EXPERIMENT 1: Survival Organic Chemistry: Molecular Models

Introduction:

The goal in this laboratory experience is for you to easily and quickly move between empirical formulas, molecular formulas, condensed formulas, Lewis structural formulas and three dimensional models of relatively simple organic compounds. To accomplish this you will use your experience and chemical intuition combined with molecular models and computer graphics in a guided laboratory exploration into the 3-dimensional structure of organic compounds.

So what, why should we spend time doing this??? Many new chemistry students find manipulating molecular models helps their understanding of the spatial relationships of atoms in molecules. Using computer graphics will also provide a new way to view and manipulate molecular models. Finally, a simple understanding of organic compounds early in the semester will provide you with structural insights which will help you better understand many of our chemical discussions in the area of chemical kinetics and acid/base chemistry.

If you go to the Assignment Page on your Personal page to the Laboratory information there are several links which will add value to your study of this material and help you answer some of the questions. Unfortunately, a plug-in is required to view some of the neater graphics at these sites. But there is still information there that can be used without using the plug-in.
Experiment #1: Pre-Laboratory Questions (Note: These questions must be completed and turned in prior to beginning this laboratory.)

Important concepts to remember: Electron configuration, octet rule, valence electrons, simple Lewis structures, covalent bond, ionic bond, polar covalent bonds, sigma and pi bonds, single, double and triple bonds, bond lengths and angles, resonance, and bond dissociation energies. Your textbook will play an important role as a reference tool in this laboratory.

Chapters and sections which will be important to refer to include:
- Chapter 15, sections 15.1 - 15.4
- Chapter 9, sections 9.1 - 9.5
- Chapter 10, sections 10.1 – 10.3
- Chapter 11, sections 10.1 – 10.2

1. Draw a Lewis electron-dot structure for each of the covalent molecules below. Include all resonance structures if they are needed to adequately represent the bonding in the molecule. Identify those compounds containing double and triple bonds. Indicate whether the compound is polar or nonpolar. In each compound indicate the magnitude of all bond angles.

<table>
<thead>
<tr>
<th></th>
<th>H₂O₂</th>
<th>CO₂</th>
<th>CO</th>
</tr>
</thead>
<tbody>
<tr>
<td>Polar</td>
<td>Yes</td>
<td>No</td>
<td>Yes</td>
</tr>
<tr>
<td>Bond Angle</td>
<td>_____</td>
<td>_____</td>
<td>_____</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>O₂</th>
<th>CH₃Cl</th>
<th>C₂H₄Cl₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>Polar</td>
<td>Yes</td>
<td>No</td>
<td>Yes</td>
</tr>
<tr>
<td>Bond Angle</td>
<td>_____</td>
<td>_____</td>
<td>_____</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>H₂CO₃</th>
<th>N₂O₅</th>
<th>BrF₃</th>
</tr>
</thead>
<tbody>
<tr>
<td>Polar</td>
<td>Yes</td>
<td>No</td>
<td>Yes</td>
</tr>
<tr>
<td>Bond Angle</td>
<td>_____</td>
<td>_____</td>
<td>_____</td>
</tr>
</tbody>
</table>
Experiment #1

2. Which of the following formulas describe ionic and/or covalent compounds?

NaCl, CO₂, CaCl₂, HCl, CH₃Br, BeCl₂, NH₄NO₃, Ba(NO₃)₂

Write a general rule for determining whether a chemical formula represents an ionic or a covalent compound.

3. Determine the empirical and molecular formula and draw the Lewis structure for a compound which is 17.34% H and 82.66% C. (NOTE: Even though I've not given you a molar mass of the unknown compound, I expect you to use your chemical intuition, (knowledge of Lewis structures) to determine the molecular formula.)
Procedure:

CHECKOUT:
Organic Model Kit

**Exploring structural features of simple organic compounds**

The goal of this part of the experiment is to get you to feel comfortable with moving between molecular formulas, Lewis structural formulas, and condensed formulas. To reach a reasonable level of comfort you will need to checkout a model kit from the freshman chemistry storeroom. Each kit should contain:

<table>
<thead>
<tr>
<th>Number</th>
<th>Color</th>
<th>Atom</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>black</td>
<td>carbon</td>
</tr>
<tr>
<td>6</td>
<td>green</td>
<td>chlorine</td>
</tr>
<tr>
<td>6</td>
<td>red</td>
<td>oxygen</td>
</tr>
<tr>
<td>2</td>
<td>blue</td>
<td>nitrogen</td>
</tr>
<tr>
<td>1</td>
<td>yellow</td>
<td>sulfur</td>
</tr>
<tr>
<td>22</td>
<td>white</td>
<td>hydrogen</td>
</tr>
</tbody>
</table>

Each packet should also contain 30 1-inch plastic connectors that represent a pair of electrons, either a lone pair or a bonding pair.

**PART I. Alkanes**

The hydrocarbon compounds with the following molecular formulas are all classified as alkanes.

CH$_4$, C$_2$H$_6$, C$_3$H$_8$, C$_4$H$_{10}$, C$_5$H$_{12}$, C$_6$H$_{14}$, C$_7$H$_{16}$, C$_8$H$_{18}$, C$_9$H$_{20}$, C$_{10}$H$_{22}$

Your TA will assign you three of the alkanes above. Your assigned alkanes are;

_____________      _____________      _____________

Write the Lewis structure, condensed structural formulas and name for each of the alkanes assigned to you.

<table>
<thead>
<tr>
<th>Condensed structural formula:</th>
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</table>

<table>
<thead>
<tr>
<th>Lewis structure:</th>
<th></th>
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</table>

Use the molecular model kit to construct several examples of alkane compounds.
Questions (use your textbook as a reference):

1. What is the general formula for an alkane?

2. What is a structural isomer? How many do each of the first seven alkanes have? Draw all of the structural (constitutional) isomers for one of the alkanes and name each isomer (your TA will tell you which one.)

   assigned alkane ____________

3. List some common physical properties of alkanes. What are some trends?

4. What is a cycloalkane? Give some examples. What is different and what is similar about the structure of a cycloalkane and an alkane with the same number of carbon atoms?
5. What are two reactions common to alkanes? (Write chemical equations to describe the reactions.)

6. What is a conformer (e.g., eclipsed, staggered and skewed)?

7. Are alkanes soluble or insoluble in water? Support your answer with a brief explanation.
PART II. Alkenes

The hydrocarbon compounds with the following molecular formulas are all classified as alkenes.

\[ \text{C}_2\text{H}_4, \text{C}_3\text{H}_6, \text{C}_4\text{H}_8, \text{C}_5\text{H}_{10}, \text{C}_6\text{H}_{12}, \text{C}_7\text{H}_{14}, \text{C}_8\text{H}_{16}, \text{C}_9\text{H}_{18}, \text{C}_{10}\text{H}_{20} \]

Your TA will assign you three of the alkenes above. Your assigned alkenes are;

_____________      _____________      _____________

Write the Lewis structure, condensed structural formulas and name for each of the alkenes assigned to you.

<table>
<thead>
<tr>
<th>Condensed structural formula:</th>
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</thead>
<tbody>
<tr>
<td>Lewis structure:</td>
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</table>

Use the molecular model kit to construct several examples of alkene compounds. Describe what you notice to be different about the structures of alkenes compared to alkanes?
Questions (use your textbook as a reference):

1. What is the general formula for an alkene?

2. What is a geometric isomer? How many do each of the first three alkenes have? Draw the Lewis structure for all of the geometric isomers for the first three alkenes and name each one.

3. List some common physical properties of alkenes. What are some trends?

4. What is a diene? Give some examples.
5. What are two reactions common to alkenes? (Write chemical equations to describe the reactions.)

PART III. Alkynes

The hydrocarbon compounds with the following molecular formulas are all classified as alkenes.

\[ \text{C}_2\text{H}_2, \text{C}_3\text{H}_4, \text{C}_4\text{H}_6, \text{C}_5\text{H}_8, \text{C}_6\text{H}_{10}, \text{C}_7\text{H}_{12}, \text{C}_8\text{H}_{14}, \text{C}_9\text{H}_{16}, \text{C}_{10}\text{H}_{18} \]

Your TA will assign you three of the alkynes above. Your assigned alkynes are;

\[ \underline{\text{Alkynes assigned to you:}} \]

Write the Lewis structure, condensed structural formulas and name for each of the alkynes assigned to you.

<table>
<thead>
<tr>
<th>Condensed structural formula:</th>
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<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Lewis structure:</td>
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</table>

Use the molecular model kit to construct several examples of alkynes compounds. Describe what you notice to be different in the structures of alkynes compared to alkenes?
Questions:

1. What is the general formula for an alkyne?

2. Draw all of the structural isomers for one of the alkynes and name each isomer (your TA will tell you which one.)
   assigned alkyne ____________

PART IV. Aromatics

The hydrocarbon compound with the following molecular formula is classified as an aromatic.

\[ \text{C}_6\text{H}_6 \]

Use the molecular model kit to construct benzene. Draw the Lewis structure and condensed structural formulas for benzene. Describe the molecular geometry of benzene.
PART V. Alcohols

The compounds with the following molecular formulas are all classified as alcohols.

\[ \text{CH}_3\text{OH}, \text{C}_2\text{H}_5\text{OH}, \text{C}_3\text{H}_7\text{OH}, \text{C}_4\text{H}_9\text{OH} \]

Write the Lewis structure, condensed structural formulas and name for each of the alcohols.

<table>
<thead>
<tr>
<th>Condensed structural formula:</th>
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<tbody>
<tr>
<td>Lewis structure:</td>
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</table>

Use the molecular model kit to construct several examples of alcohol compounds.

Questions (use your textbook as a reference):

1. What is a primary, secondary and tertiary alcohol?

2. Are alcohols soluble or insoluble in water? Support your answer with a brief explanation.

3. What is an ether? How does an ether structurally differ from an alcohol?
PART VI. Carboxylic acids

The compounds with the following molecular formulas are all classified as carboxylic acids.

\[
\text{HCOOH, CH}_3\text{COOH, C}_2\text{H}_5\text{COOH, C}_3\text{H}_7\text{COOH}
\]

Write the Lewis structure, condensed structural formulas and name for each of the carboxylic acids.

<table>
<thead>
<tr>
<th>Condensed structural formula:</th>
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<tbody>
<tr>
<td>Lewis structure:</td>
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</table>

Use the molecular model kit to construct several examples of carboxylic acids.

Questions (use your textbook as a reference):

1. What is the important functional group in the carboxylic acids?

2. Are carboxylic acids soluble or insoluble in water? Support your answer with a brief explanation.

3. What is an ester? How does an ester structurally differ from a carboxylic acid?
PART VII. Amines

The compounds with the following molecular formulas are all classified as amines.

\[ \text{CH}_3\text{NH}_2, (\text{CH}_3)_2\text{NH}, (\text{CH}_3)_3\text{N}, \text{C}_2\text{H}_5\text{NH}_2 \]

Write the Lewis structure, condensed structural formulas and name for each of the amines.

<table>
<thead>
<tr>
<th>Condensed structural formula:</th>
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<tbody>
<tr>
<td>Lewis structure:</td>
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Use the molecular model kit to construct several examples of amines.

Questions (use your textbook as a reference):

1. What is the important functional group in the amines?

2. What is a primary, secondary and tertiary amine?

3. What are amines derivatives of?

4. Are amines soluble or insoluble in water? Support your answer with a brief explanation.