MR. STONE

ELECTRONS in ATOMS
Electron Configurations

Objectives:

1. Explain the use of wave-mechanics in atomic theory.
2. Describe the wave-mechanical model of the atom.
3. Locate electrons in energy levels, sublevels, and orbitals according to the wave-mechanical model of the atom.
4. Construct orbital diagrams and write electron configurations for both neutral atoms and ions.

Recall that in the Bohr model of the atom, the electron was allowed to have only certain definite energies. Although an electron could "jump" from one energy level to another, it could not exist in the atom at any energy between these levels.

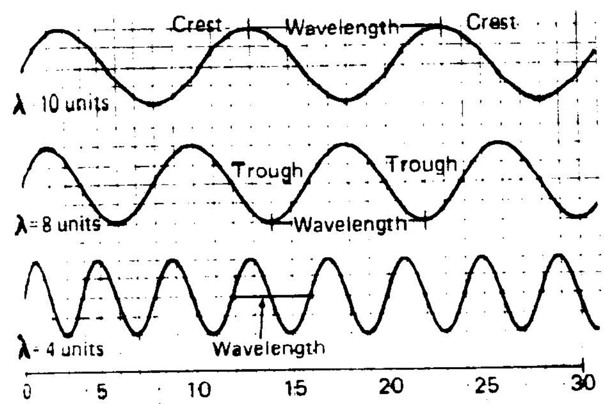
According to physical laws proposed by Issac Newton, the kinetic energy of a body always changed smoothly and continuously, not in sudden jumps. The quantum jumps of electrons proposed by Bohr were essential to explain the behavior of electrons in the atom but they did not fit into the classical theory of motion and energy proposed by Newton.

Another major difficulty with the Bohr model was that it could not be used to predict the energy levels of electrons in atoms with more than one electron.

A new theory was developed to explain the laws governing the behavior of electrons inside the atom. This new theory is called the **theory of wave mechanics** also called **quantum mechanics.**

In order to best understand this theory, you need to understand the properties and characteristics of waves.

WAVES



Properties of Waves:

frequency (f) -- the number of waves (wave peaks) that pass a point per unit of time

Frequency is symbolized by the Greek letter *nu* , **ν**. To avoid confusing *nu* with the symbol for velocity, v, we will symbolize frequency using a lower case f.

Frequency is measured using a unit called the **hertz** (Hz). By definition, a wave in which one peak passes a given point each second has a frequency of 1 hertz (1 Hz).

wavelength (λ) -- the distance between two neighboring crests or troughs or between two similar points in a set of waves

Wavelength is symbolized by the Greek letter *lambda*, **λ**.

Wavelength is commonly measured using **nm** or **Angstroms (Å)**

Å = 1×10^{-10} m　　　**nm** = 1×10^{-9} m

The wavelength and frequency of a wave are inversely related to each other:

As wavelength decreases, frequency increases.
As wavelength increases, frequency decreases.

$C = \lambda \nu$　　　C = speed of light = 3.0×10^{8} m/s

Waves have energy(E) associated with them. The energy of a wave is related to the wavelength and frequency of the wave.

$$E = hf$$

E is the symbol for energy
h is the symbol for **Planck's constant (6.6262×10^{-34} joules/second)**
f is the symbol for frequency

As frequency increases, energy increases.
As frequency decreases, energy decreases.

Electrons have wave properties associated with them. They carry their energy as wave energy. As mentioned earlier, the energy of a wave is related to its wavelength and frequency. Any change in the energy of a wave will be the result of a change of its wave characteristics of wavelength and frequency. This means that **the energy differences among the different electrons in an atom are the result of differences in wave characteristics among the electrons.**

The further an electron is from the nucleus, the more energy it posseses. What significance does this have on the wave characteristiscs of electrons?

Energy $\uparrow$, $\lambda \downarrow$, $\nu \uparrow$

What effect will the absorption of energy by an electron have on its wave properties?

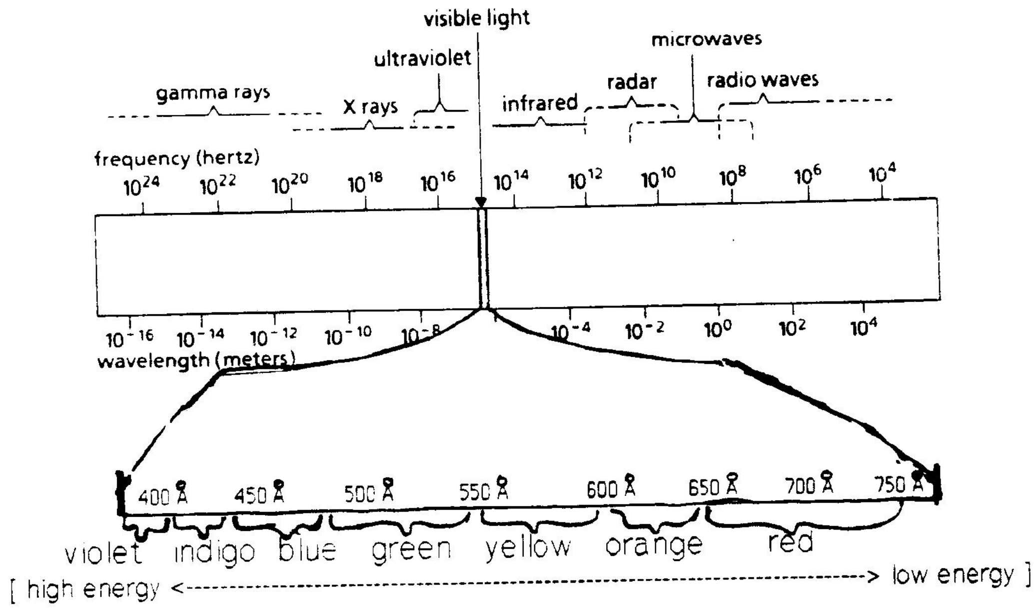
Energy $\uparrow$, $\nu \uparrow$, $\lambda \downarrow$

Keeping in mind that electrons carry their energy as wave energy, it should make sense that, **when electrons lose energy, they will give off energy in the form of wave energy.** This is why electrons emit light when they lose energy because light also carries wave energy.

What effect will the loss of energy by an electron have on its wave properties?

E $\downarrow$, $\nu \downarrow$, $\lambda \uparrow$

The Electromagnetic Spectrum



Notice that the different colors of light that are a part of the visible light spectrum all have different amounts of energy associated with them. (Recall that as wavelength decreases, frequency increases, and therefore energy increases).

The color of light emitted by an electron can give you an indication of the behavior of the electron in the atom.

Recall that the only way that an electron can lose or give away energy is by dropping from a higher energy level to a lower energy level. **The amount of energy emitted by an electron will be exactly equal to the energy difference between the amount of energy available in the energy level that it moved out of (higher level) and the amount of energy available in the energy level it has moved into (lower level). The energy of the light emitted by the electron will be exactly equal to this energy difference. Therefore the light emitted by the electron is a good indicator of how the electron is moving around in the atom.**

What color of light would you expect to be emitted by an electron making a large drop in energy levels? Why?

Violet – highest energy type of visible light

What about an electron that is making a very short drop in energy levels? Why?

red – lowest energy type of visible light

The Heisenberg Uncertainty Principal

In 1927, a German physicist named Werner Heisenberg stated that **it is impossible to know both the precise location and the precise velocity of a subatomic particle at the same time.**

The reason for this is that in order to observe a particle, a scientist must interact with it in ways that will change its velocity. For example, light would be necessary to "see" a subatomic particle but the mass and energy of a photon of light would have to collide with the subatomic particle thus changing its velocity and direction. Therefore you could not be sure what the speed and the direction of the particle were at the moment of observation thus causing uncertainty to always be associated with such an observation.

Energy Levels of the Charge-cloud Model

Even though the precise location and motion of electrons cannot be determined, the **probability** of finding an electron at a particular place at a particular time can be determined using the equations of quantum mechanics.

These equations give the probabilities for electrons inside the atom but do not enable scientists to calculate exact orbits for the electrons. They describe instead regions of space inside the atom where an electron is likely to be at any time.

The equations of wave mechanics indicate how the probability of finding an electron at a particular place within the atom changes from place to place. If these changing probabilities are plotted as points in a three-dimensional representation, there will be regions of many points showing high probability of finding an electron and regions of few points showing a low probability of finding an electron. Because these plots look like diffuse clouds with regions of low density (low probability) and high density (high probability), the resulting model is called the charge-cloud model.

The theory of wave mechanics states that a wave representing the electron must "fit" inside the atom in such a way that it meets itself without any overlap. A type of wave that does this is called a **standing wave**. Only a standing wave of 1/2 wavelength, 1 wavelength, 1.5 wavelength, 2 wavelengths, and so on can be produced. **Wavelengths will only change by factors of one-half.** The wavelength of the standing wave is therefore said to be quantized.

The wavelength describing an electron depends on the energy of the electron. There are only certain energies for which the wavelengths are just right to form standing waves in the atom. These energies at which standing waves can be produced correspond to the energy levels of the atom.

Energy Levels of the Charge-cloud Model (refer to chart)

The energy levels or shells in an atom are called **principal energy levels.**

The number of the shell or principal energy level is called the **principal quantum number** and is represented by the symbol n, where $n = 1$, $n = 2$, $n = 3$, etc.

According to wave mechanics, every atom has principal energy levels and every principal energy level has one or more **sublevels** within it. The energy of each sublevel within a given energy level is slightly different. [Keep in mind that the further away from the nucleus a sublevel is the more energy it has.]

The number of sublevels in any principal level is the same as its principal quantum number, n.

Each electron in a given sublevel has the same energy.

The sublevels are labelled **s, p, d, f, g, h, i**, etc. , where the **s** sublevel is the lowest energy sublevel available in each principal energy level.

When atoms are in the ground state, all the electrons in each principal energy level will be found in the first four sublevels (s,p,d,f). Only excited electrons can be found in g and higher sublevels.

Sublevels from different principal energy levels can overlap. [See your chart and note that the 3d sublevel has more energy than the 4s sublevel.]

Orbitals

The **orbital** is defined as a region of space in a sublevel where electrons are most likely to be found.

Each **s** sublevel has **1 orbital.**

Each **p** sublevel has **3 orbitals.**

Each **d** sublevel has **5 orbitals.**

Each **f** sublevel has **7 orbitals.**

No more than two electrons can occupy an orbital. Thus an orbital can be empty, half-filled (one electron in the orbital), or filled (two electrons in the orbital).

Principal Energy Level and the Maximum Number of Orbitals and Electrons

Principal Energy Level (*n*)	Number of Orbitals Available *s*	*p*	*d*	*f*	Total Number of Orbitals (n^2)	Maximum Number of Electrons ($2n^2$)
1	1	–	–	–	1	2
2	1	3	–	–	4	8
3	1	3	5	–	9	18
4	1	3	5	7	16	32

Note: Theoretically, the number of orbitals and possible number of electrons continue to increase for higher values of *n*. However, no atom actually has more than 32 electrons in any of its principal levels.

<u>The Shape of Orbitals</u>

All **s** orbitals, regardless of which principal energy level they are a part of, have the same shape -- **spherical.** The only difference between the **s** orbitals is that one in a higher principal energy level has a larger diameter than one in a lower level.

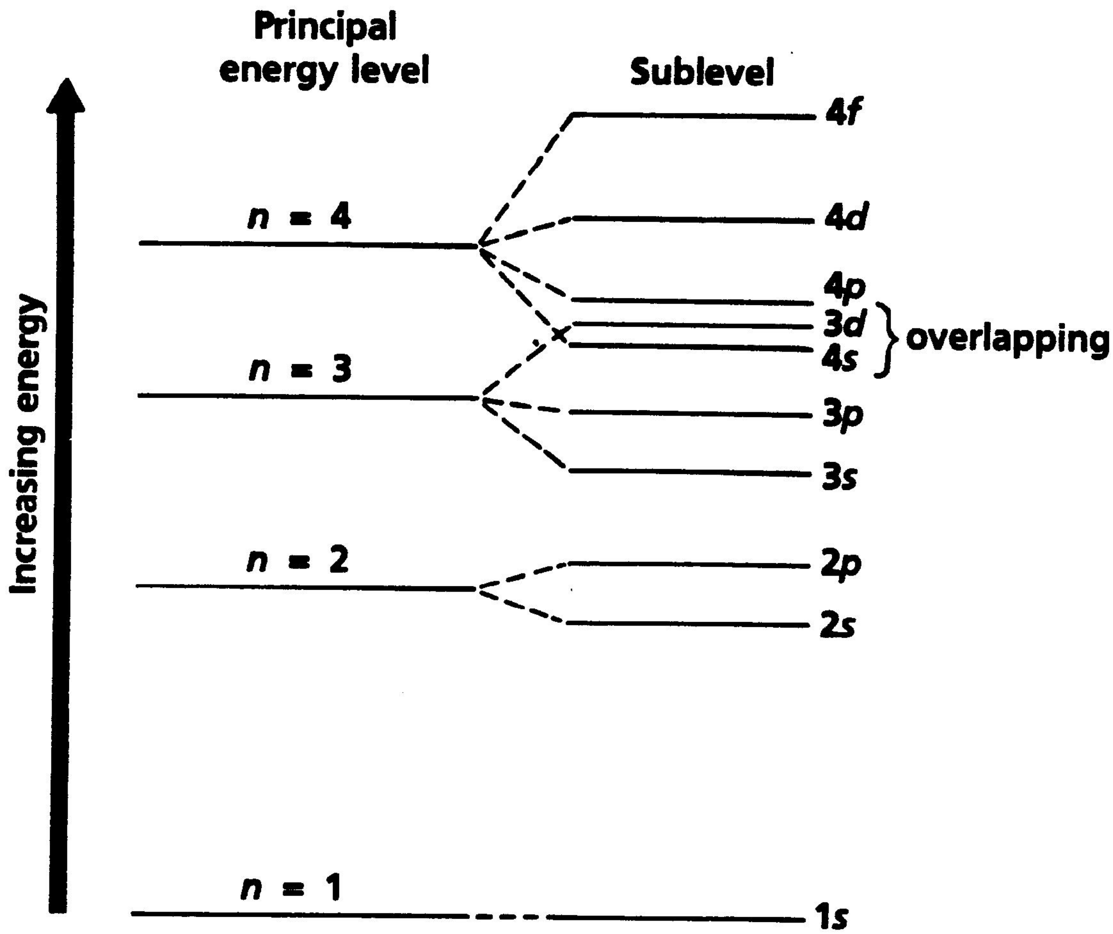
All **p** orbitals have the same shape which is described as looking like a **dumbbell** or **figure-eight**.

Sublevels Available in Each Principal Energy Level

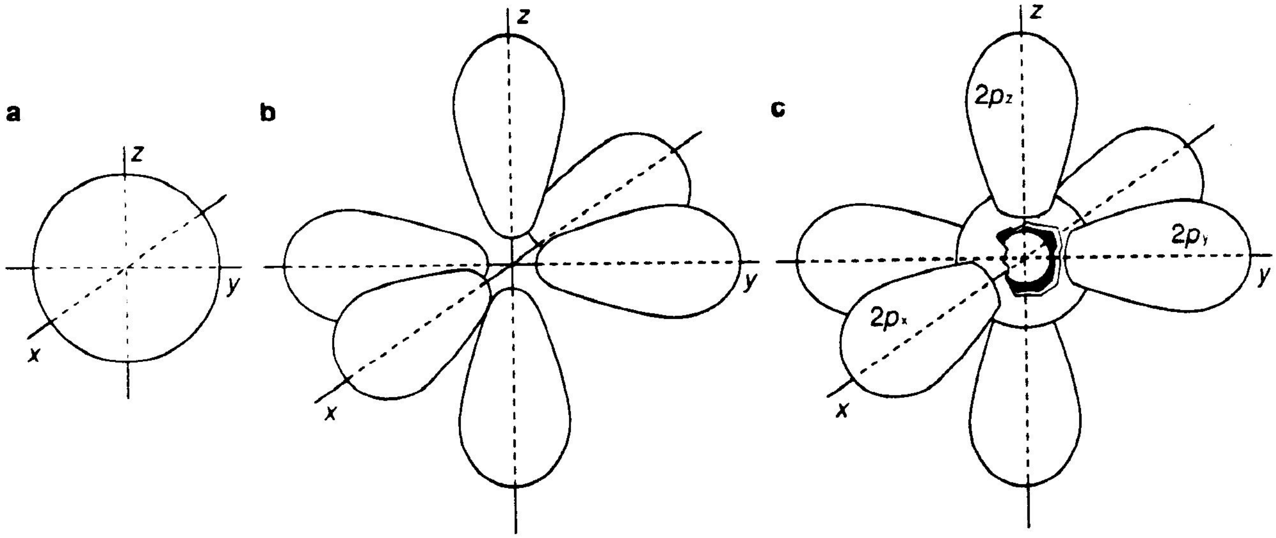
Principal Energy Level (n)	Sublevels Available
1	$1s$
2	$2s$ $2p$
3	$3s$ $3p$ $3d$
4	$4s$ $4p$ $4d$ $4f$
5	$5s$ $5p$ $5d$ $5f$ $5g$
6	$6s$ $6p$ $6d$ $6f$ $6g$ $6h$

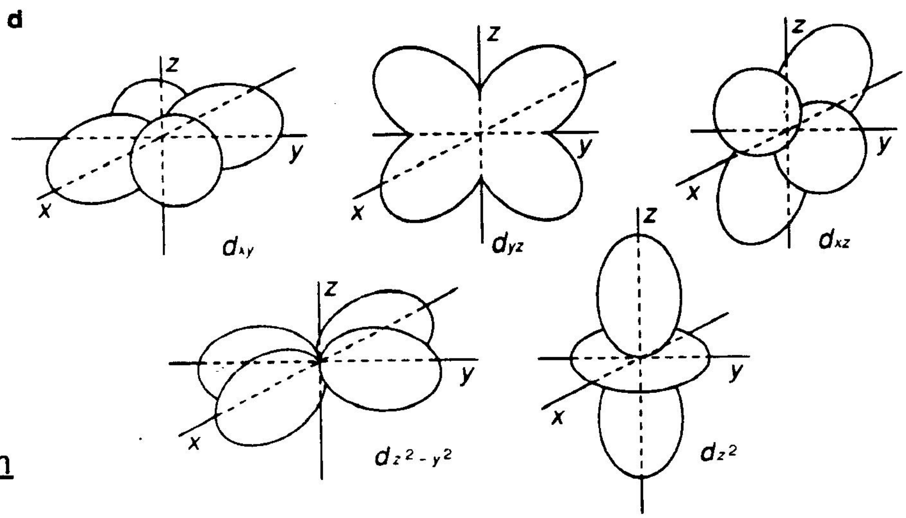
For principal energy level n, there are n sublevels. For example, for principal energy level 3, there are 3 sublevels: $3s$, $3p$, and $3d$.

The First Four Principal Energy Levels and Their Sublevels



Atomic Orbitals





Electron Spin

Electrons exhibit a property known as **spin**, a motion like that of the earth rotating on its axis.

The direction of spin is either **clockwise** or **counter-clockwise**.

Pauli exclusion principal - **in order for two electrons to occupy the same orbital they must have opposite spins**

This principal means that if one electron in an orbital is spinning clockwise, the other electron in the orbital must be spinning counter-clockwise.

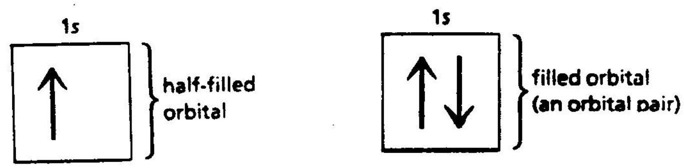
Orbital Diagrams

Orbital diagrams are used to describe the placement of electrons in atoms. These diagrams consist of boxes in which arrows are placed to symbolize electrons. A half-filled orbital is represented by a box containing a single arrow pointing either upwards or downwards. A filled orbital would be represented by a box containing two arrows, one pointing upward and the other pointing downward.

Arrows pointing **upward** symbolize electrons with **clockwise spin.**

Arrows pointing **downward** symbolize electrons with **counter-clockwise spin.**

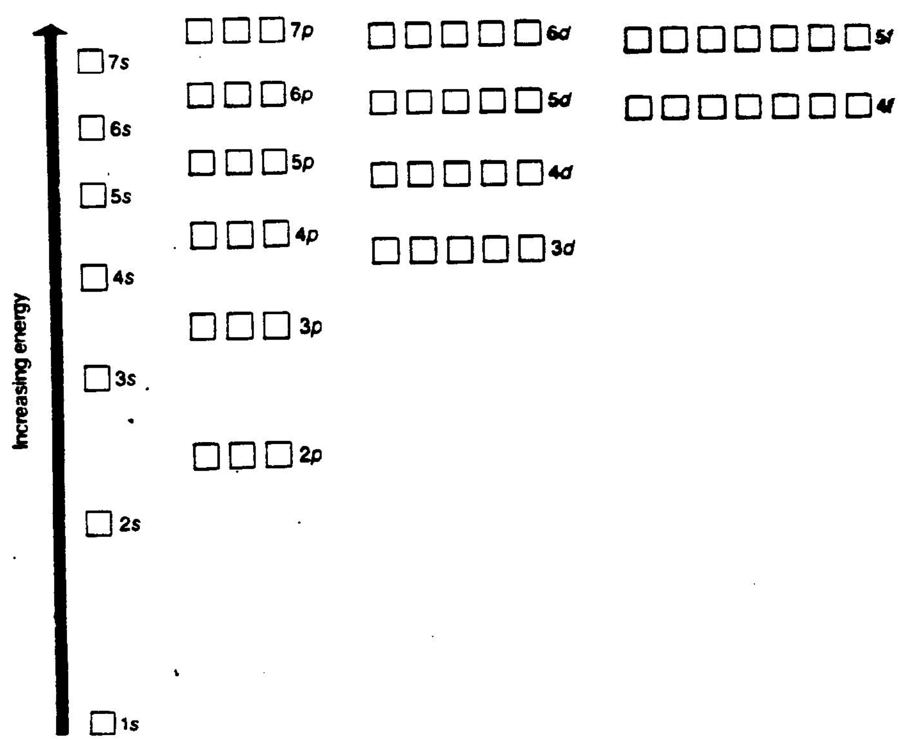
Two oppositely spinning electrons occupying the same orbital are called an **orbital pair.**



Orbital diagrams that employ the use of this box method are called **Afbau diagrams.**

Some Afbau diagrams, like the one below, show the energy relationships between the different sublevels and orbitals in the atom.

Aufbau Diagram



Other Afbau diagrams, like the one below, do not show energy relationships.

Element		1s	2s	$2p_x$	$2p_y$	$2p_z$	3s
H	______	↑					
He	______	↑↓					
Li	______	↑↓	↑				
C	______						
N	______						
O	______						
F	______	↑↓	↑↓	↑↓	↑↓	↑	
Ne	______	↑↓	↑↓	↑↓	↑↓	↑↓	
Na	______	↑↓	↑↓	↑↓	↑↓	↑↓	↑

Rules for Filling Orbitals by Electrons

1. **Afbau principle:** Electrons enter orbitals of lowest energy first
   [Each added electron enters an orbital of the lowest energy level and sublevel available.]

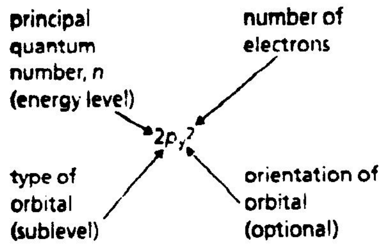
2. **Pauli exclusion principle:** Electrons in the same orbital must have opposite spins, therefore no more than two electrons can be placed in any orbital.

3. **Hund's rule:** When electrons occupy orbitals of equal energy, one electron enters each orbital until all the orbitals contain one electron with spins parallel. [Before a second electron can be placed in any orbital, all the orbitals of that sublevel must contain at least one electron.]

Writing Electron Configurations

The arrangement of the electrons among the various orbitals of an atom is called the **electron configuration** of the atom.

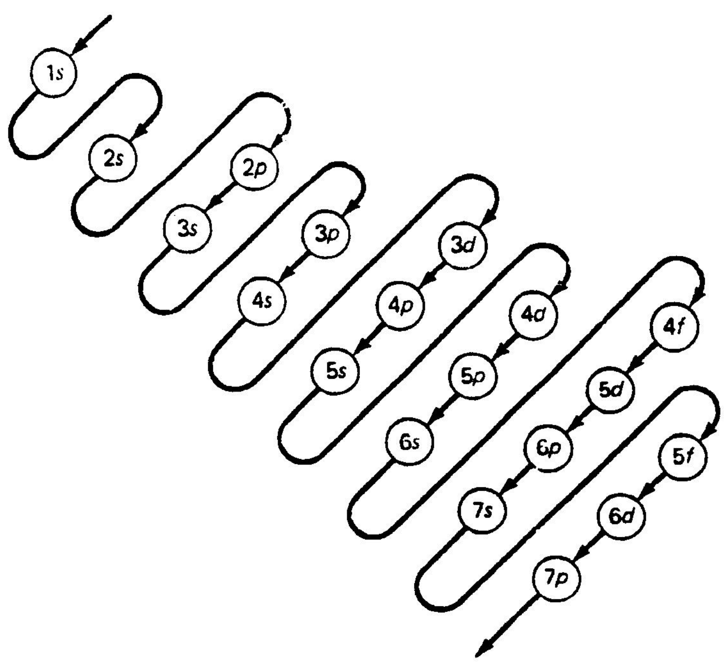
Electron configurations can be written using a special notation that tells the principal energy level, the type of sublevel, and the number of electrons in that sublevel.



For example, the electron configuration for oxygen would be $1s^2 2s^2 2p_x^2 2p_y^1 2p_z^1$

The notations for electron configurations are usually simplified to show only the total number of electrons in a sublevel. For example, the simplified electron configuration for oxygen would be $1s^2\ 2s^2\ 2p^4$.

When writing electron configurations, refer to the following chart as an aid to remembering the sequence in which orbitals fill :



The Valence Shell and Valence Electrons

Refer to the Afbau diagram, given earlier in your notes, that shows the energy relationships among the sublevels in an atom. Notice that once you pass the fourth energy level (n = 4) the overlapping of sublevels becomes more complicated. **As a result of this overlapping, the outermost principal energy level can never contain more than eight electrons.**

Whenever the p sublevel is filled (making a total of eight electrons in the principal energy level), the next electron goes into the s sublevel of the next higher level, thus starting a new shell.

The outermost principal energy level of an atom that includes at least one electron is called the **valence shell.**

The electrons in the valence shell are called **valence electrons.**

An atom cannot have more than eight valence electrons.

Valence electrons are important because they play an important role in the joining of atoms to form compounds.

From the notation for an electron configuration, you can determine the number of valence electrons and the orbitals that they occupy. Recall the notation for oxygen, $1s^2\ 2s^2\ 2p^4$. Its outermost principal energy level is n = 2. The electrons in this outermost level are oxygen's valence electrons. There are two s and four p electrons at the n = 2 level giving oxygen a total of six valence electrons.

The part of the atom exclusive of its valence electrons is called the **kernel** of the atom. The kernel of the atom includes the nucleus and all the inner energy levels of electrons.

Therefore, the kernel for oxygen would be its nucleus plus its $1s^2$ electrons.

It is important to note that electron configurations can also be written for ions and excited atoms.