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## Atomic Orbitals

Electrons tend to occupy certain locations around the nucleus of an atom. These locations are classified into Atom Orbital types based on their directional characteristics. The Atomic Orbitals involved in covalent chemical bonding are called the s, p, and d Atomic Orbitals.

### s Atomic Orbital

The s Atomic Orbital has no directional preference. The s Atomic Orbital closest to the nucleus is labeled 1s. The 1s Atomic Orbital is the lowest energy orbital. Electrons fill the lowest energy orbitals first. Hydrogen has only one electron, which occupies the 1s orbital, since this is the lowest energy orbital possible.

### p Atomic Orbital

There are three p atomic orbitals: p(x), p(y), and p(z). Each of these is dumbbell shaped, and extends along the axis indicated in brackets. The first p atomic orbital is 2p and is higher in energy than the 2s orbital.

### d Atomic Orbitals

The d atomic orbital has five directional types. The names for these orbitals are: d(xy), d(yz), d(xz), d(x<sup>2</sup> - y<sup>2</sup>), and d(x<sup>2</sup>). The names correspond to the directional characteristics of each orbital. CHEMICAL uses the symbols ', ^, ~, and " to distinguish between the five d atomic orbitals.

## **Molecular Orbitals**

Atomic Orbitals from two atoms can combine to form Molecular Orbitals, the electrons shared (covalently) between the two Atoms. Molecular Orbitals replace the Atomic Orbitals. Molecular orbitals are either Bonding or Anti-Bonding. The Bonding Orbitals are lower energy and are more commonly used for bonding. Each Molecular Orbital can hold at most two electrons.

There are only three types of Molecular orbitals: sigma, pi, and delta. Sigma orbitals are formed when the "ends" of Atomic Orbitals bond, and thus are free to rotate after bonding. Pi and delta Molecular Orbitals are by side by side bonding and thus are not free to rotate. (CHEMICAL does not include delta bonds)

## **Bonding**

Atomic and Molecular orbitals have energy states associated with them. Bonding occurs when a lower energy state occurs by sharing electrons. No more than two electrons may occupy any orbital. When many possible bonds exist the lowest energy one will dominate and determine the 3 dimensional configuration.

Typically each atom donates an electron for bonding. Sometimes one atom will donate both electrons, this is called a Dative bond. Occasionally bonding can only occur by using the higher energy anti-bonding orbitals.

The bond order is determined by the number of pairs of electrons in bonding orbitals minus the number of pairs of electrons in anti-bonding orbitals. The higher the bond order the stronger the bond.

Sometimes an electron must be moved to another orbital in order to make a dative bond. For example: in  $\text{H}_2\text{SO}_4$  two of the Oxygen atoms require dative bonding to combine with Sulfur. CHEMICAL will move an electron in order to empty one oxygen orbital for bonding with two electrons from the Sulfur atom.

**Size of Atoms**

Atoms for higher numbered elements are generally larger. Atoms get smaller going across (left to right) the periodic table. The size also varies with the type of hybrid and bonding. CHEMICAL has a built in table of atom sizes according to the orbital type and bond order.

**Ions**

Atoms that loss or gain electrons are called ions. CHEMICAL has a built in table of typical ions. Negative ions are large because they has gained an additional electron. Positive ions are small due to the loss of an electron.

**Electronegativity**

The power of attraction that an atom shows for electrons is called electronegativity. Electronegativity is a measure of the attraction of an atom for electrons in its outer shell.

## Hybrids

The s, p, and d atomic orbitals combine to form hybrids. The directional characteristic of these hybrids combine the characteristics of the composite atomic orbitals. In addition the new hybrid orbitals position themselves so as to have the maximum angle between any two orbitals.

The number after an s,p, or d indicates the number of orbitals of that type. For example: sp has two orbitals and sp<sup>2</sup> has three orbitals

### d<sup>2</sup>sp<sup>3</sup> Hybrids

When CHEMICAL forms hybrids, the electrons are re-distributed among the new orbitals. In the hybrids presented so far the distribution is done so as to spread out the electrons among all the hybrids. This forms hybrids with only one electron that can be used for covalent bonding. However, the electron distribution in some hybrids, such as d<sup>2</sup>sp<sup>3</sup> is different. These hybrids have no electrons, and require two electrons from another atom to form a covalent bond. These are called coordination compounds.



### **Flat ring structures**

The  $sp^2$  hybrid has three bonds oriented in a plane. The angle between these bonds is 120 degrees, which is the same as the angle in a six side figure. Therefore, six  $sp^2$  can combine to form a six atom ring.

However, a five sided ring has 112 degrees between its angles. In order to make five sided structures using  $sp^2$  hybrids the  $sp^2_5$  hybrid is included. This hybrid is the same as  $sp^2$ , except that the angles are changed to 112 degrees. These two bond are the default (highlighted) bonds, making five ring structure easy to make.

The angle between bond for the  $sp^3$  hybrid is not correct for either 5 or 6 ring structures. Therefore, the  $sp^3_5$  and  $sp^3_6$  bonds are provided. The  $sp^2$ ,  $sp^2_3$ ,  $sp^2_5$ ,  $sp^3_3$ ,  $sp^3_4$ ,  $sp^3_5$ , and  $sp^3_6$  hybrids form flat rings.

### **$sp^3$ Rings**

Rings can be made using the  $sp^3$  hybrids. However this structure can not be flat because the angles between bonds are not 120 degrees.

**Covalent Bonds**

Electrons tend to occupy certain locations around the nucleus of an atom. Because of the like electrical charge these orbitals tend to separate as much as possible.

**Ionic Bonds**

Atoms with an electronegativity difference of more than 0.5 volts can be attaching using ionic bonds.

**Hydrogen Bonds**

The electron from a hydrogen atom can be shared between two Oxygen, Nitrogen, or Carbon atoms. The separation between hydrogen bonded atoms is larger than the distance between Covalent or Ionic Bonds.

**Double Hydrogen bonds**

The double hydrogen bond is primarily used for combing the bases for DNA and RNA. The double hydrogen bonds must involve Oxygen, Carbon, or Nitrogen. The atoms on the two groups must be spaced correctly to form two hydrogen bonds.

**Peptide Bonds**

Peptide bonds are covalent bonds that combine amino acids. A rigid Peptide Bond Group is inserted between amino acids when forming peptide bonds.

**Ionic Bonding (Crystal Structures)**

Most crystals consist of atoms that are bonded with ionic bonds. Ionic bonds differ from covalent in that the electron is captured by one of the atoms, rather than being shared. Ionic compounds tend to form organized structures that can be described by repeating a unit cell in three dimensions.

The simplest unit cell is a cube. This is the default cell that the Matter/Crystal Dialog Boxes opens with. All sides are equal and the angles between the sides are 90 degrees. Simple crystal models can be made by placing ions at the center, corners, faces, or edges of the unit cell. More complex crystals can be made by placing ions at specified locations within the unit cell.