**Quantum-Mechanical Model**

So far we have learned three things about electrons in atoms:

1. The energy of electrons is quantized.
2. Electrons exhibit wavelike behavior.
3. It is impossible to know the exact position and momentum of an electron at any moment.

The quantum-mechanical model of an atom explains the properties of atoms by treating the electron as a wave that has quantized energy. Though it is impossible to know the exact position of electrons, the model does describe the probability that electrons will be found in certain locations around the nucleus.

## Orbitals

According to the quantum-mechanical model, electrons have no precise orbits. Instead, their motion can only be described by the probability of finding them in certain regions surrounding the nucleus. These regions are called **orbitals**.

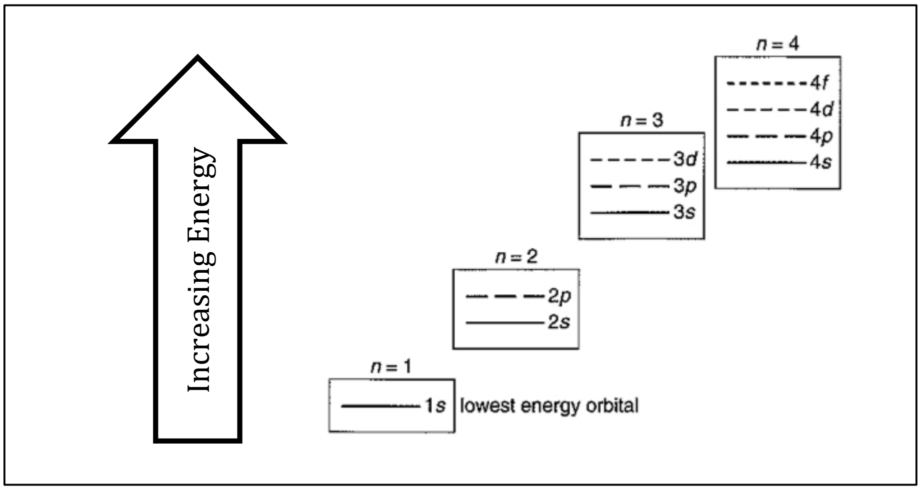
It is important to distinguish between the terms orbital (quantum-mechanical model) and orbit (Bohr model). In the Bohr model, an orbit is the actual path followed by an electron as it moves around the nucleus. In the quantum-mechanical model, an orbital is a region around the nucleus where an electron with a given energy is likely to be found.

There are several different kinds of orbitals, each having a different shape. These different kinds of orbitals are designated by the letters *s*, *p*, *d*, and *f*. All *s* orbitals are spherical, while all *p* orbitals are dumbbell shaped. The shapes of *d* and *f* orbitals are more complex.

## Orbitals and Energy

We can begin to visualize electrons with the idea of energy levels introduced by Bohr. The main or **principal energy levels** in an atom are designated by the quantum number *n*, which is called the principal quantum number.

As in the Bohr model, the energy of the electrons increases as *n* increases from 1 to 2 to 3, and so forth. Unlike the Bohr model, however, each principal energy level is divided into one or more **sublevels**. The number of sublevels in each principal energy level equals the quantum number *n* for that energy level.




As you can see in the diagram above, the sublevels are labeled with a number that is the value of the quantum number *n* and a letter (*s*, *p*, *d*, or *f*) that corresponds to the type of sublevel. For example, 2*p* is the designation of the *p* sublevel in the principal energy level 2.

Each sublevel consists of one or more orbitals. Each *s* sublevels contain a single *s* orbital, each *p* sublevel contains three *p* orbitals, each *d* sublevel contains five *d* orbitals, and each *f* sublevel contains seven *f* orbitals.

The division of the principal energy levels into sublevels and orbitals is summarized below.

| **Principal Energy Level** | **Sublevels** | **Orbitals** |
|---|---|---|
| $n = 1$ | 1s | 1s (one) |
| $n = 2$ | 2s, 2p | 2s (one) + 2p (three) |
| $n = 3$ | 3s, 3p, 3d | 3s (one) + 3p (three) + 3d (five) |
| $n = 4$ | 4s, 4p, 4d, 4f | 4s (one) + 4p (three) + 4d (five) + 4f (seven) |

**Electron Spin**

In addition to having characteristic energies, electrons also possess another important property. They behave as if they were spinning on their own axis. This spin can be either clockwise or counterclockwise.

A spinning charge creates a magnetic field. Thus, when an electron spins clockwise, it behaves like a tiny magnet whose north pole is pointing up. When it spins counterclockwise, it behaves like a tiny magnet whose north pole is pointing down.

In 1925, Wolfgang Pauli expressed the importance of electron spin in determining how electrons are arranged in atoms. The **Pauli exclusion principle** states that each orbital in an atom can hold at most 2 electrons and that these electrons must have opposite spins.

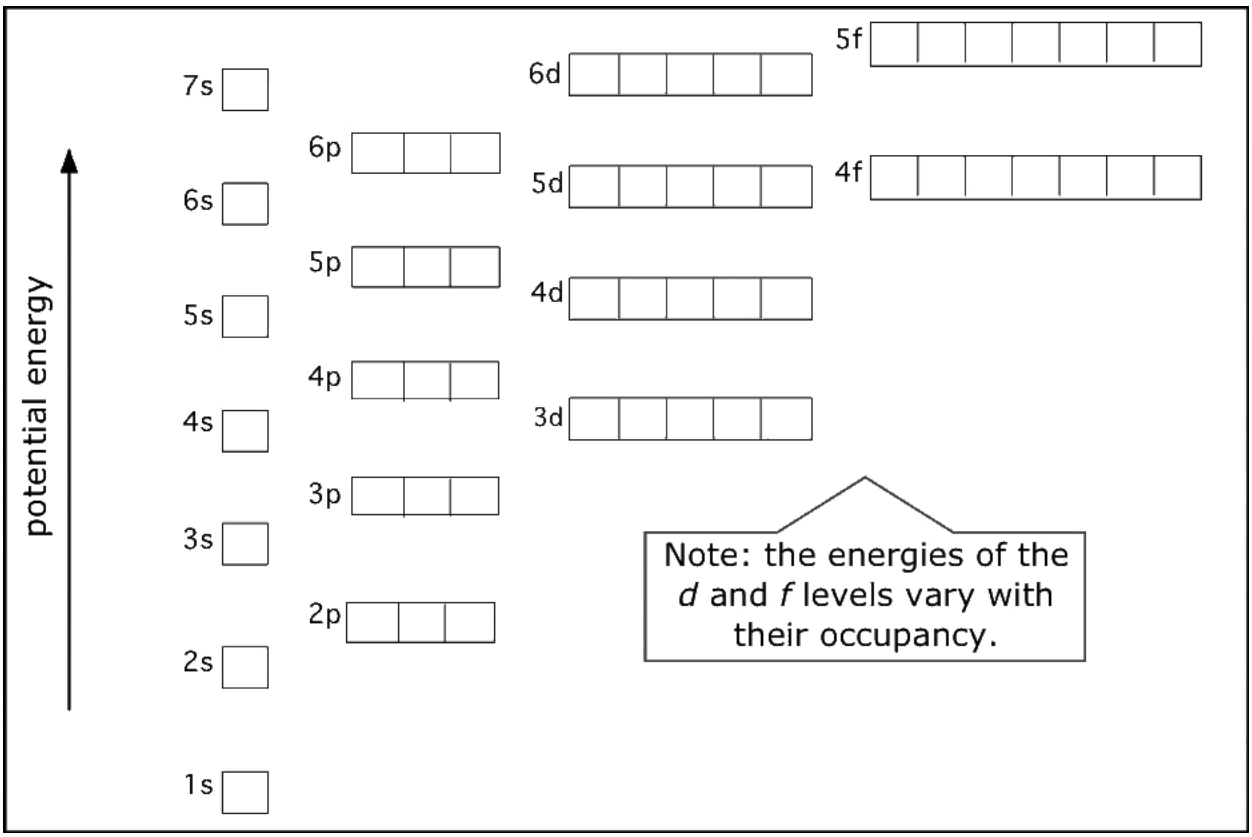
Since each orbital can hold a maximum of two electrons, there is a maximum number of electrons allowed in each sublevel in an atom, as shown below.

| Sublevel | Number of Orbitals | Maximum Number of Electrons |
|---|---|---|
| *s* | 1 | 2 |
| *p* | 3 | 6 |
| *d* | 5 | 10 |
| *f* | 7 | 14 |

## Writing Electron Configurations

The arrangement of electrons among the orbitals of an atom is called the **electron configuration** of the atom. The electron configuration describes where the electrons are found and what energies they possess.

Determining the electron configuration of an atom is easy once you know the relative energies of the orbitals. The diagram below illustrates the relative energies of the various levels, sublevels, and orbitals. Each box represents an orbital.




Notice that within each principal energy level, the *s* sublevel is always lowest in energy, followed by *p*, then *d*, and finally *f*. Also notice that above the 3*p* sublevel, the energies of the different principal energy levels begin to overlap. Thus, the 4*s* sublevel is actually lower in energy than the 3*d*.

In a later lesson, we will see how the periodic table contains within its very arrangement the energy ranking of sublevels. This means energy rankings can be easily determined, and there is no need to memorize the diagram above.

**The Aufbau Principle**

Electrons are added one at a time to the lowest energy orbitals available until all the electrons of the atom have been accounted for.

**The Pauli Exclusion Principle**

An orbital can hold a maximum of 2 electrons. To occupy the same orbital, 2 electrons must spin in opposite directions. When electrons with opposite spins occupy an orbital, the electrons are said to be paired. A single electron present in an orbital is said to be unpaired.

**Hund's Rule**

Electrons occupy equal-energy orbitals so that a maximum number of unpaired electrons result. For example, the p orbitals must be filled in the following order:

1.

| | | |
|---|---|---|
| ↑ | | |

2.

| | | |
|---|---|---|
| ↑ | ↑ | |

3.

| | | |
|---|---|---|
| ↑ | ↑ | ↑ |

4.

| | | |
|---|---|---|
| ↑↓ | ↑ | ↑ |

5.

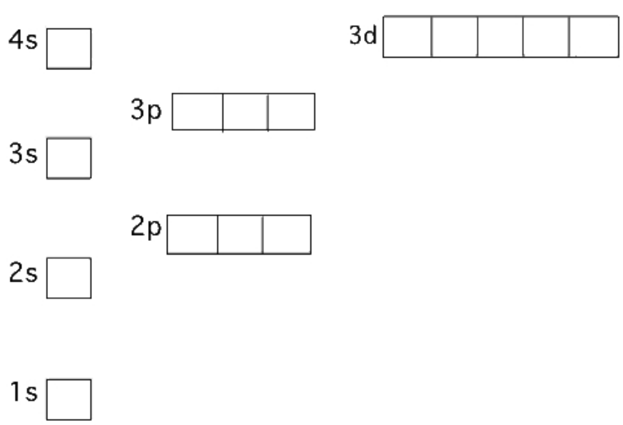
| | | |
|---|---|---|
| ↑↓ | ↑↓ | ↑ |

6.

| | | |
|---|---|---|
| ↑↓ | ↑↓ | ↑↓ |

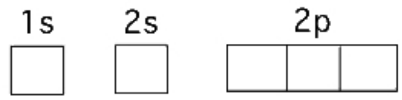
Note: The arrows in the boxes represent the electrons. A single arrow (↑) indicates an unpaired electron, spinning in one direction. A double arrow (↑↓) indicates two paired electrons, spinning in opposite directions.

**Example 1**
Determine the electron configuration for carbon.




To save space, the electron configuration is often shown by a horizontal diagram.

**Example 2**
Write carbon's electron configuration in a horizontal diagram.



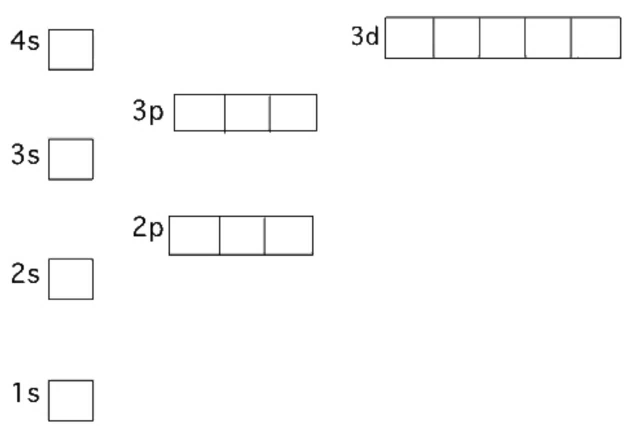

The representation in Example 2 is known as an **orbital diagram**, while the representation in Example 1 is called an **orbital energy diagram**.

Electron configurations are generally given in an even more compact form by writing the label for each occupied sublevel and adding superscripts to indicate the number of electrons in each sublevel. This is known as **sublevel notation**.

**Example 3**
Write the electron configuration for carbon in sublevel notation.

Because the superscripts represent electrons, the sum of the superscripts equals the number of electrons in the atom, which is the atomic number of the element.

**Example 4**
Complete the orbital energy diagram below for iron and then write iron's electron configuration in sublevel notation. How many unpaired electrons does iron possess?



Now that we have an understanding of electron configurations, let's examine how the colors of fireworks and neon lights are produced.

The electron configurations we have written represent ground states of atoms. When an atom is heated or supplied with energy, one of its electrons can absorb an amount of energy that corresponds to the difference between its present energy and a higher energy orbital. The atom is now in an excited state. This is an unstable state, so the electron "jumps" back to its initial energy level by emitting the extra energy in the form of light. Since the different wavelengths of light represent photons with different energies, the color of light emitted by an element depends on the energy gap between its sublevels.

Neon lights consist of sealed gas-filled tubes with electrodes at each end. As electricity passes through the tube, the gas atoms inside absorb the energy, entering an excited state. These excited atoms promptly emit the energy as visible light and return to their ground states. As long as the light is turned on, this process of electrons jumping up to excited states and returning to the ground state goes on and on.

**Example 5**
Write the electron configuration for a chlorine **ion** in sublevel notation.

**Important Note:** There are several elements on the periodic table whose electron configurations violate the normal rules. For the purposes of this course, we only need to know two of them:

| | **Expected Configuration** | **Actual Configuration** |
|---|---|---|
| Chromium | $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^4$ | $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^5$ |
| Copper | $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^9$ | $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^{10}$ |

**Worksheet**

1. What is the maximum number of electrons that can go into the following sublevels?

| | | | |
|---|---|---|---|
| a) $2s$ | c) $3p$ | e) $4f$ | g) $5d$ |
| b) $5s$ | d) $4d$ | f) $4p$ | h) $5f$ |

2. Write the electron configurations for each of the following elements. How many unpaired electrons does each possess?

| | |
|---|---|
| a) magnesium | f) chlorine |
| b) nickel | g) zinc |
| c) potassium | h) phosphorous |
| d) cobalt | i) manganese |
| e) boron | j) calcium |

3. Orbital diagrams for the ground states of two elements are shown below. Each diagram shows something that is incorrect. Identify the error in each orbital diagram and then draw the correct diagram.

a) nitrogen

| $1s$ | $2s$ | $2p$ | | |
|---|---|---|---|---|
| ↑↓ | ↑↓ | ↑↓ | ↑ | |

b) magnesium

| $1s$ | $2s$ | $2p$ | | | $3s$ |
|---|---|---|---|---|---|
| ↑↓ | ↑↓ | ↑↑ | ↓↓ | ↑↑ | ↑ |

4. Identify the elements that have the following electron configurations.

a) $1s^2 2s^2 2p^5$

b) $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^2$

c) $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^3$