**WS#5: Quantum Numbers, Orbitals, and Electron Configurations**

**Important note: Do not think of an electron as a “thing” that can be located. The electron charge is spread out in a “cloud” with regions of high charge density. The wave function describes the regions of high charge density.**

[www.angelo.edu/faculty/kboudrea/general/quantum\_numbers/Quantum\_Numbers.htm](http://www.angelo.edu/faculty/kboudrea/general/quantum_numbers/Quantum_Numbers.htm)

**Quantum Numbers and Atomic Orbitals**

By solving the Schrödinger equation (H = E), we obtain a set of mathematical equations, called **wave functions** (), which describe the probability of finding *regions of high charge density* at certain energy levels within an atom.

A wave function for an electron in an atom is called an **atomic orbital**; this atomic orbital describes a region of space in which there is a high probability of finding *regions of high charge density*. Energy changes within an atom are the result of an electron changing from a wave pattern with one energy to a wave pattern with a different energy (usually accompanied by the absorption or emission of a photon of light).

Each electron in an atom is described by four different **quantum numbers**. The first three (*n*, *l*, *ml*) specify the particular orbital of interest, and the fourth (*ms*) 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 (the distance from the nucleus of the peak in a radial probability distribution plot). 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 its *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*).

Draw a picture to show the shape of the orbitals in each subshell (also called sublevel).

 s p d (has two shapes) f (has two shapes)

1. **Magnetic Quantum Number (*ml*):  *ml* = -*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 2*l*+1 orbitals in each subshell. Thus the *s* subshell has only one orbital, the *p* subshell has three orbitals, and so on.

Draw each orbital to show the orientation about the x,y,z-axes.

px py pz

Draw all 3 p orbitals together, and you get the complete p subshell.

 p subshell

1. **Spin Quantum Number (*ms*):  *ms* = +½ or -½.**Specifies the **orientation of the spin axis** of an electron. An electron can spin in only one of two directions (sometimes called *up* and *down*).

The **Pauli exclusion principle** (Wolfgang Pauli, Nobel Prize 1945) states 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; the spins are said to be **paired**. These substances are not attracted to magnets and are said to be **diamagnetic**. Atoms with more electrons that spin in one direction than another contain **unpaired** electrons. These substances are weakly attracted to magnets and are said to be **paramagnetic**.

**Table of Allowed Quantum Numbers**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| ***n*** | ***l*** | ***ml*** | **Number oforbitals** | **OrbitalName** | **Number ofelectrons** |
| 1 | 0 | 0 | 1 | 1*s* | 2 |
| 2 | 0 | 0 | 1 | 2*s* | 2 |
|  | 1 | -1, 0, +1 | 3 | 2*p* | 6 |
| 3 | 0 | 0 | 1 | 3*s* | 2 |
|  | 1 | -1, 0, +1 | 3 | 3*p* | 6 |
|  | 2 | -2, -1, 0, +1, +2 | 5 | 3*d* | 10 |
| 4 | 0 | 0 | 1 | 4*s* | 2 |
|  | 1 | -1, 0, +1 | 3 | 4*p* | 6 |
|  | 2 | -2, -1, 0, +1, +2 | 5 | 4*d* | 10 |
|  | 3 | -3, -2, -1, 0, +1, +2, +3 | 7 | 4*f* | 14 |

**Writing Electron Configurations**

The distribution of electrons among the orbitals of an atom is called the **electron configuration**. The electrons are filled in according to a scheme known as the **Aufbau principle** ("building-up"), which corresponds (for the most part) to increasing energy of the subshells:

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

It is not necessary to memorize this listing, because the order in which the electrons are filled in can be read from the periodic table in the following fashion:



Or, to summarize:



1. In **electron configurations**, write in the orbitals that are occupied by electrons, followed by a superscript to indicate how many electrons are in the set of orbitals (e.g., H 1s1)

a) Write the electron configuration for the following elements:

Ne \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Ar\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Li\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Na\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

K\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

N\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

P\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

As\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

b) What patterns do you see?

c) Circle the part of the electron configuration that represents the valence electrons.

d) Put a box around the core electrons. The core electrons in the s & p subshells correspond to the electron configuration of a noble gas! You may use the noble gas abbreviation. For example, the electron configuration for Na can be written as [Ne]3s1

2. Another way to indicate the placement of electrons is an **orbital diagram**, in which each orbital is represented by a square (or circle), and the electrons as arrows pointing up or down (indicating the electron spin). When electrons are placed in a set of orbitals of equal energy (called degenerate orbitals), they are spread out as much as possible to give as few paired electrons as possible (**Hund's rule**).

a) Draw in the arrows to show the placement of electrons for the element P.

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 1s 2s 2p 3s 3p

How many unpaired electrons? \_\_\_\_\_\_ Is this element diamagnetic or paramagnetic?\_\_\_\_\_\_\_\_ How can you tell?

b) Make an orbital box diagram for the element Ca.

How many unpaired electrons? \_\_\_\_\_\_ Is this element diamagnetic or paramagnetic?\_\_\_\_\_\_\_\_ How can you tell?

You may also arrange the orbital box diagram like an energy diagram as shown below. Label each sublevel.

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Energy ☐☐☐

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