THE ROLES OF ELECTRONS AND NEUTRONS

Chemistry is mainly the science of how electrons behave in atoms and molecules, so we spend most of our time talking about them. However, an atom isn't an atom without protons and neutrons. Starting off, we'll think of atoms as charge-neutral, meaning that the sum of all charges, positive (the protons, charge = +1) and negative (the electrons, charge = -1) is zero. That means a neutral atom has to have and identical number of protons and electrons.

Ions

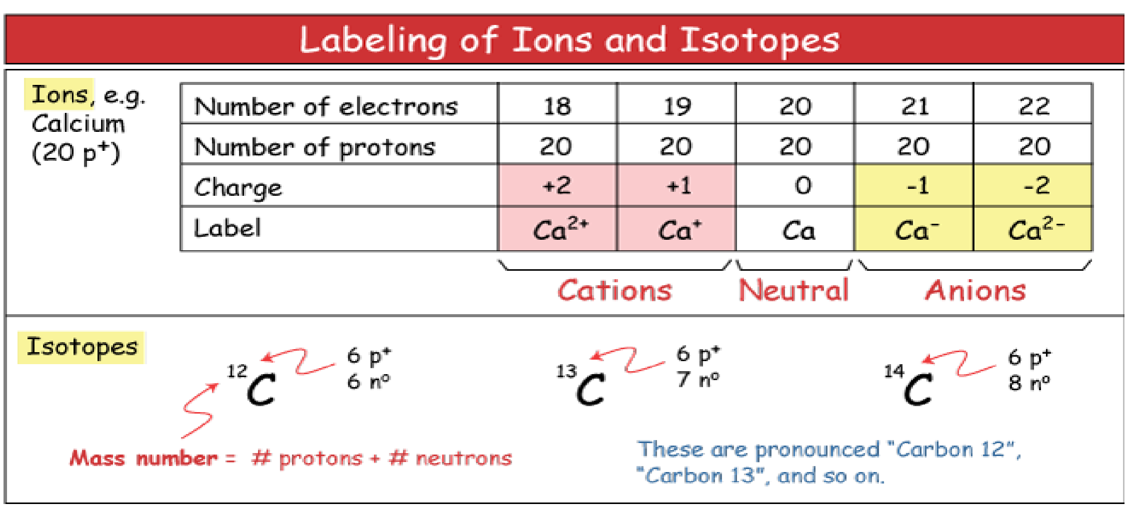
When the number of protons and electrons is not equal, we have an **ion**, a charged atom or molecule. For example, if a lithium atom (see above), which has three protons (that's what makes it a lithium atom), only has two electrons, its charge is (+3) + (-2) = +1. If a fluorine atom has 8 electrons and its complement of 7 protons (that's what makes it fluorine), its charge is (+7) + (-8) = -1. We call

Negative and positive ions **anions** and **cations**, respectively. As we will see, ions of all kinds play a crucial role in all of chemistry.

Isotopes

The number of neutrons in a nucleus can vary. In fact, most elements are composed of atoms that vary in the number of neutrons they contain. Generally, there is one number that dominates. For example, 98.8% of Carbon (6 protons) contains 6 neutrons. A little less than 1% contains 7 neutrons, and about one in every 1012 carbon atoms contains 8 neutrons (yes, that's a big number, but that's still a very detectable amount of 8-neutron carbon. We call the group of all of these versions of carbon the **isotopes** of carbon. When we refer to a isotope, we are generally referring to a version of the element with a specific number of neutrons. Extra neutrons add mass to the atom, but they only have a small effect on its chemical properties.

The identity of an element depends solely on the number of protons in its nucleus. There are specific conventions for labeling ions and isotopes.



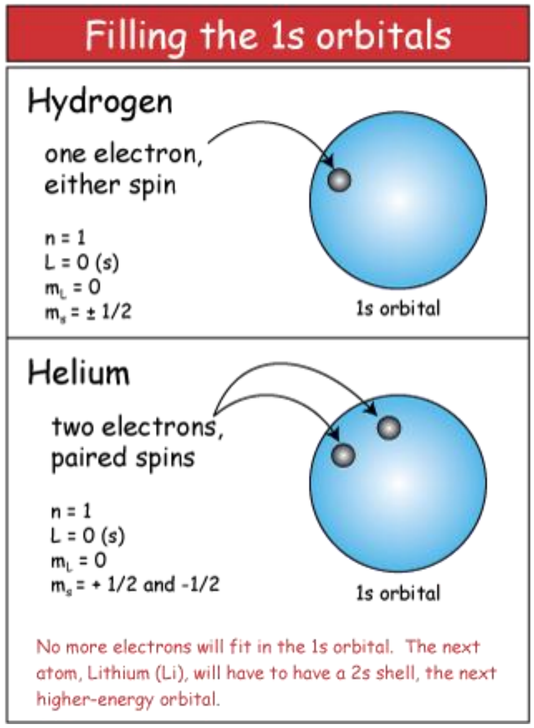
Filling orbitals

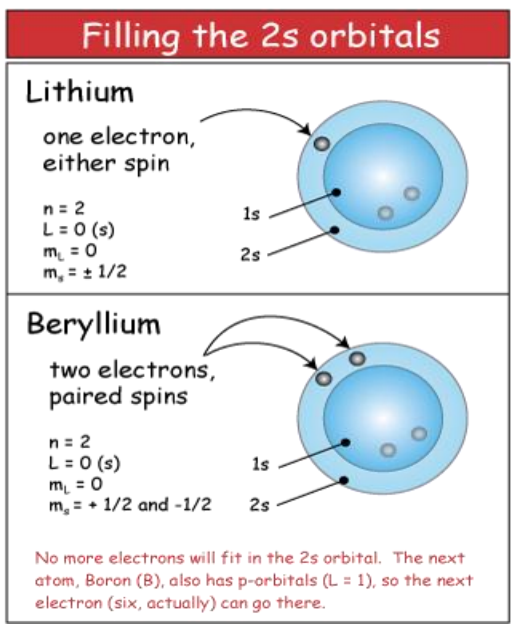
In another section, we learned about the quantum nature of electrons bound to atoms by looking at hydrogen. We can generalize this theory to any atom by simply *filling* increasingly higher-energy orbitals with electrons, one at a time, as the atoms get bigger.

Learning to fill orbitals will provide the key to understanding the periodic table of the elements, and understanding the table is the key to much of what we'll be doing in chemistry as we go along.

It will help, as we go through the next bit of material, if you remember that (1) no two electrons in an atom can have the same set of quantum numbers (n, L, m_L and m_s) and (2) we "fill" orbitals from the lowest energy upward.

For the second atom, helium (He), with two protons, we place a second electron into the 1s orbital, noting that the two electrons must have different spins (there are only two kinds). This fills the 1s shell. It can't accept any more electrons.





When we get to lithium (Li), we begin filling the second shell, which contains an s-orbital (lowest energy) and a set of p-orbitals. The s-orbital gets filled first.

Let's begin to write **electron configurations** for these atoms. The electron configuration for Li is

$$\textbf{Li: } \mathbf{1s^2, 2s^1}.$$

That means the 1s orbital contains two electrons and the 2s contains one. (The superscripts aren't mathematical powers, just counters.)

For beryllium (Be), we have

$$\textbf{Be: } \mathbf{1s^2, 2s^2}.$$

After Be, in order to add electrons (to make boron-neon), we can only add to the 2p orbitals, which can hold the next six electrons. For now, note that He had a full 1s orbital and Be has a full 2s orbital.

For elements B, C, N, O, F, Ne, we fill in the three p sub-orbitals, which can each hold two spin-paired electrons for a total of six in the p-orbital. The electron configurations are:

B: $1s^2$, $2s^2$, $2p^1$

C: $1s^2$, $2s^2$, $2p^2$

N: $1s^2$, $2s^2$, $2p^3$ ← 2p shell half filled

O: $1s^2$, $2s^2$, $2p^4$

F: $1s^2$, $2s^2$, $2p^5$

Ne: $1s^2$, $2s^2$, $2p^6$ ← 2p shell filled

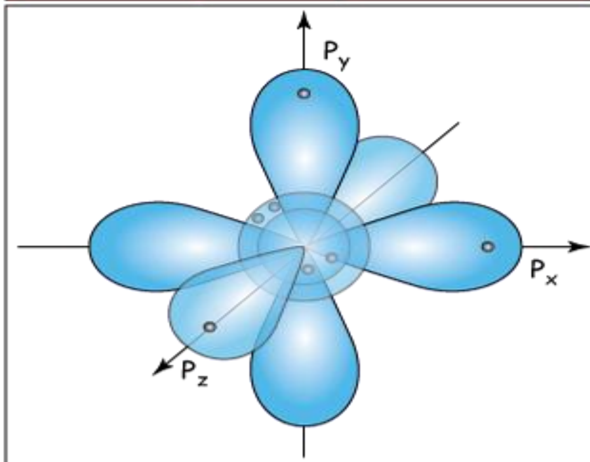
You will be tempted to ask, with all those intersecting orbitals (which may not be drawn to scale, by the way), won't the electrons collide? Don't fall into that trap. Electrons don't act like particles when bound to atoms. There is avoidance of a sort, of course. Electrons must be spin paired; the spin pairs must live in different sub-orbitals; and negatively charged electrons repel each other in any situation.

Moving on to larger atoms, we start the process over again with n=3 (we're out of orbitals in the n=2 shell). Once we work through the 3s and 3p electrons (8 in all) we start filling the 3d orbitals ... except that there's a little kink. What really happens is that energy levels are always filled by the next highest level. It turns out that there's a bit of swapping of levels from what is expected. As an example, the electron configuration of Krypton is:

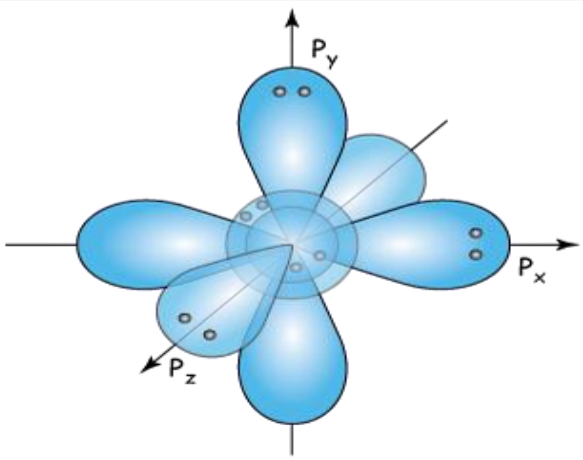
Kr: $1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^6$, $4s^2$, $3d^{10}$, $4p^6$

Notice that the 3d orbitals (5 of them) are filled between the 4s and 4p orbitals. We need to get to the bottom of that and find an easy way to remember it.

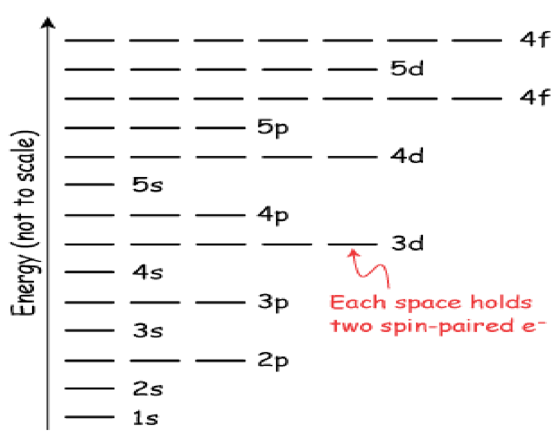
Filling the 2p orbitals



For B, C and N, electrons are placed into each of the p sub-orbitals, one at a time. The configuration of Nitrogen is shown above.



For O, F and Ne, additional electrons are placed into each of the p sub-orbitals, filling each in turn. Each p-sub orbital can hold two electrons, for a total of six. The configuration of Neon is shown above. Note that Neon has a full n=2 shell



Ordering the Energy Levels

When the Schrödinger equation is solved for the H-atom, the energy-level pattern for the upper levels does some unexpected things, and we've just got to get used to it. Take a look at the levels at the left. The levels are not necessarily spaced to scale, but the ordering is correct.

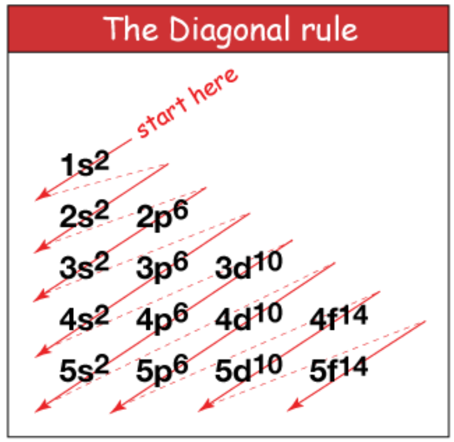
Each line in the figure represents a sub-orbital that can hold two spin-paired electrons.

Notice that the 4s level falls right between the 3p and 3d, breaking the logical sequence. It happens farther up, too. From the point of view of the Schrödinger equation, this glitch makes perfect sense but it does make things harder to remember for us ... except that there's a handy trick.

The **diagonal rule** makes remembering the energy level ordering easy. If you can remember how to write the levels in their logical order like this, then draw in the diagonal lines.

Now following the red arrows from upper right to lower left gives you the exact ordering. It's an easy way to remember.

Now given the number of electrons in an atom, you should be able to write the electron configuration.



Br^-

Xe

Na^+

Fe

Ca^{2+}

Source: http://www.drcruzan.com/Chemistry_Atoms.html