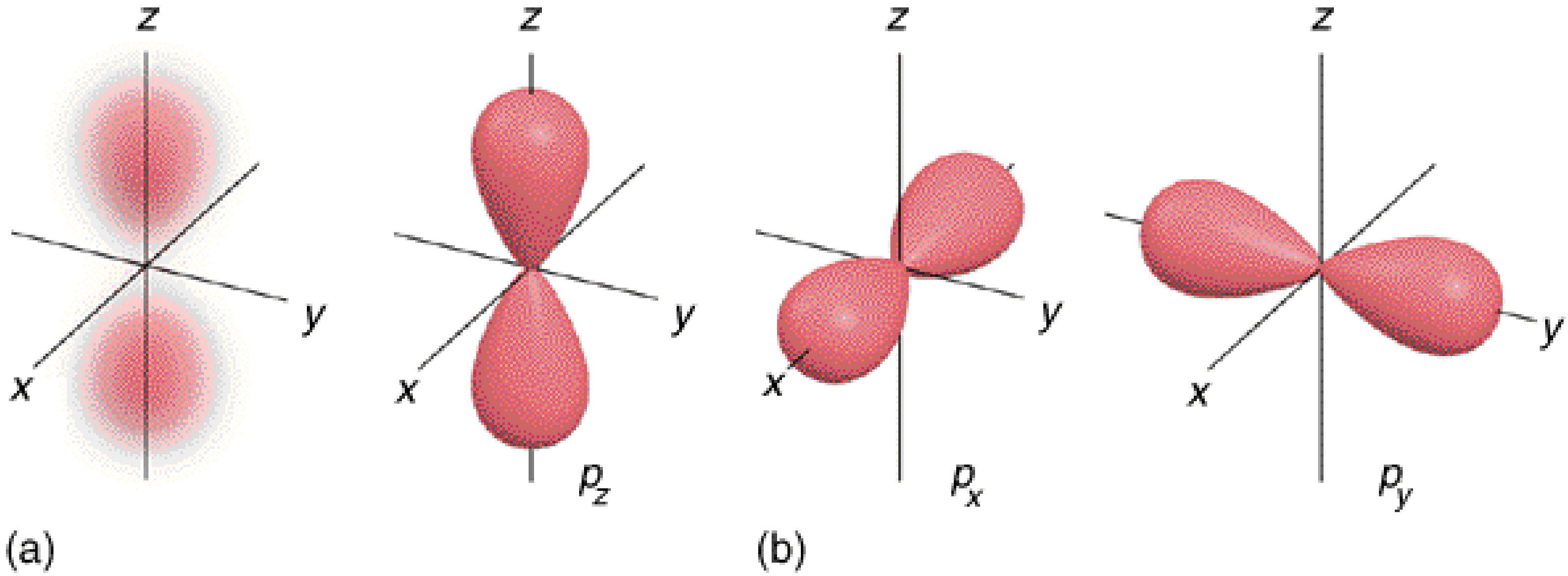
Magnetic Quantum Number, m_l. This quantum number describes the ***orientation*** of orbitals of the same shape. The magnetic quantum number has integral values between $-l$ and $+l$. However, we use **p_x** , **p_y** and **p_z** instead.

There are **3** possible *p* -orbitals		-1	0	+1	
There are **5** possible *d*-orbitals	-2	-1	0	+1	+2
There are **7** possible *f*-orbitals					

p-orbitals

The ***shape*** of a ***p-orbital*** is ***dumb-bell***, (l = 1).

Each shell, from the second shell onwards, contains ***three*** of these ***p-orbitals***, (m_l = -1   0   +1).

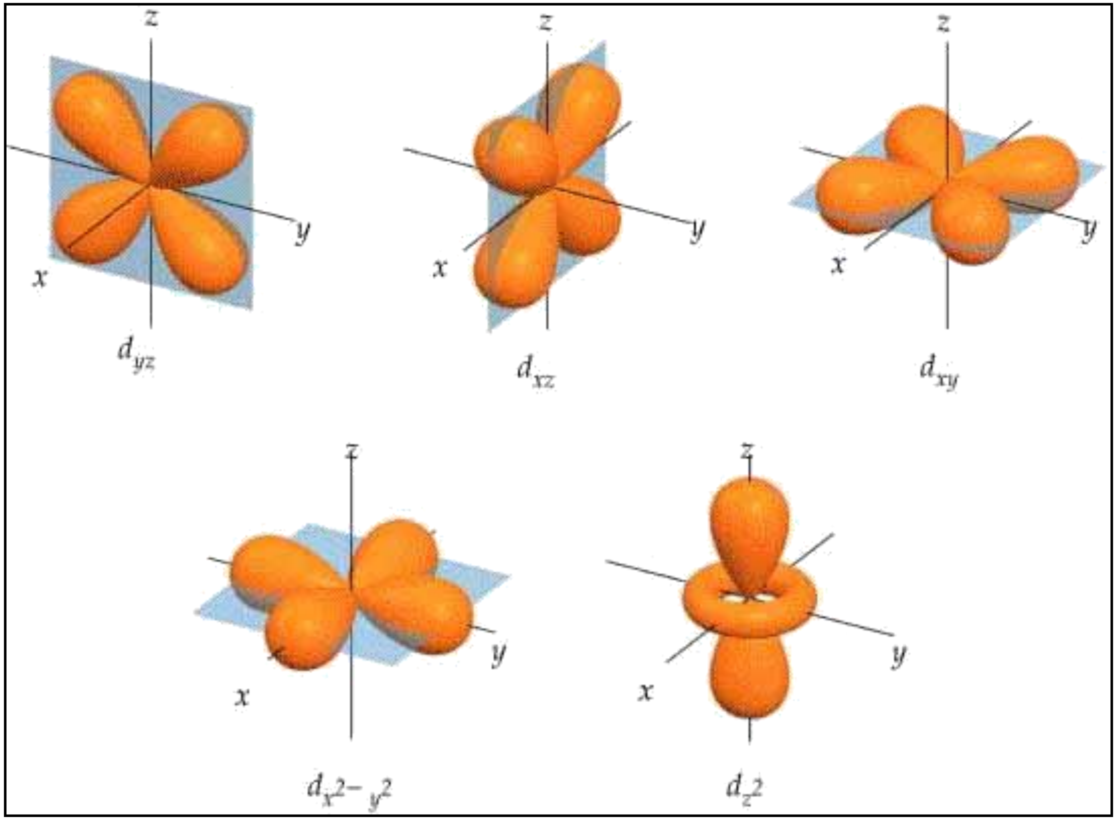


We describe their ***orientation*** as *'along the x-axis'*, $\boldsymbol{p_x}$ *'along the y-axis'*, $\boldsymbol{p_y}$ and *'along the z-axis'*, $\boldsymbol{p_z}$

d-orbitals

The ***shape*** of ***d-orbitals*** (l = 2) are more complicated.

Each shell, from the third shell onwards, contains ***five*** of these ***d-orbitals***, (m_l = -2 -1 0 +1 +2).



We describe their ***orientation*** as

'between the x-and y-axis', $\mathbf{d_{xy}}$, *'between the x-and z-axis'*, $\mathbf{d_{xz}}$, *'between the y-and z-axis'*, $\mathbf{d_{yz}}$,

'along the x- and y-axis', $\mathbf{d_{x^2-y^2}}$ and *'along the z-axis'*, $\mathbf{d_{z^2}}$

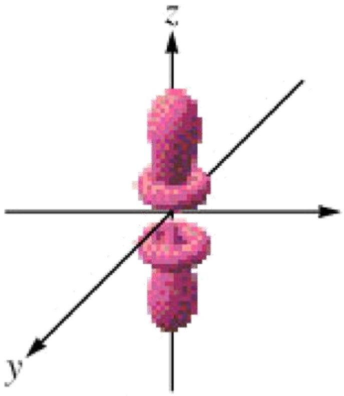
f-orbitals

The ***shape*** of ***f-orbitals*** ($l = 3$) are even more complicated.

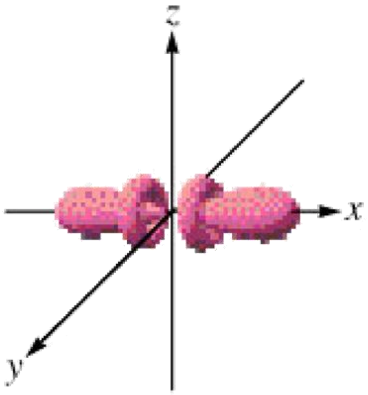
Each shell, from the fourth shell onwards, contains ***seven*** of these ***f-orbitals***, (m_l = -3 -2 -1 0 +1 +2 +3).

f-orbitals are not included in Advanced Higher so we will not have to consider their shapes or orientations, thank goodness!

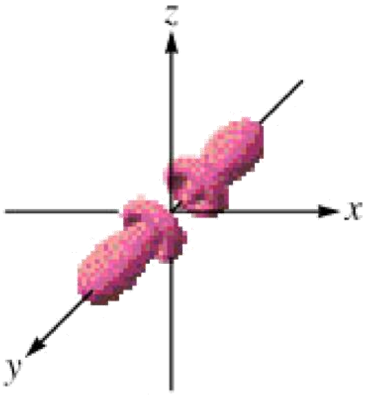
f-orbitals



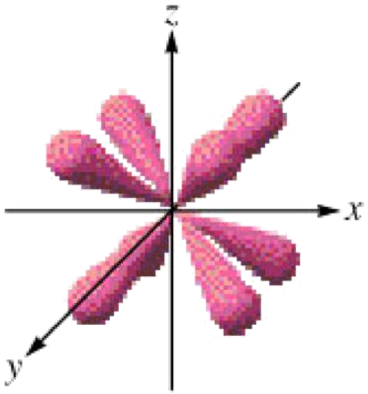
$f_{z^3-\frac{3}{5}zr^2}$



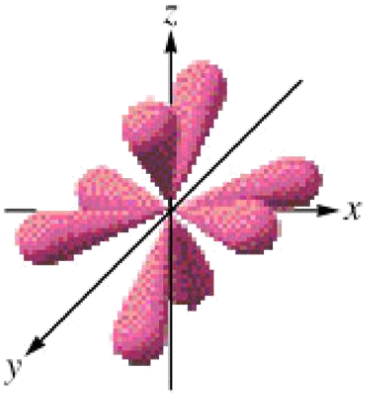
$f_{x^3-\frac{3}{5}xr^2}$



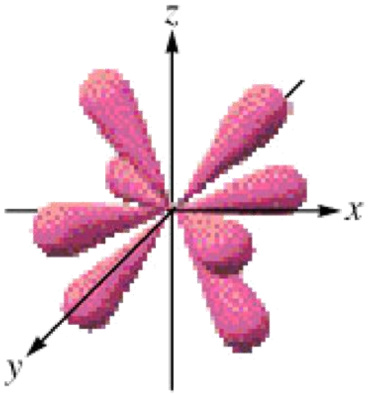
$f_{y^3-\frac{3}{5}yr^2}$



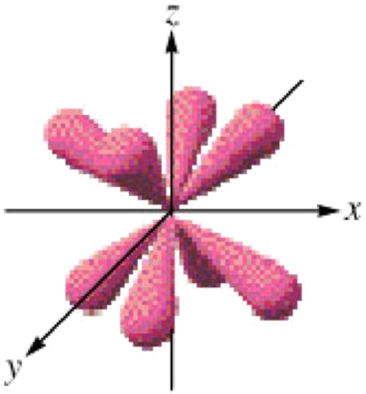
f_{xyz}



$f_{y(x^2-z^2)}$



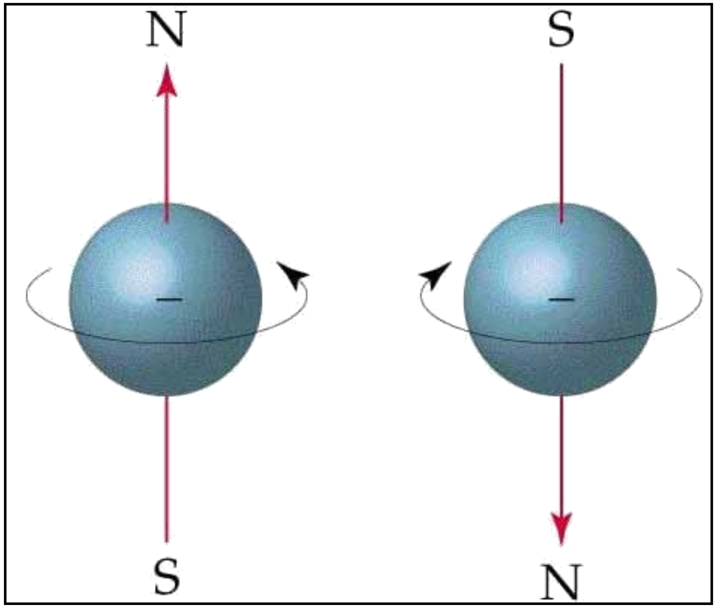
$f_{x(z^2-y^2)}$



$f_{z(x^2-y^2)}$

Couldn’t resist it !

Spin Quantum Number



Each orbital can hold up to 2 electrons.

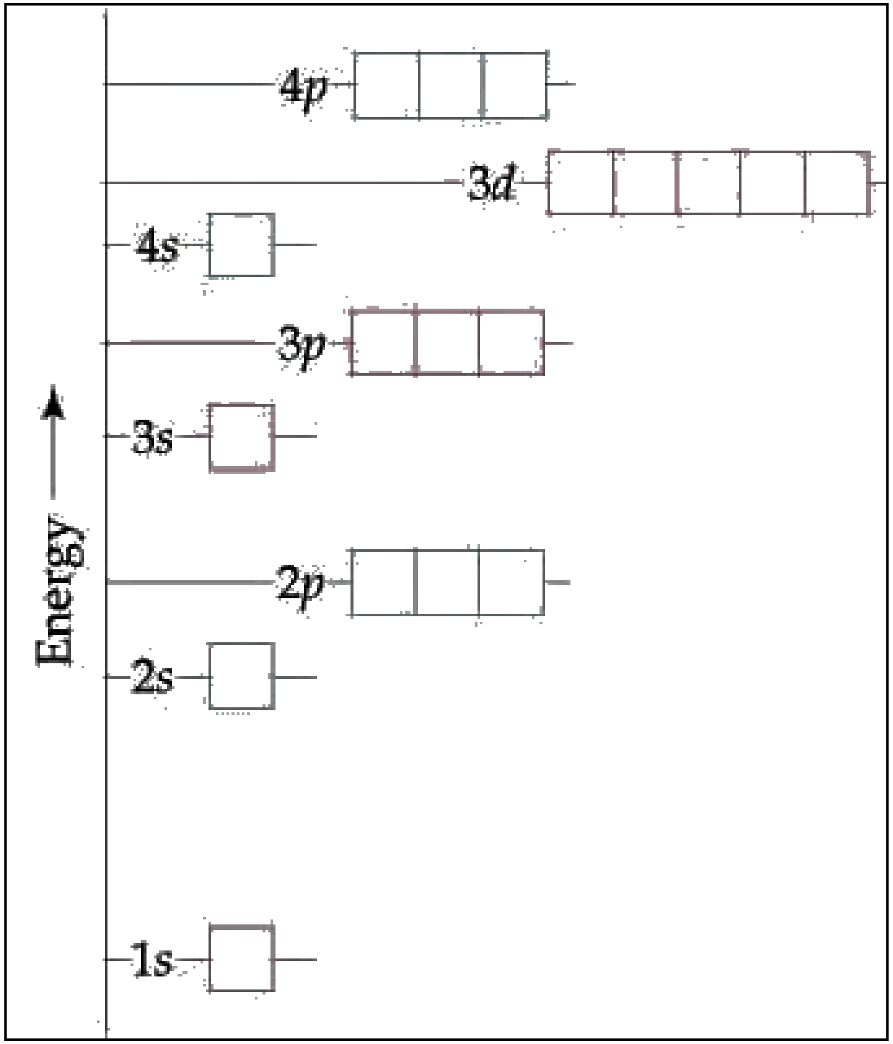
In 1920 it was realised that an electron behaves as if it has a ***spin***

A fourth quantum number was needed.

The ***spin quantum number***, m_s only has two values $+{}^1/_2$ and $-{}^1/_2$

Therefore, *up to* ***four quantum numbers***, ***n*** (***shell***), ***l*** (***shape***), $\boldsymbol{m_l}$ (***orientation***) and $\boldsymbol{m_s}$ (***spin***) are needed to ***uniquely*** describe every electron in an atom.

Energy Diagram



Orbitals can be ranked in terms of energy to yield an ***Aufbau diagram***

As ***n*** increases, note that the spacing between energy levels becomes smaller.

Sets, such as the ***2p-orbitals***, are of ***equal energy***, they are ***degenerate***

Notice that the third and fourth shells overlap

Electron Configurations 1

There are 3 rules which determine in which orbitals the electrons of an element are located.

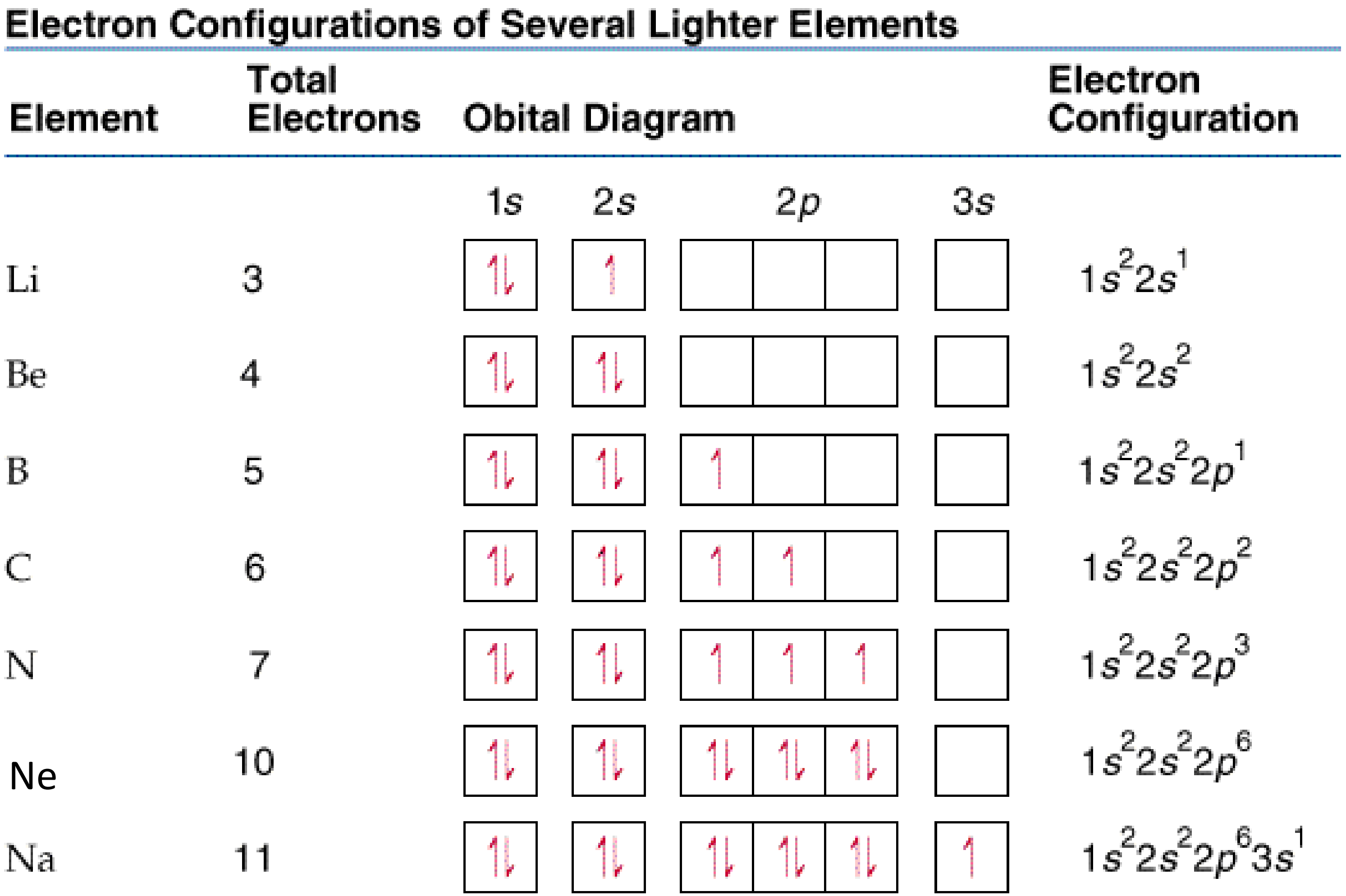
The ***Aufbau Principle*** states that ***electrons will fill orbitals starting with the orbital of lowest energy***.

For ***degenerate*** orbitals, ***electrons fill each orbital singly before any orbital gets a second electron*** (***Hund's Rule of Maximum Multiplicity***).

The ***Pauli Exclusion Principle*** states that ***the maximum number of electrons in any atomic orbital is two***……..

and ….. ***if there are two electrons in an orbital they must have opposite spins*** (rather than parallel spins).

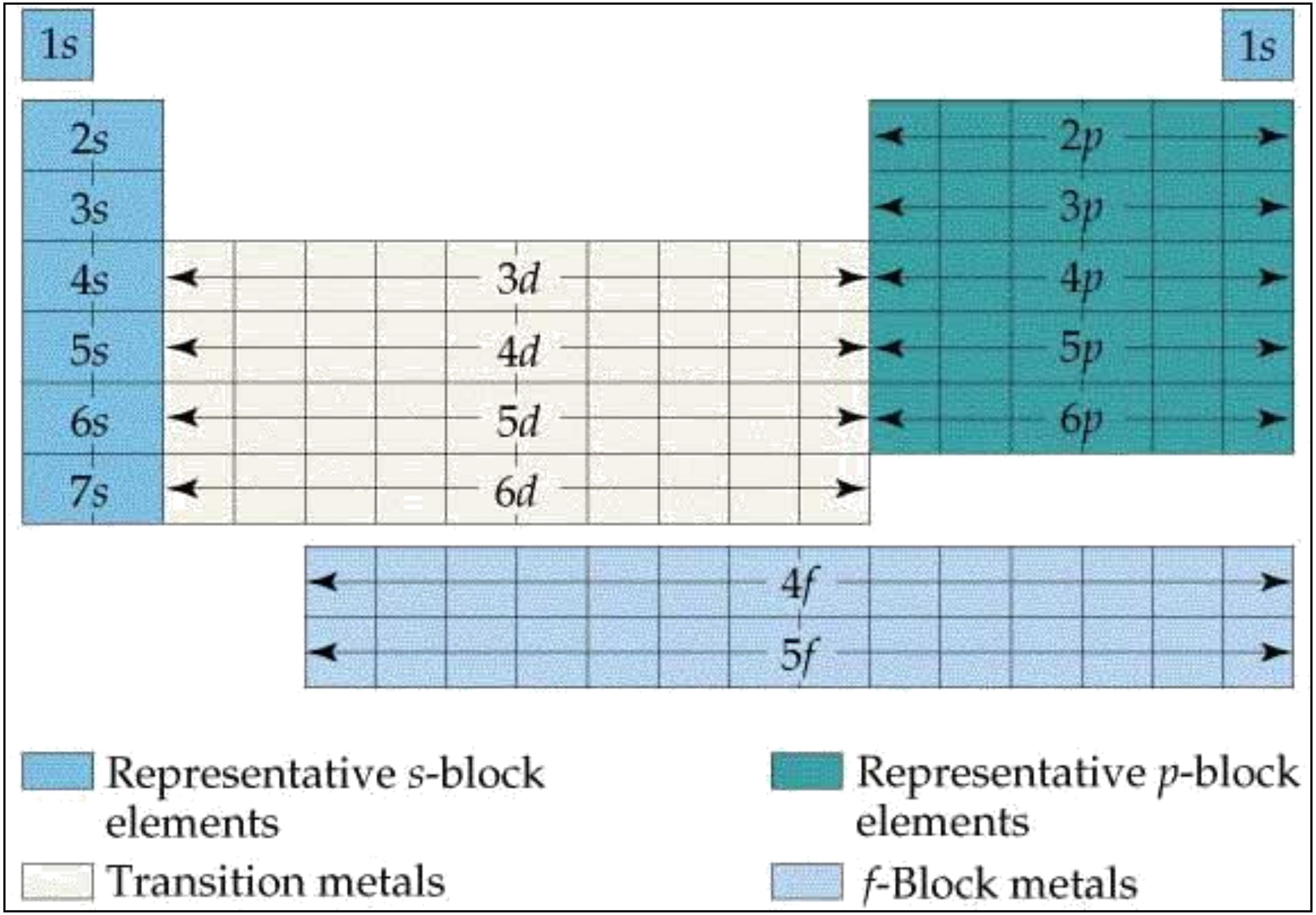
Electron Configurations 2



Electron Configurations of Several Lighter Elements

Element	Total Electrons	Obital Diagram						Electron Configuration
		1s	2s	2p			3s	
Li	3	↑↓	↑					$1s^2 2s^1$
Be	4	↑↓	↑↓					$1s^2 2s^2$
B	5	↑↓	↑↓	↑				$1s^2 2s^2 2p^1$
C	6	↑↓	↑↓	↑	↑			$1s^2 2s^2 2p^2$
N	7	↑↓	↑↓	↑	↑	↑		$1s^2 2s^2 2p^3$
Ne	10	↑↓	↑↓	↑↓	↑↓	↑↓		$1s^2 2s^2 2p^6$
Na	11	↑↓	↑↓	↑↓	↑↓	↑↓	↑	$1s^2 2s^2 2p^6 3s^1$

Periodic Table



Ionisation Energy

The first ionisation energy for an element E is the energy required to remove one mole of electrons from one mole of atoms in the gas state, as depicted in the equation

$$E(g) \rightarrow E^+(g) + e^-$$