ATOMIC STRUCTURE

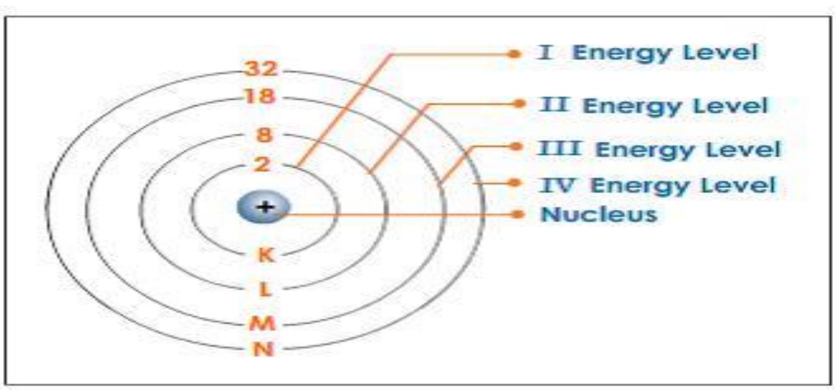
There are two ways to represent the atomic structure of an element or compound;

- Electronic Configuration
- Dot & Cross Diagrams

ELECTRONIC CONFIGURATION

Electron are not placed at fixed positions in atoms ,but we can predict approximate position of them .these position are called energy levels or shells of atoms .With electronic configuration elements are represented **numerically** by the number of electrons in their shells and number of shells.

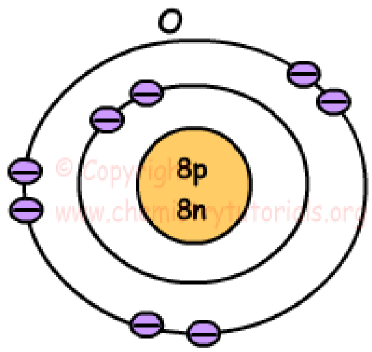
- **first shell** = K a maximum of **2** electrons
- **second shell** = L a maximum of **8** electrons
- **third shell** = M a maximum of 1**8** electrons

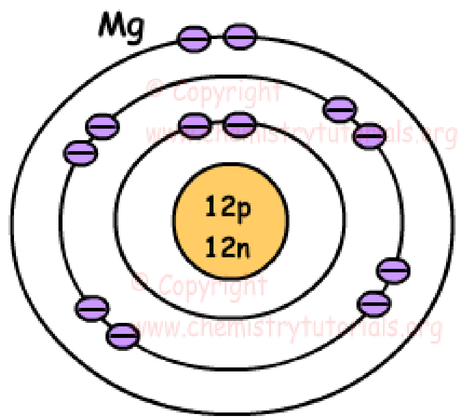


Nitrogen **configuration = 2 , 5**

- **2 in 1^{st} shell**

  5 in 2^{nd} shell





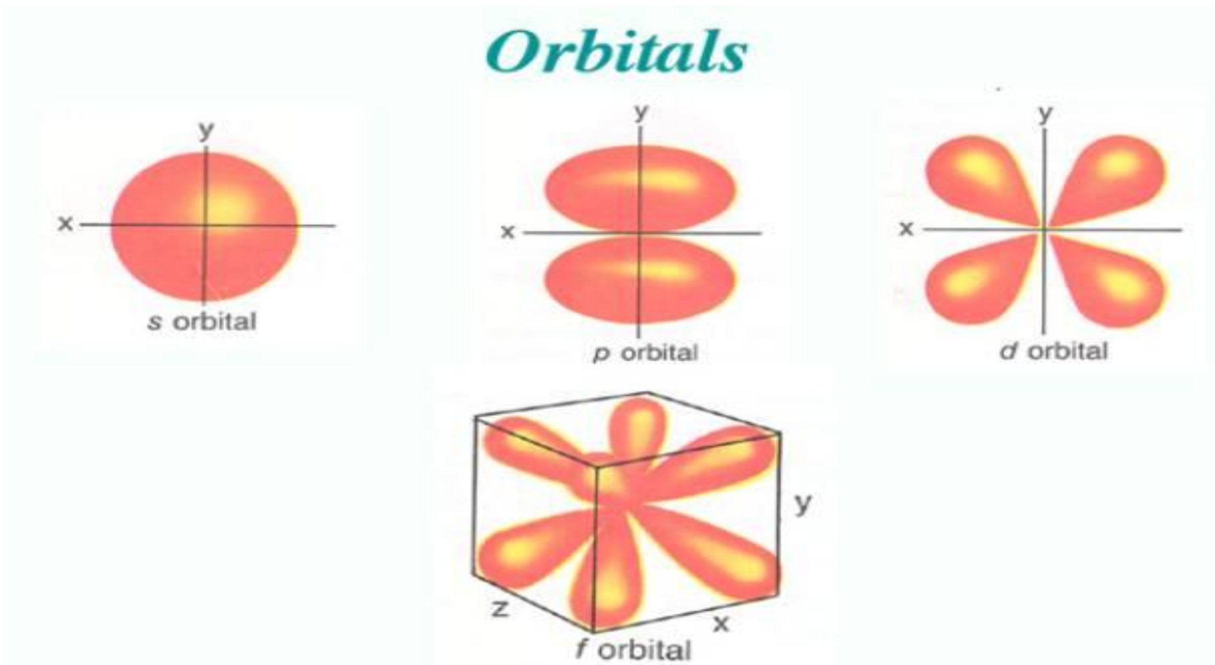
The electron configuration of an atom is a **notation** which shows how electrons are distributed in orbits. The format consists of a series of numbers, letters and superscripts.

To understand this notation we need to understand 3 concepts:

1. Orbital - a place around the nucleus where find the electron. it can hold no more than 2 electrons.

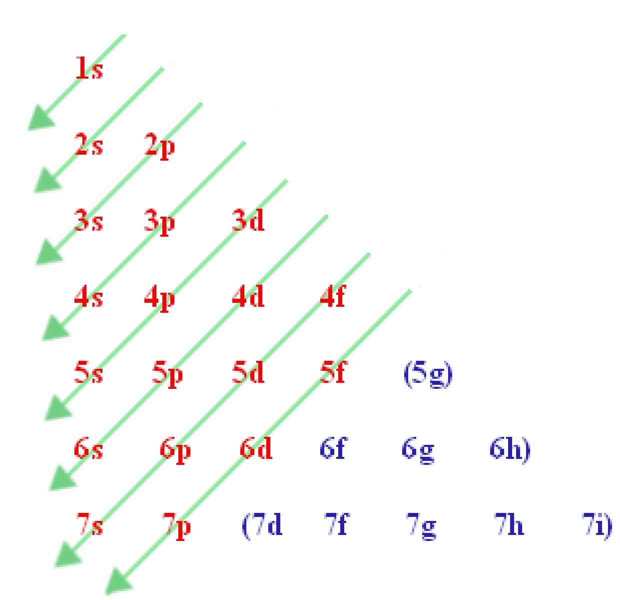
2. Sub shell - There are differently shaped orbitals. Some orbitals are round or spherical. Others are dumbbell shaped. A sub shell is just a way to organize the different orbitals.

Subshells		
Subshell	**# of Orbitals**	**Orbital Shape**
s	**1**	**spherical**
p	**3**	**dumbbell**
d	**5**	*******
f	**7**	***



3. Shell - the shell represents the orbit around a nucleus. The first shell (or orbit) is close to the nucleus. The second shell is a little farther out from the nucleus. The energy of the orbits increase as we move away from the nucleus.

Example: An electron in the 1st Shell would have less energy than an electron in the 2nd Shell.



The "1s" sub shell has the lowest energy**.** to start at the beginning of each arrow, and then follow it all of the way to the end, filling in the subshells that it passes through. In other words, the order for filling in the sub shells becomes;

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

Example :-

Write the electron configuration for Carbon. Carbon has Atomic No. = 6

A Carbon atom has 6 electrons.

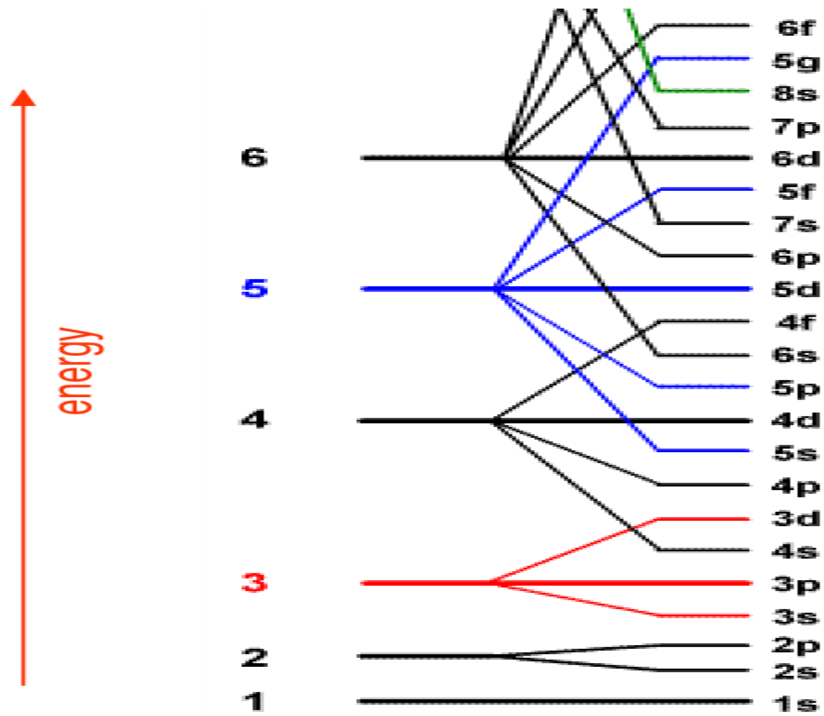
$$\mathbf{1s^2\ 2s^2\ 2p^2}$$

Quantum Numbers

Quantum numbers describe specifically the energies of electrons in atoms, but other possibilities include angular momentum, spin, etc

According to the laws of quantum mechanics, for systems with only one electron, an energy is associated with each electron configuration and, upon certain conditions, electrons are able to move from one configuration to another by emission or absorption of a quantum of energy, in the form of a photon.

Each electron in an atom is described by four different **quantum numbers**. The first three (n, l, m_l) specify the particular orbital of interest, and the fourth (m_s) specifies how many electrons can occupy that orbital



1. **Principal Quantum Number (*n*): *n* = 1, 2, 3, …, ∞**
   Specifies the **energy** of an electron and the **size** of the orbital. All orbitals that have the same value of *n* are said to be in the same **shell** (**level**).

   For a hydrogen atom with n=1, the electron is in *ground state*;

   if the electron is in the n=2 orbital, it is in an *excited state*. The total number of orbitals for a given *n* value is n^2.

2. **Angular Momentum (Secondary, Azimunthal) Quantum Number (*l*):**

   ***l* = 0, ...,(*n*-1) .**
   Specifies the **shape** of an orbital with a particular principal quantum number. The secondary quantum number divides the shells into smaller groups of

orbitals called **subshells** (**sublevels**). Usually, a letter code is used to identify ***l*** to avoid confusion with ***n***:

l	0	1	2	3	4	5	...
Letter	*s*	*p*	*d*	*f*	*g*	*h*	...

The subshell with n=2 and l=1 is the 2*p* subshell; if n=3 and l=0, it is the 3*s* subshell, and so on. The value of l also has a slight effect on the energy of the subshell; the energy of the subshell increases with l ($s < p < d < f$).

3. **Magnetic Quantum Number (m_l): $m_l = -l, ..., 0, ..., +l$.**
   Specifies the **orientation in space** of an orbital of a given energy (n) and shape (l). This number divides the subshell into individual **orbitals** which hold the electrons; there are ($2l$+1)orbitals in each subshell. Thus the *s* subshell has only one orbital, the *p* subshell has three orbitals, and so on.

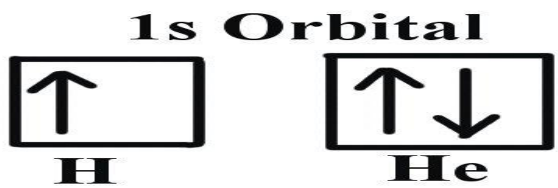
4. **Spin Quantum Number (m_s): m_s = +½ or -½.**
   Specifies the **orientation of the spin axis** of an electron.

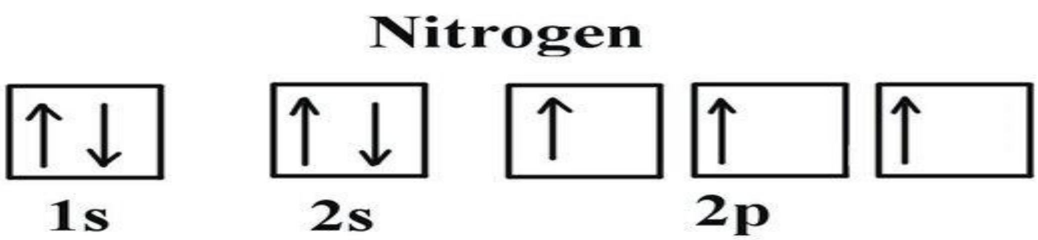
Nots :- that no two electrons in the same atom can have identical values for all four of their quantum numbers.

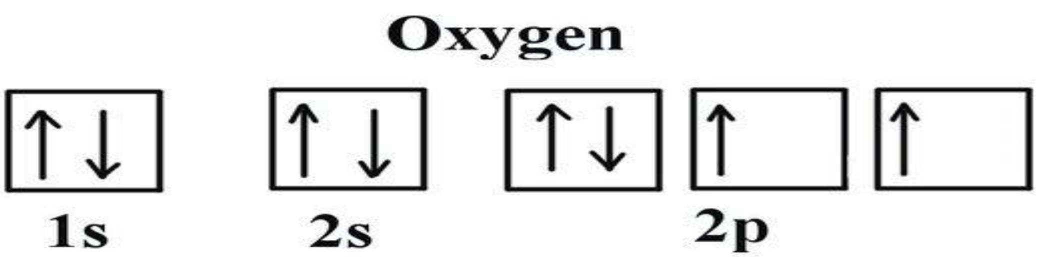
What this means is that no more than **two** electrons can occupy the same orbital, and that two electrons in the same orbital must have **opposite spins**.?

Because an electron spins, it creates a magnetic field, which can be oriented in one of two directions. For two electrons in the same orbital, the spins must be opposite to each other.

s subshell	*p* subshell	*d* subshell	*f* subshell
$\ell = 0$	$\ell = 1$	$\ell = 2$	$\ell = 3$
$m_\ell = 0$	m_ℓ= -1, 0, +1	m_ℓ= -2, -1, 0, +1, +2	m_ℓ= -3, -2, -1, 0, +1, +2, +3
One *s* orbital	Three *p* orbitals	Five *d* orbitals	Seven *f* orbitals
Two *s* orbital electrons	Six *p* orbital electrons	10 *d* orbital electrons	14 *f* orbital electrons





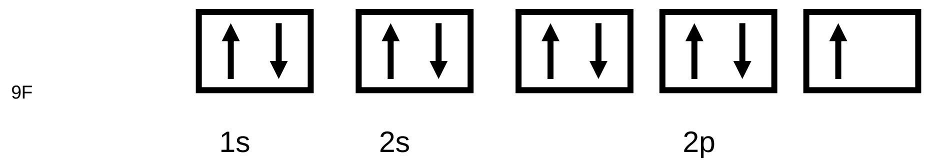


Example: The quantum numbers used to refer to the outer most valence electrons of the Carbon (C) atom, which are located in the

2p atomic orbital, are; n = 2 (2nd electron shell), ℓ = 1 (p orbital subshell), m_ℓ = 1, 0 or −1, m_s = ½ (parallel spins).

Q/ Write a set of quantum numbers for the third electron and a set for the

eighth electron of the F atom



The third electron is in the 2s orbital. Its quantum numbersare

n = ***l* =** m_l = m_s=

The eighth electron is in a 2p orbital. Its quantum numbers

Table 8.4 Partial Orbital Diagrams and Electron Configurations* for the Elements in Period 4

Atomic Number	Element	Partial Orbital Diagram (4*s*, 3*d*, and 4*p* Sublevels Only): 4*s*	3*d*	4*p*	Full Electron Configuration	Condensed Electron Configuration
19	K	[↑]	[ ][ ][ ][ ][ ]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\ 4s^1$	$[Ar]\ 4s^1$
20	Ca	[↑↓]	[ ][ ][ ][ ][ ]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\ 4s^2$	$[Ar]\ 4s^2$
21	Sc	[↑↓]	[↑][ ][ ][ ][ ]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\ 4s^23d^1$	$[Ar]\ 4s^23d^1$
22	Ti	[↑↓]	[↑][↑][ ][ ][ ]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\ 4s^23d^2$	$[Ar]\ 4s^23d^2$
23	V	[↑↓]	[↑][↑][↑][ ][ ]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\ 4s^23d^3$	$[Ar]\ 4s^23d^3$
24	Cr	[↑]	[↑][↑][↑][↑][↑]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\ 4s^13d^5$	$[Ar]\ 4s^13d^5$
25	Mn	[↑↓]	[↑][↑][↑][↑][↑]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\ 4s^23d^5$	$[Ar]\ 4s^23d^5$
26	Fe	[↑↓]	[↑↓][↑][↑][↑][↑]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\ 4s^23d^6$	$[Ar]\ 4s^23d^6$
27	Co	[↑↓]	[↑↓][↑↓][↑][↑][↑]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\ 4s^23d^7$	$[Ar]\ 4s^23d^7$
28	Ni	[↑↓]	[↑↓][↑↓][↑↓][↑][↑]	[ ][ ][ ]	$[1s^22s^22p^63s^23p^6]\ 4s^23d^8$	$[Ar]\ 4s^23d^8$

Lithium - 3 electron

Electron configuration $1S^2\ 2S^1$ $\boxed{\uparrow}$

$n = 2$ $l = 0$ $m_l = 0$ $m_s = +1/2$

Beryllium - four electrons **$1s^2$ $2s^2$** $\boxed{\uparrow\downarrow}$

n = 2
l = 0
m = 0
s = -1/2

Notice the same n, l, and m values as the third electron, but s has shifted from positive 1/2 to negative 1/2.

Boron - five electrons

Carbon - six electrons

Nitrogen - seven electrons

Oxygen - eight electrons

Fluorine - nine electrons

Neon - ten electrons

Ions

Ions are atoms (or groups of atoms) which carry an electric charge because they have

either gained or lost one or more electrons. If an atom gains electrons it becomes a negative charged. If it loses electrons, it becomes positively charged.

^{4}**Be** $\mathbf{1s^2 2s^2}$ **Be^{2+}** $\mathbf{1s^2}$

^{12}**Mg** $\mathbf{1s^2 2s^2 2p^6 3s^2}$ **Mg^{2+}** $\mathbf{1s^2 2s^2 2p^6}$

^{13}**Al** $\mathbf{1s^2 2s^2 2p^6 3s^2 3p^1}$ **Al^{3+}** $\mathbf{1s^2 2s^2 2p^6}$

The electronic structure of s- and p-block ions

Write the electronic structure for the neutral atom, and then add (for a negative ion) or subtract electrons (for a positive ion).

To write the electronic structure for Cl^-:

Cl	$1s^2 2s^2 2p^6 3s^2 3p^5$	but Cl^- has one more electron
Cl^-	$1s^2 2s^2 2p^6 3s^2 3p^6$	

To write the electronic structure for O^{2-}:

O	$1s^2 2s^2 2p^4$	but O^{2-} has two more electrons
O^{2-}	$1s^2 2s^2 2p^6$	

To write the electronic structure for Na^+:

Na	$1s^2 2s^2 2p^6 3s^1$	but Na^+ has one less electron
Na^+	$1s^2 2s^2 2p^6$	

To write the electronic structure for Ca^{2+}:

Ca	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$	but Ca^{2+} has two less electrons
Ca^{2+}	$1s^2 2s^2 2p^6 3s^2 3p^6$	

The electronic structure of d-block ions

Here you are faced with one of the most irritating facts in chemistry at this level When you work out the electronic structures of the first transition series (from scandium to zinc) using the Aufbau Principle, you do it on the basis that the 3d orbitals have a higher energy than the 4s orbital.That means that you work on the assumption that the 3d electrons are added after the 4s ones.However, in all the chemistry of the transition elements, the 4s orbital behaves as the outermost, highest energy orbital. When these metals form ions, the 4s electrons are always lost first.

You must remember this:

When d-block elements form ions, the 4s electrons are lost first.

The aufbau principle, also called the aufbau rule, states that in the ground state of an atom or ion, electrons fill subshells of the lowest available energy, then they fill subshells of higher energy. For example, the 1s subshell is filled before the 2s subshell is occupied.