Atomic structure

An atom consists of a nucleus around which the electrons orbit in **shells**. The electronic configuration of an atom shows how the electrons are arranged in the atom. So far you will have learnt the electronic configuration of atoms in the form 2, 8, 2 etc. We will look at the electronic configuration of atoms in more detail.

It is important to consider the electronic configuration of atoms because it is the electrons in an atom that participate in chemical reactions.

Every **shell** of electrons is represented by a *principal quantum number* (q.n) and consists of a group of *atomic orbitals*.

An atomic orbital is a region in space in which there is a high probability of finding an electron. Every atomic orbital can accommodate a maximum of 2 electrons. (a consequence of the Pauli exclusion principle – see below.)

Thefour types of orbital of lowest energy are called . *s, p, d* and *f.*

s orbitals occur singly.

p orbitals occur in groups of 3.

d orbitals occur in groups of 5.

f orbitals occur in groups of 7.

Every electron in an atom can be described by four quantum numbers. These numbers are derived by the solution of a very complicated equation (the Schrödinger equation) which takes into account the particle-like nature of electrons as well as their wave-like nature. The quantum numbers are:

a) the principal quantum number, *n.* This can have positive integral values of 1, 2, 3, etc.

   n =1 represents the first shell of electrons, $n = 2$ represents the second shell of electrons and so on.

   The maximum number of orbitals with a particular principal quantum number is given by n^2 e.g. the maximum number of orbitals in the third shell is $3^2 = 9$.

   The maximum number of electrons with a particular principal quantum number is given by $2n^2$ e.g. the maximum number of electrons in the third shell is $2x\ 3^2 = 18$.

b) the azimuthal quantum number, *l.* The allowable values for *l* are integral numbers 0 to n-1.

The value of l defines the type of orbital as shown in the table.

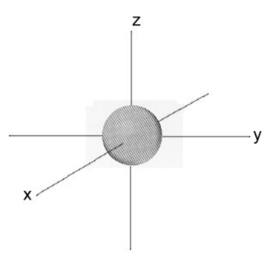
Value of l	0	1	2	3
Type of orbital	*s*	*p*	*d*	*F*

c) the magnetic quantum number, m_l. The allowable values for m_l are integral numbers from l to $-l$. The value of m_l indicates the orientation of the orbital in space.

d) the spin quantum number, m_s, which has a value of either + ½ or – ½.. The sign indicates the direction of spin of the electron.

Application of the above shows that:

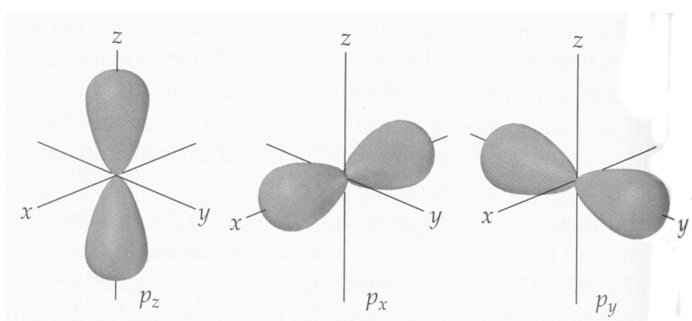
a) for $n = 1$, there is only 1 possible value of l which is $l = 0$. This corresponds to an s orbital and is described as a 1*s* orbital. The number 1 before the **s** indicates that this orbital has principal quantum number 1.



b) for n =2, there are 2 possible values for l viz. $l = 0$ and $l = 1$.

The orbital with $l = 0$ is a 2s orbital. It is very similar to the 1s orbital.

There are 3 possible values for m_l corresponding to $l = 1$. These are -1, 0 and +1. These correspond to three 2*p* orbitals. A *p* orbital is dumbbell shaped, and the three 2*p* orbitals are aligned along the x, y and z axes at right angles to each other.



The 4 orbitals in the second shell consist of one 2*s* and three 2*p* orbitals which can accommodate a maximum of 8 electrons.

c) for $n = 3$, there are 3 possible values for l viz. $l = 0$, l =1, l =2.

The orbital corresponding to $l = 0$ is a 3 *s* orbital. This is very similar to the 1s orbital.

There are 3 possible values for m_l with $l =$ 1 as shown in b). These would correspond to three 3*p* orbitals. These are very similar to the 2p orbitals.

There are 5 possible values for m_l with $l = 2$. These are 2,1,0,-1,-2. These correspond to five 3*d* orbitals. These have complicated shapes which you do not need to know.

The 8 orbitals in the third shell consist of one 3*s*, three 3*p* and five 3*d* orbitals.

d) for $n = 4$, there are 4 possible values for l viz. $l = 0$, $l =1$, $l =2$ and $l = 3$.

The orbital corresponding to $l = 0$ is a 4*s* orbital, much like the 1s.

There are 3 possible values for m_l with $l =$ 1 as shown in b). These correspond to three 4*p* orbitals, much like the 2p.

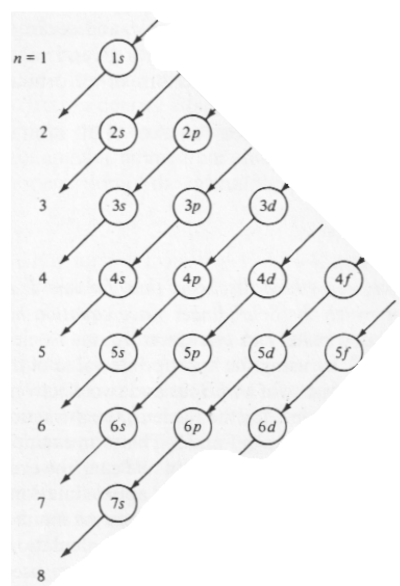
There are 5 possible values for *m* with $l = 2$. These correspond to five 4*d* orbitals, much like the 3d.

There are 7 possible values for m_l with $l = 3$. These are 3,2,1,0, -1, -2, -3. These correspond to seven 4*f* orbitals. These have even more complicated shapes than d orbitals.

The 16 orbitals in the fourth shell consist of one 3*s*, three 3*p* and five 3*d* orbitals.

A set of orbitals which have the same values of *n* and *l*, is known a **subshell.** For example, the 3d subshell, or the 2p subshell.

In working out the electronic configuration of atoms, we will apply the following principles:



a) The **Pauli exclusion principle** states that no two electrons in an atom can have all four of their quantum numbers alike. A consequence of this rule is that no atomic orbital can accommodate more than 2 electrons.

If 2 electrons occupy the same orbital, they will have the same value for *n*, *l*, and m_l but their spin quantum numbers will differ in sign.

b) The **aufbau** or **building up principle**. This states that the atomic orbitals are filled in order of increasing energy, lowest first.

The order is 1s<2s<2p<3s<3p<4s<3d<4p<5s <4d<5p<6s<4f<5d<6p<7s<5f<6d. The diagram above right makes it easier to remember this order:

c) **Hund's rule**.

One electron goes into each of a set of degenerate orbitals, with spins parallel, before any pairing occurs.

Degenerate orbitals are orbitals with the same energy level. The orbitals in a subshell are degenerate. E.g. the three 2p orbitals are degenerate, the five 4d orbitals are degenerate.