1.3: Computational Instructions

In this exercise we will learn to draw simple molecules in Avogadro, an open-access molecular visualization software package. Start by opening Avogadro on your computer by double clicking on the Avogadro icon and click on the draw button (looks like a pencil) to open the drawing menu (Figure 5).

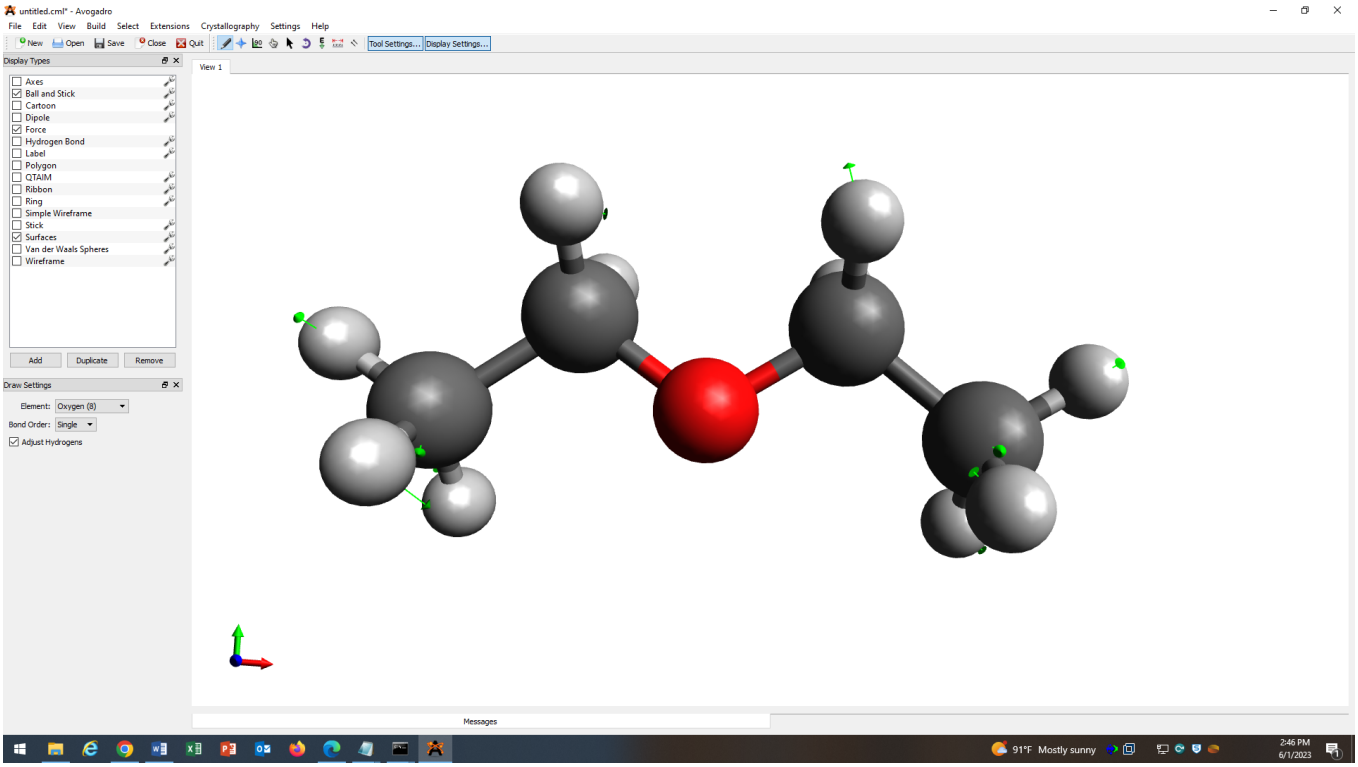

Figure 5. Avogadro with drawing menu button indicated with a red arrow and diethyl ether drawn.

From this menu you can select the atom that you would like to draw and the number of bonds that you would like it to make. Draw the structure of diethyl ether to learn how the molecular editor works. Note that with the adjust hydrogen button selected, Avogadro will automatically adjust the number of hydrogens to ensure that your molecule obeys the octet rule.

When drawing molecules your bond angles and lengths will often look different than ideal (drawing on a computer is not always easy). We can provide a more accurate geometry of your diethyl ether molecule by performing a quick optimization. You can perform this operation by clicking extensionsoptimize geometry.

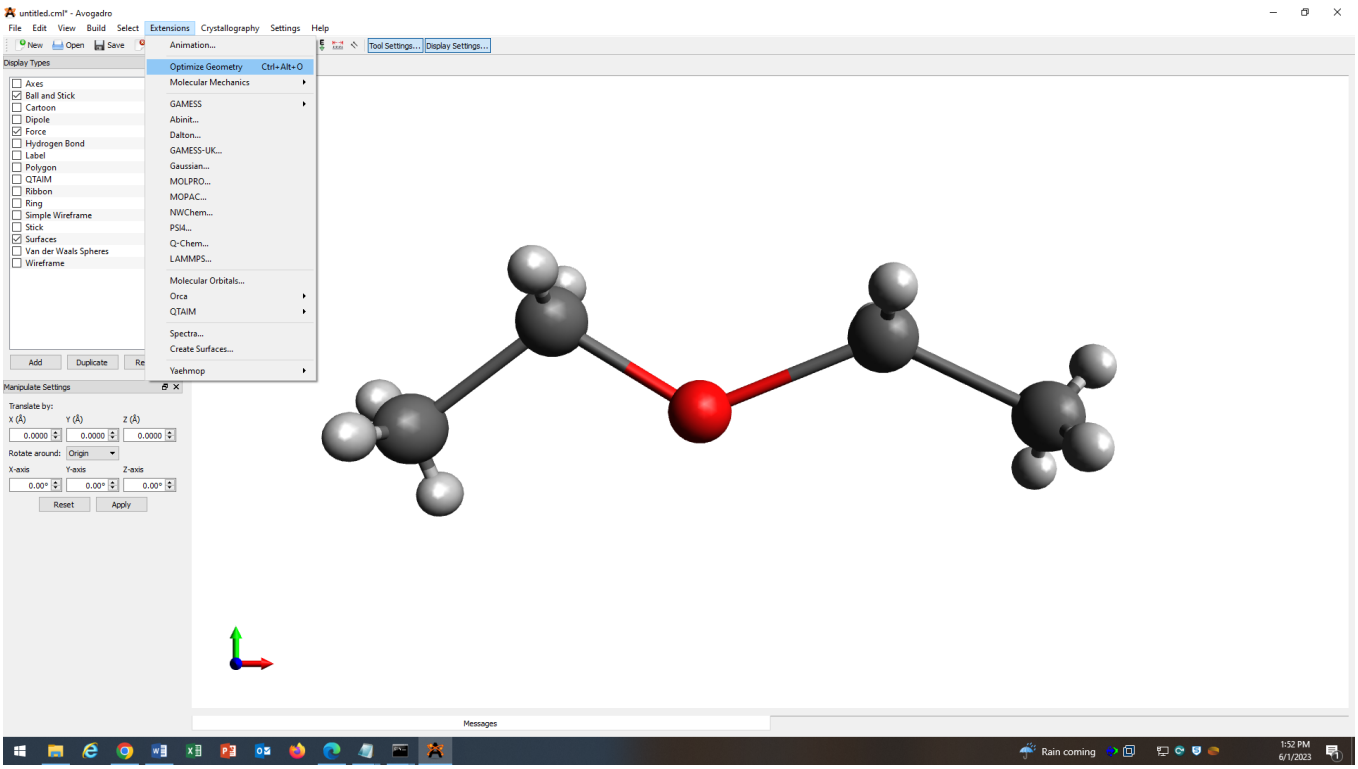

Figure 6. Avogadro with the optimize geometry option indicated.

After optimizing the geometry of your molecule, you can manipulate the molecule in three dimensions as well as measure properties such as bond lengths and angles. To rotate the molecule in three dimensions, press the navigation tool button which looks like a compass rose, as shown in Figure 7. You can then click and drag anywhere in the main display panel to rotate the molecule.

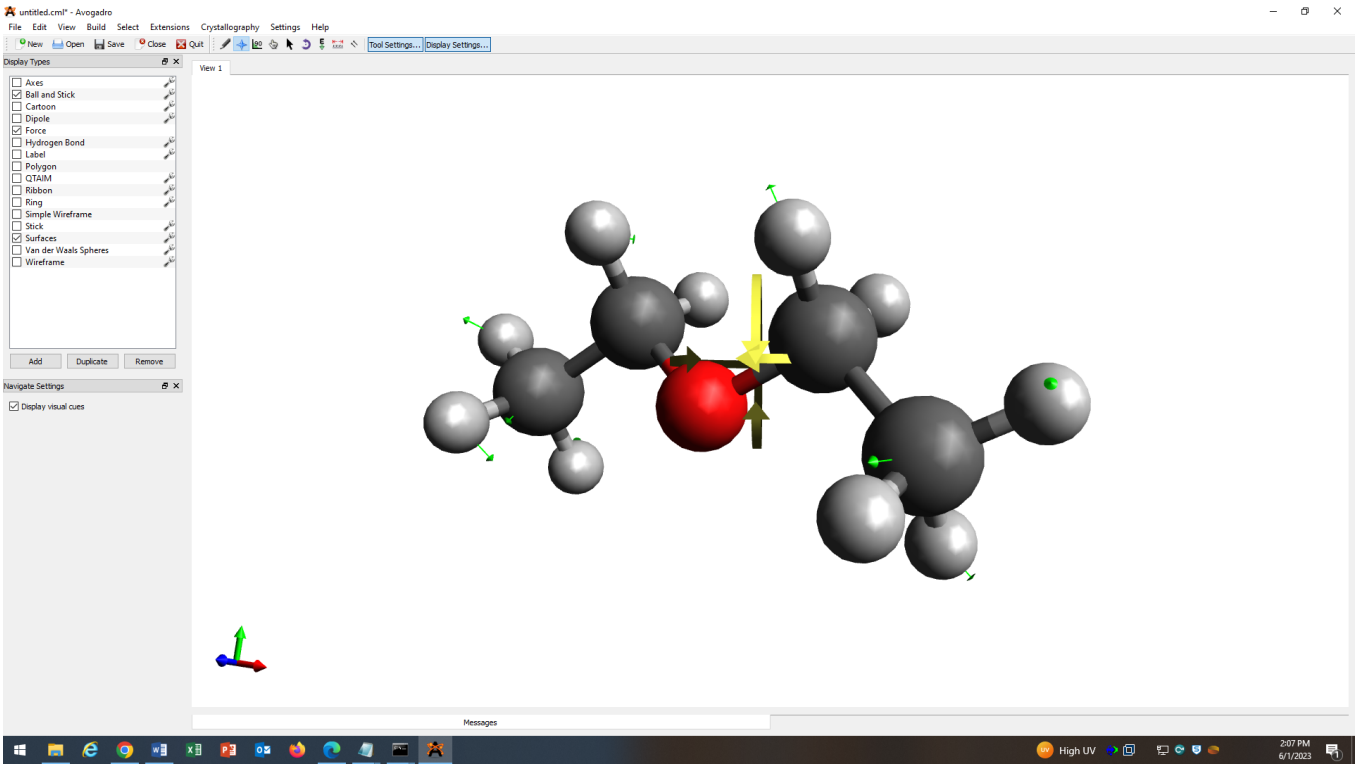

Figure 7. Avogadro with the navigation tool indicated. When rotating the molecule, the program will indicate the direction of rotation with bold yellow arrows.

To measure bond lengths, click the measurement tool, which looks like a ruler, in the main tool panel. Then left click on the two atoms (one after the other) that you would like to measure. When you have measured the length of interest you can reset the measurement tool by right clicking anywhere in the main display panel. To measure a bond angle, click the three atoms (one right after another) composing the angle that you would like to measure. The angle will appear on the bottom left of the main display panel as well as the individual bond lengths for atom 1 to atom 2 and atom 2 to atom 3. For example, we can measure the $C-O-C$ bond angle of diethyl ether using this method to find a bond angle of 111.7°.

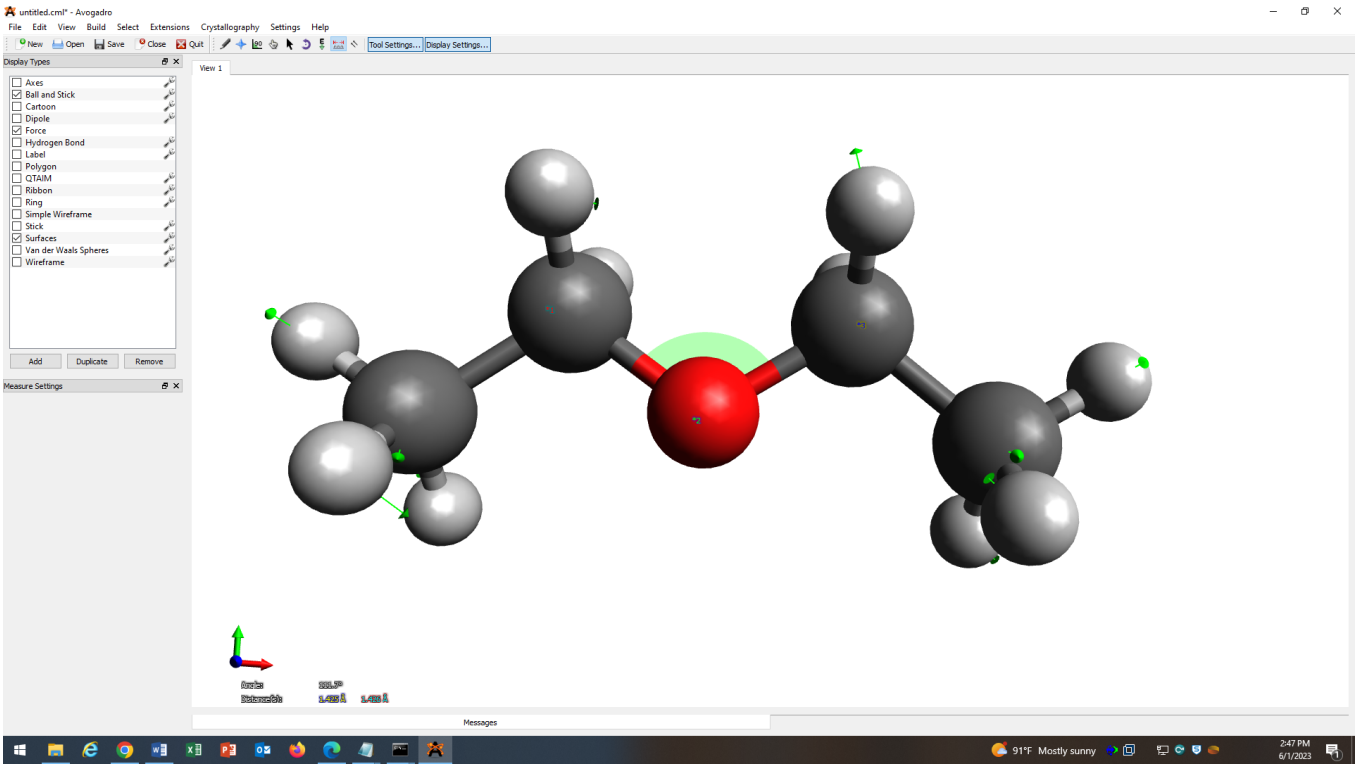

Figure 8. Avogadro with the measurement tool (Blue Arrow) open displaying the oxygen-carbon-oxygen bond angle of diethyl ether. The bond lengths for the carbon-oxygen bonds and the $C-O-C$ bond angle are shown at the bottom left of the screen (Red Arrow).

References

1. Hanwell, M. D.; Curtis, D. E.; Lonie, D. C.; Vandermeersch, T.; Zurek, E.; Hutchison, G. R. Avogadro: An Advanced Semantic Chemical Editor, Visualization, and Analysis Platform. *J. Cheminformatics* **2012**, *4* (1), 17. https://doi.org/10.1186/1758-2946-4-17.
2. Avogadro: An Open-Source Molecular Builder and Visualization Tool. http://avogadro.cc/