VSEPR and the Avogadro Program

Let your mouse rest on any of these buttons to bring up a short explanation of the tool.

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| **Button** | **Located** | **What it does** |
| Tool Settings… | On the top panel to the right. | This shows you options for the Tool you have currently selected. You will want to click this and leave this side panel up. |
| Draw Tool | Image of a pencil on the button. One button to the right of “Quit”. | Creates new atoms.  **Element** – choose which element you want to add.  **Bond Order** – choose which type of bond is created with new atoms. If necessary, you can always click on a bond to change the type of bond while the “Draw Tool” is selected.  **Adjust Hydrogens** – if checked, it will automatically add hydrogens to new atoms. |
| Navigation Tool | Blue “plus” or compass picture. One button to the right of Draw Tool. | Moves the molecule around. Left-click rotates, middle-click zooms in and out, and right-click slides the molecule. |
| Manipulation Tool | White glove picture. 4th button to the right of “Quit”. | Moves an individual atom around while keeping the rest of the molecule stationary. Left-click slides the atom left, right, up or down, while middle-click slides it in or out. |
| Selection Tool | Black mouse arrow picture. One button to the right of the Manipulation Tool. | Selects parts of the molecule. Click and drag to select several parts. Click and drag on open space to un-select. |
| Auto Rotation Tool | Dark purple curving arrow picture. One button to the right of the Selection Tool. | Click and drag in a direction to start rotating the molecule. You can adjust the speed of the rotation with the sliders on the left. |
| Auto Optimization Tool | E with a down arrow under it. One button to the right of the Auto Rotation Tool. | Click the “Start” button on the left to optimize and find the VSEPR Theory shape of any molecule. Click “Stop” to end the optimization. Remember to always run this Tool when finding the VSEPR Shape, measuring bond angles, or measuring bond lengths.  Note: you can also optimize by going to “Extensions 🡪 Optimize Geometry”. |
| Measure Tool | Ruler with small red arrows above it. One button to the right of the Auto Optimization Tool. | Select individual atoms in a specific order to measure either bond length or bond angle. These measurements will be shown at the bottom of your screen. |
| Display Settings… | Far right of the top toolbar. | Brings up various display options. One important one is that “Dipole” is checked if you are looking for the polarity of a molecule. |
| Molecule Properties… | View 🡪 Properties 🡪 Molecule Properties… | Shows various properties for the molecule. One important thing to see is the “Estimated Dipole Moment”. If this is zero, then the molecule is non-polar, otherwise, it is polar. |

**Part 1: Creating Molecules**

One downside to this program is that it assumes you know which atoms are connected in a molecule, because you can’t just type in a formula. Therefore, we will begin by drawing some simple Lewis Diagrams and then creating them in Avogadro.

For each of the following molecules, *draw the Lewis Diagram* on this paper, create the structure in Avogadro, and then draw the atom as best you can from Avogadro. Make sure you use auto-optimization before you draw the structure. You may draw a sketch of the molecule or you may draw it using lines and triangles to represent depth and dimension.

1. CH­4
2. CS­2
3. CH2O
4. C2H6
5. C2H4 (Tip: use the C2H6 model, have “Adjust Hydrogens” checked, and click on the bond between the two Carbons to make it a double bond.)
6. C2H5OH (Note: this has several stable angles—try to make one that is easy to draw.)
7. BCl2OH

**Part 2: The Van Der Waals Surface**

Go to “Display Settings…” and check the box labeled “Van Der Waals Spheres”. You can actually edit the display by clicking on the wrench to the right of the name so that the Spheres are transparent and you can see the ball and stick model behind it.

Van Der Waals Spheres are a close approximation of the actual “size” of an atom or molecule. The type of model we have been using is often called a “ball and stick” model, and both models have their advantages.

1. Draw the Van Der Waals Spheres for water: H2O. You may have to rotate the molecule around to get a good sketch-able image of the molecule.
2. What are some advantages of the Van Der Waals Spheres model?
3. What are some advantages of the ball-and-stick model?

**Part 3: Dipoles and Polarity**

Go to “Display Settings…” and turn on the “Dipole” display. This is a little red arrow that will show up if the molecule is polar. The arrow points in the direction that the electrons spend their time, in other words, where there is a partial negative charge (δ-). For this exercise, you will first determine whether or not the molecule is polar (no arrow or a very, very small arrow means that it is non-polar), and then you will draw the partial charges (if it is polar): δ- on the side of the molecule in the direction of the arrow and δ+ on the other side of the molecule. Don’t forget to auto-optimize each molecule before drawing!

1. PH3
2. SCl2
3. O2H2
4. C3H8
5. P(OH)3

Bonus: Create your own cool molecule, write the chemical formula here: \_\_\_\_\_\_\_\_\_\_, and then draw it!

Bonus II: Diamond is entirely made of Carbon, where each Carbon has 4 other carbons around it (a tetrahedral shape!). Create a segment of diamond in Avogadro and show Mr. Newman! You may want to Google “diamond” to find some pictures of the structure. (Tip: use the “Adjust Hydrogens” to see where the carbons should go!)