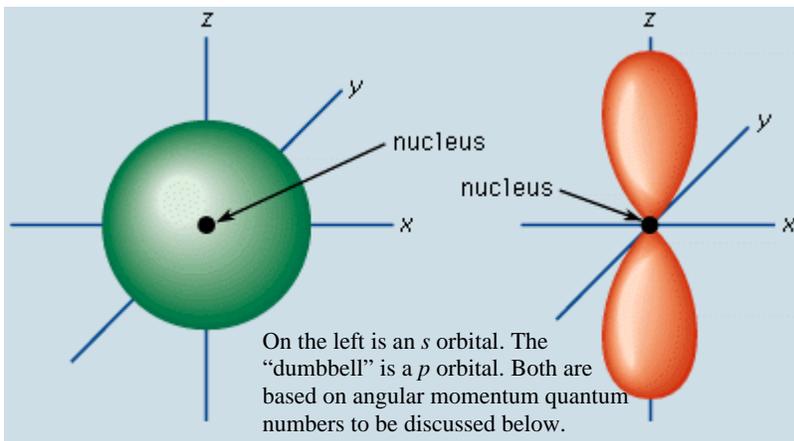**Electron Configuration (detailed shell diagrams)**

From a high school discussion of electrons and the so-called Bohr-Rutherford model, it is easy for many misconceptions to arise. For one, the electron does **not** move in a circular orbit around the nucleus. It is **not** like a planet either. It does **not** move along an elliptical path. Its precise movement is really unknown. What complicates the matter on this scale is that although electron has mass, it also has wave-like properties that cannot be ignored. This leads to the unpopular idea that we can never be certain of an exact route or position for an electron.

Furthermore, when we draw shell diagrams, the shells represent energy levels. The diagrams create the false impression that all electrons in that shell are identical. In reality, each energy level consists of n^2 number of **orbitals**, where n is the principal **quantum number**.

Before we move on, let's define these two terms. A *quantum, E,* is a discrete bundle of energy proportional to its frequency, ν. ($E = h\nu$, where h = Planck's constant). Due to their wave-like nature, electrons cannot have just any amount of energy: they are limited to having certain integral amounts. The principal quantum number also determines how far from the nucleus electrons are. Understandably, being less tightly bound to the nucleus is associated with having more energy. An *orbital* in chemistry and physics, is a mathematical expression, called a wave function. It describes properties characteristic of no more than two electrons in the vicinity of the nucleus, or in the case of molecules, of a system of nuclei. Since there are two electrons per orbital, the total number of electrons for any given energy level equals $2n^2$. Quantum mechanics is based on probability, and an orbital can be thought of as a three dimensional region in which there's a 90 to 95% chance of finding an electron. The two electrons within an orbital are also different. They have a different spin quantum number, m_s. The **Pauli exclusion principle** states that no two electrons within an atom have the same set of quantum numbers, just like no two people have the same social insurance number, even though they may be from the same family.

On the left is an *s* orbital. The "dumbbell" is a *p* orbital. Both are based on angular momentum quantum numbers to be discussed below.

In order to assign atoms electronic configurations (detailed shell diagrams), we have to discuss the angular momentum quantum number l, which has values that range from 0 to n -1 for each value of n.

For each value of l, a letter is used to represent the corresponding type of atomic orbital. The table summarizes these depictions.

l's value	0	1	2	3	4
Letter for orbital-type	s (origin: spherically symmetric)	p	d	f	g

The angular momentum quantum number determines the shape of the orbital, as seen in the diagram above. But there is a third quantum number that will determine how many orbitals each type will have. We are referring to the magnetic quantum number, m_l. This has integral values that lie between l and –l. For example, $l = 0$ for s-type orbitals, so m_l can only equal zero. So for a given n, there is only one orbital for s . Next, p orbitals have $l =1$, which means that m_l *can equal -1, 0* or 1. Thus at any level for n, there are three orbitals of p type. Similarly there are five for d, seven for f, and nine for g. If you want a formula, then there are **2l +1** orbitals for each orbital type with a **4l + 2** number of electrons.
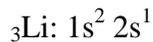
n	l	Orbital	m_l	#of orbitals	Number of electrons	Total e⁻ = 2n²
1	0	1s	0	1	2	2
2	0	2s	0	1	2	8
	1	2p	-1,0,1	3	6	
3	0	3s	0	1	2	18
	1	3p	-1,0,1	3	6	
	2	3d	-2,-1,0,1,2	5	10	
4	0	4s	0	1	2	32
	1	4p	-1,0,1	3	6	
	2	4d	-2,-1,0,1,2	5	10	
	3	4f	-3,-2,-1,0,1,2,3	7	14	
5	0	5s	0	1	2	50
	1	5p	-1,0,1	3	6	
	2	5d	-2,-1,0,1,2	5	10	
	3	5f	-3,-2,-1,0,1,2,3	7	14	
	4	5g	-4,-3,-2,-1,0,1,2,3,4	9	18	
6	0	6s	0	1	2	72
	1	6p	-1,0,1	3	6	
	2	6d	-2,-1,0,1,2	5	10	
	3	6f	-3,-2,-1,0,1,2,3	7	14	
	4	6g	-4,-3,-2,-1,0,1,2,3,4	9	18	
	5	6h	-5,-4,-3,-2,-1,0,1,2,3,4,5	11	22	
7	0	7s	0	1	2	98
	1	7p	-1,0,1	3	6	
	2	7d	-2,-1,0,1,2	5	10	
	3	7f	-3,-2,-1,0,1,2,3	7	14	
	4	7g	-4,-3,-2,-1,0,1,2,3,4	9	18	
	5	7h	-5,-4,-3,-2,-1,0,1,2,3,4,5	11	22	
	6	7i	-6-5,-4,-3,-2,-1,0,1,2,3,4,5, 6	13	26	

The chart below reveals (there are exceptions) the order in which these orbitals are filled.
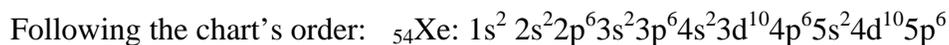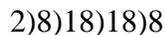
1s				
2s	2p			
3s	3p	3d		
4s	4p	4d	4f	
5s	5p	5d	5f	5g
6s	6p	6d	6f	6g
7s	7p	7d	7f	7g
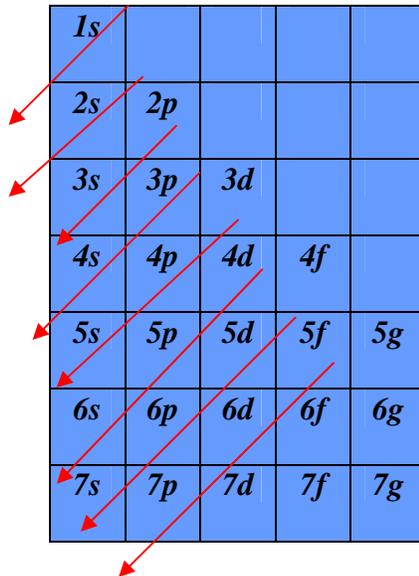
Examples:

1. Lithium has three electrons. Two are in the *1s* orbital and the third will be in the *2s* orbital, so we write:

$$_3\text{Li: } 1s^2\, 2s^1$$

2. Let's do something bigger like Xe:

Following the chart's order: $_{54}\text{Xe: } 1s^2\, 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6$
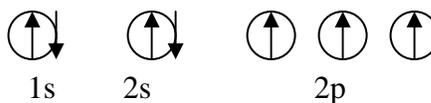
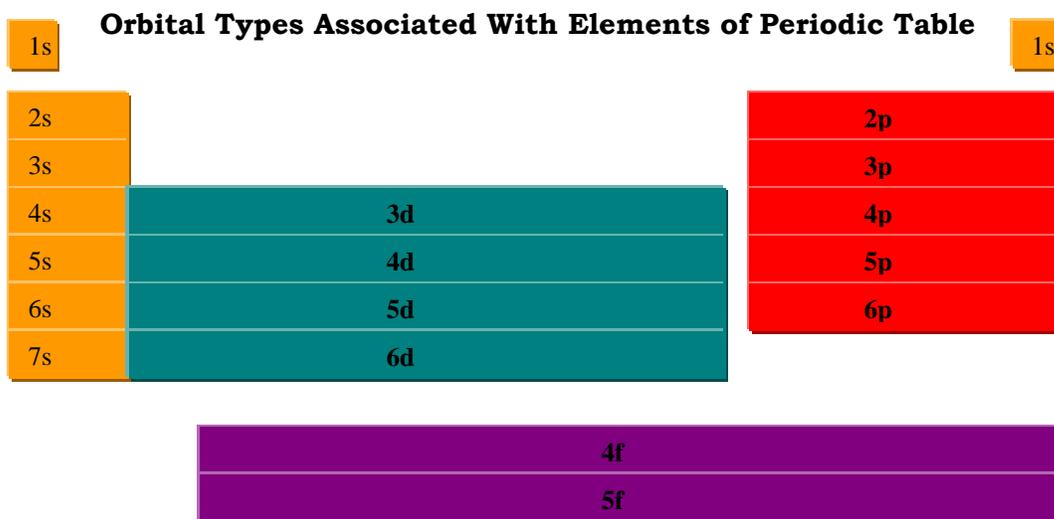This is what's behind the simplified Bohr-Rutherford model:

2)8)18)18)8

The next question is: in what order do we place electrons within the p, d, and f orbitals? We apply **Hund's Rule** which states that the lowest energy arrangement(and therefore the most stable) is the one having the *maximum number of unpaired electrons* allowed by the Pauli exclusion principle.

Let's apply it to nitrogen which is $1s^2\, 2s^2 2p^3$.

The three electrons in p will according to Hund's rule apply three different orbitals, rather than fill the first and half-fill the second.

⊕↑↓   ⊕↑↓   ⊕↑ ⊕↑ ⊕↑

1s   2s   2p

Orbital Types Associated With Elements of Periodic Table

1s				1s

2s		2p

3s		3p

4s	3d	4p

5s	4d	5p

6s	5d	6p

7s	6d	

4f
5f

Example 2

Give the full set of quantum numbers for all of calcium's electrons.

	1s	2s	2p			3s	3p			4s
Quantum number	⇅	⇅	⇅	⇅	⇅	⇅	⇅	⇅	⇅	⇅
n	1	2	2	2	2	3	3	3	3	4
l	**0**	**0**	**1**	**1**	**1**	**0**	**1**	**1**	**1**	**0**
m	0	0	-1	0	1	0	-1	0	1	0
s	$\pm\frac{1}{2}$	$\pm\frac{1}{2}$	$\pm\frac{1}{2}$	$\pm\frac{1}{2}$	$\pm\frac{1}{2}$	$\pm\frac{1}{2}$	$\pm\frac{1}{2}$	$\pm\frac{1}{2}$	$\pm\frac{1}{2}$	$\pm\frac{1}{2}$

As the 3p's get filled, they do so in the following order because of Hund's rule:

{3,1,-1,+½}, {3,1,0,+½}, {3,1,1,+½} so that the most electrons are spinning in the same direction and then we get {3,1,-1,-½}, {3,1,0,-½}, {3,1,1,-½}

Implications For Chemical Bonding

H_2 and the Covalent Bond

Two hydrogen atoms can share an electron to form the molecular form of hydrogen, H_2.
How does this happen, and what does quantum chemistry have to do with it?
If both electrons have a spin quantum number of $+ \frac{1}{2}$, the atoms cannot come together to form a molecular orbital because no two electrons can have the same quantum numbers. But if they have opposite spins, then all is fine.
When they come together they do so spatially in the sense that they will spend a lot (but not all) of their time in a small region between the two hydrogen nuclei. The shared region is called a **covalent bond** and both nuclei, positive in charge, are attracted to the negatively charged electrons.
But because the electrons are not confined to that in-between area, when compared to the original space occupied when part of a single atom, they are now covering a larger volume. Since the electron has wave-like properties and a wavelength, λ, the larger radius of its covered region increases its wavelength. This in turn decreases its momentum, p, because $p = h/\lambda$ (h = Planck's constant). Of course the same is true of H_2 other electron, and since their total momentum is lower, the electrons also have less energy now in bonded form than when they were part of separate atoms. This is the reason why H_2 is more stable (has less energy) than 2 H atoms and why the conversion: $2 H \rightarrow H_2$ is exothermic.

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