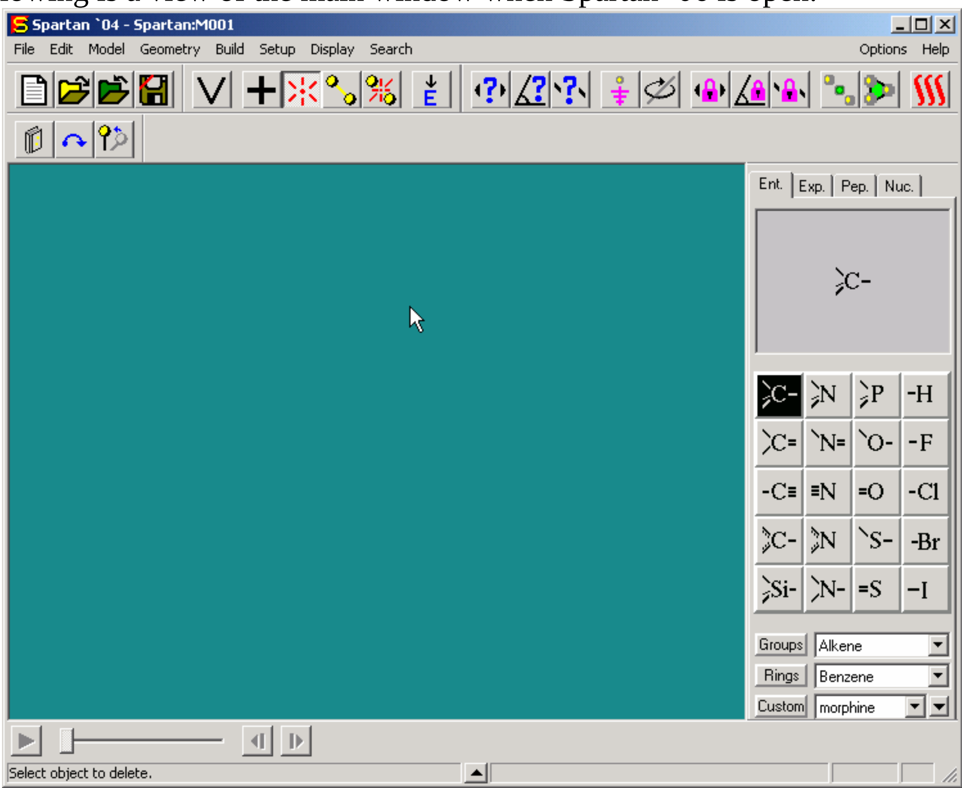
Molecular Modeling using Spartan ‘06

The purpose of this laboratory is to help you visualize different types of bonds found within and between biologically relevant molecules. This first page is a guide to some of the basic functions of Spartan ’06. Subsequent pages provide step-by-step directions to help you construct and analyze several different molecules. Use the data you find to complete the worksheet at the end of this document. Once you have completed this exercise you may build more molecules on your own.

The following is a view of the main window when Spartan ’06 is open:

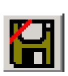


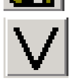
The icons in the tool bar at the top are displayed below:

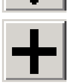
 **New**- Opens new molecule window

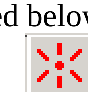
 **Open**- Opens previously saved window

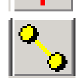
 **Close**- Closes current window without closing program

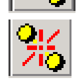
 **Save**- Saves current window

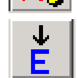
 **View**- Finalized molecule

 **Add**- Allows addition of new atoms to current molecule

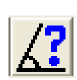
 **Remove**- Removes atoms

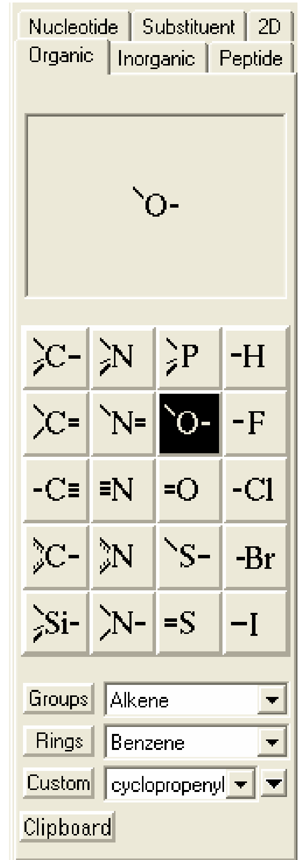
 **Add Bond**

 **Remove Bond**

 **Minimize**- Calculates most stable structure

 **Distance**- measure length of bond between two selected atoms

 **Angles**- measure angle between three selected atoms



Begin by using your lecture notes to answer questions 1 and 2 of the Chemistry and Molecular Modeling Worksheet. When you're ready, use the following instructions to open Spartan '06.

- Double click Spartan '06 icon on desktop
- Click on the **New** icon ( ), the entry model kit will appear at the right of the screen (shown at right).

1) Let's begin by exploring bonds between hydrogen and oxygen atoms. To do this you will build and analyze a water molecule (H_2O)

- Click the **Add** ( ) icon on the top toolbar.
- Click on the button displaying an oxygen atom with two single bonds on the entry model kit.
- Click on the main screen. An oxygen atom with two available single bonds will appear.
- Click the hydrogen button from the entry model kit.
- Add a hydrogen atom to each of the available single bonds by clicking on each bond (available bonds should appear yellow on the main screen).
- Now that your molecule is built, click the **Minimize** ( ) icon on the top toolbar to put your molecule in its most stable form.
- Click the **View** ( ) icon to finalize your molecule.
- Once finalized, look at several different representations of your molecule by using the "Model" menu at the top of the screen and selecting from different views such as "wire," "ball and wire," "tube," or "space filling," from the dropdown menu.
- Return to "ball and spoke" view.
- Left click, hold, and drag the mouse on the main molecule screen to rotate the molecule in three dimensions. Right click, hold, and drag the mouse to move the molecule to a different location on the screen. Right click, hold, and drag the mouse while holding down the shift key to zoom in and out.
- Next we will examine the polarity of the O-H bonds in water, but in order to do this you must first save the molecule you have built by going to File>Save As. Name this file "H2O" and save it to the desktop.
- Now click on Setup>Surfaces. In the Surfaces window that pops up, click "Add". Use the drop-down menus to set Surface to "density", Property to "potential", and Resolution to "medium". This calculation will determine which parts of the molecule will interact most favorably with positive charges. Click OK and close the Surfaces window.
- Next click on Setup>Submit. A window will pop-up, indicating that Spartan has begun calculating the electrostatic potential of the molecule. Click OK. You may have to wait briefly while Spartan completes the calculations. When the window indicating that the calculations are complete appears, click OK.

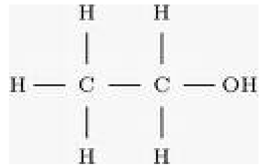
- To view the electrostatic potential of various portions of the molecule, click Display>Surfaces. Click on the yellow box next to “density” and close the Surfaces window.
- Now set the color scheme by clicking on Display>Properties. Then click on the water molecule and set the Property Range on the left (red) to -261 and the Property Range on the right (blue) to 246.
- While leaving the Surface Properties window open, rotate the molecule to view all surfaces of it, and notice that some portions of the molecule are red, indicating that they interact favorably with positive charges (such as sodium ions). Are such parts of the molecule more likely to be electron-poor or electron-rich?
- Blue parts of the molecule repulse positive charges. Are such parts of the molecule likely to be electron-poor or electron rich?
- To view the ball and spoke model and the electrostatic potential map simultaneously, use the drop-down menu in the Surface Properties window to set the Style to “Transparent”. Rotate the molecule as desired to gain the information needed to answer questions 3-5 on the worksheet.

2) Now let’s examine a covalent bond that forms between identical atoms, namely the double bond between the oxygen atoms in O_2.
- Begin by closing the H2O file ( ) and opening a new molecule window ( ).
- Click the **Add** ( ) icon on the top toolbar.
- Click on the button displaying an oxygen atom with a double bond (=O) on the entry model kit.
- Complete the molecule by adding the same type of oxygen atom to the available (yellow) double bond.
- Use the **Minimize** ( ) icon on the top toolbar to put your molecule in its most stable form.
- Save this file as O2, then calculate and map its electrostatic potential by following the same steps as you did for water (be sure to set the Property Range to -261 to 246). After viewing the molecule, use what you learned to answer questions 6 and 7 on the worksheet.

3) Now let’s examine a covalent bond that forms between atoms with similar electronegativity, namely the bonds between carbon and hydrogen atoms in the simple molecule methane (CH_4).
- Begin by closing the O2 file ( ) and opening a new molecule window ( ).
- Click the **Add** ( ) icon on the top toolbar.
- Click on the entry model kit button displaying a carbon atom with four single bonds.
- Complete the molecule by adding a hydrogen atom to each available (yellow) single bond.
- Use the **Minimize** ( ) icon on the top toolbar to put your molecule in its most stable form.
- Save this file as CH4 , then calculate and map its electrostatic potential by following the same steps as you did for water (be sure to set the Property Range to -261 to 246). When finished re-open the H2O and O2 files, and display the

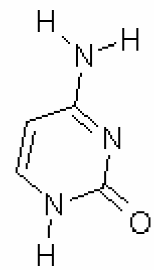
electrostatic potential map for each molecule. Compare the structures and color scheme of each molecule, and use what you learned to answer questions 8-10 on the worksheet.

4) Now let's explore a larger molecule with several different types of bonds, specifically C-H, C-C, C-O, and O-H bonds. To do this you will build and analyze a molecule of ethanol (shown to the right).



- Begin by closing the H2O, O2, and CH4 files () and opening a new molecule window ().
- Click the **Add** () icon on the top toolbar.
- Click on the button displaying a carbon atom with four single bonds on the entry model kit.
- Click on the main screen. A carbon atom with four available single bonds will appear. Attach another carbon atom to one of these available (yellow) bonds by clicking on it.
- Click on the button displaying an oxygen atom with two single bonds on the entry model kit.
- Add an oxygen atom to one of the carbon atoms by clicking on one of the available (yellow) bonds.
- Add a hydrogen atom to each of the remaining available (yellow) single bonds.
- Now that your molecule is built, click the **Minimize** () icon on the top toolbar to put your molecule in its most stable form.
- Rotate this structure to view it in its entirety.
- Save the molecule you have built by going to File>Save As. Name this file "ethanol" and save it to the desktop.
- Now click on Setup>Surfaces. In the Surfaces window that pops up, click "Add". Use the drop-down menus to set Surface to "density", Property to "potential", and Resolution to "medium". This calculation will determine which parts of the molecule will interact most favorably with positive charges. Click OK and close the Surfaces window.
- Next click on Setup>Submit. A window will pop-up, indicating that Spartan has begun calculating the electrostatic potential of the molecule. Click OK. You may have to wait briefly while Spartan completes the calculations. When the window indicating that the calculations are complete appears, click OK.
- To view the electrostatic potential of various portions of the molecule, click Display>Surfaces. Click on the yellow box next to "density" and close the Surfaces window.
- To view the ball and spoke model and the electrostatic potential map simultaneously, click on Display> Properties. Then click on the water molecule, and use the drop-down menu to set the Style to "Transparent". Rotate the molecule as desired to gain the information needed to answer questions 11 and 12 on the worksheet.

5) Now let's move on and look at an even more complicated structure. During this part of the lab we will also explore how two small molecules can interact via hydrogen bonds. To begin this part of the exercise, you will first need to construct the nitrogenous base cytosine, a component of DNA.

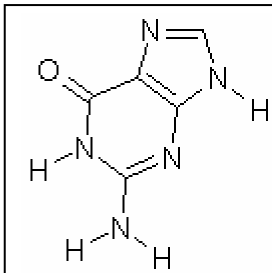


cytosine

- Begin by closing the ethanol file () and opening a new molecule window ().
- Click the **Add** () icon on the top toolbar.
- Click on the button displaying a nitrogen atom with three single bonds on the entry model kit.
- Click on the main screen. A nitrogen atom with three available single bonds will appear. This corresponds with the bottom-most atom in the picture of cytosine provided above. We'll continue building this molecule by proceeding in a clockwise fashion around the ring.
- Go back to the entry model kit and click on the button displaying a carbon atom with a double bond and two single bonds. Add this carbon atom to one of the available (yellow) bonds of your nitrogen atom.
- Add the same type of carbon to the available (yellow) <u>double</u> bond of the first carbon atom you attached.
- Keep building this linear chain of atoms by adding the same type of carbon (one double bond and two single bonds) to one of the available (yellow) single bonds of the last carbon you added. Now you should have a chain of four atoms, specifically, a single nitrogen followed by three carbon atoms.
- Next add the second nitrogen atom that will be found in the ring, by going back to the entry model kit and clicking on the nitrogen button which has a double bond and a single bond. Add this nitrogen atom to the available (yellow) <u>double</u> bond of the last carbon you added.
- Again, go back to the entry model kit and click on the carbon button with two single bonds and a double bond. Add one such carbon to the available single bond of the most recently added nitrogen.
- Click the **Minimize** () icon on the top toolbar to better visualize all the atoms and bonds you have built thus far.
- Close the ring by clicking on the "Add Bond" button () at the top of the page. Next click on one of the available single bonds from your first nitrogen atom and then the available single bond from your last carbon atom.
- Click the **Minimize** () icon on the top toolbar to better visualize the ring. Is the ring six-sided? And does it have all the necessary atoms in the appropriate order as shown in the diagram above?
- Now add the remaining atoms to your cytosine molecule.
- Go to the entry model kit and click on the button corresponding to oxygen with a double bond. Add one such oxygen to the available (yellow) double bond of your molecule.
- Use the appropriate buttons on the entry tool kit to add the $–NH_2$ and other remaining atoms.
- Now that your molecule is built, click the **Minimize** () icon on the top toolbar to put your molecule in its most stable form.

- Click the **View** (✓) icon to finalize your molecule.
- Once finalized, look at several different representations of your molecule, rotating it and zooming in and so you can see all of its relevant features.
- Save the molecule you have built by going to File>Save As. Name this file “cytosine” and save it to the desktop.
- Now click on Setup>Surfaces. In the Surfaces window that pops up, click “Add”. Use the drop-down menus to set Surface to “density”, Property to “potential”, and Resolution to “medium”. This calculation will determine which parts of the molecule will interact most favorably with positive charges. Click OK and close the Surfaces window.
- Next click on Setup>Submit. A window will pop-up, indicating that Spartan has begun calculating the electrostatic potential of the molecule. Click OK. You may have to wait briefly while Spartan completes the calculations. When the window indicating that the calculations are complete appears, click OK.
- To view the electrostatic potential of various portions of the molecule, click Display>Surfaces. Click on the yellow box next to “density” and close the Surfaces window.
- To view the ball and spoke model and the electrostatic potential map simultaneously, click on Display> Properties. Then click on the water molecule, and use the drop-down menu to set the Style to “Transparent”. Rotate the molecule as desired to gain the information needed to answer question 13 on the worksheet.
- Do NOT close the cytosine document.

4) Now open the Spartan document titled “guanine”. This document can be found on the desktop of the computer you are using.



guanine

- Now click on Setup>Surfaces. In the Surfaces window that pops up, click “Add”. Use the drop-down menus to set Surface to “density”, Property to “potential”, and Resolution to “medium”. This calculation will determine which parts of the molecule will interact most favorably with positive charges. Click OK and close the Surfaces window.
- Next click on Setup>Submit. A window will pop-up, indicating that Spartan has begun calculating the electrostatic potential of the molecule. Click OK. You may have to wait briefly while Spartan completes the calculations. When the window indicating that the calculations are complete appears, click OK.
- To view the electrostatic potential of various portions of the molecule, click Display>Surfaces. Click on the yellow box next to “density” and close the Surfaces window.
- To view the ball and spoke model and the electrostatic potential map simultaneously, click on Display> Properties. Then click on the water molecule, and use the drop-down menu to set the Style to “Transparent”.
- If necessary, right click, hold, and drag the mouse to pull the guanine molecule to a part of the screen that is away from the cytosine. Rotate the guanine as desired to gain the information needed to answer question 14 on the worksheet.

- With both the guanine and cytosine files open, take a moment to refresh your memory about what a hydrogen bond is, referring to your lecture notes if necessary. Record your answer on the worksheet.
- Within the structure of double-stranded DNA, cytosine and guanine form three hydrogen bonds with each other. In Spartan, orient the cytosine and guanine molecules so that you can easily visualize where the three hydrogen bonds will form. What do you notice? Does red in one molecule line up with blue in the other? Print out this image, write on it to indicate where the hydrogen bonds form, then staple this page to your worksheet. Turn in both documents.

Name:___________________________

Chemistry and Molecular Modeling Worksheet

1. Carbon, hydrogen, nitrogen, and oxygen are the most common elements making up the human body. What is the difference in electronegativity between…

   …carbon and hydrogen?

   …carbon and oxygen?

   …carbon and nitrogen?

   …oxygen and hydrogen?

   …nitrogen and hydrogen?

2. Water readily dissolves table salt (NaCl). In a salt solution, which atom of a water molecule (hydrogen or oxygen) will be attracted to a sodium ion (Na^+) from the salt? Why?

3. The electrostatic potential of a molecule, or part of a molecule, is a measure of how favorably the atom(s) under study interact with (or are attracted to) positive charges. Which atom of a water molecule, hydrogen or oxygen, will interact favorably with (be attracted to) positive charges? Why?

   Which atom of a water molecule, hydrogen or oxygen, will interact unfavorably with (be repulsed from) positive charges? Why?

4. When looking at the electrostatic potential map for water, what color is this surface near the oxygen atom?

   Given that red shading indicates portions of the molecule that interact favorably with positive charges, do you think this part of the molecule is electron-rich or electron-poor? Briefly explain your answer.

5. When looking at the electrostatic potential map for water, what color is this surface near the hydrogen atoms?

   Given that blue shading indicates portions of the molecule that repulse positive charges, do you think this part of the molecule is electron-rich or electron-poor? Explain your answer.

6. Molecular oxygen (O_2) is formed when two oxygen atoms are covalently attached to each other through a double bond. How many electrons are shared between two atoms involved in a double bond? How many electrons are donated from each atom? (feel free to use your lecture notes or textbook to look up this answer!)

7. Describe the electrostatic potential map for molecular oxygen. (what do you notice? does the molecule have red parts? blue parts? is it all basically the same color?) What does this tell you about the nature of O_2? Is this molecule polar or nonpolar?

8. Methane (CH4) is formed when one carbon atom is covalently attached to four hydrogen atoms. How many electrons are shared between two atoms involved in a single bond? How many electrons are donated from each atom? (feel free to use your lecture notes or textbook to look up this answer!)

9. Describe the electrostatic potential map for methane. (what do you notice? does the molecule have red parts? blue parts? is it all basically the same color?) What does this tell you about the nature of methane? Is this molecule polar or nonpolar?

10. When comparing the structures of water, molecular oxygen, and methane, which molecule is the most polar (i.e.- has red and blue parts)? Which molecule is the least polar?

How do these results correlate with the differences in electronegativity that you calculated when answering question #1?

11. When looking at the electrostatic potential map for ethanol, which atom will interact most favorably with positive charges (i.e.- which atom has a “red” electrostatic potential?

Which atom will repulse positive charges (i.e.- which atom has a “blue” electrostatic potential?

12. Which bond in this molecule is the most polar? In other words, which bond is between an atom with a “red” electrostatic potential and a “blue” electrostatic potential?

Which bonds appear to be the least polar?

What color is used to represent nonpolar portions of the molecule?

13. What color is being used to represent the electrostatic potential of the nitrogen atom that doesn't have any hydrogens directly bonded to it? What does this tell you about this atom? Is it electron-rich or electron poor? Will this nitrogen attract or repulse positive charges?

14. Which hydrogens in the structures of cytosine and guanine are the most likely to repulse positive charges (i.e.- which have the "bluest" electrostatic potential?)?... the hydrogen atoms bonded to carbon atoms or the hydrogen atoms bonded to nitrogen atoms? Why do you think this might be the case?

15. What is the definition of a hydrogen bond?

16. In DNA, three hydrogen bonds form between guanine and cytosine. Indicate where these bonds form on the print-out of the structures from Spartan.