Beginning Exercises with Molecular Models

For our first exercises with Molymod models, we will work in 10 groups with each group getting the following parts:

14 **black** 4-hole **carbon** atoms (natural configuration, tetrahedral – sp^3 – 109.5°)
6 black 3-hole trigonal carbon atoms (short double bond + 2 single bonds)

29 **white** hemispherical **hydrogen** domes (normal representation of hydrogen atoms)
3 white 2-hole spherical hydrogen atoms (for weak hydrogen bonds as in DNA or ice)

12 **red** 2-hole **oxygen** atoms (normal representation of oxygen, angular - 105°)
2 red 4-hole oxygen atoms (used for CO and O_3, tetrahedral – sp^3 – 109.5°)

5 **blue** 3-hole pyramidal **nitrogen** atoms (natural configuration, pyramidal – 107°)
3 blue 3-hole triangular nitrogen atoms (various special cases like in amino acids in blood)
2 blue 4-hole tetragonal nitrogen atoms (for nitro groups, tetrahedral – sp^3 – 109.5°)

1 **purple** 3-hole **phosphorous** atoms (natural configuration, pyramidal – 107°)
2 **purple** 5-hole **phosphorous** atoms (for phosphates, trigonal bi-pyramidal)

2 **green** 1-hole (or 6-hole) **chlorine** atoms (natural configuration)

2 **silver** 6-hole **metal** atoms (Na in NaCl, Fe in heme, Mg in chlorophyll, Co in vitamin B-12)

1 **yellow** 2-hole **sulfur** atoms (natural configuration, angular - 105°)

22 gray rigid 20 mm normal bonds (open structures that can display multiple bonding)
22 gray 35 mm flexible bonds (double bonds in open structures)
50 clear 1 mm rigid bonds (used with hydrogen domes and in short bonding structures)

The actual atoms have no visible light color since they are about 1000 times smaller than the wavelength of visible light, but these atom colors help us keep track of which atom is which.

Please be careful not to lose any parts. Any that fall on the floor should be immediately retrieved.

We will learn how to make a wide variety of molecules based on molecular diagrams. An 11-page handout with the initial page entitled "Some Simple Molecules" will be used for many of our exercises.

The first lab day with these will focus on basic rules of how to use these atoms and bonds, starting with the following molecules built with longer bonds that clearly distinguish between single and multiple bonds:

1. **Water molecule H_2O** built with a 2-hole oxygen atom with two hemispherical hydrogen domes connected by two short bonds. All holes are used. The end result looks like a Mickey Mouse head.

2. **Hydrogen peroxide H_2O_2** built like water but with an additional oxygen atom. It is used as a bleaching agent and disinfectant. Hydrogen peroxide decomposes to water and oxygen giving off heat.

3. **Hydrogen sulfide H_2S** built with a 2-hole yellow sulfur atom and two hemispherical hydrogen domes using short bonds. Famous for being the agent of rotten egg smell.

4. **Oxygen molecule O_2** built with two oxygen atoms connected by a pair of flexible bonds. In reality, the oxygen atoms are closer to each other and the fact that double bonds are involved would not be

obvious. (That closeness could be simulated by just connecting the oxygen atoms by a single short bond and ignoring the extra holes in each atom.)

5. **Carbon dioxide molecule CO_2** built with a 4-hole carbon atom connected to two oxygen atoms by two pairs of flexible bonds. The oxygen atoms are separated by an unrealistically large distance, but the double bond is clearly shown. All holes are used.

6. **Carbon monoxide CO** built with a 4-hole carbon atom and a four-hole oxygen atom, using 3 flexible bonds. One hole in each of the atoms is not used.

7. **Ozone O_3** built with a 4-hole oxygen atom and two 2-hole oxygen atoms with the 4-hole atom in between the 2-hole atoms. One 2-hole atom is connected by a pair of flexible bonds, but the other is connected with a single long, rigid bond. The double bond rapidly switches (resonates) between the two outer atoms.

8. **Chlorine Cl_2** built with two green chlorine atoms connected by a single short or long rigid bond. (If a 6-hole green chlorine atom is used, the remaining 5 holes are not used.)

9. **Nitrogen N_2** built with two 3-hole pyramidal nitrogen atoms and connected by 3 flexible bonds. Only nitrogen-fixing bacteria are able to break this strong triple bond; animals and plants cannot.

10. **Hydrazine N_2H_4** built with a single bond connecting the two 3-hole pyramidal nitrogens and 4 hydrogen domes on the remaining holes. Hydrazine is used as a rocket fuel. It is highly toxic and dangerously unstable.

11. **Ammonia NH_3** built with a 3-hole pyramidal nitrogen atom and three hydrogen domes connected by short bonds.

12. **Phosphine PH_3** built with a 3-hole pyramidal phosphorus atom and three hydrogen domes connected by short bonds.

13. **Phosphoric acid H_3PO_4** built with a 5-hole phosphorus surrounded by four oxygen atoms, one connected by a double bond using a pair of flexible bonds and the others by single bonds using long rigid bonds. Each single-bond oxygen also is attached to a hydrogen dome using a short bond. It is called an acid because it will lose some of its hydrogens if placed in water. The oxygens with the missing hydrogens then will have a negative charge. Phosphate ions PO_4^{-3} help hold DNA together, are part of cell membranes, and are key to energy transfer in living systems.

14. **Phosgene $COCl_2$** built with a 4-hole carbon, 2-hole oxygen, and two chlorine atoms. Two flexible bonds form a double bond between the carbon and oxygen atom. The remaining holes in the carbon atom are connected by rigid single bonds to the chlorine atoms. (If a 6-hole chlorine atom is used, 5 holes will be unused.) Phosgene was the poison gas used by the Germans in WWI that killed 85,000 allied soldiers.

The following molecules belong to a chemical group called **alkanes**, all of which have names ending in -ane and which have **all single bonds** between their carbon atoms. Their general formula is C_nH_{2n+2}, starting with methane where n=1 and a formula of CH_4.

15. **Methane CH_4** built with a single 4-hole carbon and four hydrogen domes connected by short bonds.

16. **Ethane C_2H_6** built with two 4-hole carbon atoms connected together with a single bond (short or long rigid). The remaining 6 holes in the carbon atoms are connected to hydrogen domes.

17. **Propane C_3H_8** built as a chain of three 4-hole carbon atoms and 8 hydrogen domes connected to the remaining 8 holes. Note that the middle carbon can only have 2 hydrogens. Propane can be stored under pressure as a liquid at room temperature and is used for heating.

18. **Butane C_4H_{10}** is like propane, but with yet another carbon atom in the chain with two additional hydrogen domes. It is also a liquid under pressure at room temperature and used for heating.

We will later build **heptane C_7H_{16}** and **octane C_8H_{18}**, the common constituents of **gasoline**. They are also alkanes with 7 and 8 carbon atoms, respectively.

There is another chemical group called **alkenes** which are similar to the alkanes except that they contain **at least one double bond**. Their names end in **-ene** and the ones with just one double bond have the general formula C_nH_{2n}. The simplest is ethylene with n=2 which we will now build.

19. **Ethylene C_2H_4** built with two 4-hole carbon atoms connected by a pair of flexible bonds making a **double bond** between them. The remaining empty holes are connected to 4 hydrogen domes with short bonds. When all groups have made an ethylene molecule, we will connect them together to make a polymer known as **polyethylene**. Each ethylene molecule connects to the next by breaking its double bond and using the free hole for the connecting rigid bond.

There is a third chemical group, the **alkynes** that have at least one **triple bond** between two carbon atoms. The simplest example is acetylene.

20. **Acetylene C_2H_2** built with two 4-hole carbon atoms connected by three flexible bonds. The remaining holes are connected to hydrogen domes using short bonds. An oxygen-acetylene torch produces a flame that can be used to melt and weld steel.

Many molecules that involve 5- or 6-sided rings. Here are 4 examples.

21. **Cyclohexane C_6H_{12}** built with six 4-hole carbon atoms connected in a ring with rigid bonds. The remaining holes are filled with short bonds to 12 hemispherical hydrogen domes.

22. **Benzene C_6H_6** also built with six 4-hole carbon atoms connected by pairs of flexible double bonds alternating with rigid single bonds. The remaining holes are filled with short bonds to 6 hydrogen domes. In actuality, the single and double bonds "resonate" between atoms so that the effect is an average of 1-1/2 bonds between carbon atoms. This is known as an aromatic structure because often molecules with such bonding have a distinct fragrance. Benzene is a carcinogen, but before that was known it was common in chemistry labs as an "unknown" to be determined by various tests that sometimes included smell or taste.

23. **Toluene C_7H_8** is benzene with an attached methyl group ($-CH_3$) in place of one of its hydrogens. Toluene is a solvent common in paint thinners.

24. **Trinitrotoluene $C_6H_2(NO_2)_3CH_3$** is toluene with three nitro groups ($-NO_2$) in place of three of the remaining hydrogens in a symmetric manner. Each nitro group is made with a 4-hole nitrogen atom connected by a single bond to the ring, a double bond to one oxygen, and a single bond to the second oxygen. One hole on that last oxygen is empty. Unfortunately, we do not have enough 4-hole nitrogen atoms and we must pretend that a 4-hole purple atom is actually blue. Trinitrotoluene is the well-known explosive TNT.

Hydrocarbons and Combustion

Burning (oxidizing) methane to produce water and carbon dioxide

The following chemical reaction equation describes the burning of 6.022×10^{23} molecules of methane:

$$\mathbf{CH_4 + 2\,O_2 \Rightarrow 2\,H_2O + CO_2 + 0.89\,MJ}$$

This special number, 6.022×10^{23}, is called a mole and its unit is abbreviated as "mol." It is a number that we will learn later is closely connected with the masses given in the Periodic Table of Elements. The equation above states that 1 mol of methane when burned with 2 mol of oxygen molecules produces 2 mol of water, 1 mol of carbon dioxide, and gives off 0.89 MJ of heat.

Make a methane molecule and two oxygen molecules, then to simulate the burning process, rearrange their atoms to make two water molecules and one carbon dioxide molecule. You start with 1 carbon atom, 4 hydrogen atoms, and 4 oxygen atoms, and after the rearrangement, you still end up with the same number of each kind of atom. They are just with new partners. This is what a chemical reaction does. Combustion reactions like this give off heat energy, but other types of reactions might absorb heat. No atoms are destroyed or created, they are just rearranged.

The molecules on the left side are called the **reactants** and those on the right side are called the **products**, but the equation could be reversed in which case the reactants would be water and carbon dioxide. All reactions can go both ways, but many like this one need to be forced in some manner to go "backwards." Plants are able to use sunlight and very complicated mechanisms to change carbon dioxide and water into hydrocarbon molecules.

Burning gasoline to power engines

Regular gasoline is a hydrocarbon mixture of normal **heptane** $\mathbf{C_7H_{16}}$ (**n-heptane**) and a version of **octane** $\mathbf{C_8H_{18}}$ called **iso-octane** (**2,2,4-trimethylpentane**).

To build n-heptane, we connect 7 carbon atoms together in a chain using the short, clear bonds, and add hydrogen domes to all the remaining holes.

Iso-octane is more complicated. It has 8 carbon atoms, but they are not all in a zig-zag chain, but rather some are sticking out sideways. That is generally what “iso-” means in chemistry.

To build 2,2,4-trimethylpentane, we first connect 5 carbons together in a chain, add 3 hydrogen domes to each end, two in the middle, and one onto one of the 4 remaining holes of the carbons on either side of the middle carbon.

The three remaining empty holes will be connected to **methyl groups**, $\mathbf{-CH_3}$. They are like methane but with one hydrogen missing. This leaves an empty hole for bonding to another molecule.

To complete building 2,2,4-trimethylpentane, we connect the three methyl groups to the empty holes in the 5-carbon pentane chain using short, clear bonds. All its holes should now be filled.

In order to burn one mole of n-heptane molecules, 11 oxygen molecules are required. The combustion equation must deal with whole n-heptane, oxygen, water, and carbon dioxide molecules without losing any atoms. That leads to the following equation:

$$\mathbf{C_7H_{16} + 11\,O_2 \Rightarrow 8\,H_2O + 7\,CO_2 + 4.82\,MJ}$$

Unfortunately, unless we combine resources with another group's atom collection, we don't have enough oxygen. So, let's just pretend we did it with the production of 8 water molecules and 7 carbon dioxide molecules.

The equation for burning iso-octane is

$$\mathbf{2\,C_8H_{18} + 25\,O_2 \Rightarrow 18\,H_2O + 16\,CO_2 + 10.92\,MJ}$$

In order to write this equation while still using whole O_2 molecules, it was necessary to burn two iso-octane molecules.

CO_2 production comparison between methane and gasoline
Methane produced 0.89 MJ of energy per mole of CO_2 produced. The value for gasoline is smaller, about 0.69 MJ per mole of CO_2 produced. That is one reason why it is preferable to burn methane instead of gasoline. Other reasons methane is preferable have to do with reduced production of **carbon monoxide CO** and **nitrogen oxides NO** and **NO_2** as air pollution.

CO production during combustion
Carbon monoxide is produced when hydrocarbons or carbon (as charcoal) are burned without sufficient oxygen. With excess fuel and inadequate oxygen, the carbon is only partially oxidized; only one oxygen atom is combined with each carbon instead of two. Carbon monoxide is a deadly, odorless gas that combines with our blood in a manner that prevents the blood from carrying oxygen to our brain and muscles. Modern gasoline engines have oxygen sensors and computers that monitor the fuel/oxygen ratio and minimize carbon monoxide production.

CO is not very stable and therefore is a highly reactive molecule. (Generally, molecules that are highly reactive have unconventional bonding, and when building them, we need to use atoms with more or fewer than the normal number of holes.)

Production of nitrogen oxides during combustion
Air is 78% N_2 and 21% O_2, but N_2 is ordinarily not very reactive. At high temperatures such as during lightning or inside of an internal combustion engine, the available heat encourages the endothermic (head absorbing) reaction of nitrogen with oxygen to produce nitrogen oxides:

$$\mathbf{N_2 + O_2 + heat \Leftrightarrow 2\,NO} \quad \text{then} \quad \mathbf{2\,NO + O_2 + heat \Leftrightarrow 2\,NO_2}$$

Nitrogen dioxide NO_2 is a poisonous reddish gas that gives smog a reddish tinge. In general, a complicated mixture of these and other gases react with sunlight to produce **photochemical smog**.

To make nitrogen dioxide with models, we can use a **pyramidal** nitrogen atom and connect it with a double bond to one oxygen and a single bond to another. The two oxygens, however, are equivalent so the double and single bonds are said to alternate (**resonate**) between the two oxygens.

To make **nitric oxide NO** with models, we can use a pyramidal nitrogen atom and connect it with a double bond to an oxygen atom. This leaves an open bonding hole (electron) in the nitrogen which alternates (resonates) between the nitrogen and oxygen. NO can therefore be said to have 2.5 bonds between its atoms.

As with carbon monoxide, the peculiar bonding of these nitrogen oxide molecules make them highly reactive when they encounter other molecules.

Alcohols

Alcohols are made from hydrocarbons by adding one or more **hydroxyl groups, – OH**, in place of hydrogens. The hydroxyl group is made using an oxygen atom with only one hydrogen attached. The remaining bond hole in the oxygen is used to attach the hydroxyl group to a molecule.

For example, **methyl alcohol CH_3OH** (also called **methanol**) is made by replacing one hydrogen in methane by a hydroxyl group. As you do this with the model atoms, you will see that it doesn't matter which hydrogen is replaced since all hydrogens are equivalent.

Sometimes someone with little knowledge of chemistry will obtain methanol (also known as wood alcohol) and drink it. The result is that they are blinded for life! When ingested it becomes formic acid and drinking as little as 10 mL can destroy the optic nerve and 30 mL can cause death.

We can use additional hydroxyl groups to replace other hydrogen atoms in methane making the less common molecules **methanediol $CH_2(OH)_2$**, **methanetriol $CH(OH)_3$**, and **methanetetraol $C(OH)_4$**. In each case, however, it doesn't matter which hydrogens are replaced because they are all equivalent.

Ethanol alcohol C_2H_5OH (also called **ethanol**) is an alcohol made by replacing one hydrogen in ethane with a hydroxyl group. Again, it doesn't matter which hydrogen because all are equivalent. Ethanol is the alcohol produced by microbes during **fermentation** when making alcoholic drinks.

Ethylene glycol $HO(CH_2)_2OH$ or **$C_2H_6O_2$**, (**1,2-ethanediol**) is formed by replacing hydrogens on each end of an ethane molecule with hydroxyl groups. It has been used as an antifreeze and coolant fluid, but is sweet tasting and toxic. Children and pets have been poisoned by drinking it. So, under government dictate, manufactures have now added a bitter tasting molecule (**denatonium benzoate**) to ethylene glycol when sold as antifreeze and to methanol when sold as windshield washer fluid. Denatonium benzoate is also added to ethyl alcohol sold as denatured alcohol. An alternate antifreeze fluid, **propylene glycol**, with a natural bitter taste is also being used.

Binding energies do not allow the two hydroxyl groups to be added to the same carbon in ethane; they must be added at opposite ends.

Propanol CH_3-$(CH_2)_2$-OH (also called **n-propanol**, **1-propanol**) and **isopropyl alcohol** $(CH_3)_2$-CH-OH (also called **propan-2-ol**) are both alcohols of propane, but propanol has its hydroxyl group at an end and iso-propanol has it added to the middle carbon. Finally, we have met a molecule where the location for adding the hydroxyl group matters; a different chemical is formed when it is added at an end of propane (n-propanol) than when it is added in the middle (isopropyl alcohol). n-propanol has important industrial applications, but is not used at home whereas isopropyl alcohol is used as a topical antiseptic and convenient solvent for home use. It is toxic, however, if ingested.

Alcohols can be made from cyclohexane and benzene by replacing a hydrogen by a hydroxyl group. The result is **cyclohexanol $C_6H_{11}OH$** and **phenol C_6H_5OH**, respectively. Both of these are important in the manufacture of plastics, and phenol is especially import in the manufacture of many more complicate organic chemicals.

Carbohydrates

Many important molecules have chemical formulas of the form $C_m(H_2O)_n$. Where *m* and *n* are integers, and often *m*=*n*. These and some similar molecules are called **carbohydrates**. The most important types of carbohydrates are **sugars** (for short-term energy storage in plants and animals), **starches** (for long-term energy storage in plants), **glycogen** (for long-term energy storage animals), **cellulose** (for structural material in plants), and **chitin** (for exoskeletons of insects and crustaceans).

Like many molecules, sugars can be **left-** and **right-handed**. On earth, nearly all living things use right-handed sugars.

Sugars also form into loops when in water, but they can do that in two different ways, making **α-rings** and **β-rings**. Simple sugars, called **monosaccharides**, can link up to form **disaccharides** and **polysaccharides**. These will be discussed as we build some of them on pages 5 and 6 of the molecular structure diagram handout.

In the remainder of this note, all page numbers will all refer to that 11-page handout.

Lipids

Another important class of biological molecules are **lipids**, generally known as **fats**. We will make some **fatty acids** and a **triglyceride** following page 3. Lipids naturally form cell wall structures.

Amino Acids

Amino acids are the basic elements from which proteins are made following the recipes in our DNA. We will make the 21 important biological amino acids shown on the top of page 7. We will then make a famous 9-amino acid polypeptide called oxytocin shown at the bottom of page 7.

Amino acids also come in left- and right-handed versions, but on earth the left-handed form dominates.

Nucleic Acids and DNA

The 5 basic nucleic acids used to form DNA and RNA are shown on page 9 along with two layers of DNA. We will build 5 layers of DNA.

Other Interesting Molecules

Pages 4, 8, 10, and 11 contain other interesting molecules such as plastics, explosives, and hormones.