An Atomic Model

Our present model of the atom is based on the concept of energy levels for electrons within an atom and on the mathematical interpretation of detailed atomic spectra. The requirements for our model are:

1. Each electron in a particular atom has a unique energy that depends on the relationship between the negatively charged electron and both the positively charged nucleus and the other negatively charged electrons in the atom.

2. The energy of an electron in an atom can increase or decrease, but only by specific amounts, or quanta.

Energy Levels

We picture an atom as a small nucleus surrounded by a much larger volume of space containing the electrons. This space is divided into regions called principal energy levels, numbered 1, 2, 3, 4, ... , outward from the nucleus.

Each principal energy level can contain up to 2n2 electrons, where n is the number of the level. Thus, the first level can contain up to 2 electrons, 2(12) = 2; the second up to 8 electrons, 2(22) = 8; the third up to 18, 2(32) = 18; and so on. Only seven energy levels are needed to contain all the electrons in an atom of any of those elements now known.

As stated earlier, the energy associated with an energy level increases as the distance from the nucleus increases. An electron in the seventh energy level has more energy associated with it than does one in the first energy level. The lower the number of the principal energy level, the closer the negatively charged electron in it is to the positively charged nucleus and the more difficult it is to remove this electron from the atom.

Sublevels and Orbitals

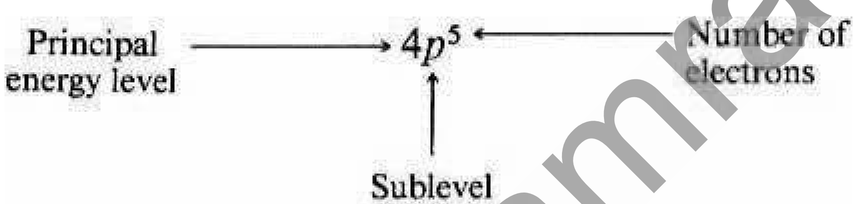
When an electron is in a particular energy level, it is more likely to be found in some parts of that level than in others. These parts are called orbitals. Orbitals of equivalent energy are grouped in sublevels. Each orbital can contain a maximum of two electrons. When in a magnetic field, the two electrons in a particular orbital differ very slightly in energy because of a property called electron spin. The theory of electron spin states that the two electrons in a single orbital spin in opposite directions on their axes, causing an energy difference between them. (Like many models, this explanation is an oversimplification, but for the purpose of this course it is a useful description.)

Each principal energy level has one sublevel containing one orbital, an s orbital that can contain a maximum of two electrons. Electrons in this orbital are called s electrons and have the lowest energy of any electrons in that principal energy level. The first principal energy level contains only an s sublevel; therefore, it can hold a maximum of two electrons.

Each principal energy level above the first contains one s orbital and three p orbitals. A set of three p orbitals, called the p sublevel, can hold a maximum of six electrons. Therefore, the second level can contain a maximum of eight electrons - that is, two in the s orbital and 6 in the three p orbitals.

Each principal energy level above the second contains, in addition to one s orbital and three p orbitals, a set of five d orbitals, called the d sublevel. The five d orbitals can hold up to 10 electrons. Thus, the third level holds a maximum of 18 electrons: 2 in the s orbital, 6 in the three p orbitals, and 10 in the five d orbitals. The fourth and higher levels also have an f sublevel, containing seven f orbitals, which can hold a maximum of 14 electrons. Thus, the fourth level can hold up to 32 electrons: 2 in the s orbital, 6 in the three p orbitals, 10 in the five d orbitals, and 14 in the seven f orbitals.

To distinguish which s, p, d, or f sublevel we are talking about, we precede the letter by the number of the principal energy level. For example, the s sublevel of the second principal energy level is designated 2s; the s sublevel of the third principal energy level is designated 3s; and so on. The number of electrons occupying a particular sublevel is shown by a superscript after the letter of the sublevel. The notation means that five electrons are contained in the p sublevel of the fourth energy level.

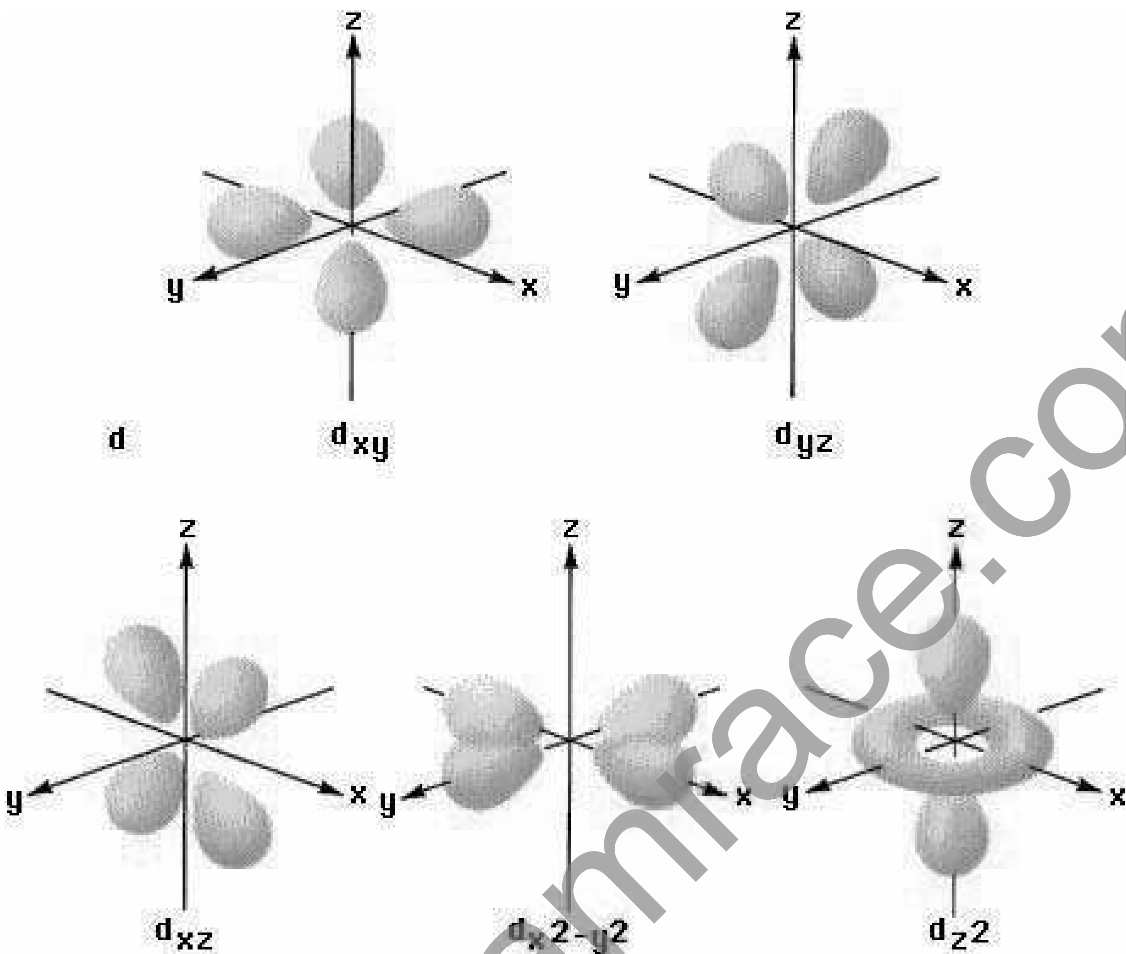


Orbital shapes and sizes

Each orbital has a unique shape and size. In these diagrams, the nucleus is at the origin of the axes. The s orbitals are spherically symmetrical about the nucleus and increase in size as distance from the nucleus increases. The 2s orbital is a larger sphere than the 1s orbital, the 3s orbital is larger than the 2s orbital, and so on.

The three p orbitals are more or less dumbbell-shaped, with the nucleus at the center of the dumbbell. They are oriented at right angles to one another along the x, y, and z axes, hence we denote them as px, py, and pz. Like the s orbitals, the p orbitals increase in size as the number of the principal energy level increases; thus a 4p orbital is larger than a 3p orbital.

The five d orbitals are denoted by dxy, dyz, dxz, dx2-y2, and dx2. Notice that these shapes are more complex than those of p orbitals, and recall that the shapes of p orbitals are more complex than those of s orbitals. Clearly, the shape of an orbital becomes more complex as the energy associated with that orbital increases. We can predict that the shapes of f orbitals will be even more complex than those of the d orbitals.



One further, important note about orbital shapes: These shapes do not represent the path of an electron within the atom; rather, they represent the region of space in which an electron of that sublevel is most apt to be found. Thus, a p electron is most apt to be within a dumbbell-shaped space in the atom, but we make no pretense of describing its path.

The energy of an electron versus its orbital

Within a given principal energy level, electrons in p orbitals are always more energetic than those in s orbitals, those in d orbitals are always more energetic than those in p orbitals, and electrons in f orbitals are always more energetic than those in d ortitals. For example, within the fourth principal energy level, we have:

$$\underset{\text{Increasing energy}}{\xrightarrow{4s < 4p < 4d < 4f}}$$

In addition, the energy associated with an orbital increases as the number of the principal energy level of the orbital increases. For instance, the energy associated with a 3p orbital is always higher than that associated with a 2p orbital, and the energy of a 4d orbital is always higher than that associated with a 3d orbital. The same is true of s orbitals:

$$\xrightarrow[\text{Increasing energy}]{1s < 2s < 3s < 4s < 5s}$$

Each orbital is not a region of space separate from the space of other orbitals. This is implicit in Figures 5.5, 5.6, and 5.7. If all those orbitals were superimposed on one another, you would see that a great deal of space is included in more than one orbital. For example, a 3p electron can be within the space assigned to a 3d or 3s orbital as well as within its own 3p space.

Our Model and the Spectra of Different Elements

According to our model of the atom, electrons are distributed among the energy levels and orbitals of the atom according to certain rules, and each electron has a unique energy determined by the position of its orbital. When an atom absorbs the right amount of energy, an electron moves from its original orbital to a higher-energy orbital that has a vacancy. Similarly, when an atom emits energy, the electron drops to a lower-energy orbital that has a vacancy. For example, an electron in a 3s orbital can drop to the 2p orbital, the 2s orbital, or the 1s orbital. The energy emitted by an electron in dropping to a lower-energy orbital is released in the form of radiation and determines the lines in the spectrum of the element.

When all the electrons of an atom are in the lowest possible energy states (meaning that the energy levels have been filled in order of increasing energy), the atom and its electrons are in the ground state. If one of these electrons moves to a higher energy level, the atom is in an excited state.

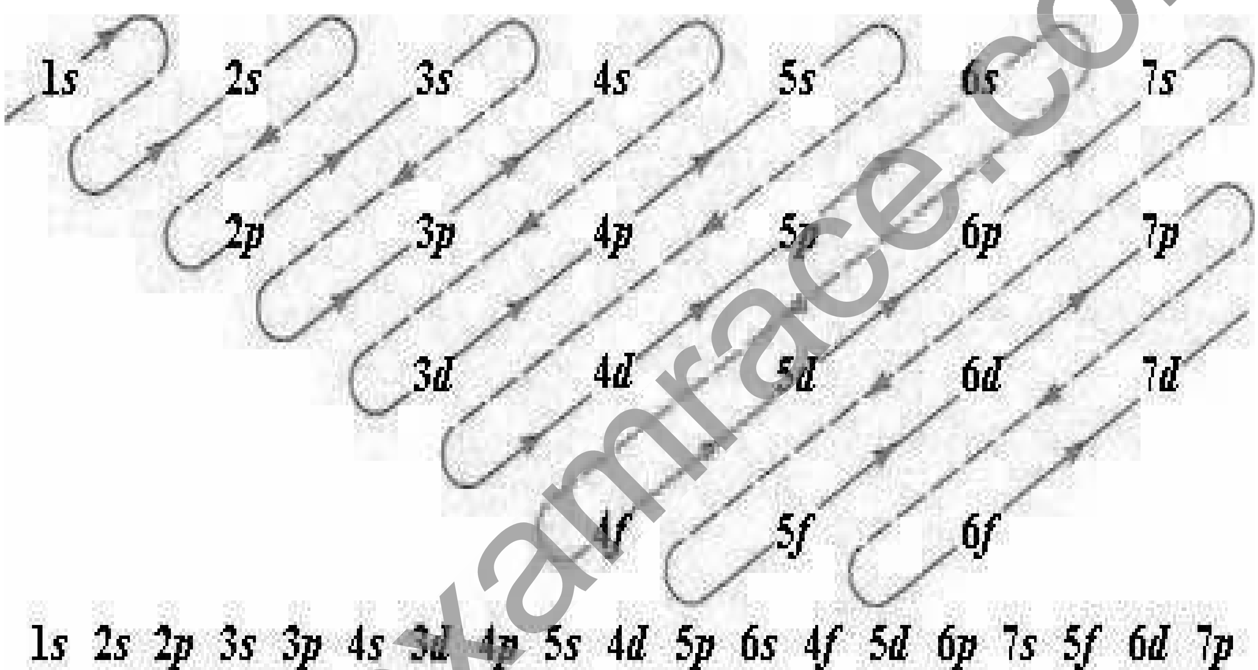
We know that each element has a unique spectrum. These spectra show that the energy differences among the electrons in an atom vary from one element to another. What causes this variation?

Recall that the nucleus of an atom is positively charged, that electrons carry a negative charge, and that oppositely charged bodies attract one another. The atoms of one element differ from those of another element in the number of protons in the nucleus and, consequently, in the charge on the nucleus. The attraction for an electron, and therefore its energy, will differ from one element to the next according to differences in nuclear charge. In addition, the atoms of one element contain a different number of electrons than do atoms of any other element. The energy of each electron within the atom depends not only on its interaction with the positively charged nucleus, but also on its interaction with the other electrons in the atom. Therefore, the energies of the electrons of one element will differ from the energies of the electrons of another element. Considering these two variables--nuclear charge and number of electrons--we can see that each element must have a unique spectrum derived from its unique set of electron energy levels.

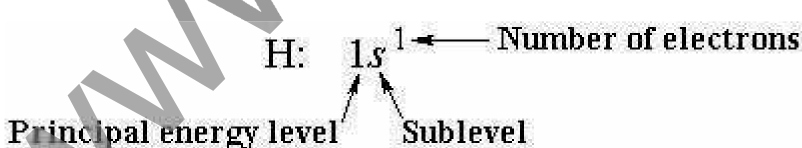
The Electron Configurations of Atoms

The electron configuration of an atom shows the number of electrons in each sublevel in each energy level of the ground-state atom. To determine the electron configuration of a particular atom, start at the nucleus and add electrons one by one until the number of electrons equals the number of protons in the nucleus. Each added electron is assigned to the lowest-energy sublevel available. The first sublevel filled will be the 1s sublevel, then the 2s sublevel, the 2p sublevel, the 3s, 3p, 4s, 3d, and so on. This order is difficult to remember and often hard to determine from energy-level diagrams.

A more convenient way to remember the order is to use Figure given below. The principal energy levels are listed in columns, starting at the left with the 1s level. To use this figure, read along the diagonal lines in the direction of the arrow. The order is summarized under the diagram.



An atom of hydrogen (atomic number 1) has one proton and one electron. The single electron is assigned to the 1s sublevel, the lowest-energy sublevel in the lowest-energy level. Therefore, the electron configuration of hydrogen is written:



For helium (atomic number 2), which has two electrons, the electron configuration is:

He: 1s2

Two electrons completely fill the first energy level. Because the helium nucleus is different from the hydrogen nucleus, neither of the helium electrons will have exactly the same energy as the single hydrogen electron, even though all are in the 1s sublevel. The element lithium (atomic number 3) has three electrons. In order to write its electron configuration, we must first determine (from Figure 5.9) that the 2s sublevel is next higher in energy after the 1s sublevel. Therefore, the electron configuration of lithium is:

Li: 1s22s1

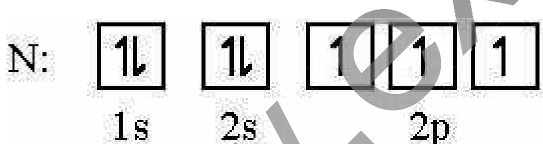
Boron (atomic number 5) has five electrons. Four electrons fill both the 1s and 2s orbitals. The fifth electron is added to a 2p orbital, the sublevel next higher in energy (Figure 5.9). The electron configuration of boron is:

B: 1s22s22p1

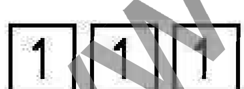
Box Diagrams of Electron Configuration

If an atom has a partially filled sublevel, it may be important to know how the electrons of that sublevel are distributed among the orbitals. Research has shown that unpaired electrons (a single electron in an orbital) are in a lower energy configuration than are paired electrons (two electrons in an orbital). The energy of the electrons in a sublevel would then be lower with half-filled orbitals than with some filled and some empty. We can show the distribution of electrons by using box diagrams, where each box represents an orbital and the arrows within the boxes represent the electrons in that orbital. The direction of the arrow represents the spin of the electron. (Recall from Section 5.3B that two electrons in an orbital spin in opposite directions on their axes.) Therefore, if an orbital contains two electrons, its box will contain two arrows, one pointing up and the other down.

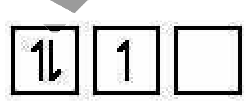
Using a box diagram, we show the electron configuration of nitrogen as:



Notice that the 2p electrons are shown as



rather than



which would mean that, of the three p orbitals, one is filled, one is half-filled, and one is empty.