# Making Molecular Models

Molecular models are excellent tools for teaching about atoms, molecules and crystals. Models can be made using Styrofoam atoms connected by small wooden dowels; gumdrop candies and toothpicks; or using expensive commercial molecular modeling parts as we will be doing.

Styrofoam balls come in various sizes, but don't hold their connecting dowels very well and need to be painted to distinguish different atoms. Gumdrop candies come in multiple colors, hold the toothpicks pretty well, but are not reusable week-to-week or year-to-year. Also, ants can become a problem when using gumdrops!

Commercial models, particularly Molymod, are used by colleges and professionals because they come in standard colors; have realistic bond numbers and angles; are reusable for decades; and can be washed. I am very cost-sensitive, but feel that buying Molymod kits (*http://www.indigo.com/models/molymod-molecular-model-kits.html*) and extra parts (*http://www.indigo.com/models/molymod-molecular-model-components.html*) is worth the extravagance. We will use my personal collection of Molymod parts in our lab activities. Be sure to pick up any that fall on the floor.

When I helped at a small local school in a classroom with 6, 7, and 8 graders, the students were quick to build interesting molecules like Aspirin. My grandchildren easily learned how to build various molecules with the 8-year old building sucrose. (It is true, however, that they spend quite a bit of time building doggies, bracelets, necklaces, and miscellaneous unidentifiable creations.)

## Molymod Parts

The MolyMod molecular modeling kits have atoms with varying colors and number of bond connections. The color associations of different kinds of atoms are not strict since there are far more different types of atoms than MolyMod colors. In fact, actual atoms are too small to have detectable colors; the colors used in the models reflect tradition, not reality. The most common atoms types (with their indigo.com part numbers) are listed in the following table where bold-faced entries indicate atoms with holes matching their normal valences:

| | | | |
|---|---|---|---|
| **60150E** | **white 19 mm dome** | **1-hole** | **hydrogen** |
| 60210E | white 17 mm sphere | 2-holes, 180º | hydrogen |
| 60220E | black | 2-holes, 180º | carbon |
| 60310E | black | 3-holes, 120º | carbon |
| **60400E** | **black** | **4-holes, 109.5º** | **carbon** |
| 60511E | black | 5-holes, 120º, 90º | carbon |
| 60514E | brown | 5-holes, 120º, 90º | boron |
| 60103E | red 20 mm sphere | 1-hole | oxygen |
| 60121E | red 23 mm sphere | 1-hole | oxygen |
| 60211E | red 17 mm sphere | 2-holes, 180º | oxygen |
| **60200E** | **red 23 mm sphere** | **2-holes, 105º** | **oxygen** |
| 60402E | red 23 mm sphere | 4-holes, 109.5º | oxygen |
| 60203E | blue 23 mm sphere | 2-holes, 105º | nitrogen |
| **60300E** | **blue 23 mm sphere** | **3-holes, 107º** | **nitrogen** |
| 60311E | blue 23 mm sphere | 3-holes, 120º | nitrogen |
| 60401E | blue 23 mm sphere | 4-holes, 109.5º | nitrogen |
| 60512E | blue 23 mm sphere | 5-holes, 120º, 90º | nitrogen |
| **60201E** | **yellow 23 mm sphere** | **2-holes, 105º** | **sulfur** |
| 60613E | yellow 23 mm sphere | 6-holes, octahedral | sulfur |
| 60403E | yellow 23 mm sphere | 4-holes, 109.5º | sulfur |
| **60120E** | **green 23 mm sphere** | **1-hole** | **chlorine** |
| 60612E | green 23 mm sphere | 6-holes, octahedral | chlorine |
| **60115E** | **purple 17 mm sphere** | **1-hole** | **iodine** |
| 60407E | purple 23 mm sphere | 4-holes, 109.5º | phosphorus |
| **60510E** | **purple 23 mm sphere** | **5-holes, 120º, 90º** | **phosphorus** |
| **60114E** | **orange 17 mm sphere** | **1-hole** | **bromine** |
| 60404E | gray 23 mm sphere | 4-holes, 105º | metals |
| 60610E | gray 23 mm sphere | 6-holes, octahedral | metals |

The following types of bonds are available:

| | | | |
|---|---|---|---|
| 61015E | clear 1 mm | rigid | for compact models & hydrogen domes |
| 61020E | gray 3 mm "V" style | flexible | for strained compact bonds |
| 61012E | gray 20 mm | rigid | for single bonds in open models |
| 61013E | gray 35 mm | flexible | for double and triple bonds in open models |
| 61014E | purple 35 mm | flexible | for van der Waals hydrogen bonds |

## Double and Triple Covalent Bonds

In nearly all molecules, carbon has 4 bonds with tetrahedral symmetry. That is, its four bonds point to four of the eight corners of a cube surrounding the atom. Sometimes, however, two or even three bonds go to the same neighboring atom. These are called double and triple bonds. Two atoms connected by a single bond can easily rotate around the bond, but those connected by a double or triple bond cannot.

Nitrogen has three bonds, oxygen two bonds and hydrogen one bond. The number of bonds is related to the number of electrons in the outermost electron shell of the atom.

As we construct models, we will learn how in methane, $CH_4$, ethane, $C_2H_6$, and in a hydrogen molecule, $H_2$, all bonds are single, while in $O_2$ the two oxygen atoms are connected by a double bond. In ethylene, $C_2H_4$, the bond connecting the carbon atoms is a double bond. In acetylene, $C_2H_2$, the bond connecting the carbon atoms is a triple bond.

We will also see how in benzene, chlorophyll, and heme, and many other "aromatic" molecules, loops made up of alternating single and double bonds lead to flat molecules that interact rather well with light.

## Types of Molecular Models - Compact and Open

Molecular Models can be made in a compact form (semi-space filling) that uses only the short bonds or in an open form that uses long bonds and explicitly shows double and triple bonds.

The compact form has an average scale factor of about 1.3 cm = 100 pm. Put differently the model molecules are about 130,000,000 times actual size. On this scale a typical grain of salt would be a cube with about 40 km on a side.

The open form has internuclear distances that have a scale factor of about 2.5 cm = 100 pm. The atoms are separated by distances about 250,000,000 times actual size.

Double and triple bonds are easily seen in the open type of molecular models, but in the compact models, a double bond to a carbon atom is faked by using a 3-hole trigonal carbon atom. In compact models involving oxygen, the double bond is faked by using a 1-hole oxygen atom.

The compact models have more realistic spacing between atoms, but the open models have more realistic bonding. So both types are needed to understand the chemistry of molecules.

One can mix the two types by building open models with all hydrogen atoms connected as in the compact models. That looks a little prettier and still shows the multiple bonds. That is the approach we use.

# Ionic Molecules

**Ions** are atoms with an imbalance of charge – too many or too few electrons. Ionic molecules are molecules with an imbalance of charge.

In pure water at room temperature, nearly all molecules retain their $H_2O$ structure, but 1 out of 556 million of those has split apart into its ions, $H^+$ and $OH^-$ . The $OH^-$ ions are called **hydroxyl** (or **hydroxide**) ions. The $H^+$ immediately joins with a nearby $H_2O$ molecule to form the ion $H_3O^+$ called **hydronium**.

Normally, oxygen has two bonds, but the oxygen in $OH^-$ only has a single bond, the one connecting it to its H atom. As a result, it has an unpaired electron and therefore a negative charge. To represent the $OH^-$ ion with our model oxygen atom, one of the two holes will be left unconnected. There are other occasions where we need to represent an $O^-$ ion and will also do so by leaving an empty hole on the oxygen.

On the other hand, the $H_3O^+$ has an extra proton ( $H^+$ ion) that became attached without bringing an additional electron. The net result is that the hydronium ion has a positive charge, and we will need an oxygen atom with an additional hole. For that, we can use a 4-hole red ball and pretend it is a 3-hole oxygen atom.

There is a similar problem with $NH_3$ (ammonia) molecules in water. Any free $H^+$ ion (or one from a $H_3O^+$ ion) will join with $NH_3$ to make $NH_4^+$ ions. Normally our N atoms have three holes, but to make an $NH_4^+$ ion, we need to use an N atom with an additional hole. This will also be the case whenever we have a molecule with an N atom connected by 4 single bonds or a double bond and two single bonds. For those cases, we can will use a 4-hole blue ball with its holes in a tetrahedral geometry. On other occasions, $NH_3$ may have lost a proton and become a $NH_2^-$ ion. In that case, we will use our 3-hole trigonal N atom, but leave one hole unattached.

Another common ion is the carbonate ion $CO_3^{--}$ . Here, the carbon atom is double bonded to one oxygen and single-bonded to the other two oxygens which will each have an unattached hole. The phosphate ion $PO_4^{3-}$ is like carbonate except that it has one oxygen with a double bond and the other three with single bonds. Phosphate atoms are represented by a purple ball with of 5 holes.

Ozone, $O_3$ , is not an ion, but has a significant separation between negative and positive charges. It can be represented as a central oxygen atom of positive charge connected by a double bond to one of its other oxygen atoms and a single bond to the other. The central atom therefore needs to be represented like the oxygen in $H_3O^+$ , a 4-hole red ball is used with one hole ignored.

# Supply of Molymod Parts

| Quantity | Element | Color | Holes | Type of Bond | Size (mm) | Part # | |
|---|---|---|---|---|---|---|---|
| 10 | Hydrogen | White | 1 | | 17 | 60110E | |
| 400 | Hydrogen | White | 1 | | 19 | 60150E | |
| 64 | Hydrogen | White | 2 | Linear – 180º | 17 | 60210E | Hydrogen bonds |
| 6 | Carbon | Black | 2 | Linear – sp – 180º | 23 | 60220E | $BeCl_2$,$CO_2$ |
| 190 | Carbon | Black | 3 | Trigonal – $sp^2$ – 120º | 23 | 60310E | Compact w/dbl bond |
| 184 | Carbon | Black | 4 | Tetrahedral – $sp^3$ – 109.5º | 23 | 60400E | Ice |
| 12 | Carbon | Black | 5 | Trigonal bi-pyramidal – $sp^2d$ | 23 | 60511E | graphite |
| 60 | Nitrogen | Blue | 2 | Angular - 105º | 23 | 60203E | Purines, $NO_2^-$ |
| 54 | Nitrogen | Blue | 3 | Trigonal – $sp^2$ – 120º | 23 | 60311E | Peptide bond |
| 52 | Nitrogen | Blue | 3 | Pyramidal – 107º | 23 | 60300E | $N_2$, R-$NH_2$, $NH_3$ |
| 32 | Nitrogen | Blue | 4 | Tetrahedral – $sp^3$ – 109.5º | 23 | 60401E | R-$NO_2^-$ R-$NH_3^+$, $NH_4^+$ |
| 4 | Nitrogen | Blue | 5 | Trigonal bi-pyramidal – $sp^3d$ | 23 | 60512E | no examples |
| 24 | Oxygen | Red | 1 | | 23 | 60121E | $O^-$ |
| 10 | Oxygen | Red | 1 | | 20 | 60103E | $O^-$ |
| 20 | Oxygen | Red | 2 | Linear | 17 | 60211E | O hydrogen bond |
| 150 | Oxygen | Red | 2 | Angular - 105º | 23 | 60200E | $H_2O$ |
| 32 | Oxygen | Red | 4 | Tetrahedral – $sp^3$ – 109.5º | 23 | 60402E | CO, $O_3$ |
| 10 | Phosphorus | Purple | 1 | | 17 | 60115E | |
| 10 | Phosphorus | Purple | 3 | Pyramidal – 107º | 23 | 60301E | $PH_3$, $PCl_3$ |
| 35 | Phosphorus | Purple | 4 | Tetrahedral – $sp^3$ – 109.5º | 23 | 60407E | $PO_4^{3-}$ |
| 32 | Phosphorus | Purple | 5 | Trigonal bi-pyramidal – $sp^3d$ | 23 | 60510E | $PCl_5$ |
| 12 | Sulfur | Yellow | 2 | Angular - 105º | 23 | 60201E | $SO_2$ sulfur bridge |
| 4 | Sulfur | Yellow | 4 | Tetrahedral – $sp^3$ – 109.5º | 23 | 60403E | |
| 14 | Sulfur | Yellow | 6 | Octahedral | 23 | 60613E | HCTZ |
| 18 | Chlorine | Green | 1 | | 23 | 60120E | |
| 18 | Chlorine | Green | 6 | Octahedral | 23 | 60612E | NaCl |
| 12 | Bromine | Orange | 1 | | 17 | 60114E | |
| 12 | Iodine | Purple | 1 | | 17 | 60115E | |
| 2 | Metal | Grey | 2 | Angular – 105º | 23 | 60202E | Selenocysteine |
| 2 | Metal | Grey | 4 | Tetrahedral – $sp^3$ – 109.5º | 23 | 60404E | |
| 23 | Metal | Grey | 6 | Octahedral | 23 | 60610E | NaCl |
| 670 | Short Bonds | Clear | | Space filling bond | 1 | 61015E | |
| 60 | H bond | Purple | | van der Waals hydrogen bond | 35 | 61014E | |
| 330 | Standard Bond | Grey | | Standard medium bond | 20 | 61012E | |
| 232 | Flexible Bond | Grey | | Double/Triple bond | 35 | 61013E | |
| 140 | "V" Links | Grey | | Short flexible links | 3 | 61020E | |
| 8 | Tool | Cream | | Short bond removal tool | | 61002 | |
| 2 | Tool | Cream | | Push Tool | | 61001 | |