In Class#1: Lewis (Electron dot) Structures and Structural Formulas

The study of organic chemistry involves almost exclusively molecular substances, i.e., compounds in which the bonds connecting the atoms are covalent. In a covalent bond one or more electron pairs are shared by two atoms. To show covalent bonds in a molecule, begin with the electron dot structures for the individual atoms and then put all the atoms together so that each atom achieves a completely filled outer shell. Remember that a completely filled outer shell contains 8 electrons. Sometimes we call this a ‘full octet’ or the octet rule. An exception to this rule is hydrogen which contains 2 electrons.

Example: Draw a Lewis structure for water H₂O. Note that H₂O is sometimes referred to as a molecular formula. We begin with each hydrogen has 1 electron and the oxygen has 6 electrons:

\[
\begin{array}{c}
\vdots \\
\text{O} \\
\vdots \\
\text{H} \\
\text{H} \\
\end{array}
\]

In order to make a point, let’s be a little ridiculous and put two hydrogen atoms together: H:H. Now we have 2 happy hydrogen atoms (filled outer shells), but one unhappy oxygen atom and no water! Of course, the right structure is:

\[
\begin{array}{c}
\vdots \\
\text{H} \\
\vdots \\
\text{H} \\
\text{O} \\
\end{array}
\]

Since you can count the shared electrons when looking at both atoms in the bond, all three atoms now have completely filled outer shells and we have a good Lewis structure for water. Another way to represent water is to replace each shared pair with a dash. This is referred to as a structural formula:

\[
\begin{array}{c}
\text{H} \\
\text{H} \\
\text{O} \\
\end{array}
\]

It’s also acceptable to leave out the lone pair electrons in structural formulas but we will leave them in for this assignment.

Exercise 1: Draw the Lewis structure and structural formulas for (be sure to include lone pair electrons):

\[
\begin{align*}
\text{NH}_3 & \quad \text{CH}_4 \\
\text{CH}_4\text{O} & \quad \text{CH}_5\text{N}
\end{align*}
\]
Lewis structures are not used that often in organic chemistry, but structural formulas are very important. Fortunately, there is an easy way to draw structural formulas without first drawing a Lewis structure. Most of the elements in organic compounds consistently form the same number of bonds in neutral compounds. The following table gives the normal number of bonds for some of the most common elements found in organic compounds:

<table>
<thead>
<tr>
<th>Element</th>
<th>No. of covalent bonds</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>1</td>
</tr>
<tr>
<td>C</td>
<td>4</td>
</tr>
<tr>
<td>N</td>
<td>3</td>
</tr>
<tr>
<td>O</td>
<td>2</td>
</tr>
<tr>
<td>Cl, F, Br, I</td>
<td>1</td>
</tr>
</tbody>
</table>

**Exercise 2:** Using the table draw structural formulas for the following compounds (be sure to include lone pair electrons):

- CH₃Cl
- C₂H₆
- C₃H₈
- C₂H₇N

So far all of the covalent bonds have been single bonds. As you probably remember, we can also have double and triple covalent bonds. For example, draw the Lewis structure for an oxygen molecule, O₂.

The two oxygen atoms can form one covalent bond as follows:

\[
\text{O}::\text{O}^\cdot + \cdot\text{O}: \rightarrow \cdot\text{O}: \cdot\text{O}::
\]

However, each atom now has only 7 electrons in the outer shell. So, another pair must be shared:
Now each oxygen atom has 8 electrons in the outer shell. This is known as a double bond, consisting of two shared pairs of electrons. The structural formula looks like this:

\[ \ddot{O} = \ddot{O} \]

Note that this structure is consistent with our table for the normal number of covalent bonds for oxygen. We can use the same table for drawing structural formulas for compounds that have double and triple bonds.

**Exercise 3:** Draw structural formulas for the following (be sure to include lone pair electrons):

\[ \text{N}_2 \quad \text{C}_2\text{H}_4 \]

\[ \text{C}_2\text{H}_2 \]

**Part 2: Shapes of organic molecules using molecular models**

Now let's extend our study of organic molecular structures to the use of molecular models. The following table gives the color of the balls corresponding to each element. You might want to check to see that the number of holes in each colored ball corresponds to the number of bonds that each of the elements normally forms.

<table>
<thead>
<tr>
<th>Element</th>
<th>Color</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>white</td>
</tr>
<tr>
<td>C</td>
<td>black</td>
</tr>
<tr>
<td>N</td>
<td>blue</td>
</tr>
<tr>
<td>O</td>
<td>red</td>
</tr>
<tr>
<td>Cl</td>
<td>green</td>
</tr>
<tr>
<td>Br</td>
<td>orange</td>
</tr>
<tr>
<td>I</td>
<td>purple</td>
</tr>
</tbody>
</table>

**Exercise 4:** Make a model of a hydrogen molecule $\text{H}_2$. (Use the shorter gray bonds for single bonds.)

Now draw the structural formula for $\text{H}_2$. 
Does the structural formula look similar to the model?

**Exercise 5:** Make a model of methane, CH₄.

Now draw the structural formula. Does it look the same as the model?

Most likely you answered no. (It’s OK if you said yes) Methane is not a flat molecule, as the structural formula seems to indicate. The structural formulas we have been drawing usually do not accurately represent the actual three-dimensional shape of the molecules. This is OK as long as we are aware of this limitation.

The Geometry of the carbon atom in methane is considered ‘Tetrahedral’. Speculate on why in reality, methane is tetrahedral as opposed to a ‘flat’ molecule.

**Exercise 6:** Make a model of methanol, CH₃OH. Draw the structural formula for methanol. Do they look identical?

**Note:** We could have written the molecular formula for methanol as CH₄O. Writing it as CH₃OH makes it more clear what the actual bonding is. So, often molecular formulas will be written in a more clear way like this.

**Exercise 7:** Make a model of propane, C₃H₈. Then draw the structural formula.

**Exercise 8:** Make a model ethylene, C₂H₄. Here you will need to use the longer, more flexible gray bonds for the double bond. Ask for help if you’re not sure how to do this. Then draw the structural formula.

What would you consider the geometry of the carbon atoms are in ethylene as Flat or tetrahedral?
Part 3: Isomers & Conformations

Exercise 9: Make a model of C$_2$H$_6$O. Now make another one that is different from the first one! Draw the structural formulas for each.

These two structures are examples of isomers, compounds with the same molecular formula but different structures. More specifically, the two different C$_2$H$_6$O compounds are structural (or constitutional) isomers – compounds with the same molecular formula but with different connections among their constituent atoms. There is an easy way to tell if two structures are structural isomers. If you must break and make new bonds in order to convert one structure into the other, than they are isomers. The concept of isomers is very important in organic chemistry and biochemistry.

Exercise 10: Take one of the models of C$_2$H$_6$O. Are there any ways that you can change its shape without breaking any bonds? Hopefully you said yes! In most molecules, you can rotate the atoms about many of the single bonds. When you do this, you are usually changing the shape of the molecule. These different shapes are referred to as different conformations of the compound. However, different conformations do not represent different compounds. A conformation is analogous to a human taking on different yoga poses; still the same person (2 legs, 2 arms connected in the same way) but is changing positions.

Exercise 11: Draw structural formulas for all of the structural isomers of C$_4$H$_{10}$. (Hint: There are two. You may find it helpful to build models to solve this exercise.)
**Exercise 12:** Draw structural formulas for all of the structural isomers of C$_5$H$_{12}$. (Hint: There are three.)

**Exercise 13:** Draw structural formulas for all of the structural isomers of C$_3$H$_7$Cl.

**Exercise 14:** Draw structural formulas for all of the isomers of C$_4$H$_8$. (Hint: There are six. Using models can be very helpful with this one.)