Atoms and orbitals

A brief history
The idea of an atom first originated with the Greeks. The thinking was that if one were to cut an object with a knife, one would get pieces that are smaller than the original. Keep this process up and one gets smaller and smaller pieces. It seemed logical that if one continued this process long enough one would reach a point where one has a piece that cannot be cut further. They called these pieces “atomos” which means indivisible. Later in the early 19\textsuperscript{th} century John Dalton gave this idea a shot in the arm by proposing that matter is composed of atoms and that these atoms are the basic units of chemical reactions.

Later Dalton's atom was found to not be indivisible after all. It was discovered that atoms contain little bits of matter called \textit{electrons} that orbit a very small region called the \textit{nucleus} as shown below.

The electrons occupy almost all the space while the nucleus hogs up the mass. Later the nucleus itself was found to be occupied with bits of matter, namely the \textit{proton} and \textit{neutron}.

The problem with this view of the atom is that it is physically unstable as the electrons would end up crashing into the nucleus. Correcting this meant restricting the energies that the electrons can have, and this meant that electrons can exist in one of an allowed orbits as shown on the next page.
This is called the *Bohr model*.

A better view of the atom comes when we bring in *Quantum Mechanics*. Here we can still think of the electrons moving around the atom, but with a position and behavior that is unknown. While the mathematics for this can be formidable, the gist of the outcome is that we define regions where the electron is most likely to be found via experiment. These regions are called *orbitals* en-lieu or the atomic orbits above. These orbitals come in different flavors called s, p, d, f, ... For the physics aficionados the different orbitals correspond to the different angular momentum of the electron. Each orbital type comes in different configurations as shown below. The reason for the different sub-types is that multiple electrons might occupy a given orbital, and so (since electrons push away from each other) we need orbitals that can accommodate this.

Depictions of the different orbitals are shown below. These images have points scattered in such a fashion as to approximate the shape of the orbitals. In the center is a point representing the nucleus.

*S orbital* (Spherical shape)
**P orbitals** (Dumbbell shaped in three orientations)

![P orbitals diagram]

**D orbitals**: Dumbbell with a ring around it.

![D orbitals diagram]

**D orbitals**: Four lobes

![D orbitals diagram]
Spin city and maximum occupancy
As a consequence of Quantum Mechanics it turns out that bits of matter, such as electrons, obey what is called the Pauli exclusion principle. Simply stated, this states that no two identical objects can occupy the same state at the same time. This is something like in our everyday world where two objects cannot occupy the same place at the same time. So since, for example, the P orbital has three possible states within it then there must be at most three electrons in a P orbital. Ah, but the problem is that experiments show that in fact 6 electrons can occupy P orbitals. To account for this we introduce the notion of spin as an extension of an object's state. One can imagine that the spin is something a kin to an orbiting planet that spins as it rotates clockwise or counterclockwise in its orbit.

Electron configuration
So now let us apply what has been learned to the arrangement of electrons in an atom. We can imagine that we begin with a nucleus and then add one electron at a time until the atom is filled in. So we will begin at \( n = 1 \) and the s orbital for that state. Then we would go onto \( n = 2 \) and the s and p orbitals for that state etc. In so doing we must remember Hund's Rule that is that electrons want to fill in all the same spin before doubling up.

As an example consider Nitrogen with 7 electrons. Let us build up this atom from the lowest energy level on up.

\( n = 1: \)

Possible states, s orbital:

\[
\begin{array}{c}
1s \\
\end{array}
\]

Fill in the electrons that will fit:

\[
\begin{array}{c}
\uparrow \downarrow \\
1s \\
\end{array}
\]

\( n = 2: \)

Possible states, s & p orbital:

\[
\begin{array}{cccc}
\_ & \_ & \_ & \_ \\
2s & 2p \\
\end{array}
\]

Fill in the remaining 5 electrons:

\[
\begin{array}{cccc}
\uparrow \downarrow & \uparrow & \uparrow & \uparrow \\
2s & 2p \\
\end{array}
\]
So the arrangement of electrons in Nitrogen can be written as 
   \[ 1s^22s^22p^3 \]
The superscripts designate the number of electrons in each orbital.

As another example consider that of Silicon with 14 electrons.
n = 1:
   Possible states, s orbital:
   
   \[ 1s \]
   Fill in the electrons that will fit (First two electrons):
   \[ \uparrow \downarrow \]
   \[ 1s \]

n = 2:
   Possible states, s & p orbital:
   
   \[ 2s \quad \quad 2p \]
   Fill in the maximum number of electrons: (Bringing us up to 10 electrons total)
   \[ \uparrow \downarrow \quad \uparrow \downarrow \quad \uparrow \downarrow \quad \uparrow \downarrow \]
   \[ 2s \quad 2p \]

n = 3:
   Possible orbitals, s , p and d
   
   \[ 3s \quad 3p \quad 3d \]
   Fill in the orbitals with the remaining electrons 4 electrons:
   \[ \uparrow \downarrow \quad \uparrow \quad \uparrow \quad \uparrow \quad 3d \]
   \[ 3s \quad 3p \quad 3d \]

So the configuration would be \[ 1s^22s^22p^33s^23p^2 \]. As a final example consider Chromium with 24 electrons.
n = 1:
Possible states, s orbital:

Possible states, s & p orbital:

Fill in the maximum number of electrons:

Fill in the s & p orbitals. The d orbital is a higher energy and will be filled later.

n = 4:

Possible orbitals, s, p, d and f (not included). Also include the 3d orbital.

Now fill in the remaining 6 electrons

So the configuration for Chromium is \(1s^22s^22p^63s^23p^64s^23d^4\).
Practice Set: Express the configuration for the following (solutions at end).

1. Mg
2. Ga
3. S

The configuration shortcut

The above is a valid, if not cumbersome, process. However there is a much faster approach that mimics the same physical processes and is obtainable using the periodic table. The reason is that the arrangement of the periodic table arises from the configuration of the electrons.

Consider the basic regions of the periodic table below.

The different parts of the periodic table correspond to the different orbitals. Moreover the rows, for the most part, correspond to the n levels. The exceptions are as follows:

- The d-orbitals have an n-value one less than the row number.
- The f-orbitals have an n-value two less than the row number.

So to construct an electron configuration simply go down row-by-row in the table, accumulating orbitals as you go, until the desired atom is reached. As an example let us visit Gallium.
So the configuration is $1s^22s^22p^63s^23p^64s^23d^{10}4p^1$. As a further simplification we can note that we have built up to Argon (completing the orbitals) before pressing onto Gallium. So we can adopt the shorthand notation.

$[\text{Ar}]4s^23d^{10}4p$

Practice Set: Express the configuration for the following (solutions below).

4. As
5. Rb
6. U

Solutions:

1. Mg: $1s^22s^22p^63s^2$
2. Ga: $1s^22s^22p^63s^23p^64s^23d^{10}4p^1$
3. S: $1s^22s^22p^63s^23p^4$
4. As: $1s^22s^22p^63s^23p^64s^23d^{10}4p^3$ or $[\text{Ar}]4s^23d^{10}4p^3$
5. Rb: $1s^22s^22p^63s^23p^64s^23d^{10}4p^65s^1$ or $[\text{Kr}]5s^2$
6. U: $1s^22s^22p^63s^23p^64s^23d^{10}4p^55s^24d^{10}5p^66s^25d^{10}4f^{14}6p^67s^26d^{1f}^3$ or $[\text{Rn}]7s^26d^{1f}^8$

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