# *Structure and Bonding Theories*

**Electron Dot Symbols**

A method of gaining understanding of the way in which atoms can bond is to depict the **valence**, or outer shell, electrons around the chemical symbol for an element in a way that shows how many bonds the atom is likely to form. Writing what are known as electron dot symbols for the elements does this. The electrons are placed around the atom on one of each of the four sides. There will be a maximum of 2 electrons per side and the electrons are placed following an analog of Hund's rule: one electron per side until each has one then they are paired up. Following this rule will give us an indication of how many bonds a particular element can form. The electron dot symbol for Hydrogen is the simplest:

H·

Helium would look like:

He:

This doesn't follow the above rule because 2 electrons fill the valence shell for Helium. Carbon would look like:

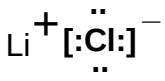
The presence of unpaired electrons is an indication of the number of bonds it is likely to form. Hydrogen is likely to form only one bond. Carbon is likely to form 4 bonds but there are exceptions though. Helium is not likely to form any bonds. This knowledge can help us to decide which atoms are bonded to which other atoms. This means that we can now draw electron dot structures of molecules. **Electron dot structures** (or **Lewis Dot Structures**) are two-dimensional representations of the bonding in molecules. When we have an idea of the bonding that is present in a molecule we can then make decisions about the molecule such as how the atoms are arranged in three-dimensional space and whether or not the molecule is polar.

**Electron Dot Structures**

An electron dot structure allows us to determine the bonding in a molecule. It will show us which atoms are connected to each other. Once this information is obtained we can use it to determine other properties of the molecule.

The simplest electron dot structures are those for the binary ionic compounds. These are comprised only of the electron dot symbols for the ions. All metals lose electrons to form ions. This is represented by the electron dot symbol for the element without any electrons. We are talking about only the main group elements. For instance, lithium will lose its 1 2s electron to form an ion. It therefore will have no valence electrons to

represent in the symbol. All non-metals gain electrons to form ions. This is represented in the electron dot symbol by a completely filled octet of electrons around the atom. When a non-metal gains electrons, it gains enough electrons so that it has the same electron configuration as the nearest noble gas. This means that the valence shell of a non-metal ion will contain eight electrons. The symbol for the non-metal ion will be enclosed in square brackets. This indicates that all of the electrons belong to the ion and none of them are shared. The symbol for the metal ion is placed first with the symbol for the non-metal ion placed next to it.



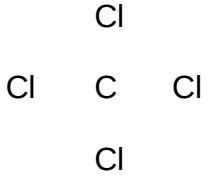
Covalent compounds are almost as easy. Do draw the electron dot structure for a covalently bonded compound we have to follow a few rules.

1. Determine the skeletal structure of the compound. This will involve determining the central atom. The central atom is going to be the atom that forms the most number of bonds. If there are two atoms that form the same number of bonds, the atom that is least **electronegative** will be the central atom. All of the other atoms will be arranged around the central atom.
2. Count the number of valence electrons in the compound. If it is a polyatomic ion, add one electron for each negative charge and subtract an electron for each positive charge.
3. Connect all the outer atoms to the central atom by single bonds (use a single line). A single bond is two electrons.
4. Give all of the outer atoms an octet by placing the appropriate number of electron pairs around each atom. Any left over electron are placed in pairs on the central atom.
5. If the central atom does not have an octet, convert lone pairs on the outer atoms to form double or triple bonds until the central atom has an octet.

Example:

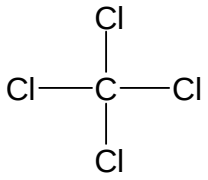
$CCl_4$

Step one: The central atom is going to be Carbon because it can form the most number of bonds and it is the least electronegative.

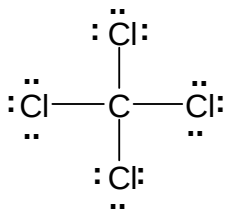


Step two: There are 32 valence electrons.

Step three: Connect the outer atoms to the central atom by single bonds.




Step four: Give the outer atoms octets.




all atoms have octets at this point and there are no more electrons. We are done with this structure.

**Electronegativity**

Electronegativity is the tendency of an atom to attract electrons to it when it is covalently bonded to another atom. The trend of electronegativity in the periodic table is that Fluorine is the most electronegative element and Cesium is the least. As we move away from fluorine in the periodic table, electronegativity decreases.

Electronegativity can also be used to determine polarity. We will discuss this aspect of molecules after we can determine the molecular geometry.

**Resonance structures**

Sometimes we are able to draw more than one correct electron dot structure for a molecule. When we look at formal charges there is no way to distinguish between the two structures. Here is an example:


Both of these structures are correct. When this happens the molecule is said to have **resonance**. Resonance lends stability to a molecule. The two structures above are called **resonance structures**.

**Molecular Structure**

Once we are able to determine which atoms are bonded to each other and the number of lone pairs on the central atom we can then make a determination about the shape of the molecule. This is done using a model known as **VSEPR**, or **Valence Shell Electron Pair Repulsion**. This model postulates that the electron groups, or pairs, will repel each other and get as far away as they can from each other around the central atom. This results in the molecule having a particular shape. There are two kinds of geometries we can talk about. The first is called the **electron pair geometry**, which shows us how the groups of electrons are arranged around the central atom. The second is called the **molecular geometry**, which shows us how the atoms are arranged in three-dimensional space.

**Electron Pair Geometry**

There are three kinds of electron pair geometry. This depends solely on the number of groups of electrons around the central atom. We need to remember that multiple bonds (i.e., double and triple bonds) count as one group of electrons. The number of groups of electrons determines the electron pair geometry:

| Number of electron groups | Electron Pair Geometry |
|---|---|
| 2 | Linear |
| 3 | Trigonal Planar |
| 4 | Tetrahedral |

These are the **ONLY** three electron pair geometries. The electron pair geometry leads to the molecular geometry.

**Molecular Geometry**

Molecular geometry can be derived from the electron pair geometry. If we ignore the lone pairs (but not their effect on the other electron groups) and just look at where the atoms are we are looking at the molecular geometry.

| Total $e^-$ groups | # of lone pairs | Electron Pair Geometry | Molecular Geometry |
|---|---|---|---|
| 2 | 0 | Linear | Linear |
| | 1 | Linear | Linear |
| 3 | 0 | Trigonal Planar | Trigonal Planar |
| | 1 | Trigonal Planar | Bent |
| 4 | 0 | Tetrahedral | Tetrahedral |
| | 1 | Tetrahedral | Trigonal Pyramidal |
| | 2 | Tetrahedral | Bent |

As we can see from the table, the electron pair geometry and the molecular geometry is the same if the number of lone pairs is zero. This makes sense because if there are no

lone pairs on the central atom, there is an atom wherever there is an electron group. When there are one or more lone pairs the molecular geometry differs from the electron pair geometry.

**Molecular Polarity**

Now that we are able to determine the shapes of molecules, we can also determine if the molecule is **polar** or not. A molecule is polar if there is a separation of charge in the molecule. This arises due to the difference in electronegativity in the atoms comprising the molecule. Each bond that is between two atoms of differing electronegativity is polar. The degree of polarity depends on the magnitude of the electronegativity difference.

The polarity of the molecule depends on the arrangement of the polar bonds in space, in other words, the molecular geometry. If the polar bonds are arranged symmetrically around the central atom they will cancel each other out and the molecule will be non-polar. If they are not symmetrically arranged, they will not cancel out and the molecule will be polar.

We can determine if they are symmetrically arranged by a simple test. If we rotate the molecule around a bond such that we change the positions of the atoms and the molecule looks the same it is symmetric and therefore it is non-polar. If the molecule looks different, it is polar.