






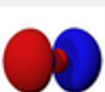







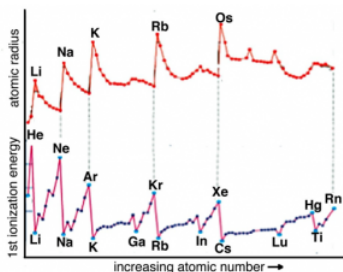
2.7: Quantum Numbers

Quantum numbers (whose derivation we will not consider here) provide the answer to our dilemma. Basically we can describe the wave function for each individual electron in an atom by a distinct set of three quantum numbers, known as n , l , and ml . The principal quantum number, n , is a non-zero positive integer ($n = 1, 2, 3, 4$, etc.). These are often referred to as electron shells or orbitals, even though they are not very shell- or orbital-like. The higher the value of n , the higher the overall energy level of the electron shell. For each value of n there are only certain allowable values of l , and for each value of l , only certain allowable values of ml . Table 2.7.1 (next page) shows the allowable values of l and ml for each value of n are shown. There are a few generalizations we can make. Three quantum numbers, n , l , and ml , describe each orbital in an atom and each orbital can contain a maximum of two electrons. As they are typically drawn, each orbital defines the space in which the probability of finding an electron is 90%. Because each electron is described by a unique set of quantum numbers, the two electrons within a particular orbital must be different in some way.^[18] But because they are in the same orbital they must have the same energy and the same probability distribution. So what property is different? This property is called spin. The spin quantum number, m_s , can have values of either $+\frac{1}{2}$ or $-\frac{1}{2}$. Spin is responsible for a number of properties of matter including magnetism.

Hydrogen has one electron in a $1s$ orbital and we write its electron configuration as $1s^1$. Helium has both of its electrons in the $1s$ orbital ($1s^2$). In lithium, the electron configuration is $1s^2 2s^1$, which tells us that during ionization, an electron is being removed from a $2s$ orbital. Quantum mechanical calculations tell us that in $2s$ orbital there is a higher probability of finding electrons farther out from the nucleus than the $1s$ orbital, so we might well predict that it takes less energy to remove an electron from a $2s$ orbital (found in Li) than from a $1s$ orbital (found in H). Moreover, the two $1s$ electrons act as a sort of shield between the nucleus and the $2s$ electrons. The $2s$ electrons feel what is called the effective nuclear charge, which is smaller than the real charge because of shielding by the $1s$ electrons. In essence, two of the three protons in the lithium nucleus are counterbalanced by the two $1s$ electrons. The effective nuclear charge in lithium is $+1$. The theoretical calculations are borne out by the experimental evidence—always a good test of a theory.

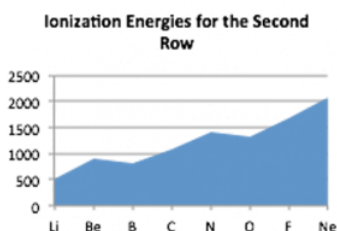
Table 2.7.1 Elemental electron shell organization

	$s(l = 0)$	$p(l = 1)$			$d(l = 2)$			
	$m = 0$	$m = 0$	$m = \pm 1$		$m = 0$	$m = \pm 1$		$m = \pm 2$
	s	p_z	p_x	p_y	d_{z^2}	d_{xz}	d_{yz}	d_{xy} $d_{x^2-y^2}$
$m = 1$								
$m = 2$								
$m = 3$								



At this point, you might start getting cocky; you may even be ready to predict that ionization energies across the periodic table from lithium to neon (Ne) will increase, with a concomitant decrease in atomic radius. In the case of atomic radius, this is exactly what we see in the figure – as you go across any row in the periodic table the atomic radius decreases. Again, the reason for both these trends is that same: that is, each electron is attracted by an increasing number of protons as you go from Li to Ne, which is to say that the effective nuclear charge is increasing. Electrons that are in the same electron shell do not interact much and each electron is attracted by all the unshielded charge on the nucleus. By the time we get to fluorine (F), which has an effective nuclear charge of $9 - 2 = +7$, and neon ($10 - 2 = +8$), each of the electrons are very strongly attracted to the nucleus, and very difficult to dislodge. Meaning that the size of the atom gets smaller, and the ionization energy gets larger^[19]

As you have undoubtedly noted from considering the graph, the increase in ionization energy from lithium to neon is not uniform: there is a drop in ionization energy from beryllium to boron and from nitrogen to oxygen. This arises from the fact that as the number of electrons in an atom increases the situation becomes increasingly complicated. Electrons in the various orbitals influence one another and some of these effects are quite complex and chemically significant. We will return to this in a little more detail in Chapter 3 and at various points through the rest of the book.



If we use the ideas of orbital organization of electrons, we can make some sense of patterns observed in ionization energies. Let us go back to the electron configuration. Beryllium (Be) is $1s^2 2s^2$ whereas Boron (B) is $1s^2 2s^2 2p^1$. When electrons are removed from Be and B they are removed from the same quantum shell ($n = 2$) but, in the case of Be, one is removed from the 2s orbital whereas in B, the electron is removed from a 2p orbital. s orbitals are spherically symmetric, p orbitals have a dumbbell shape and a distinct orientation. Electrons in a 2p orbital have lower ionization energies because they are on average a little further from the nucleus and so a little more easily removed compared to 2s electrons. That said, the overall average atomic radius of boron is smaller than beryllium, because on average all its electrons spend more time closer to the nucleus.

The slight drop in ionization potential between nitrogen and oxygen has a different explanation. The electron configuration of nitrogen is typically written as $1s^2 2s^2 2p^3$, but this is misleading: it might be better written as $1s^2 2s^2 2p_x^1 2p_y^1 2p_z^1$, with each 2p electron located in a separate p orbital. These p orbitals have the same energy but are oriented at right angles (orthogonally) to one another. This captures another general principle: electrons do not pair up into an orbital until they have to do so.^[20] Because the p orbitals are all of equal energy, each of them can hold one electron before pairing is necessary. When electrons occupy the same orbital there is a slight repulsive and destabilizing interaction; when multiple orbitals of the same energy are available, the lowest energy state is the one with a single electron in an orbital. Nitrogen has all three 2p orbitals singly occupied and therefore the next electron, which corresponds to oxygen, has to pair up in one of the p orbitals. Thus it is slightly easier to remove a single electron from oxygen than it is to remove a single electron from nitrogen, as measured by the ionization energy.

To pull together a set of seriously obscure ideas, the trends in ionization energies and atomic radii indicate that electrons are not uniformly distributed around an atom's nucleus but rather have distinct distributions described by the rules of quantum mechanics. Although we derive the details of these rules from rather complex calculations and the wave behavior of electrons, we can cope with them through the use of quantum numbers and electron probability distributions. Typically electrons in unfilled shells are more easily removed or reorganized than those in filled shells because atoms with unfilled shells have higher effective nuclear charges. Once the shell is filled, the set of orbitals acts like a shield and cancels out an equal amount of nuclear charge. The next electron goes into a new quantum shell and the cycle begins again. This has profound implications for how these atoms react with one another to form new materials because, as we will see, chemical reactions involve those electrons that are energetically accessible: the valence electrons.

We could spend the rest of this book (and probably one or two more) discussing how electrons are arranged in atoms but in fact your average chemist is not much concerned with atoms as entities in themselves. As we have said before, naked atoms are not at all common. What is common is combinations of atoms linked together to form molecules. From a chemist's perspective, we need to understand how, when, and where atoms interact. The electrons within inner and filled quantum shells are "relatively inert"

which can be translated into English to mean that it takes quite a lot of energy (from the outside world) to move them around. Chemists often refer to these electrons as core electrons, which generally play no part in chemical reactions; we really do not need to think about them much more except to remember that they form a shield between the nucleus and the outer electrons. The results of their shielding does, however, have effects on the strong interactions, commonly known as bonds, between atoms of different types, which we will discuss in Chapters 4 and 5. Reflecting back on Chapter 1, we can think about the distinction between the London Dispersion Forces acting between He atoms and between H_2 molecules versus the bonds between the two H atoms in a H_2 molecule.

Bonds between atoms involve the valence electrons found in outer, and usually partially filled, orbitals. Because of the repeating nature of electron orbitals, it turns out that there are patterns in the nature of interactions atoms make—a fact that underlies the organization of elements in the periodic table. We will come back to the periodic table once we have considered how atomic electronic structure influences the chemical properties of the different elements.

? Questions

Questions to Answer

- Try to explain the changes in ionization potential as a function of atomic number by drawing your impression of what each atom looks like as you go across a row of the periodic table, and down a group.

Questions to Ponder

- How does the number of valence electrons change as you go down a group in the periodic table? How does it change as you go across a row?
- How do you think the changes in effective nuclear charge affect the properties of elements as you go across a row in the periodic table?

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