Hands-on Modeling of Molecular Structure and Chemical Bonding

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1. Overview
This unit is consists of mostly on hands-on experiences in which students learn the basics of molecular structure and chemical bonding using ball-and-stick molecular modeling kits and molecular modeling software.

2. Objectives
1. Build molecules with single, double and triple bonds.
2. Relate how valence electrons of atoms affect the molecular structure of compounds.
3. Learn concept of computer modeling of molecular structure and chemical bonding.

3. Key Concepts
Valence of Atom, Molecule, Carbon Chemistry, Chemical Bond, Chemical Group

4. Subjects
Chemistry, Computer Applications

5. Duration
2 class periods (40-50 minutes)

6. Setting
Classroom equipped with computers and internet access to download Avogadro program

7. Introduction
The most fundamental concept in chemistry is chemical bonding – the way atoms interact to form various chemical compounds. The beginning of 21st century is marked by the significant progress in computer based modeling of chemical reactions and larger scale processes. The current project serves as an introduction for students to computer based molecular design. Exploring virtual (computer based) and hands-on (molecular modeling kits) modeling of molecules, students will learn the fundamental concepts and practical application of molecular modeling. At first, the students will work in small groups to create virtual molecules using molecular modeling software. They will start from creating an arbitrary set of organic atoms (C, H, N, O) in the Avogadro program. Then, using the program they will compute the stable structures, corresponding to a given set of atoms, and come up with the computationally predicted molecular structures. Using these structures students will be able to identify molecular formulas of the compounds, types of chemical bonds found in the structure and important structurally-dependent chemical properties. They will learn the concept of bond order and determine the similarities and differences between saturated and unsaturated chemical bonds. The culminating activity includes construction of computationally predicted molecules using a molecular model kit. Finally, the students will discuss the properties of created models recognizing specific functional groups, such as methyl groups and ring structures. The students will learn the properties and common uses of some organic compounds they created, as well as learn basics of computer based molecular design, chemical structure and bonding.

8. Indiana State Science Standards Met

The Nature of Science and Technology

8.1 Students design and carry out increasingly sophisticated investigations. They understand the reason for isolating and controlling variables in an investigation. They realize that scientific knowledge is subject to change as new evidence arises. They examine issues in the design and use of technology, including constraints, safeguards, and trade-offs.
8.1.1 Recognize that and describe how scientific knowledge is subject to modification as new information challenges prevailing theories and as a new theory leads to looking at old observations in a new way. (Core Standard)
8.1.3 Recognize and describe that if more than one variable changes at the same time in an experiment, the outcome of the experiment may not be attributable to any one of the variables. (Core Standard)
8.1.8 Explain that humans help shape the future by generating knowledge, developing new technologies, and communicating ideas to others. (Core Standard)

Scientific Thinking

8.2 Students use computers to organize and compare information. They perform calculations and determine the appropriate units for the answers. They weigh the evidence for or against an argument, as well as the logic of the conclusions.
8.2.4 Use technological devices, such as calculators and computers, to perform calculations.
8.2.5 Use computers to store and retrieve information in topical, alphabetical, numerical, and keyword files and create simple files of students' own devising.
8.2.7 Participate in group discussions on scientific topics by restating or summarizing accurately what others have said, asking for clarification or elaboration, and expressing alternative positions. (Core Standard)

The Physical Setting

8.3 Students collect and organize data to identify relationships between physical objects, events, and processes. They use logical reasoning to question their own ideas as new information challenges their conceptions of the natural world.
8.3.8 Explain that all matter is made up of atoms which are far too small to see directly through an optical microscope. Understand that the atoms of any element are similar but are different from atoms of other elements. Further understand that atoms may stick together in well-defined molecules or may be packed together in large arrays. Also understand that different arrangements of atoms into groups comprise all substances. (Core Standard)
8.3.9 Demonstrate, using drawings and models, the movement of atoms in a solid, liquid, and gaseous state. Explain that atoms and molecules are perpetually in motion. (Core Standard)
8.3.11 Describe how groups of elements can be classified based on similar properties, including highly reactive metals, less reactive metals, highly reactive non-metals, less reactive non-metals, and some almost completely non-reactive gases. (Core Standard)
8.3.15 Identify different forms of energy that exist in nature. (Core Standard)

The Mathematical World

8.5 Students apply mathematics in scientific contexts. Students use mathematical ideas, such as symbols, geometrical relationships, and the use of key words and rules in logical reasoning, in the representation and synthesis of data.
8.5.3 Demonstrate that mathematical statements can be used to describe how one quantity changes when another changes.

Common Themes
8.7 Students analyze the parts and interactions of systems to understand internal and external relationships. They investigate rates of change, cyclic changes, and changes that counterbalance one another. They use mental and physical models to reflect upon and interpret the limitations of such models.
8.7.1 Explain that a system usually has some properties that are different from those of its parts but appear because of the interaction of those parts.
8.7.2 Explain that even in some very simple systems, it may not always be possible to predict accurately the result of changing some part or connection.
8.7.3 Use technology to assist in graphing and with simulations that compute and display results of changing factors in models.
8.7.4 Explain that as the complexity of any system increases, gaining an understanding of it depends on summaries, such as averages and ranges, and on descriptions of typical examples of that system.
8.7.6 Recognize that and describe how symmetry may determine properties of many objects, such as molecules, crystals, organisms, and designed structures.

9. Materials

- Gumdrops and toothpicks OR Student Molecular Modeling Kit, Arbor Scientific: http://www.amazon.com/Student-Molecular-Modeling-Kit/dp/B000701AWK
- Molecular Modeling Software–Avogadro 1.0 free download from: http://avogadro.openmolecules.net/wiki/Get_Avogadro

10. Preparation

This activity will require installation of Avogadro 1.0 program on the computers and teaching students about carbon bonding. A full list of structures used in this lesson can be found in Appendix A.

11. Activities

11.1 Explore Concept of Covalent Bonding

Procedures:

1. Using electron dot diagrams students will predict molecular structures for covalently bonded molecules including hydrocarbons.
2. Students will note that two electrons compose a single bond, four electrons compose a double bond, and six electrons compose a triple bond.
3. When given a molecular formula, students will draw the corresponding structural formula and vice versa.

Questions:

1. Using the structural formula of a hydrocarbon such as methane, identify how many electrons (and bonds) are shared by each hydrogen atom and each carbon atom.
2. Explain the differences in electron configuration and bonding between an alkane, an alkene, and an alkyne.

11.2 Explore Molecular Structure Using Molecular Modeling Kit

Procedures:

1. Using provided pictures with chemical formulas (See Appendix A,B), students will identify atoms, chemical bonds and groups.
2. Using molecular modeling kit and structural formula provided, students will build plastic 3D models of the molecules.

3. Observing and comparing structures built, students will note graphical representations of the molecules with their 3D plastic models.
4. Using Avogadro 1.0 software, students will draw molecules and manipulate them to observe behavior and energy.

Questions:

1. Using a picture of a structural formula of the molecule, identify which chemical elements it contains.
3. Using a picture of a structural formula, determine how many chemical bonds atoms of carbon, nitrogen, oxygen and hydrogen can form in given molecules.
4. Using a picture of a structural formula, identify rings (cycles) in the molecules. What types of chemical bonds can you find in these rings?
5. Using a 3-D model of a molecule, describe what type of bond (single, double, or triple) is more flexible.
6. Is it possible to rotate a part of the molecule (chemical group) around a single bond, double or triple bond?
7. Is C_6H_6 (benzene) ring rigid or flexible?
8. What you can conclude about stability of benzene molecule based on your observations?

11.3 Explore Molecular Structure Using Molecular Modeling Software

Procedures:

1. Using 3D plastic models from the previous section now build these molecules using Avogadro computer program.
2. Find optimal structure of the molecule using "Optimization Tool" of the Avogadro program.
3. Explore computer model of the molecule using "ball-and-stick" and "space fill" visualization modes
4. Observe how the addition or removal of atoms affects the molecular structures. Use the "Optimization Tool" to predict the shape of the molecule.

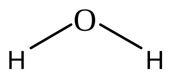
Questions:

1. Using "space fill" visualization mode what can you conclude about the sizes of carbon and hydrogen atoms?
2. Is your plastic 3D model of a molecule different from its computer representation?
3. Is the structure obtained after computer optimization different from your initial guess and your 3D plastic model? What differences can you see?
4. What happens if you remove a hydrogen atom from the molecule?
5. What happens if you add a hydrogen atom to the molecule with a double or triple bond?
6. What happens if you remove a carbon atom from the molecule?
7. How do the molecules respond to deformations (stretching, rotating, etc.) in their structures?
8. Compare the flexibility and rigidity of different types of molecules.
9. What are the advantages and disadvantages of computer modeling of molecules?

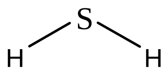
12. Appendices

Appendix A: Molecular Structures Used in the Lesson
Appendix B: Gumdrop Compounds Lesson
Appendix C: Optimizing Chemical Structures, Day #1
Appendix D: Optimizing Chemical Structures, Day #2
Appendix E: Avogadro Program Tutorial
Appendix F: Pre/Post Instructional Survey

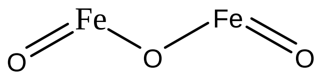
Appendix A: Molecular Structures Used in the Lesson



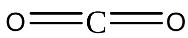
Water



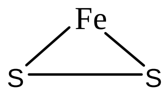
Hydrogen sulfide



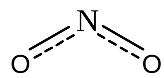
Iron(iii) oxide



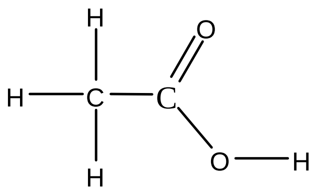
Carbon dioxide



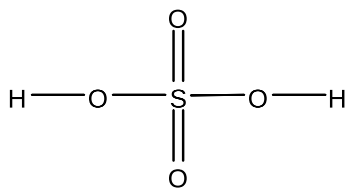
Iron sulfide



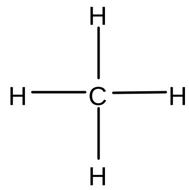
Nitrogen dioxide



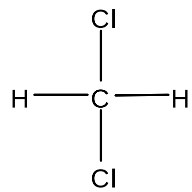
Acetic acid



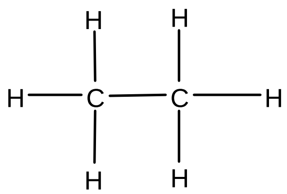
Sulfuric acid



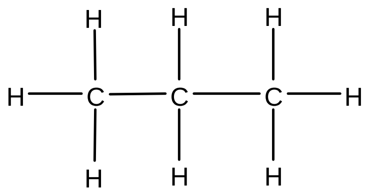
Methane



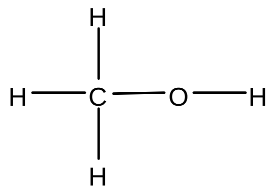
Dichloromethane



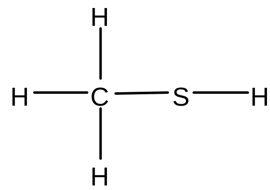
Ethane



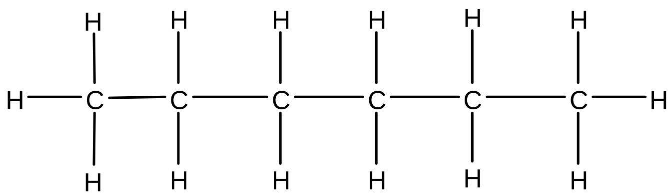
Propane



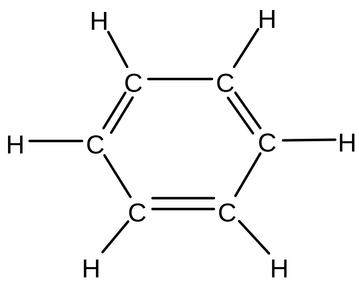
Methanol



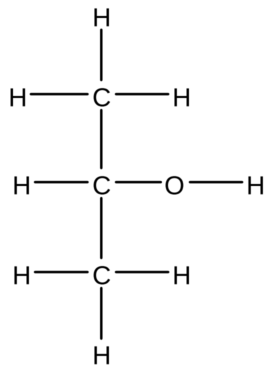
Thiomethanol



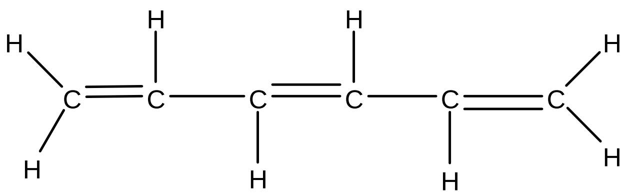
Hexane



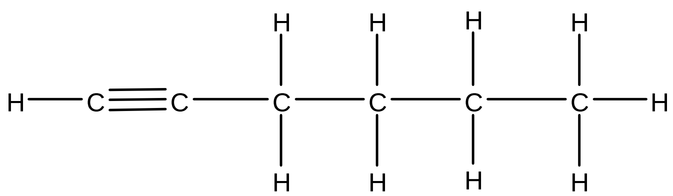
1,3,5-Cyclohexatriene
(Benzene)



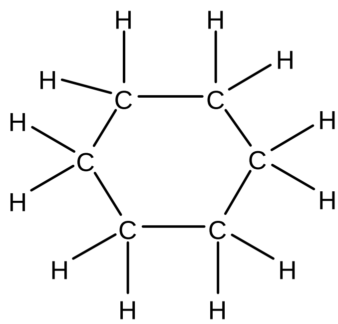
Isopropyl alcohol



1,3,5-Hexatriene



1-Hexyne



Cyclohexane

Appendix B: Gumdrop Compounds Lesson

GUMDROP COMPOUNDS Name ______________________

RED= ______ PURPLE=__________ ORANGE=_________ BLACK= ______
GREEN= ___ WHITE= _________ YELLOW= _________

READ the following FORMULAS, make the MODEL, then DRAW it.

FORMULA	DRAWING
H_2O Water	
H_2S Hydrogen sulfide (smells like rotten eggs)	
Fe_2O_3 Iron(iii) oxide (rust)	
CO_2 Carbon dioxide	
FeS_2 Iron sulfide	

(fool's gold)	
FORMULA	DRAWING
$C_2H_4O_2$ Acetic acid (vinegar)	
CH_4 Methane (natural gas)	
C_3H_8 Propane (gas for central heating)	
H_2SO_4 Sulfuric acid (battery acid)	
NO_2 Nitrogen dioxide (reddish-brown toxic gas)	
C_3H_7OH Isopropyl alcohol (rubbing alcohol)	

Appendix C: Optimizing Chemical Structures, Day #1

Optimizing Organic Compounds **Name___________________________**
Molecule #1: Ethane

Directions	Work Space
Step 1: Molecular Formula C_2H_6	What atoms are in this molecule? How many of each type of atom?
Step 2: Draw the Structural Formula of C_2H_6 in this box.	What do you notice about the bonds between the atoms?
Step 3: Build the molecule using your modeling kit Draw the molecule you built using black circles for carbon and white circles for hydrogen in this box.	How is the molecule you built similar to the molecule you drew? How is the molecule you built different than the molecule you drew?
Step 4: Draw the molecule on the computer. This is your prediction of what the molecule looks like and behaves in the real world.	What do you notice about your drawing compared to the molecule you built?
Step 5: Optimize the molecule you drew on the computer. This is what the molecule looks like and how it can behave in the real world.	What do you notice about your drawing before you optimized it on the computer and after you optimized it on the computer? How close was your predicted drawing with the actual drawing? What is the energy of the optimized molecule? ______
Step 6: Play around with your molecule…	Is it possible to rotate one carbon group? ____ What do you notice? Stretch out the two carbon atoms. Click on the bond between the two carbon atoms. What happens to the structure? Is it possible to rotate the carbon group now? ____

	What do you notice?

Molecule #2: Hexane

Directions	Work Space
Step 1: Molecular Formula C_6H_{14}	What atoms are in this molecule? How many of each type of atom?
Step 2: Draw the Structural Formula of C_6H_{14} in this box.	What do you notice about the bonds between the atoms?
Step 3: Build the molecule using your modeling kit Draw the molecule you built using black circles for carbon and white circles for hydrogen in this box.	How is the molecule you built similar to the molecule you drew? How is the molecule you built different than the molecule you drew?
Step 4: Draw the molecule on the computer. This is your prediction of what the molecule looks like and behaves in the real world.	What do you notice about your drawing compared to the molecule you built?
Step 5: Optimize the molecule you drew on the computer. This is what the molecule looks like and how it can behave in the real world.	What do you notice about your drawing before you optimized it on the computer and after you optimized it on the computer? How close was your predicted drawing with the actual drawing? What is the energy of the optimized molecule? ______
Step 6: Play around with your molecule… Do you notice anything about the energy of the molecule as you move it around?	Is it possible to rotate one carbon group? _____ What do you notice? Stretch out the two carbon atoms. Click on the bond between the two carbon atoms. What happens to the structure? Is it possible to rotate the carbon group now? _____ What do you notice?

Molecule #3: Cyclohexane

Directions	Work Space
Step 1: Molecular Formula C_6H_{12}	What atoms are in this molecule? How many of each type of atom?
Step 2: Draw the Structural Formula of C_6H_{12} in this box. Remember the carbons are in a ring.	What do you notice about the bonds between the atoms?
Step 3: Build the molecule using your modeling kit Draw the molecule you built using black circles for carbon and white circles for hydrogen in this box.	How is the molecule you built similar to the molecule you drew? How is the molecule you built different than the molecule you drew?
Step 4: Draw the molecule on the computer. This is your prediction of what the molecule looks like and behaves in the real world.	What do you notice about your drawing compared to the molecule you built?
Step 5: Optimize the molecule you drew on the computer. This is what the molecule looks like and how it can behave in the real world.	What do you notice about your drawing before you optimized it on the computer and after you optimized it on the computer? How close was your predicted drawing with the actual drawing? What is the energy of the optimized molecule? ______
Step 6: Play around with your molecule… Do you notice anything about the energy of the molecule as you move it around?	Is it possible to rotate one carbon group? _____ What do you notice? Stretch out the two carbon atoms. Click on the bond between the two carbon atoms. What happens to the structure? Is it possible to rotate the carbon group now? _____ What do you notice?

Molecule #4 1,3,5-Hexatriene (3 double bonds on alternating carbons)

Directions	Work Space
Step 1: Molecular Formula C_6H_8	What atoms are in this molecule? How many of each type of atom?
Step 2: Draw the Structural Formula of C_6H_8 in this box.	What do you notice about the bonds between the atoms?
Step 3: Build the molecule using your modeling kit Draw the molecule you built using black circles for carbon and white circles for hydrogen in this box.	How is the molecule you built similar to the molecule you drew? How is the molecule you built different than the molecule you drew?
Step 4: Draw the molecule on the computer. This is your prediction of what the molecule looks like and behaves in the real world.	What do you notice about your drawing compared to the molecule you built?
Step 5: Optimize the molecule you drew on the computer. This is what the molecule looks like and how it can behave in the real world.	What do you notice about your drawing before you optimized it on the computer and after you optimized it on the computer? How close was your predicted drawing with the actual drawing? What is the energy of the optimized molecule? ______
Step 6: Play around with your molecule… Do you notice anything about the energy of the molecule as you move it around?	Is it possible to rotate one carbon group? _____ What do you notice? Stretch out the two carbon atoms. Click on the bond between the two carbon atoms. What happens to the structure? Is it possible to rotate the carbon group now? _____ What do you notice?

Molecule #5 1,3,5-cyclohexatriene aka **Benzene** (6 carbon ring, 3 double bonds on alternating carbons)

Directions	Work Space
Step 1: Molecular Formula C_6H_6	What atoms are in this molecule? How many of each type of atom?
Step 2: Draw the Structural Formula of C_6H_6 in this box.	What do you notice about the bonds between the atoms?
Step 3: Build the molecule using your modeling kit Draw the molecule you built using black circles for carbon and white circles for hydrogen in this box.	How is the molecule you built similar to the molecule you drew? How is the molecule you built different than the molecule you drew?
Step 4: Draw the molecule on the computer. This is your prediction of what the molecule looks like and behaves in the real world.	What do you notice about your drawing compared to the molecule you built?
Step 5: Optimize the molecule you drew on the computer. This is what the molecule looks like and how it can behave in the real world.	What do you notice about your drawing before you optimized it on the computer and after you optimized it on the computer? How close was your predicted drawing with the actual drawing? What is the energy of the optimized molecule? ______
Step 6: Play around with your molecule… Do you notice anything about the energy of the molecule as you move it around?	Is it possible to rotate one carbon group? ____ What do you notice? Stretch out the two carbon atoms. Click on the bond between the two carbon atoms. What happens to the structure? Is it possible to rotate the carbon group now? ____ What do you notice?

Questions

1. How do the double bonds affect the flexibility of the molecules? Think about the 6 carbon straight chain with only single bonds (hexane) compared with the six carbon straight chain with three double bonds (1,3,5-Hexatriene).

2. The more covalent bonds a structure has, the more energy is it has. When these bonds are broken, energy is released.

   A carbon-hydrogen bond has 414 kJ/mole of energy.
   A carbon-carbon single bond has 347 kJ/mole of energy.
   A carbon-carbon double bond has 620 kJ/mole of energy.
   A carbon-carbon triple bond has 812 kJ/mole of energy.

   Which molecule would make a better fuel (release more energy when burned) hexane, 1,3,5-hexatriene, or 1-Hexyne? Calculate the energy of the three molecules using the information about bond energies above.

Energy of hexane:

Energy of 1,3,5-hexatriene:

Energy of 1-Hexyne:

3. If a compound has 6 carbons many different types of molecules can be built. Use the space below to sketch out some of the possible structural formulas.

4. Based on your drawings above, what does the possibility of drawing so many different types of compounds with six carbons tell you about the ubiquitous nature of carbon in living things?

Appendix D: Optimizing Chemical Structures, Day #2

Optimizing Organic Compounds **Name___________________________**

Molecule #1: Methane to Dichloromethane

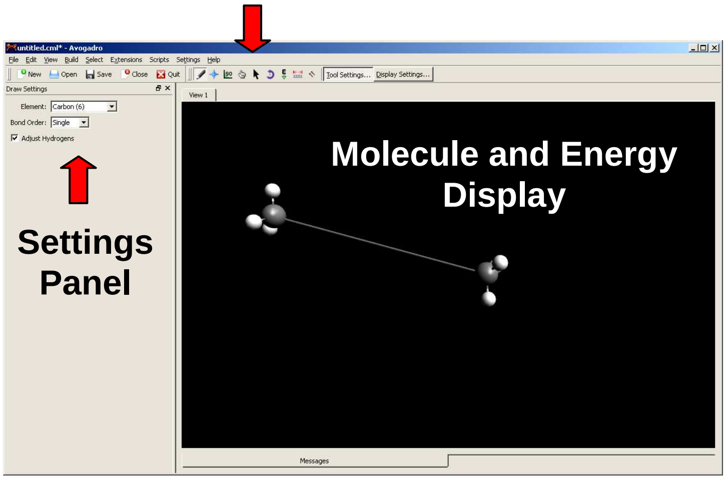
Directions	Work Space
Step 1: Molecular Formula CH_4	What atoms are in this molecule? How many of each type of atom?
Step 2: Draw the Structural Formula of CH_4 in this box.	What do you notice about the bonds between the atoms?
Step 3: Build the molecule using your modeling kit Draw the molecule you built using black circles for carbon and white circles for hydrogen in this box.	Substitute two chlorine atoms (green) for two hydrogen atoms. Draw the molecule using the correct color for chlorine. What is the formula for the new structure?
Step 4: Draw the molecule on the computer. This is your prediction of what the molecule looks like and behaves in the real world.	What do you notice about your drawing compared to the molecule you built?
Step 5: Optimize the molecule you drew on the computer. This is what the molecule looks like and how it can behave in the real world.	What do you notice about your drawing before you optimized it on the computer and after you optimized it on the computer? How close was your predicted drawing with the actual drawing? What is the energy of the optimized molecule? _____

Molecule #2 and #3: Methane to Methanol to Thiomethanol

Directions	Work Space
Step 1: Molecular Formula CH_4	What atoms are in this molecule? How many of each type of atom?
Step 2: Draw the Structural Formula of CH_4 in this box.	What do you notice about the bonds between the atoms?
Step 3: Build the molecule using your modeling kit Draw the molecule you built using black circles for carbon and white circles for hydrogen in this box.	Substitute an alcohol group (-OH) for one of the hydrogen atoms. Draw the molecule using the correct color for oxygen (red) and hydrogen. What is the formula for the new structure?
Step 4: Draw the molecule on the computer. This is your prediction of what the molecule looks like and behaves in the real world.	What do you notice about your drawing compared to the molecule you built?
Step 5: Optimize the molecule you drew on the computer. This is what the molecule looks like and how it can behave in the real world.	What do you notice about your drawing before you optimized it on the computer and after you optimized it on the computer? How close was your predicted drawing with the actual drawing? What is the energy of the optimized molecule? ______
Step 6: In the molecule you just built, substitute a sulfur atom (yellow) for the oxygen atom in methanol. You have now made thiomethanol. Draw the molecule you just built on the computer and then optimize it.	Do you notice any differences between the optimization of methanol and the optimization of thiomethanol? What can you conclude from this?

Appendix E: Avogadro Program Tutorial

Avogadro Program Tutorial



Toolbar

click icon to activate the tool

Draw Tool

- Create atoms and bonds : Left Mouse Click and Drag
- Select Atom Type: Use Settings Panel
- Delete Atom Right Mouse Click
- Zoom Molecule: Middle Mouse (or Scrollbar)

Navigation Tool

- Rotate Molecule: Left Mouse Click and Drag
- Move Molecule : Right Mouse Click and Drag
- Zoom Molecule: Middle Mouse (or Scrollbar)

Manipulation Tool

- Move atom: Left Mouse Click and Drag
- Move Whole Molecule: Right Mouse Click and Drag
- Zoom Molecule: Middle Mouse (or Scrollbar)

Auto Optimization Tool

- Optimize Molecule: On the Settings Panel: Click "START" button
- Terminate Optimization: On the Settings Panel: Click "STOP"
- Energy is printed in the left top corner of the on the screen during the optimization.

Appendix F: Pre/Post Instructional Survey

Pre/Post Survey Name ______________________

Please answer the following questions as best as you can.

Strongly Agree Disagree

1. I understand what single, double and triple bonds are. 5 4 3 2 1

Explain the difference between these bonds: ____

2. I understand what a structural formula is. 5 4 3 2 1

Explain what a structural formula is: ____

3. I feel confident using computer to draw molecules. 5 4 3 2 1

Explain how you gained this confidence: ____

4. I understand the meaning of optimizing molecules on the computer.
5 4 3 2 1

Explain what you think optimizing molecules means: ____

5. I understand that molecules arrange their atoms to adapt to the "best" energy for the molecule.
5 4 3 2 1

Explain how energy changes during optimization to obtain the "best" energy:

____

6. I feel confident using plastic models to show chemical structures.
5 4 3 2 1

Explain how you gained this confidence: ____

7. The correct structural formula for a compound with the formula C_2H_6 is:

8. The correct structural formula for a compound with the formula CH_3SH is:

9. One thing I like about learning about chemistry this week is: ______________________________

10. A question I still have about the lessons this week is: ____