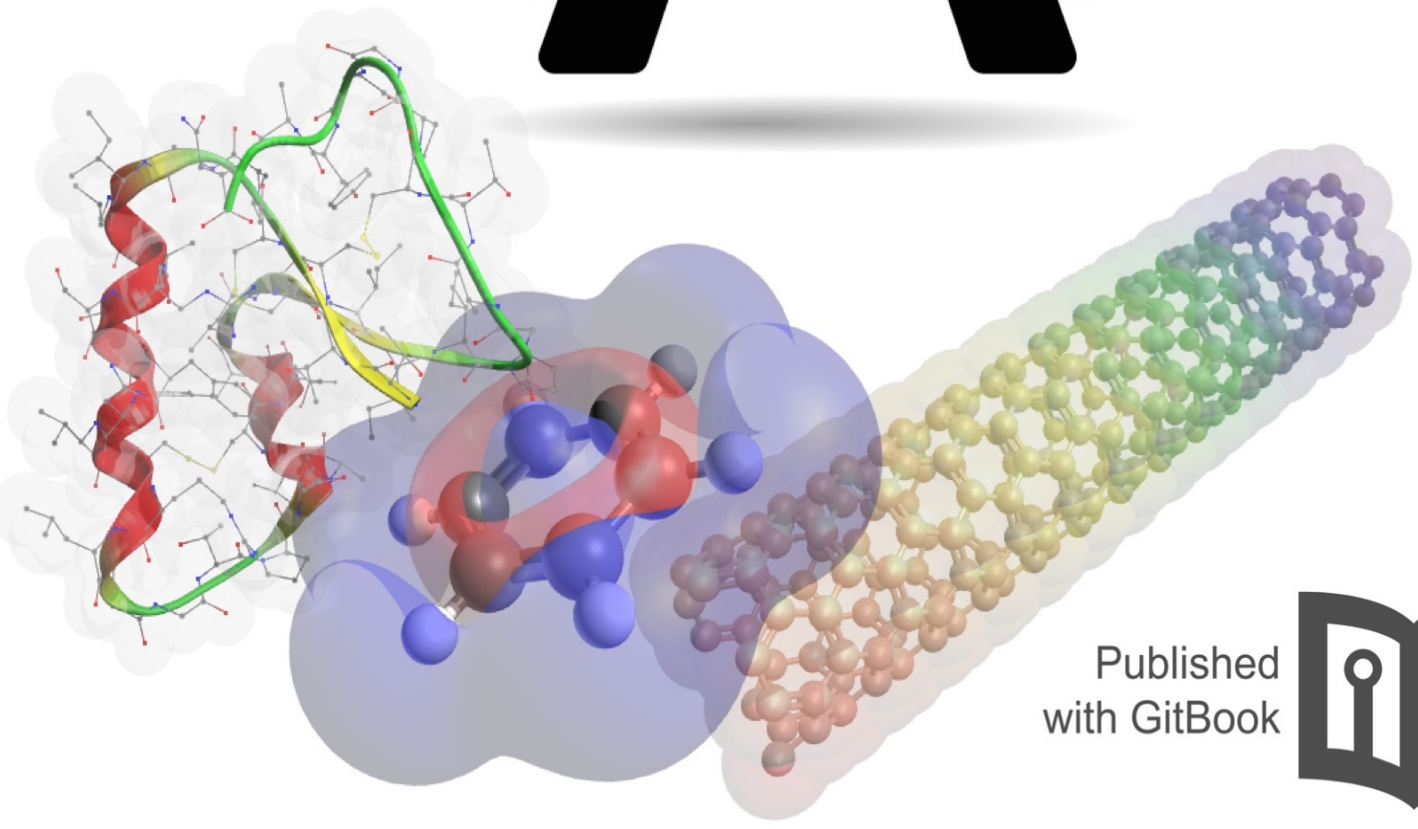
Learning Avogadro

The Molecular Editor



Published
with GitBook

Table of Contents

Avogadro: Molecular Editor and Visualization

Avogadro is a free, open source molecular editor and visualization tool, designed for use on Mac, Windows, and Linux in computational chemistry, molecular modeling, bioinformatics, materials science, and related areas. It offers flexible high quality rendering and a powerful plugin architecture.

More about Avogadro, including development details and downloads can be found at http://avogadro.cc

Thanks

This book would not be possible without the help and effort of many people, including Avogadro developers, translators, and users world-wide.

Funding for the Avogadro manual was provided by the University of Pittsburgh Department of Chemistry.

-Taylor Cornell and Geoffrey Hutchison

Summer 2015

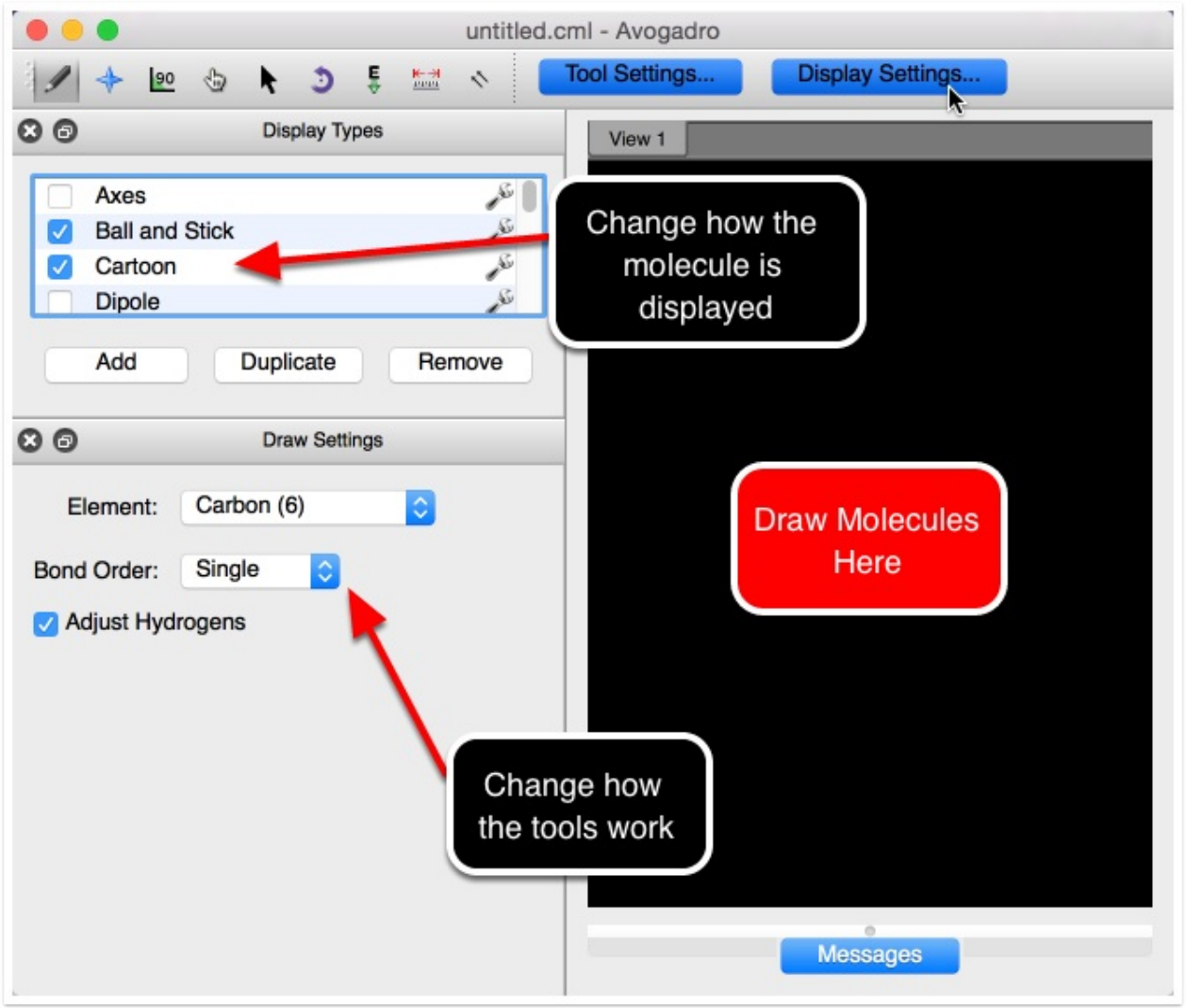
Pittsburgh, Pennsylvania

Introduction

Avogadro is a "molecular editor," designed to be easy to use to construct and view molecules and materials in 3D. It runs on Windows, Linux, and Mac.

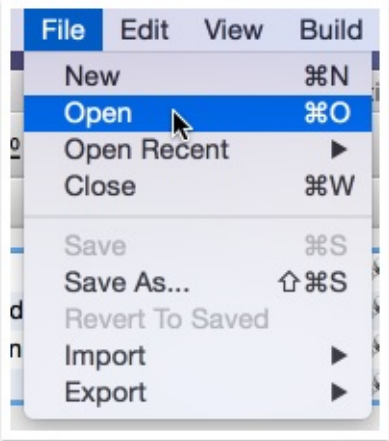
This manual was largely made on a Mac, but the interface should be very similar on any computer.

When you initially open Avogadro you will be presented with a screen such as the one shown below.

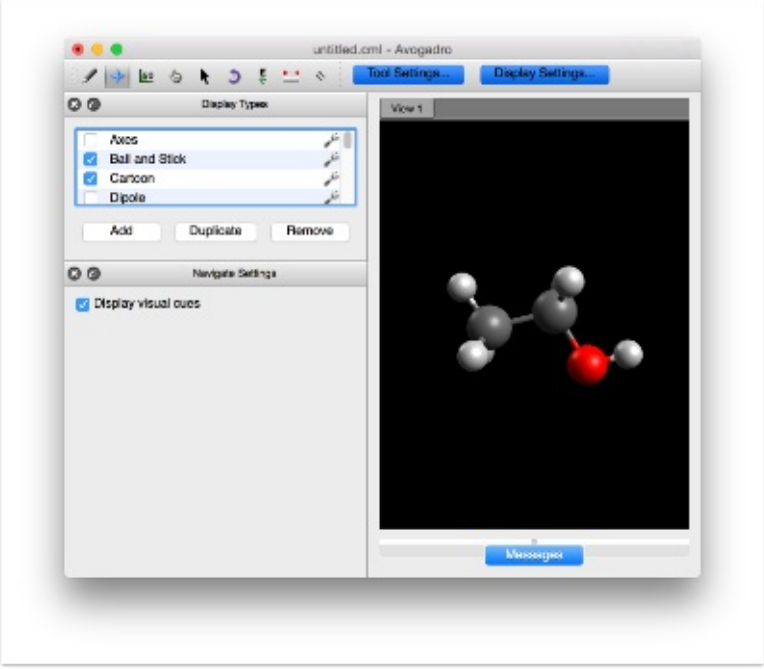


Opening a File

The first thing you will probably want to do is open a file and navigate around the molecule. To do this click on the `File` menu and select `Open...`.



You can then look through the files on your disk and find an appropriate chemical file. Thanks to Open Babel, a large number of file types are supported including CML, XYZ, SDF, Mol2, PDB etc. Several example molecules are supplied with Avogadro.



The screen shot above shows the ethanol.cml file opened up and displayed using the default Ball and Stick display type. Notice that when a new file is opened Avogadro switches from the Draw Tool to the Navigate Tool, which allows you to view the molecule without editing it.

Navigation

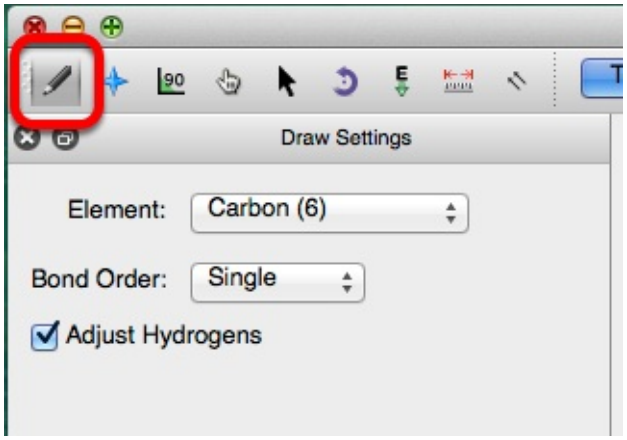
You can zoom in/out using the scroll wheel on your mouse or holding down the middle mouse button and moving the mouse cursor up/down. You can rotate the view by holding down the left mouse button and moving the mouse cursor. You can also translate the view by holding down the right mouse button and moving the mouse cursor.

Note: if your mouse only has one or two buttons you can also use the modifier keys (shift and control) along with the left mouse button to perform actions where you would normally use the middle or right mouse buttons respectively.

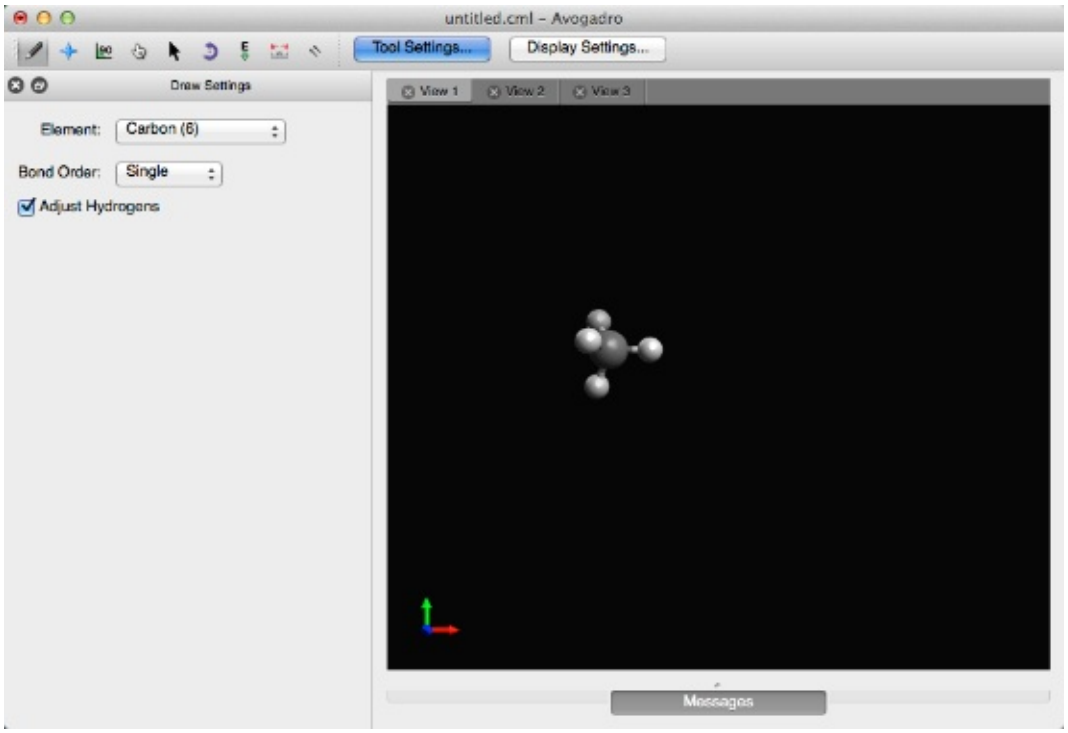
Drawing Molecules

Creating a Molecule

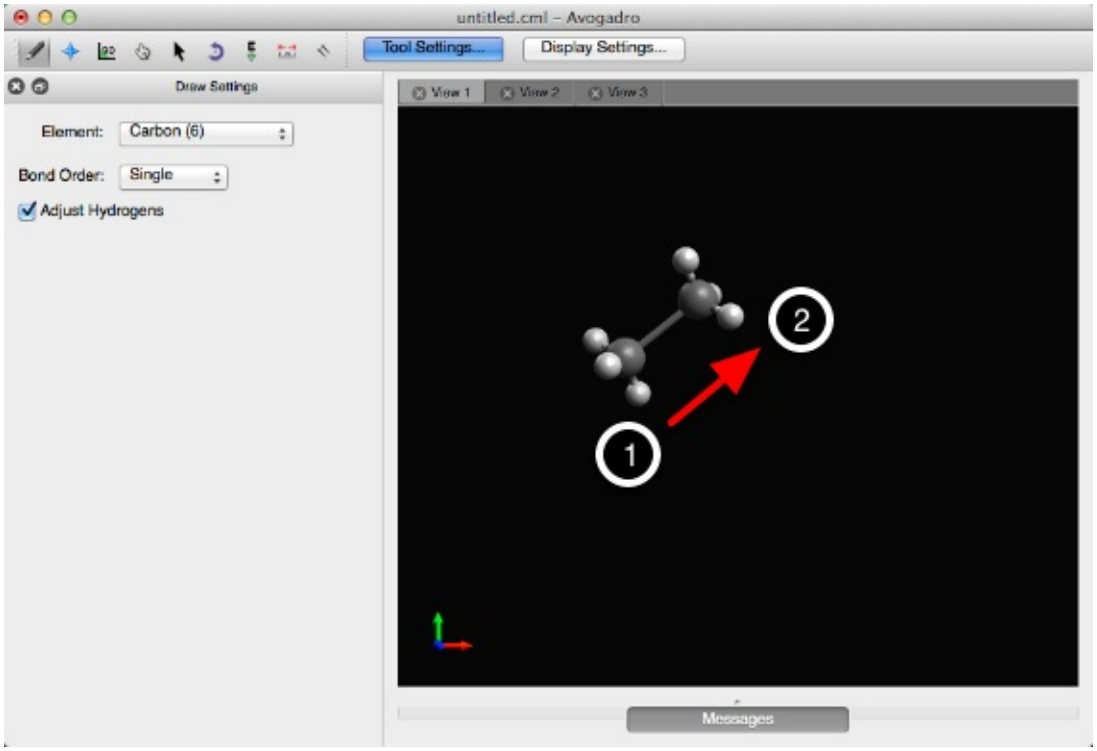
Molecules can be built and edited with the draw tool.



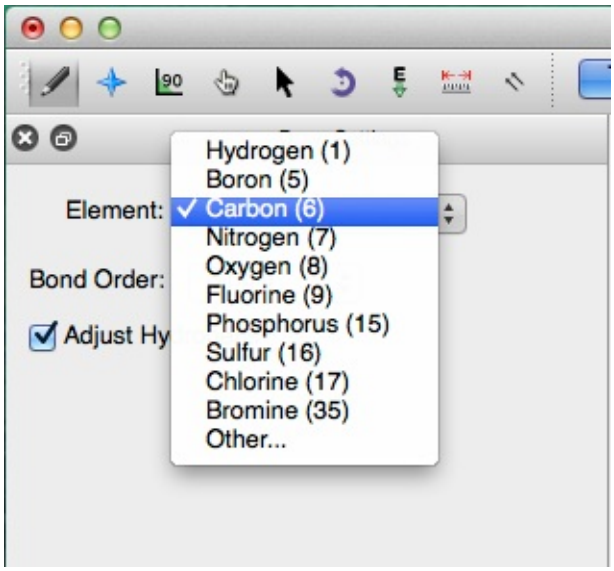
You can begin creating a molecule by left clicking on the black display. This will generate a carbon atom. Right clicking on the atom will delete it.



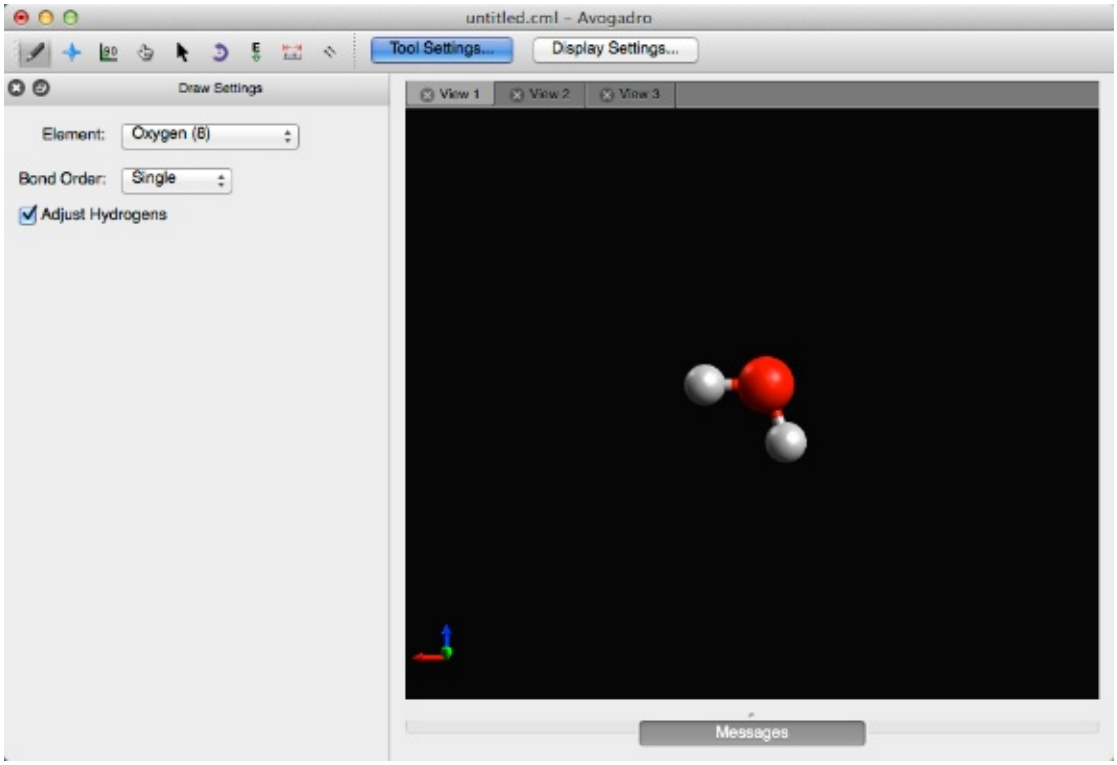
Left clicking and dragging the mouse will generate a bond to another carbon atom.



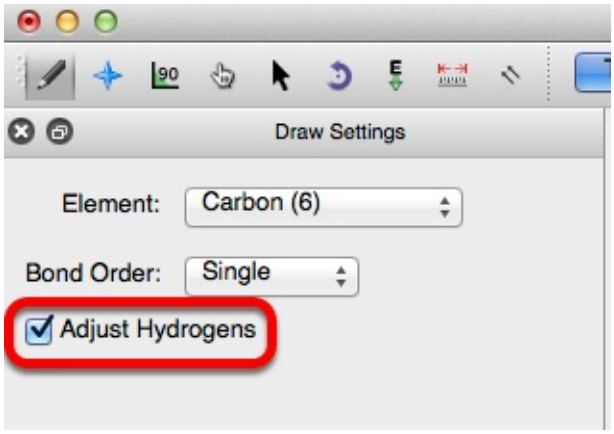
Different elements can be selected from the Element drop down menu. Typing the atomic symbol (e.g., "A-s" for Arsenic) is a shortcut for changing the selected element.



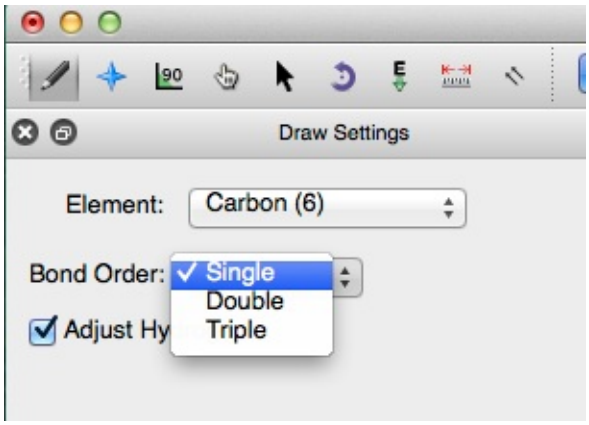
For example, if you wanted to create water, you can type in "O", or select "Oxygen (8)" from the drop down menu and click on the black display.



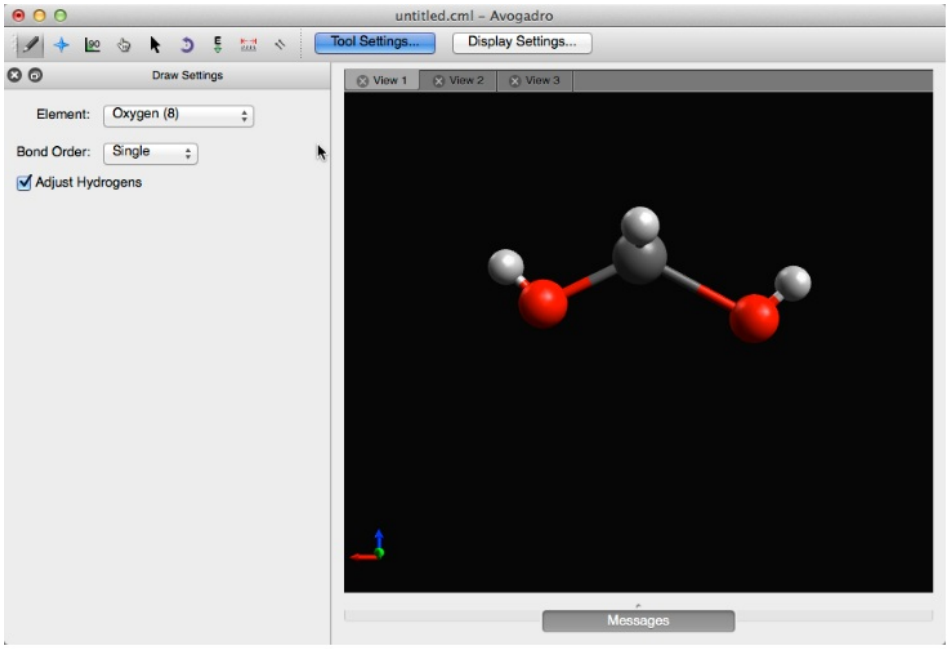
If the "Adjust Hydrogens" box is checked, hydrogens in the molecule are automatically adjusted to satisfy valency (as shown above).

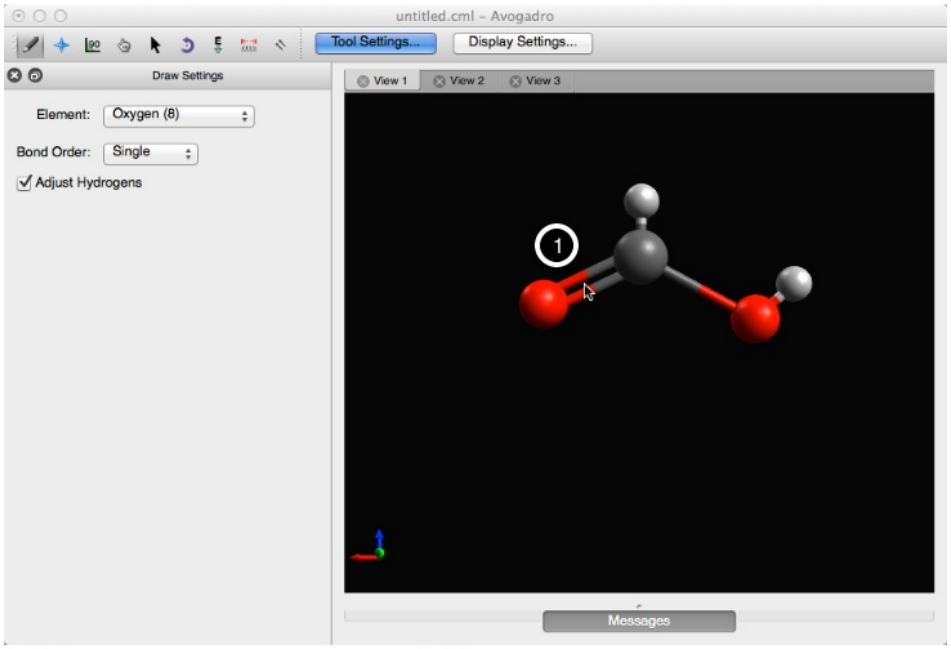


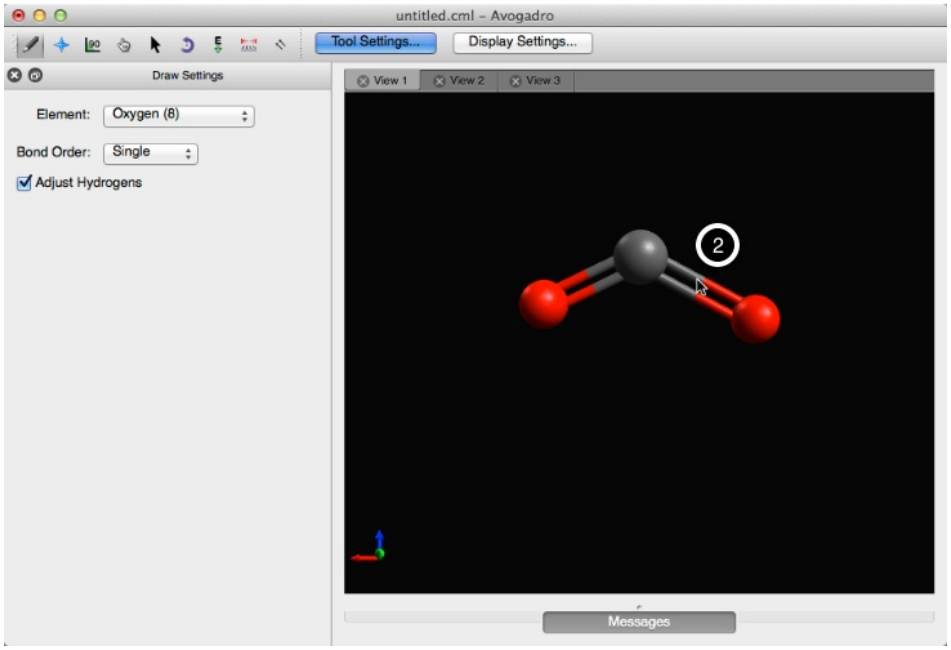
Bond order can be changed through the Bond Order drop down menu, or by typing the numbers "1", "2", or "3". Bonds can also be added to a molecule by left clicking on a bond that has already been created (this process cycles through single, double, and triple bonds). Right clicking on a bond will delete the bond, and the atom it's bonded to.



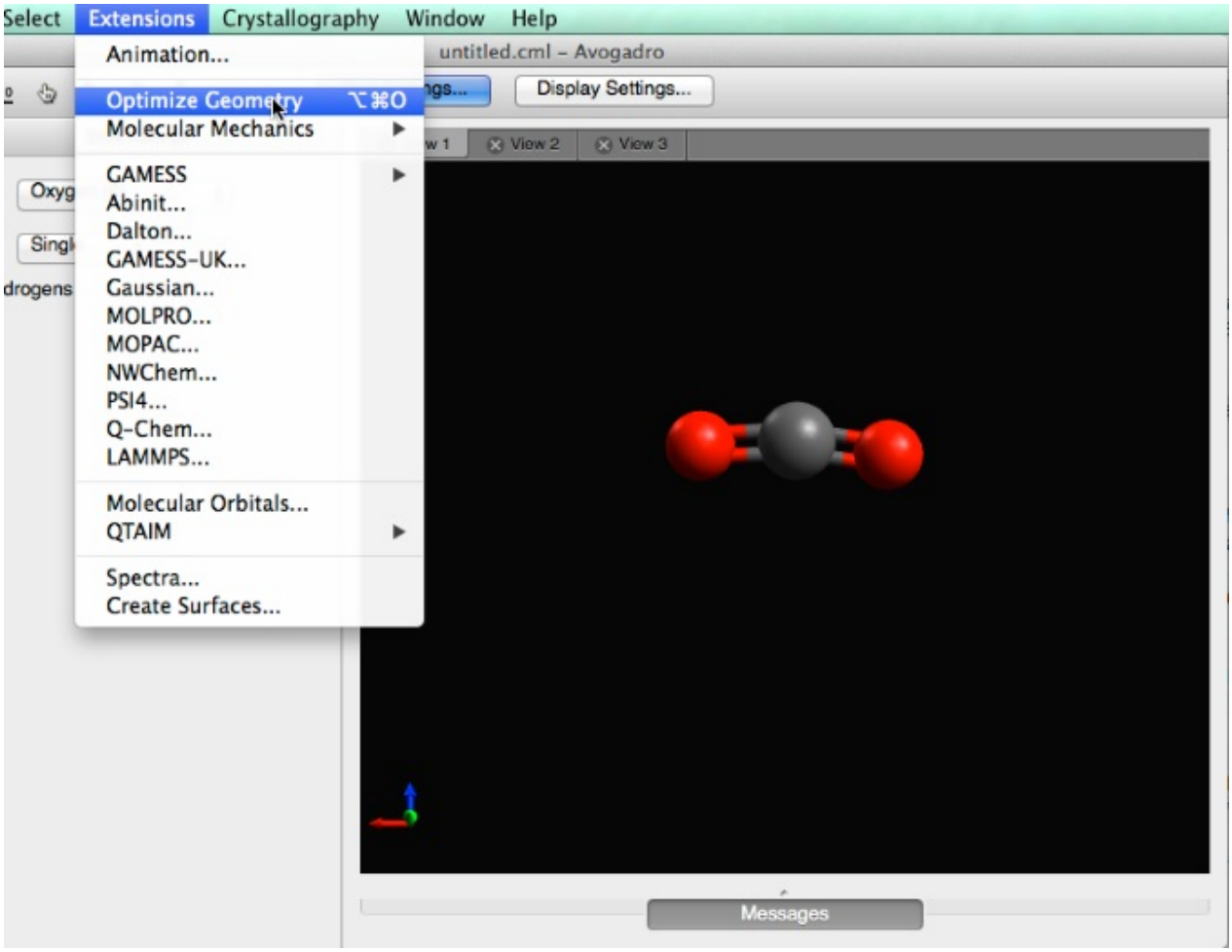
For example, to create carbon dioxide, the general structure ("O-C-O") needs to be drawn, and then by left clicking the bonds in the molecule, double bonds will be created.


untitled.cml – Avogadro
Tool Settings...
Display Settings...
Draw Settings
Element: Oxygen (8)
Bond Order: Single
Adjust Hydrogens
View 1
View 2
View 3
Messages


untitled.cml – Avogadro
Tool Settings...
Display Settings...
Draw Settings
Element: Oxygen (8)
Bond Order: Single
Adjust Hydrogens
View 1
View 2
View 3
1
Messages


untitled.cml – Avogadro
Tool Settings...
Display Settings...
Draw Settings
Element: Oxygen (8)
Bond Order: Single
Adjust Hydrogens
View 1
View 2
View 3
2
Messages

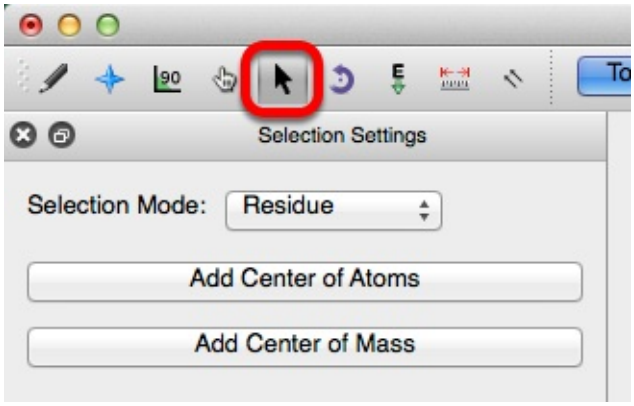
Under the "Extensions" menu, the geometry of a molecule can be optimized by selecting "Optimize Geometry".



You now know the basics on drawing a molecule!

Making Selections

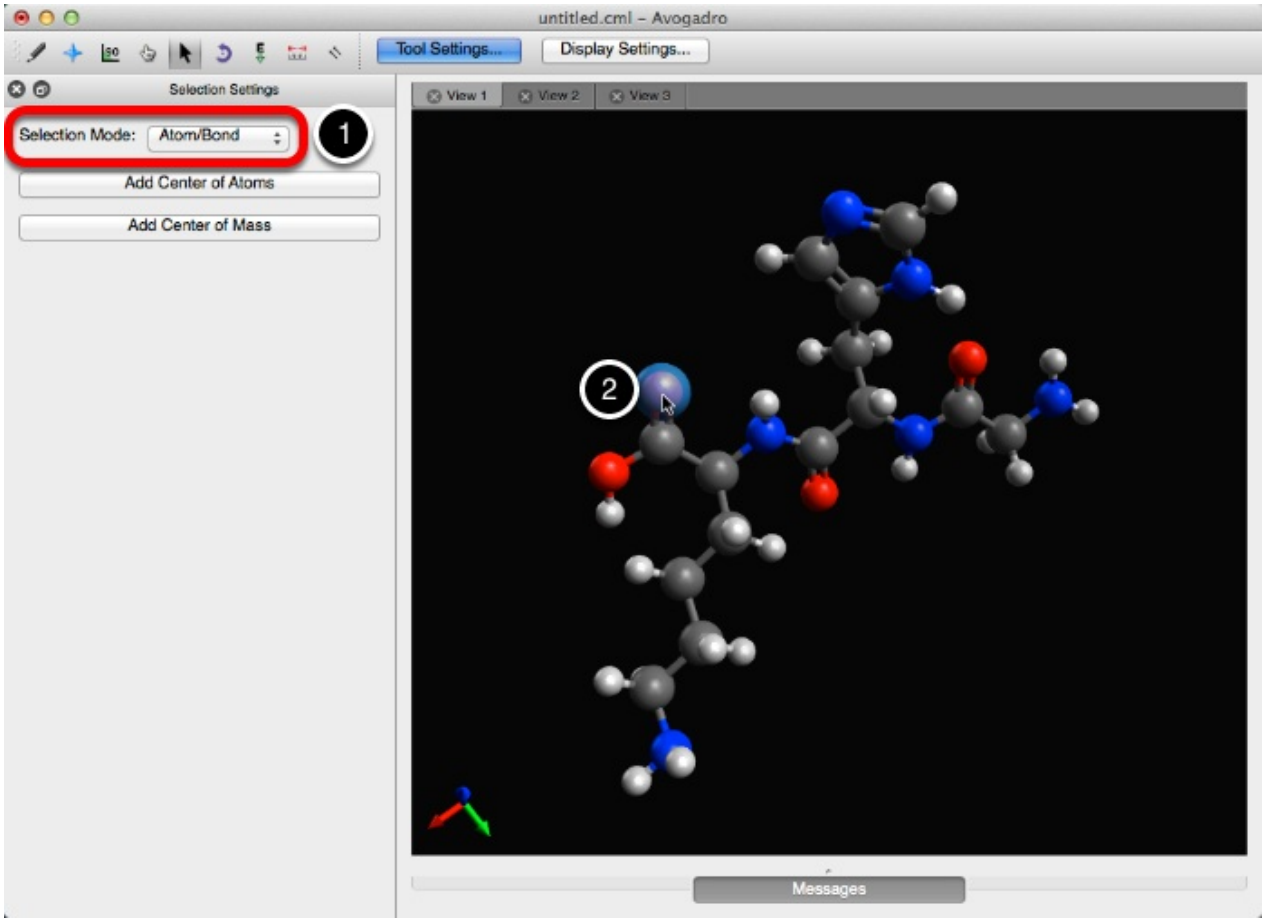
The selection tool allows the indiviual selection of atoms, bonds, or fragments.



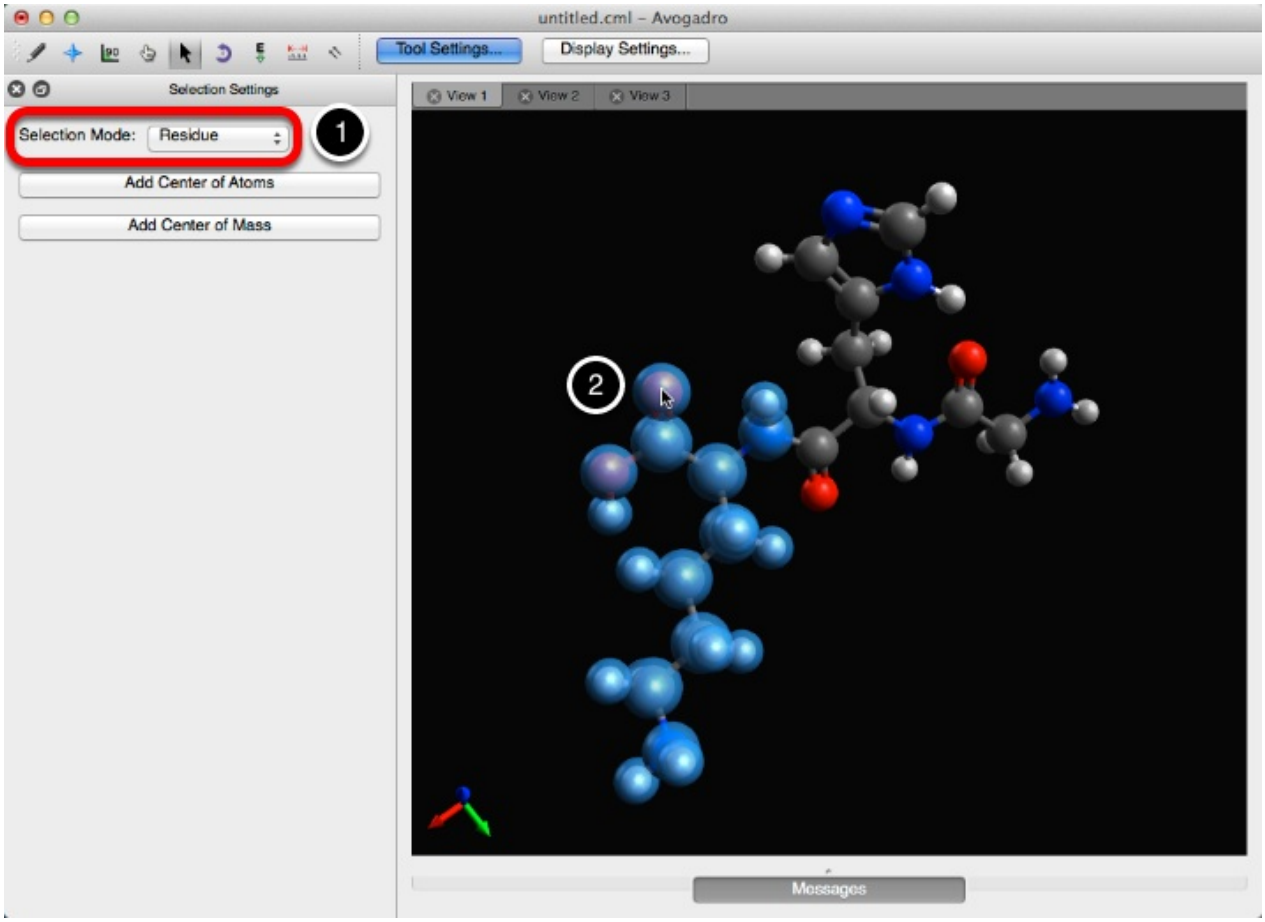
There are three types of selection modes: "Atom/Bond", "Residue", and "Molecule".

The "Atom/Bond" selection mode provides you with the ability to select a single atom within a molecule. This is achieved by left clicking the atom. Pressing down the "Shift" button on your keyboard allows the selection of multiple atoms.

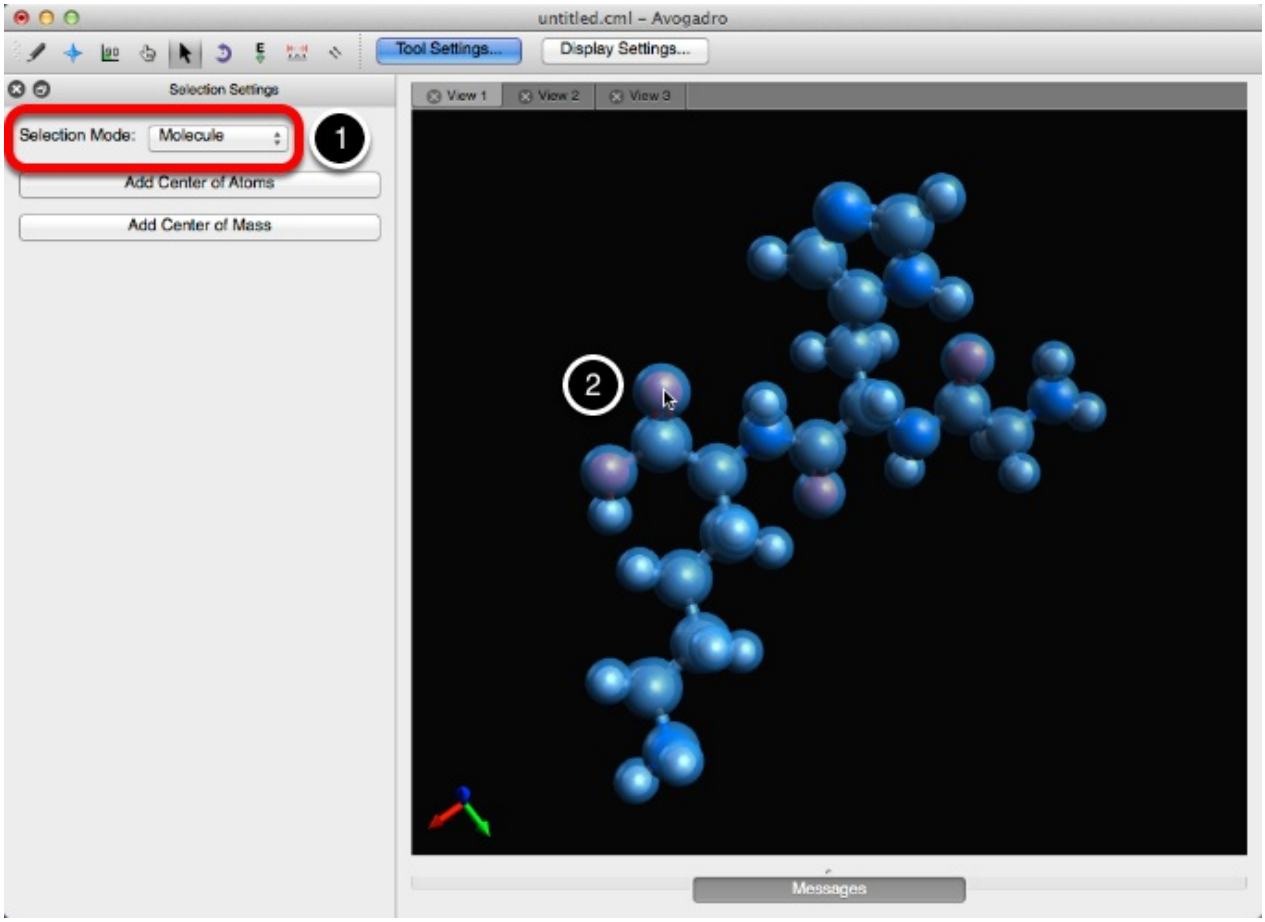
Right clicking on the black display will clear the selection made.



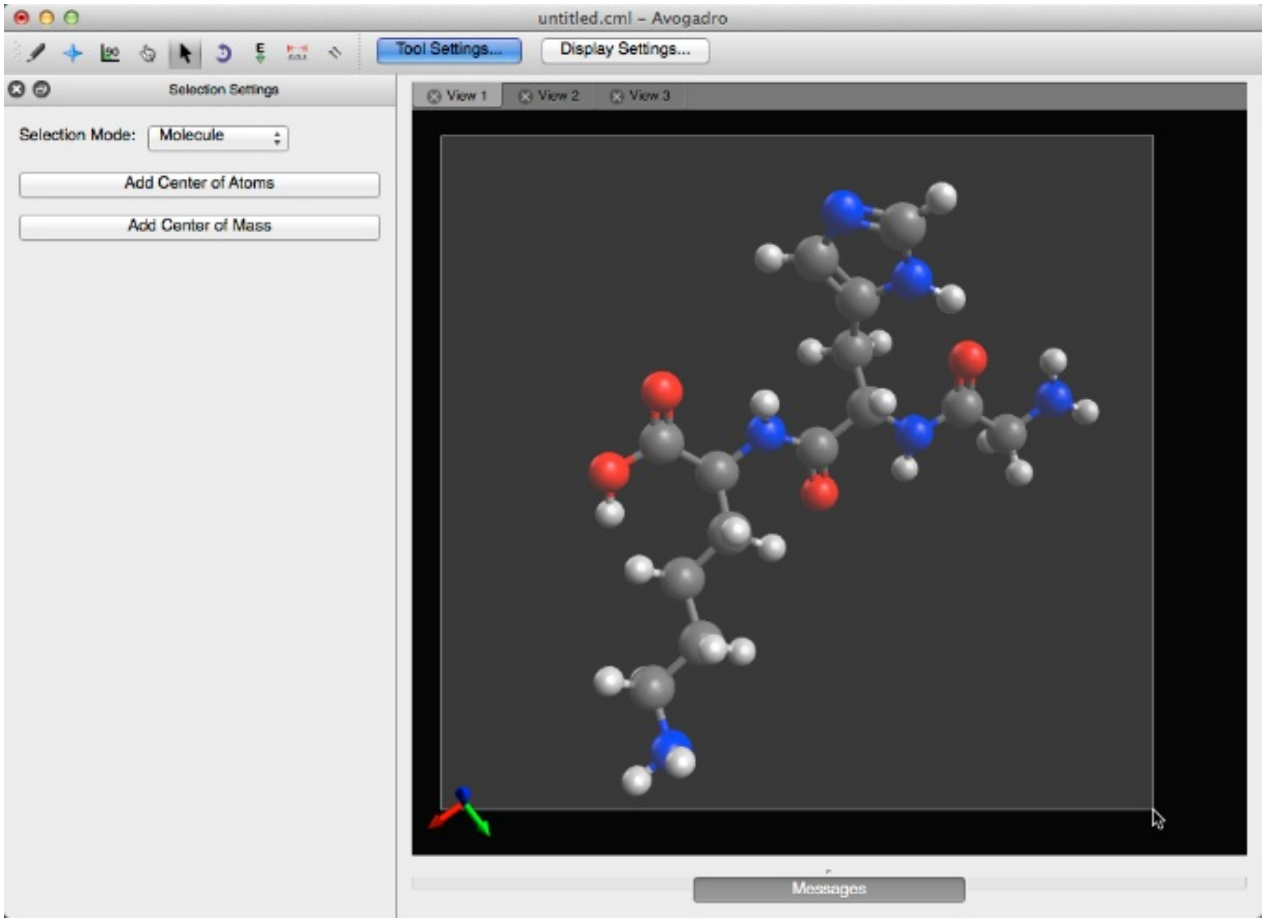
The "Residue" selection mode will select an entire residue within the molecule, by clicking on a single atom in the residue.



The "molecule" selection mode will select the entire molecule by clicking on an atom. Double clicking the molecule will also select the entire molecule.



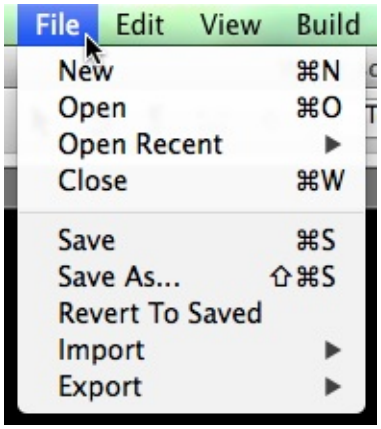
Molecules can also be selected by clicking and dragging your cursor across the display.



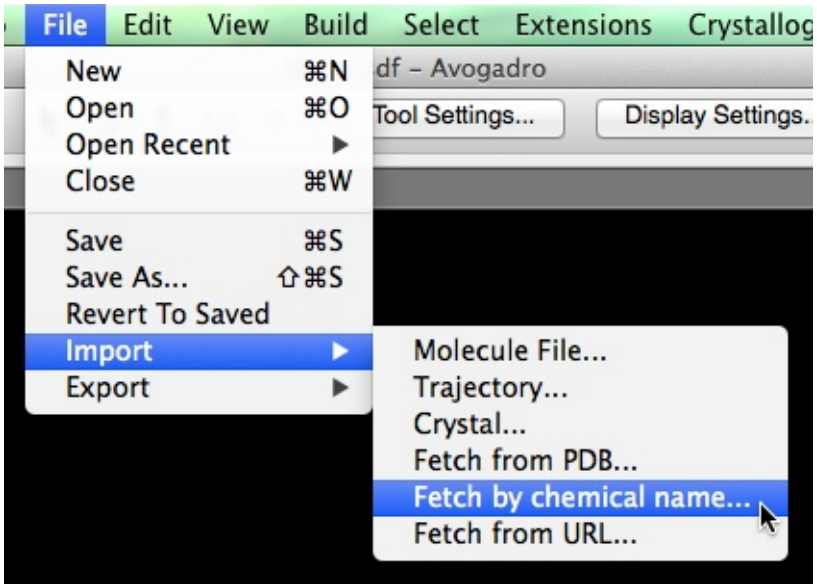
For more information refer to the Selection Tool section.

Importing Molecules by Name

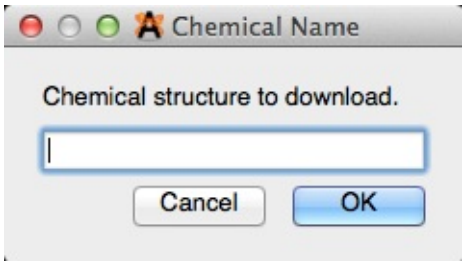
Select the "File" menu.



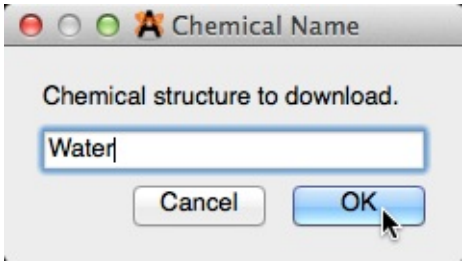
Then select "Import", and "Fetch by chemical name..."



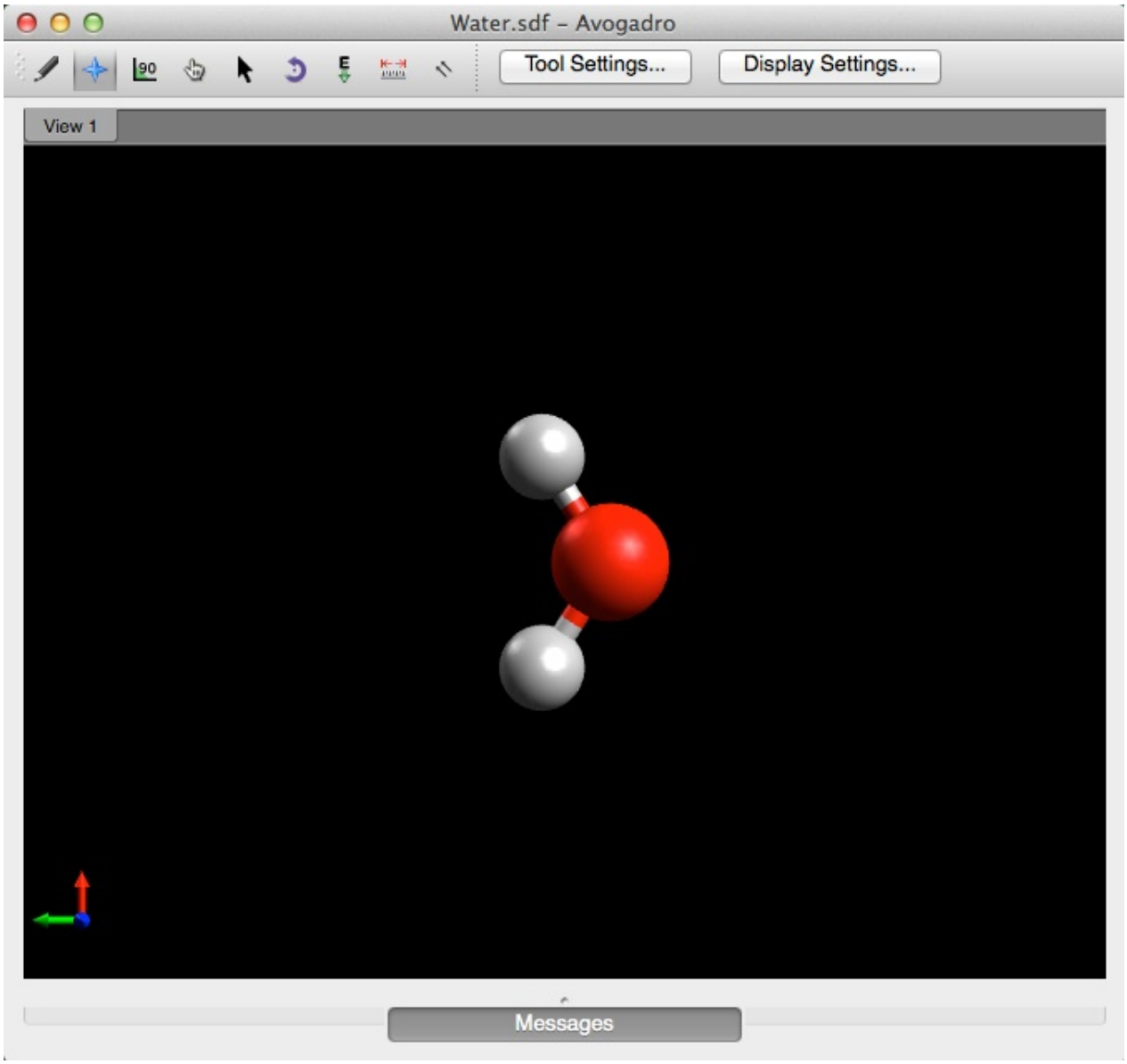
A dialog box will pop up (depicted below), where you can type in any chemical name.



Avogadro will import the molecule into the viewing screen after you click "OK".



It may take a few seconds or even a minute to download the molecule online. Avogadro uses the NIH "Chemical Resolver" http://cactus.nci.nih.gov/chemical/structure to convert the name into a molecular structure.

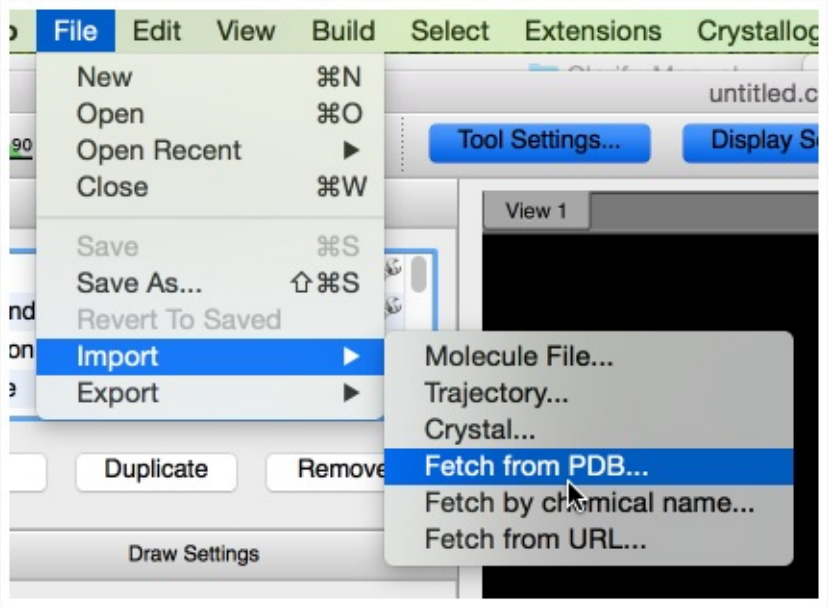


Importing from the Protein Data Bank (PDB)

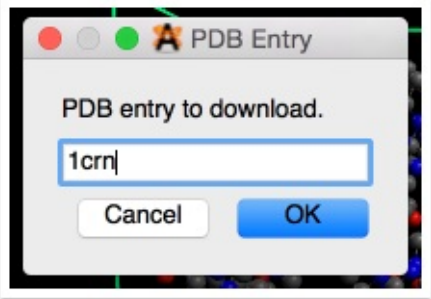
You can read PDB files that you download yourself from http://www.rcsb.org/ or access the PDB code yourself.

Importing directly

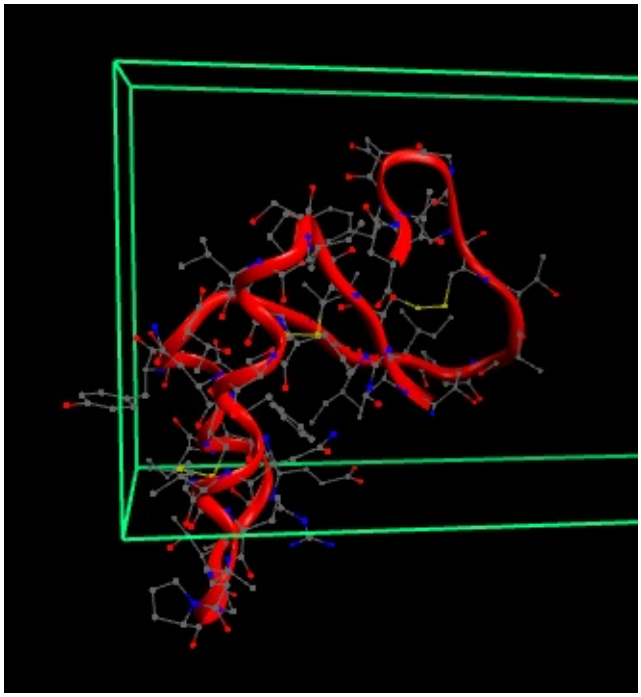
Older versions of Avogadro have a bug with direct access to the PDB (since the website has moved) but using v 1.2.0, you can again use File > Import > Fetch from PDB... to download proteins.



A dialog will come up and allow you to enter a PDB code (e.g., 1CRN for crambin)



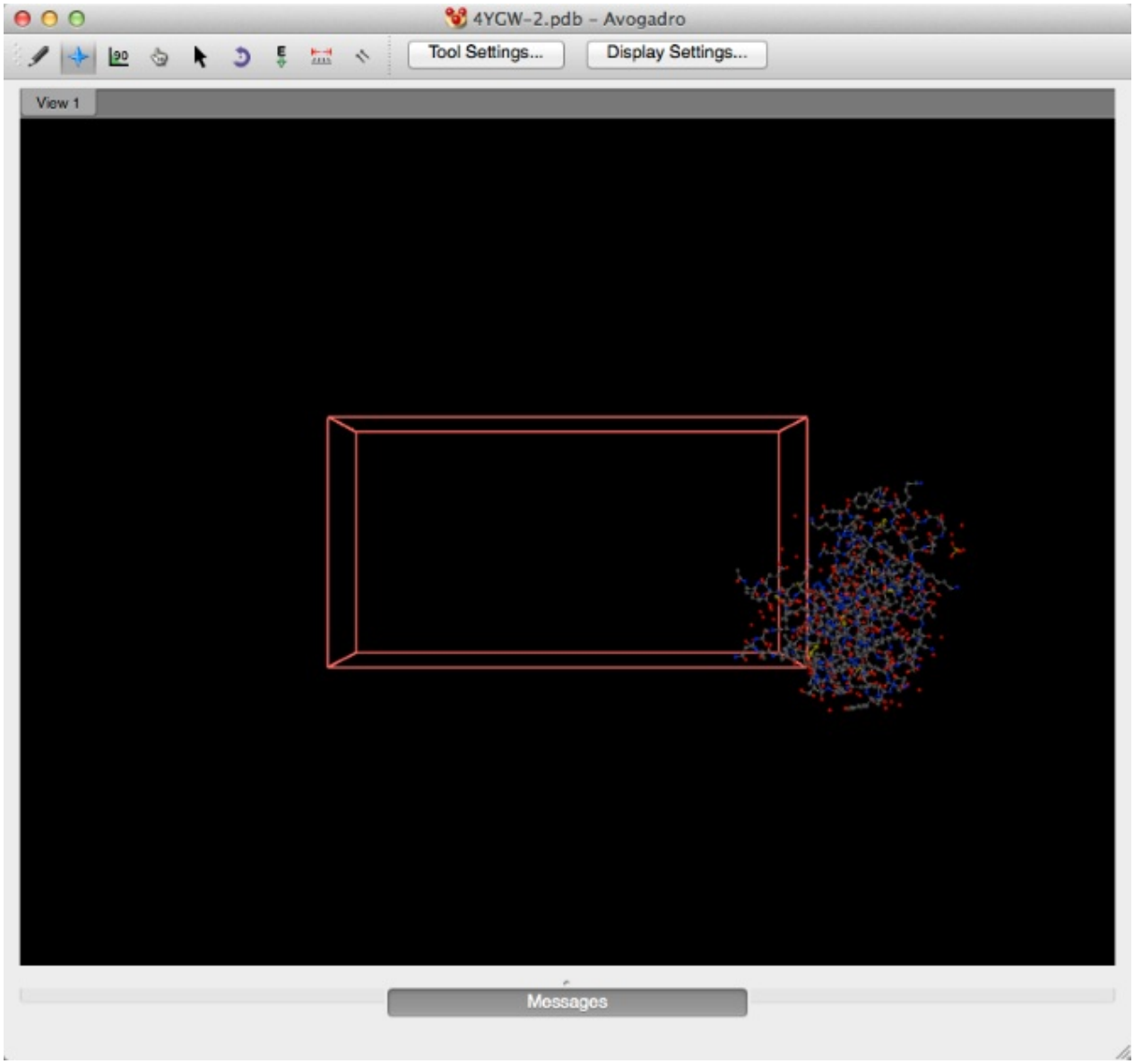
There it is... the PDB data direct from the website.



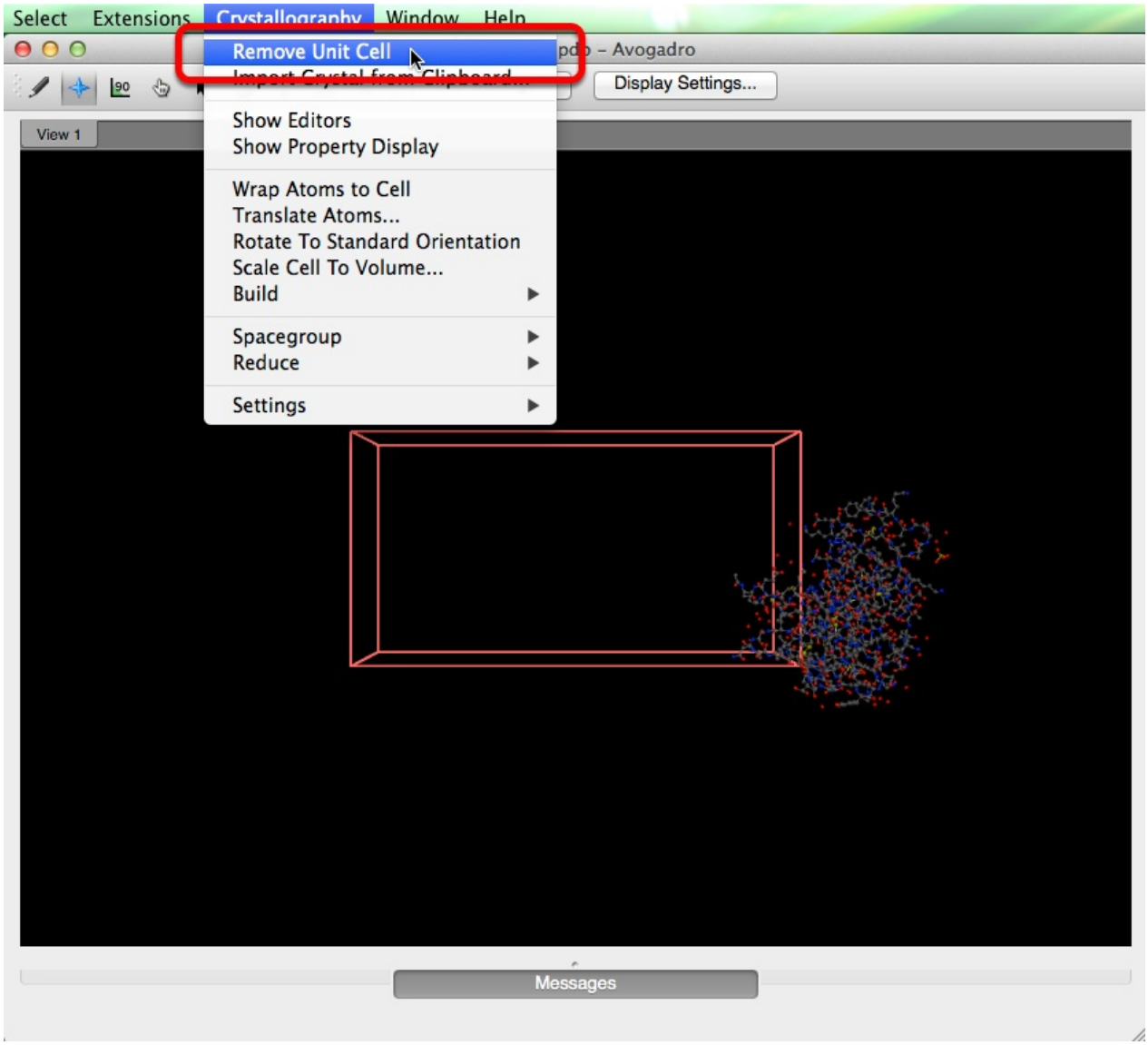
Reading a Downloaded PDB file

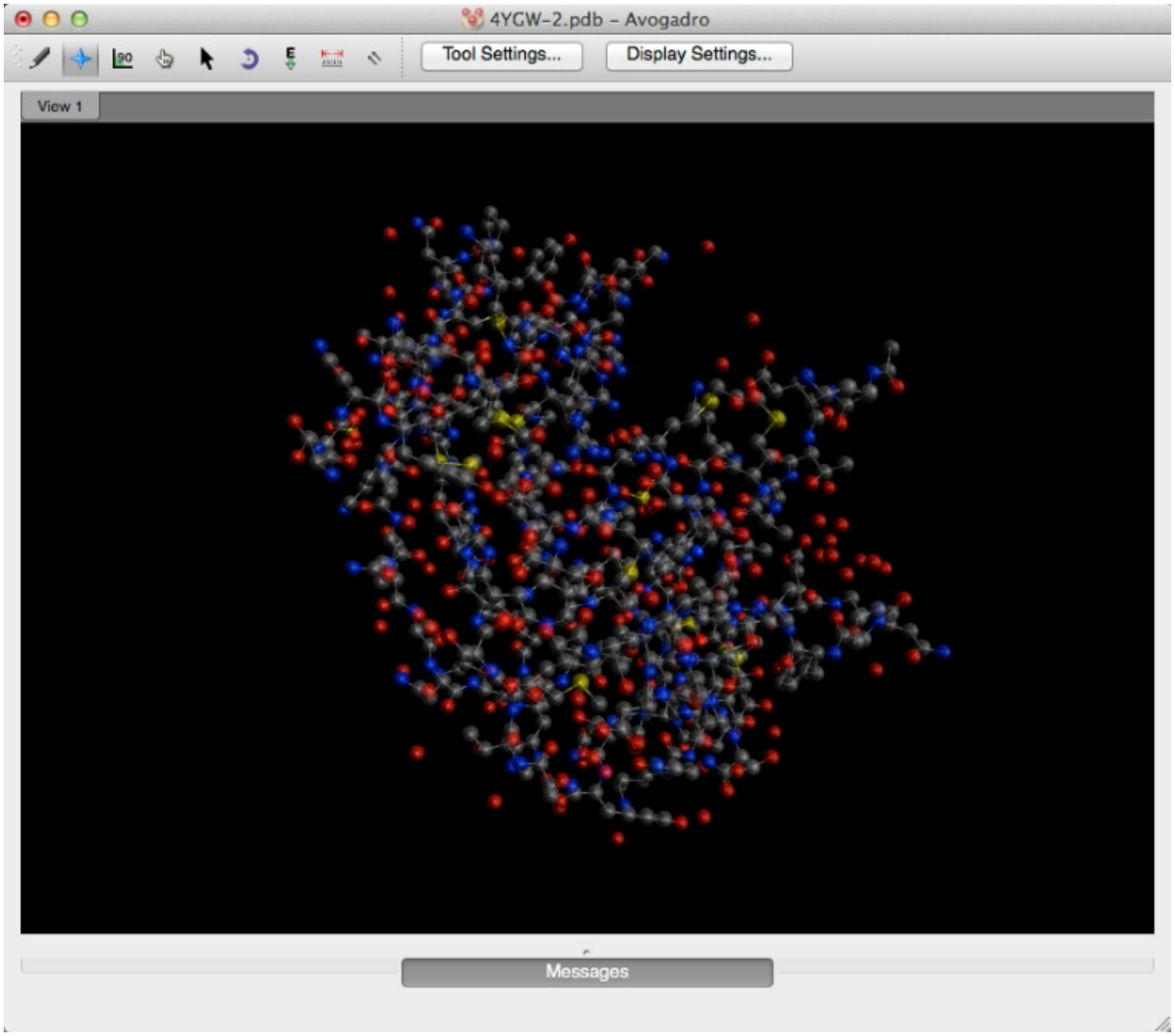
If the direct import doesn't work, you can also use the website yourself. Go to http://www.rcsb.org/ and select a protein, then download the "PDB File (text)" format of the file. From your downloads folder you can either drag and drop the file onto an Avogadro display screen, or drag and drop the file over the Avogadro application icon.

Dragging and dropping the file will open the PDB import with a unit cell (Avogadro displays unit cells for all PDB imports).



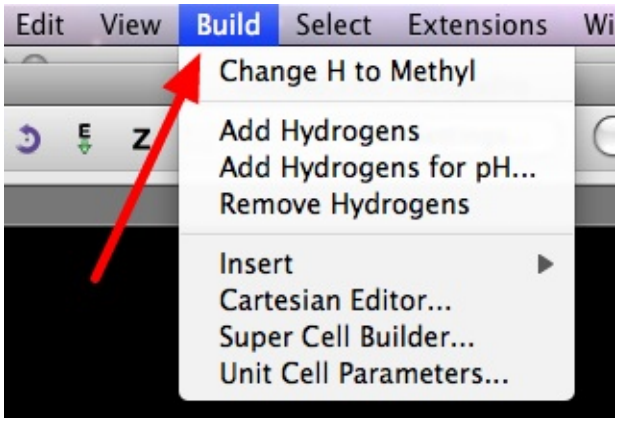
If the unit cell is unwanted, you can remove the unit cell under the "Crystallography" menu by selecting "Remove Unit Cell".


Select
Extensions
Crystallography
Window
Help
Remove Unit Cell
Import Crystal from Clipboard...
Show Editors
Show Property Display
Wrap Atoms to Cell
Translate Atoms...
Rotate To Standard Orientation
Scale Cell To Volume...
Build
Spacegroup
Reduce
Settings
Display Settings...
View 1
Messages

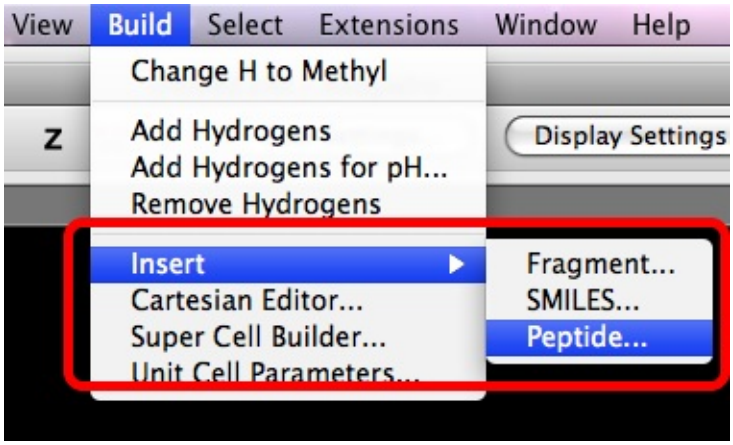

4YGW-2.pdb – Avogadro
Tool Settings...
Display Settings...
View 1
Messages

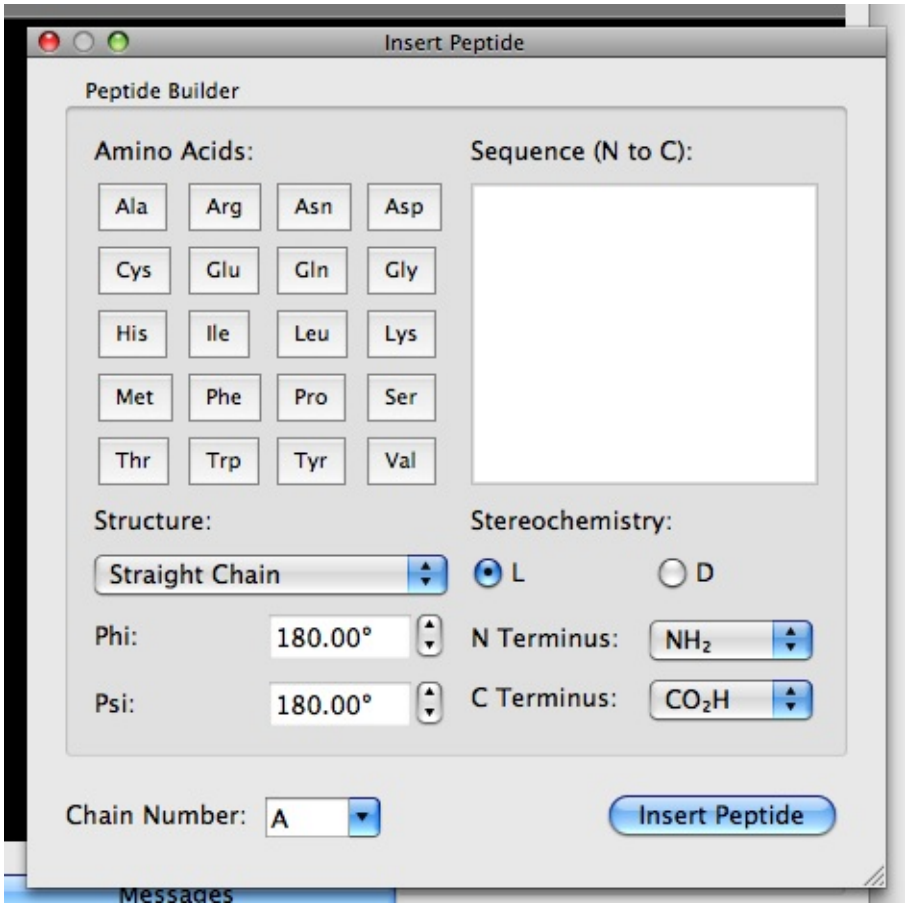
Building a Peptide

A walkthrough on how to create a custom peptide model in Avogadro.

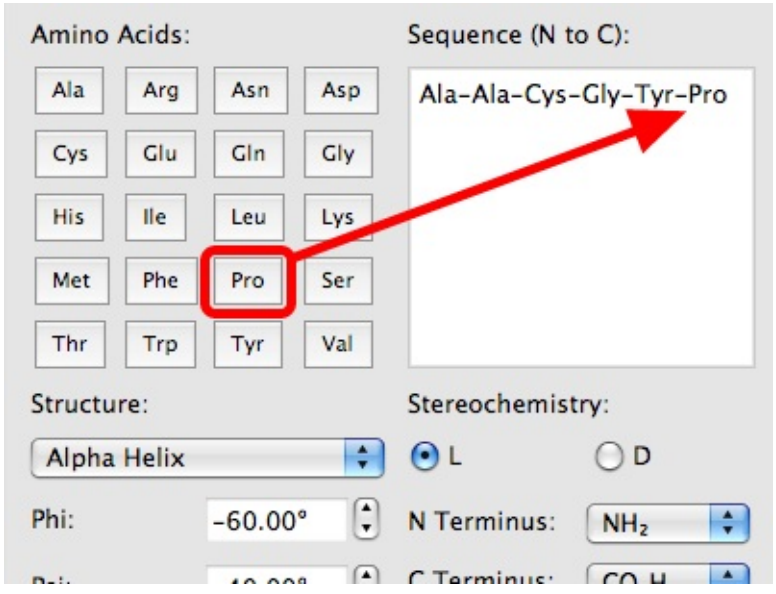


Select the “Build” menu.

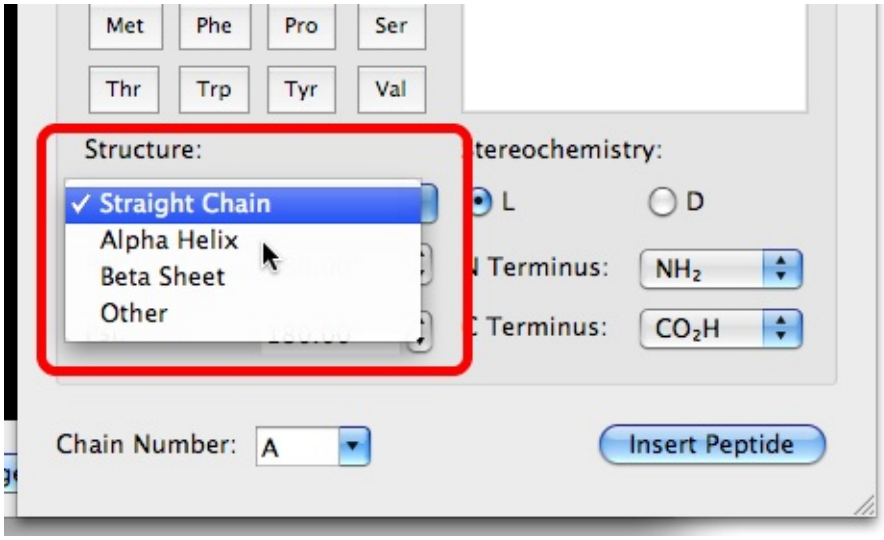




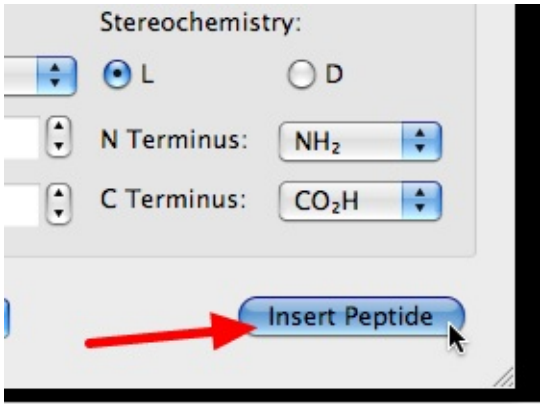
Bring up the peptide builder window. You can select amino acids to insert into the new peptide.



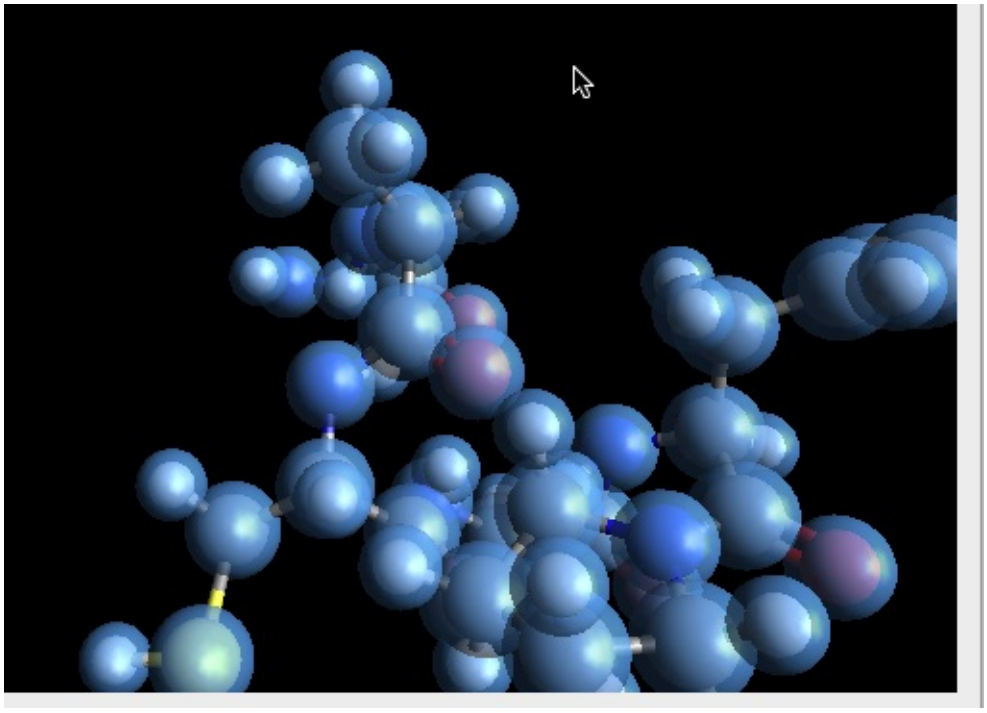
As you click on particular amino acids, they will be added to the sequence on the right. The peptide will build up as a sequence, starting from the N terminus. Of course you can also type the residues directly or paste from an online database.

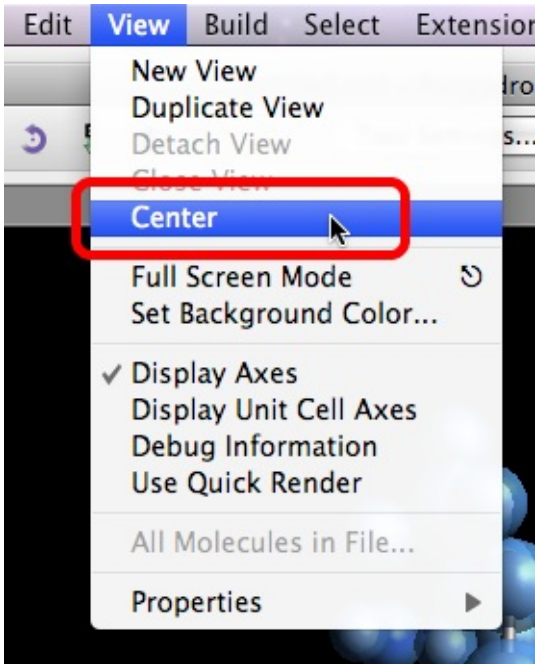


You can pick the secondary structure



Click to insert the sequence into the main window. The new oligopeptide will be selected automatically, and the manipulate tool will allow you to translate and rotate the chain into the position you want.

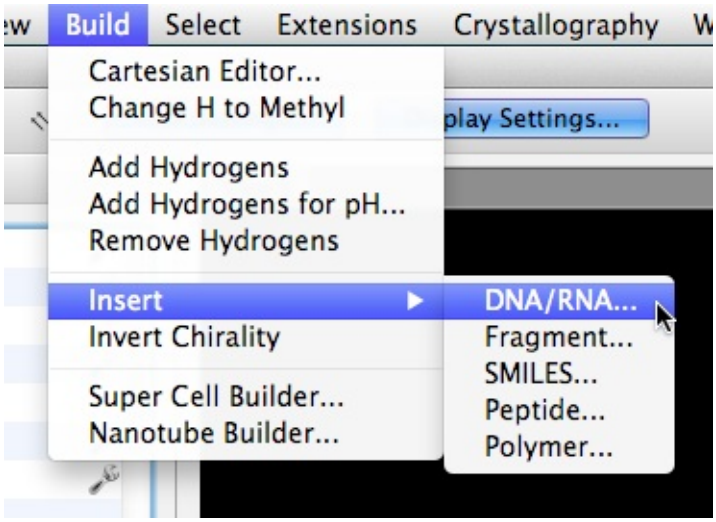




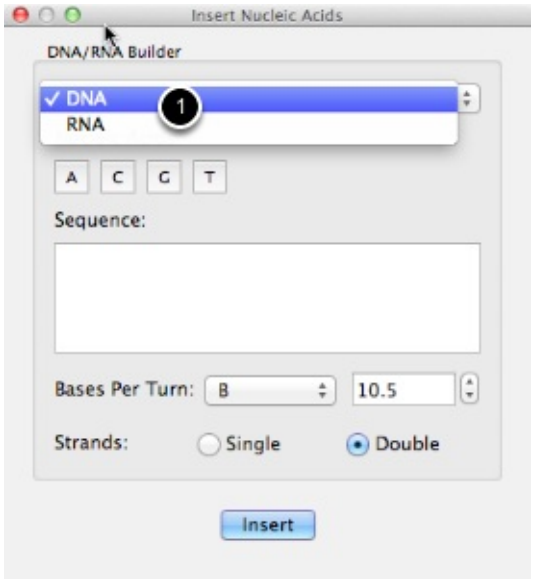
You may wish to re-center the view, since the new peptide may be large.

Building DNA/RNA

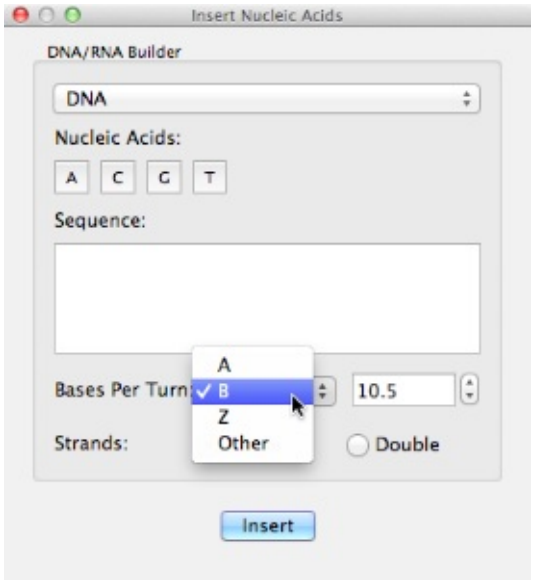
Avogadro now has a builder for nucleic acid sequences and this walk-through will show you how to use it.



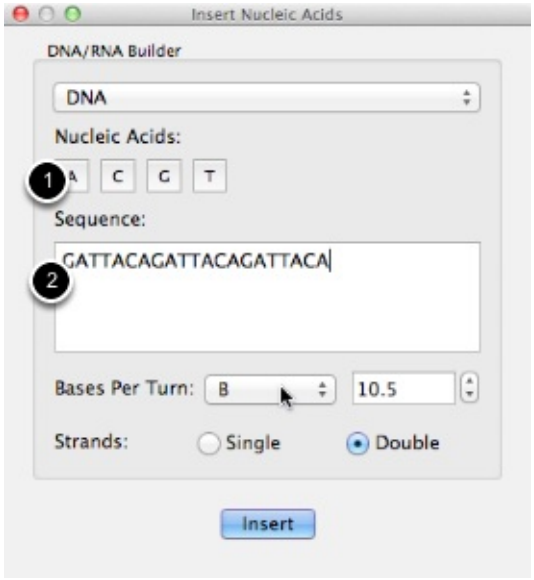
The DNA/RNA builder is under the "Build" menu and "Insert" submenu.



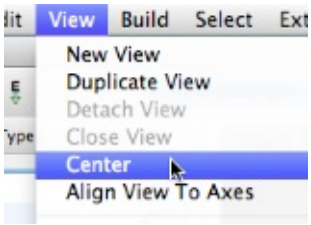
Select either DNA or RNA (1) and the rest of the window will update accordingly.



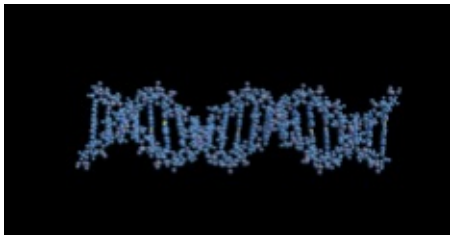
You can also control the number of bases per turn as shown (with defaults for A-DNA, B-DNA, Z-DNA, or RNA).



You can enter the sequence either by clicking the buttons, or by typing the one-letter codes directly. For DNA sequences (as shown here), you can insert either single-stranded or double-stranded DNA.



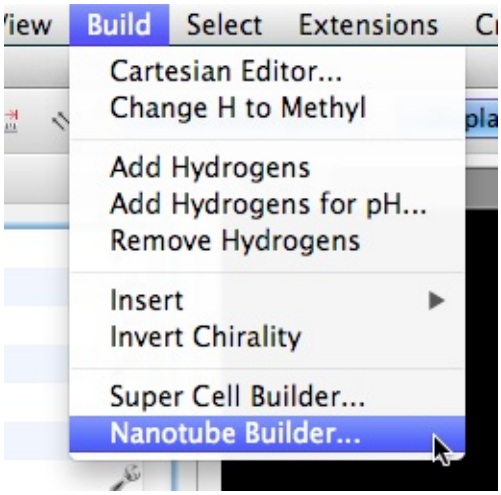
You may wish to re-center the view or align the view to axes to see the whole molecule.



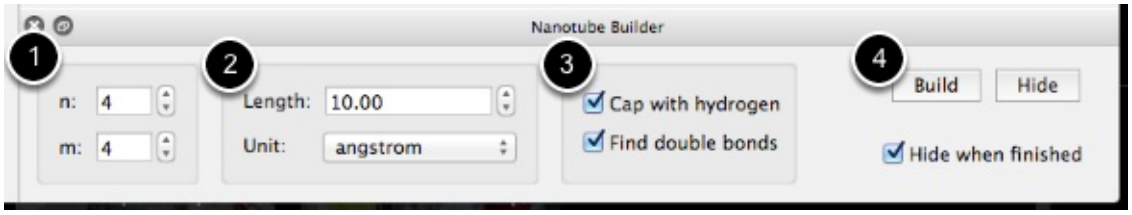
There we go -- the well-known DNA double-helix!

Building Carbon Nanotubes

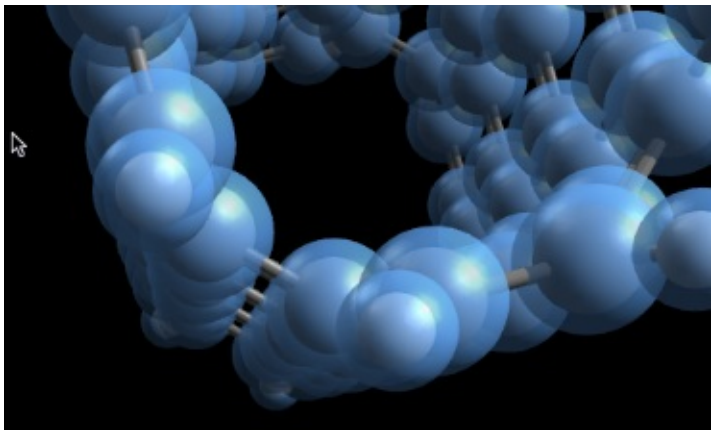
Avogadro 1.1 includes a new nanotube builder, based on the well-known TubeGen code and website from the Doren group at U. Delaware. (http://turin.nss.udel.edu/research/tubegenonline.html)



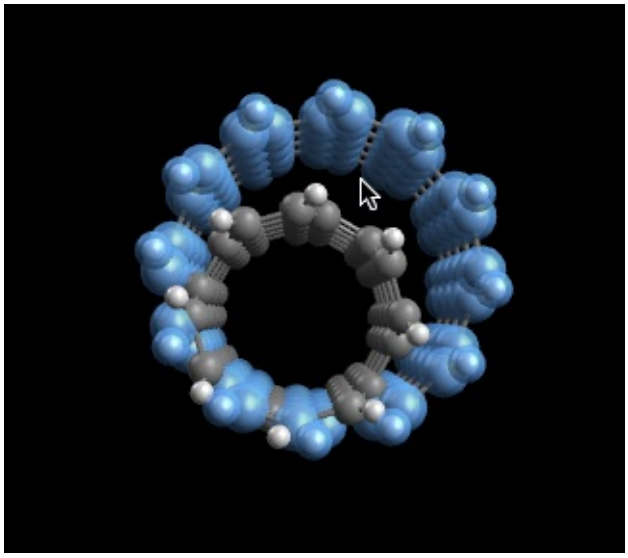
Under the Build menu, there's a new option for the nanotube builder. At the moment only single-walled nanotubes (SWNT) can be built in one step, although it's easy to generate several nested tubes for multi-walled (MWNT) as shown here.



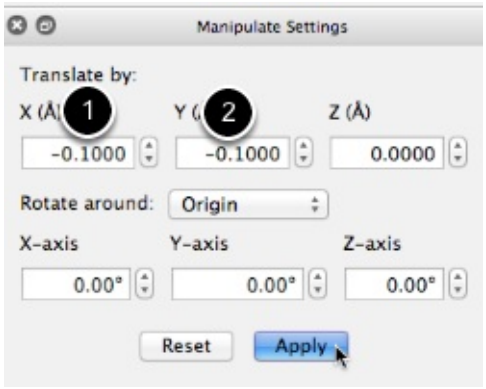
The builder will show up at the bottom of the Avogadro window. You can set the n,m indexes to determine the type of nanotube (1) the length of the tube (2), in Angstrom, bohr, picometers, nanometers, or periodic unit cells (e.g., if you wish to do a calculation with periodic boundar conditions), and how to terminate the nanotube (3). **NOTE**: determining double bonds can be time-consuming on large nanotubes.



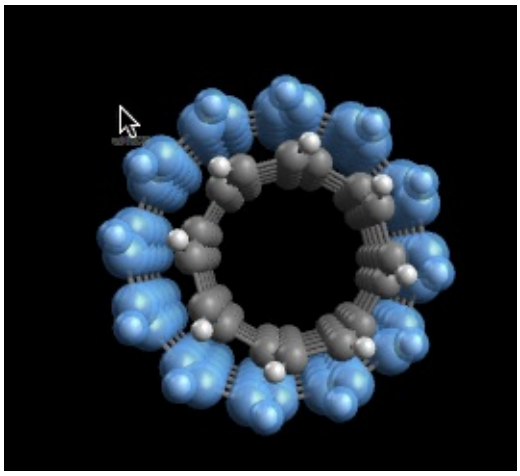
The nanotube will be generated aligned along the z-axis, so you may want to re-center the view.



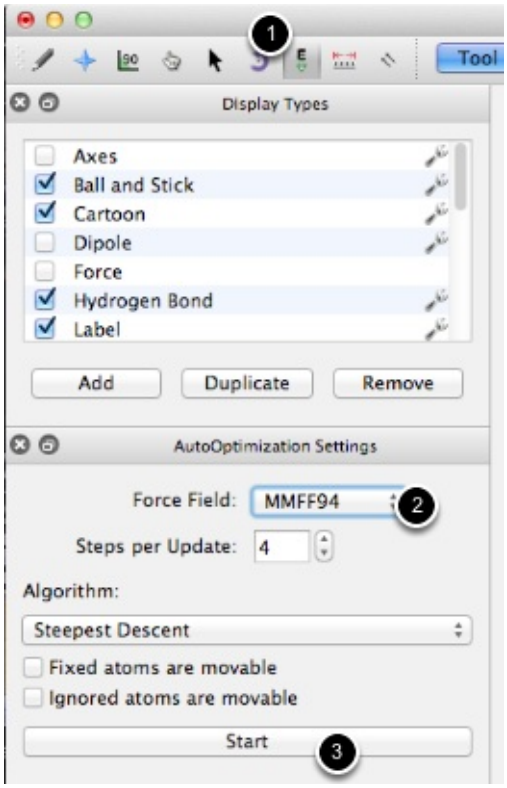
Here, we've added a 6,6 nanotube after inserting our 4,4 nanotube. We'll need to re-center the tube to produce a more accurate double-walled system.



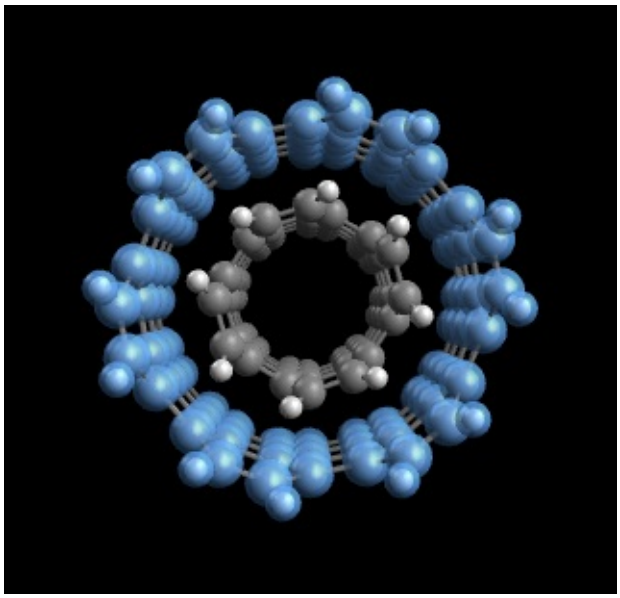
Here, we use the manual translation options, new in Avogadro 1.1, to “nudge” the 6,6 nanotube in the XY plane to properly center around the 4,4 nanotube.



Here we’ve nudged the 6,6 tube into an approximately correct position. We’ll now use Avogadro’s built-in force fields and the Auto-Optimize tool to relax the structure.



We (1) select the Auto-Optimize tool to allow interactive minimization of the nanotubes, and (2) select the MMFF94 force field. Other forcefields would also likely work well. Finally (3) start the optimization.

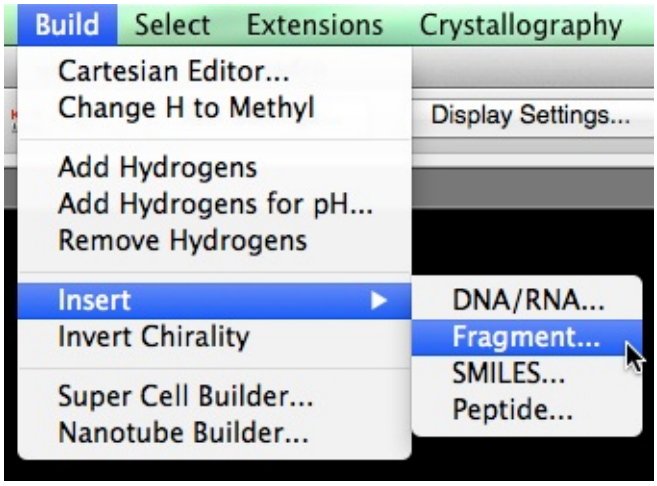


After a few steps, you can see a nicely relaxed double-walled nanotube. You could repeat the process as desired.

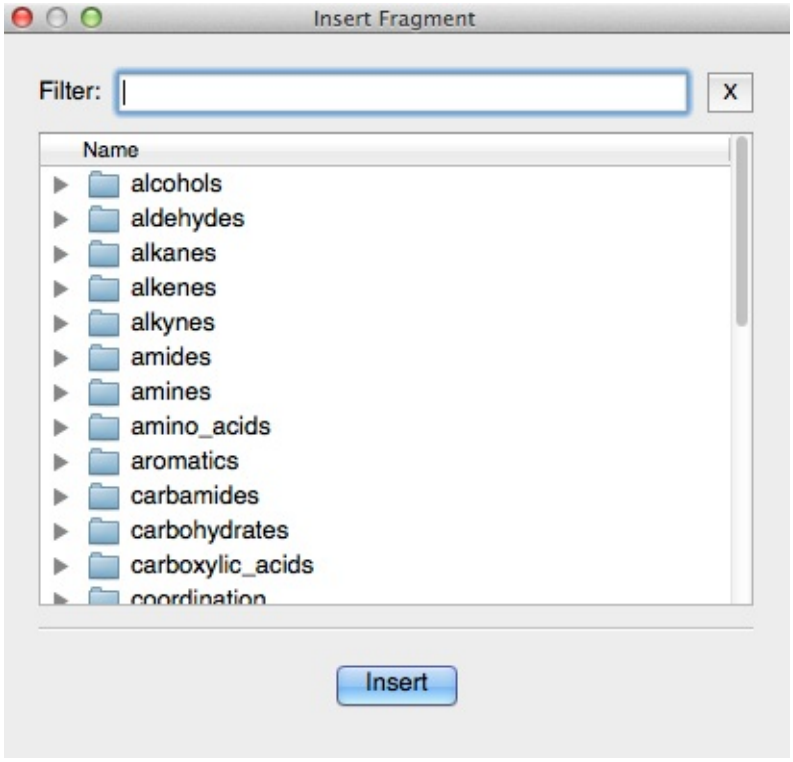
Insert Fragments

Avogadro includes over 300 common molecules and molecular fragments to make building larger structures easy.

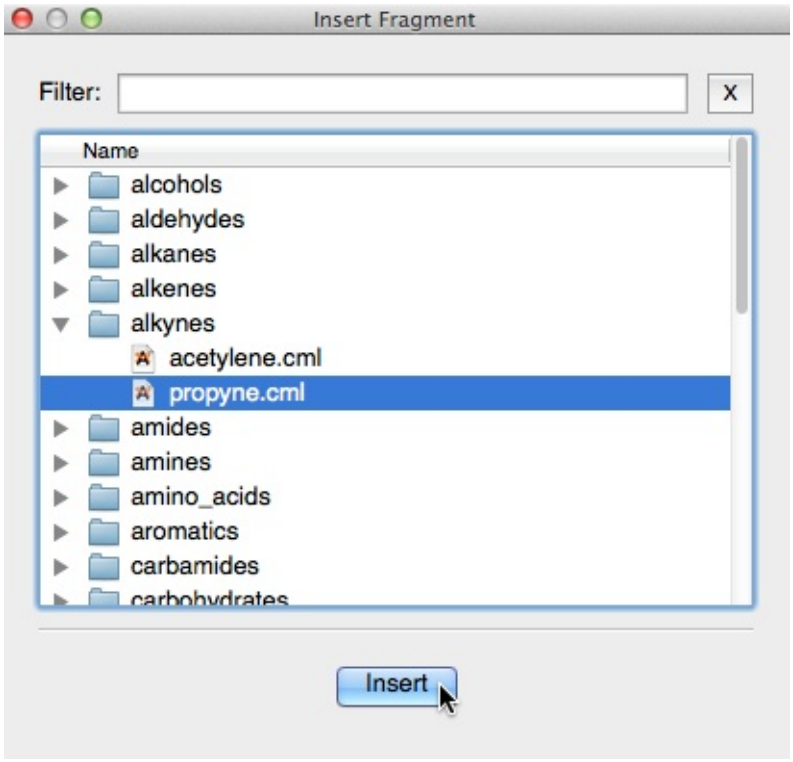
Under the "Build" menu, hold your cursor over "Insert", and then select "Fragment...".



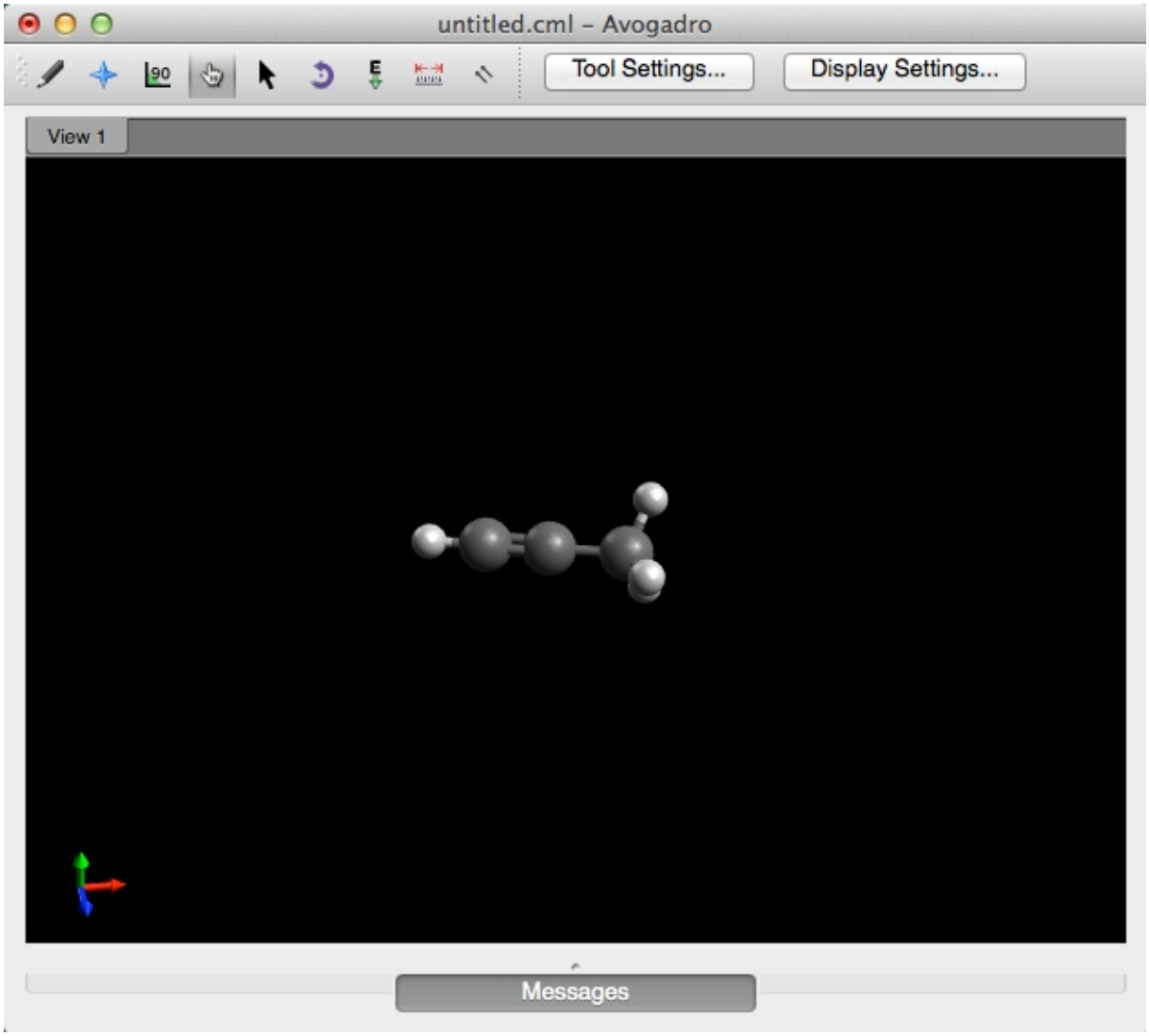
A database of fragments will then pop up (shown below). You can filter the selection if need be.



After you've made your fragment selection, click "Insert".



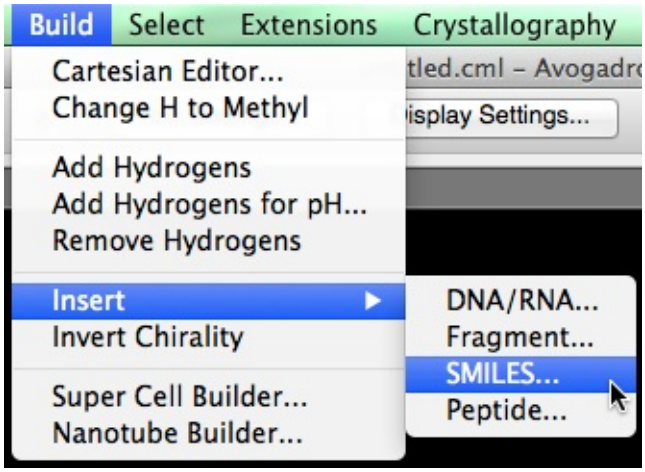
The fragment will be inserted and the Manipulate tool will be selected so you can move the new fragment around the window.


untitled.cml – Avogadro
Tool Settings...
Display Settings...
View 1
Messages

Building with SMILES

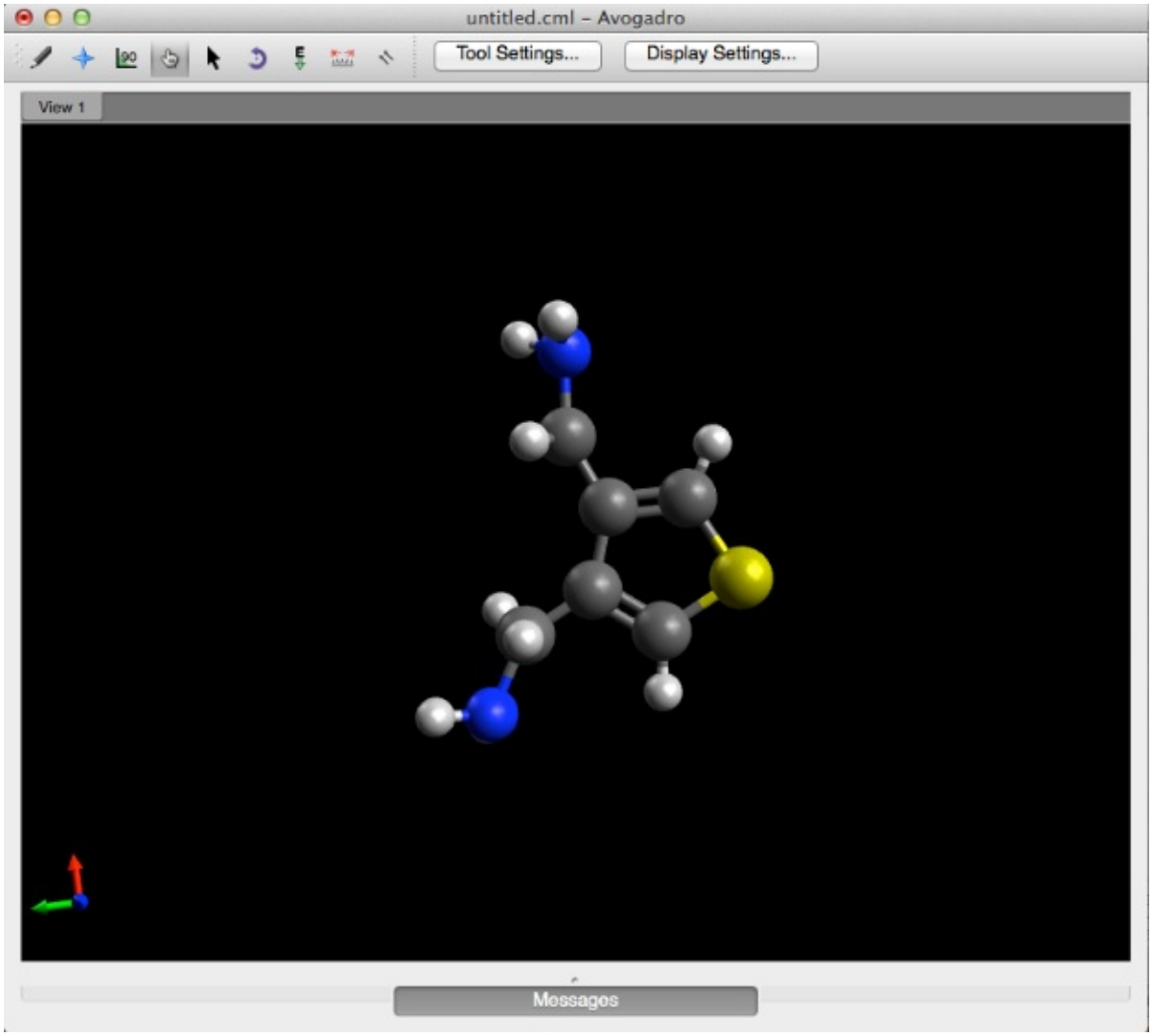
SMILES (Simplified molecular-input line-entry system) allows you to build molecules through a string of text. If you have a SMILES string (e.g., copied from a paper or website) or prefer to enter one for a complicated molecule, Avogadro will build a 3D geometry from the SMILES.

Under the "Build" menu, hold your cursor over "Insert", and select "SMILES...".



Enter your SMILES fragment, and select "OK".

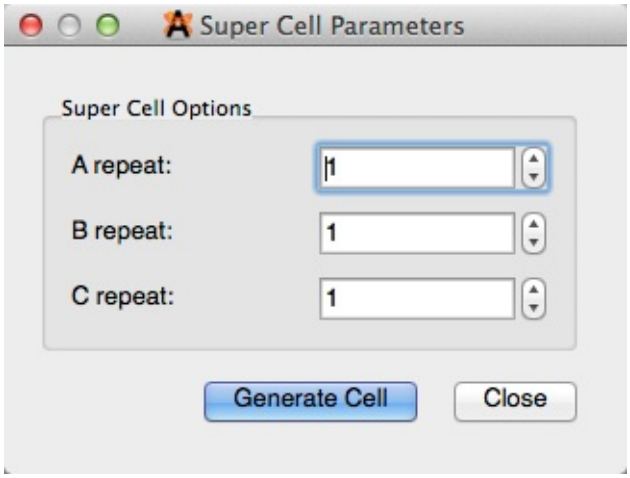
There it is..


untitled.cml – Avogadro
Tool Settings...
Display Settings...
View 1
Messages

Super Cell Builder

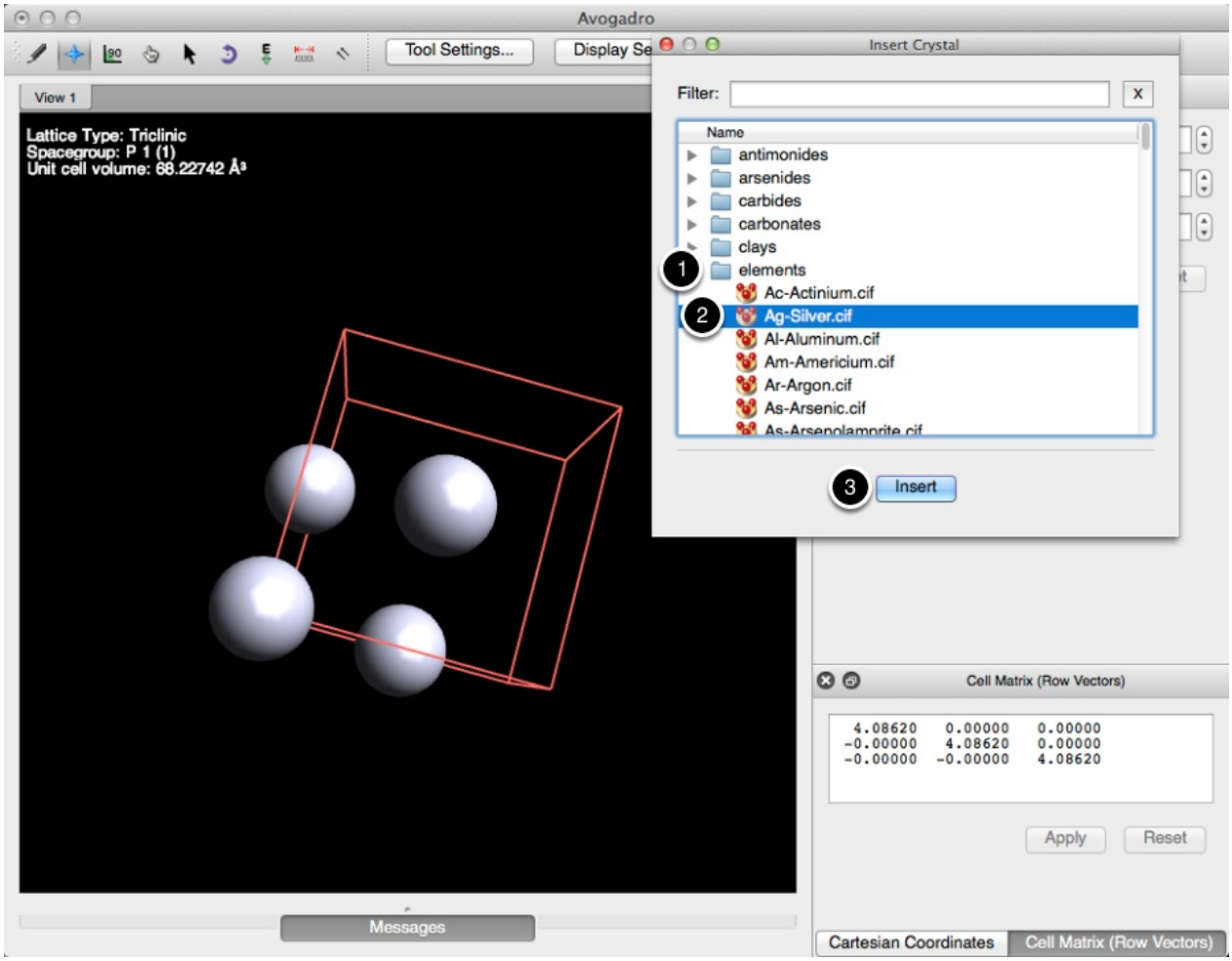
Once a crystal surface has been built, the Super Cell Builder can expand atoms within a space group, replicate the unit cell, and perform simple bonding.

When "Super Cell Builder..." is selected under the "Build" menu, the dialog box below pops up. This dialog box will allow you to replicate a unit cell that has already been created (if need be, a unit cell can be created by selecting "Add Unit Cell" under the "Crystallography" menu).

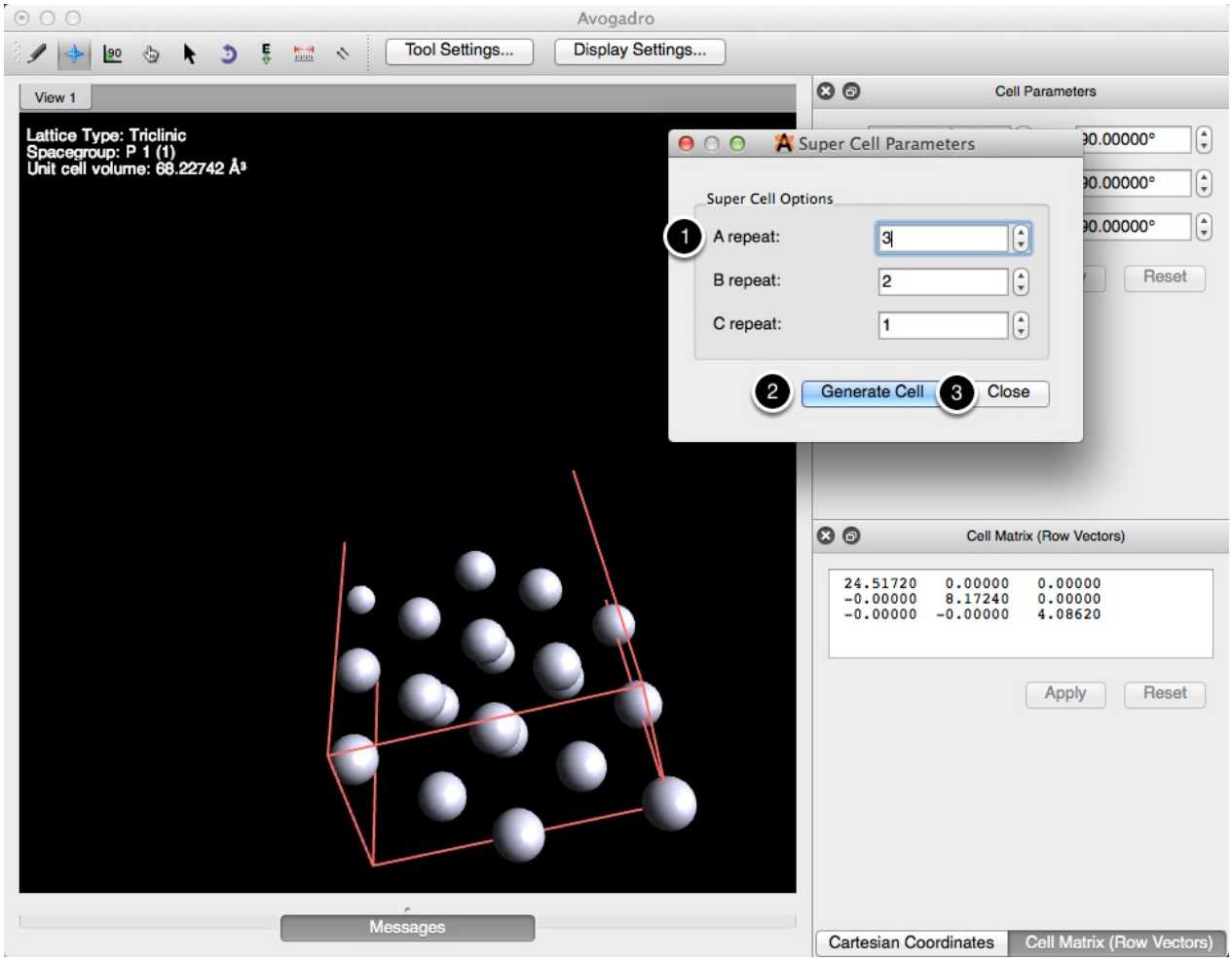


Creating a Surface

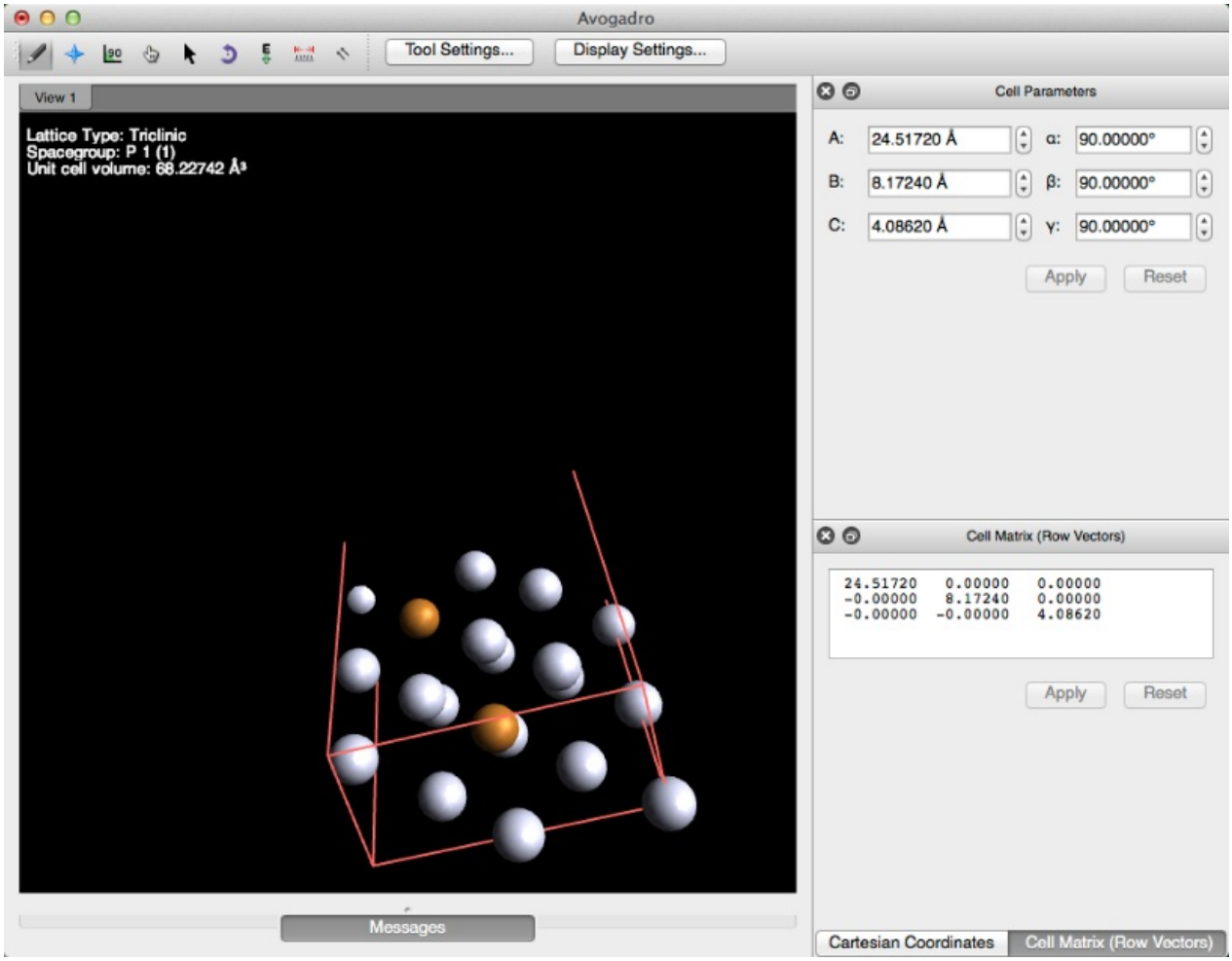
One way supercell can be utilized is by creating a surface. Below is an elemental unit cell comprised of silver. This cell was imported through the "File" menu, under "Import", "Crystal...". When the dialog box appears follow the procedure displayed below.



A unit cell can then be replicated to make a *slab* or a surface. For this example, the parameters were edited as shown in the image below. After editing the parameters, clicking "Generate Cell" will expand your surface.



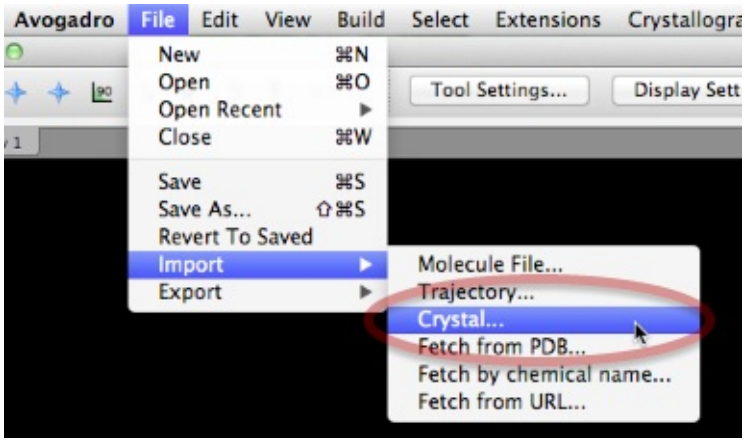
A surface can then be *modified* by introducing impurities. Here, copper impurities were added to the silver surface. This file can now be exported to another program to determine, through calculations, how the impurities will impact the surface.


Avogadro
Tool Settings...
Display Settings...
View 1
Lattice Type: Triclinic
Spacegroup: P 1 (1)
Unit cell volume: 68.22742 Å³
Messages
Cell Parameters
A: 24.51720 Å
B: 8.17240 Å
C: 4.08620 Å
α: 90.00000°
β: 90.00000°
γ: 90.00000°
Apply
Reset
Cell Matrix (Row Vectors)
24.51720 0.00000 0.00000
-0.00000 8.17240 0.00000
-0.00000 -0.00000 4.08620
Apply
Reset
Cartesian Coordinates
Cell Matrix (Row Vectors)

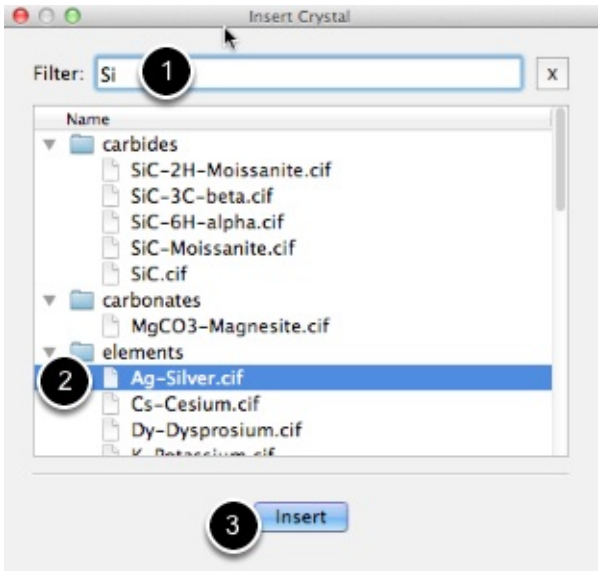
Building a Crystal Surface (Slab)

Build up a crystal surface, e.g., Pt <111> for a defined Miller Plane.

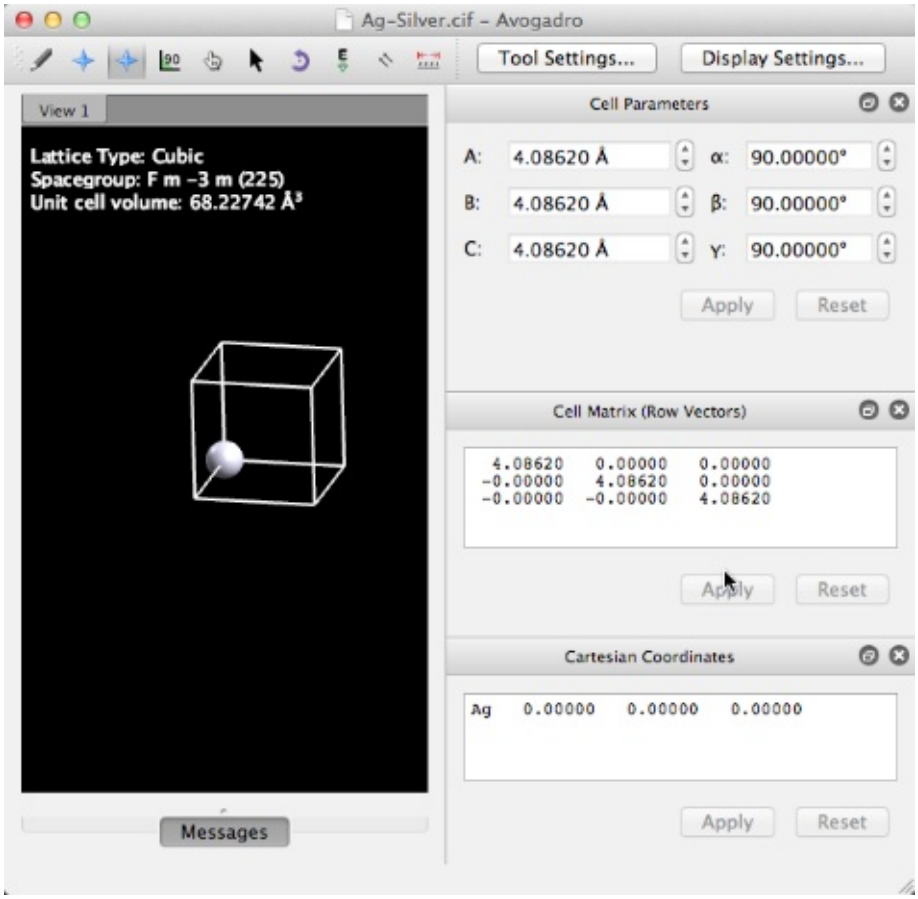
Import the appropriate crystal structure.



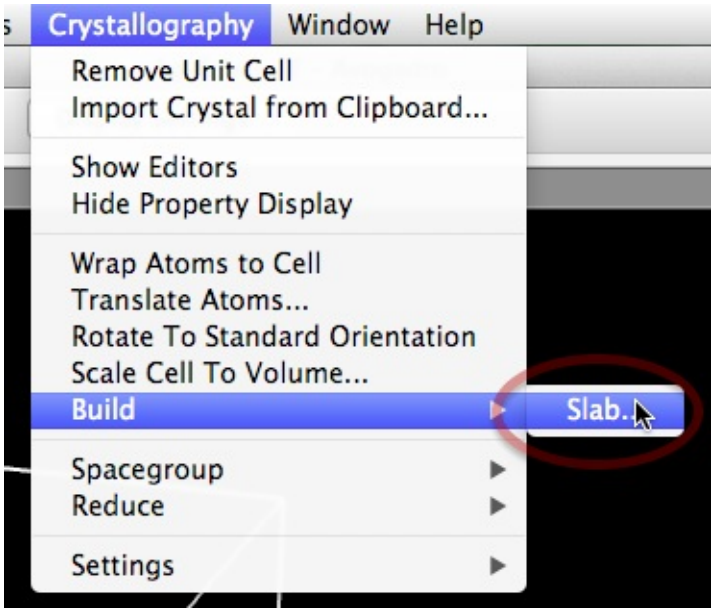
Either open a CIF file with the crystal structure needed, or import one from the built-in Avogadro crystal library. The tutorial will assume you import a structure from the Avogadro library. Choose File > Import > Crystal to bring up the library.



Either browse through the crystals, or type a filter -- by element or name. Click "Insert" to import the selected structure.



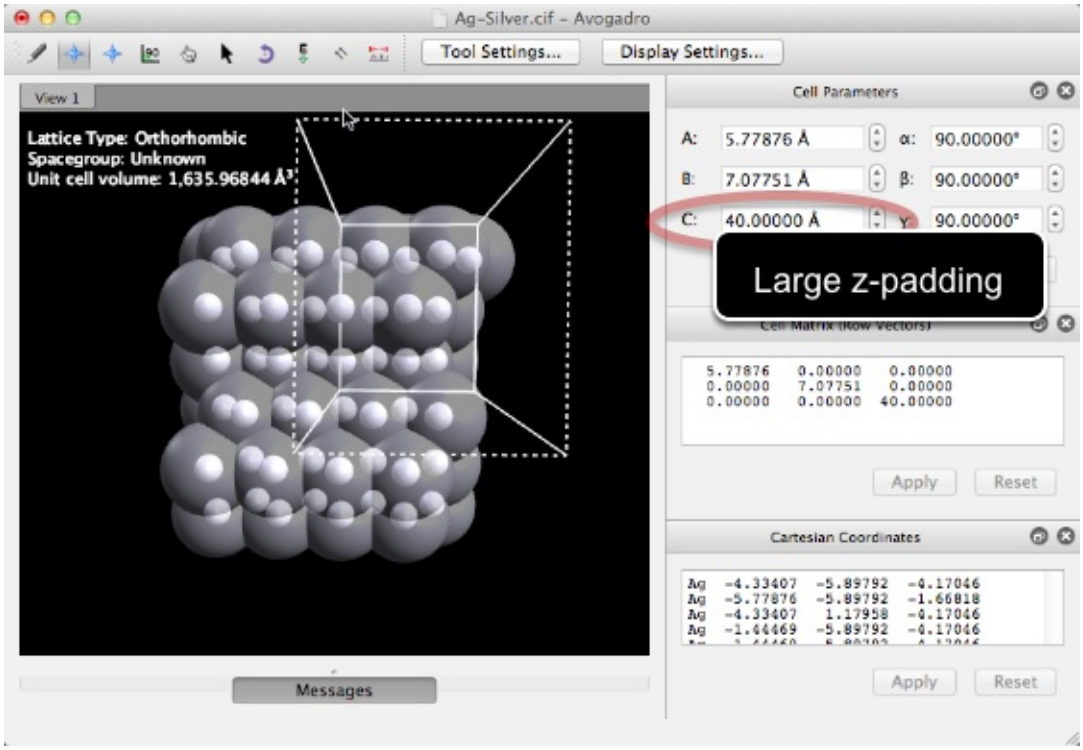
Importing a crystal will show the asymmetric unit cell (e.g., one atom for Silver here).



To build a specified surface (e.g., Ag <121>) choose Crystallography > Build > Slab... to bring up the slab builder settings. Future crystal builders (e.g., nanoparticles, supercells) will also appear in this menu.

Specify the indices of the Miller plane desired (for hexagonal unit cells, all 4 indices will appear), and choose the dimensions in either distances or repeating cells of the resulting surface. The generated surface is aligned in the XY plane, and a specified thickness will be cleaved in the z-axis below the XY plane. This feature allows easy alignment between a

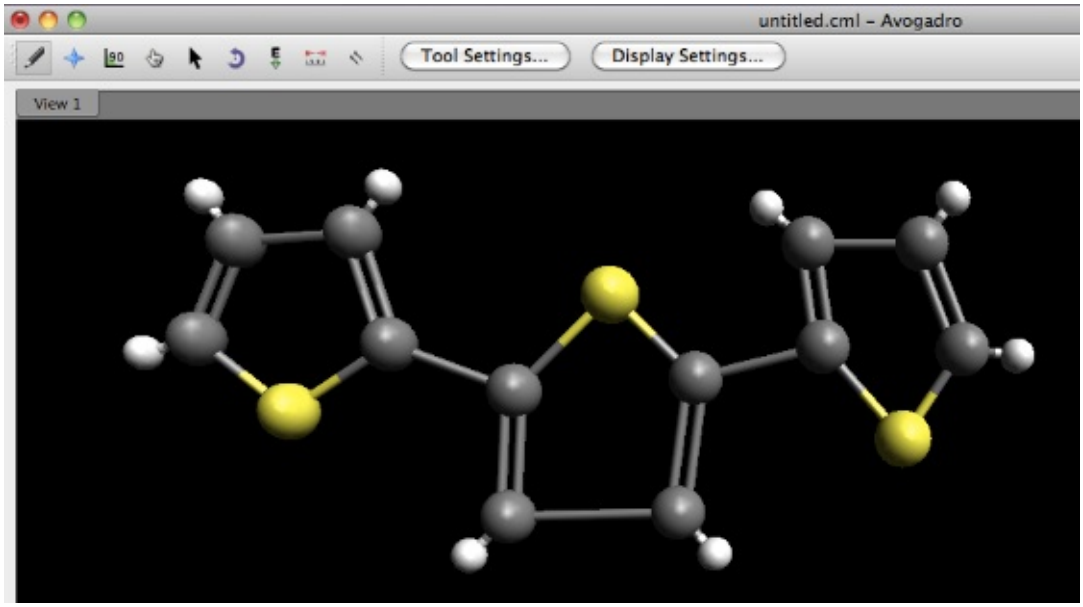
new surface and a molecule for surface interaction calculations. Click "Build" to start the surface generation.



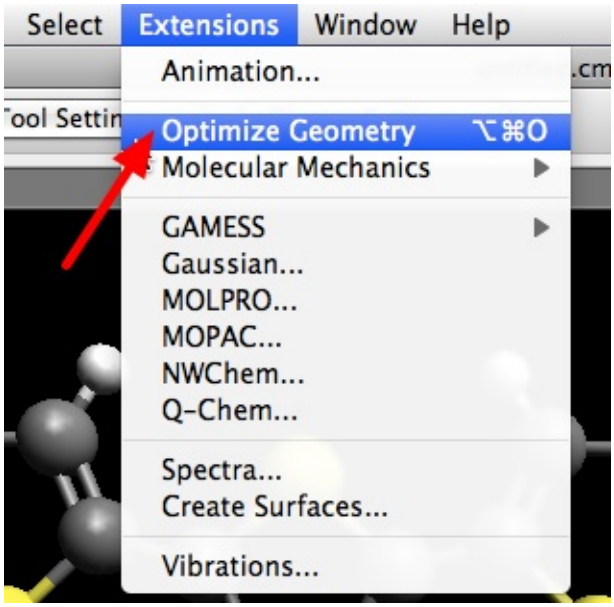
After clicking "Build," Avogadro will generate a large supercell, align, rotate, and cleave the designated surface. This may take some time, depending on the size of the crystal cell. Here translucent van der Waals spheres are used to illustrate the corrugation of the Ag <121> surface. The resulting surface is a 2x2 supercell, with a large spacing (40 Å) in the z-axis.

Building a Polymer Unit Cell

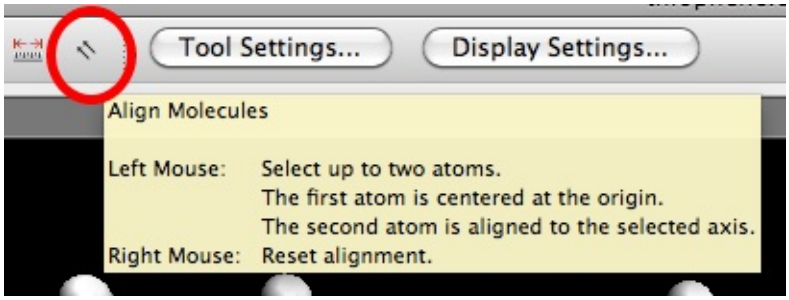
A walk-through on creating a unit cell (of a polymer) using Avogadro and the Align tool. This specific example uses Gaussian, but translation vectors for other programs can be performed similarly.



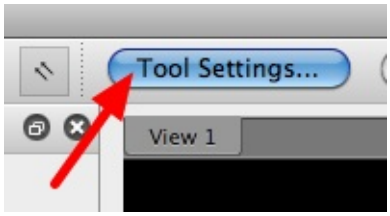
Build out the molecule for the unit cell. Notice that while the repeat unit here is 2 rings, we have built 3 rings. This way, we will properly model the bond which spans two unit cells.



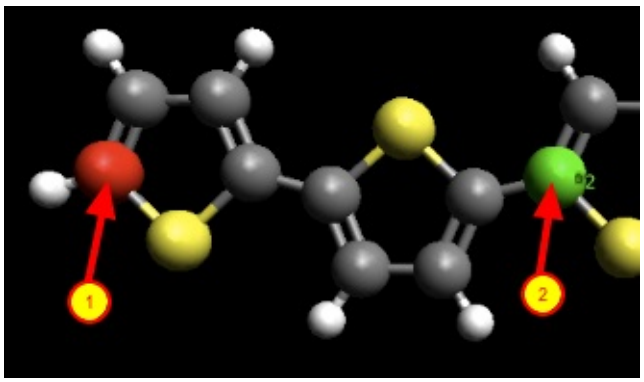
Optimize the geometry of the molecule.



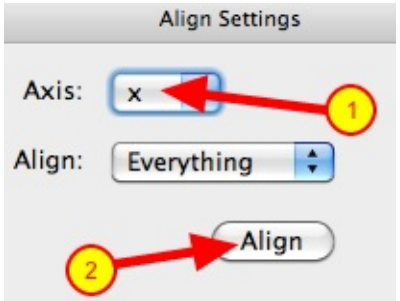
Switch to the Align tool to translate and orient the unit cell coordinates.



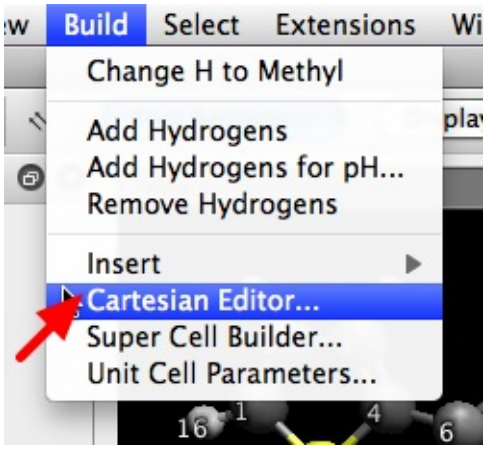
Make sure to open the Tool Settings window, which will allow you to work with the Align tool.



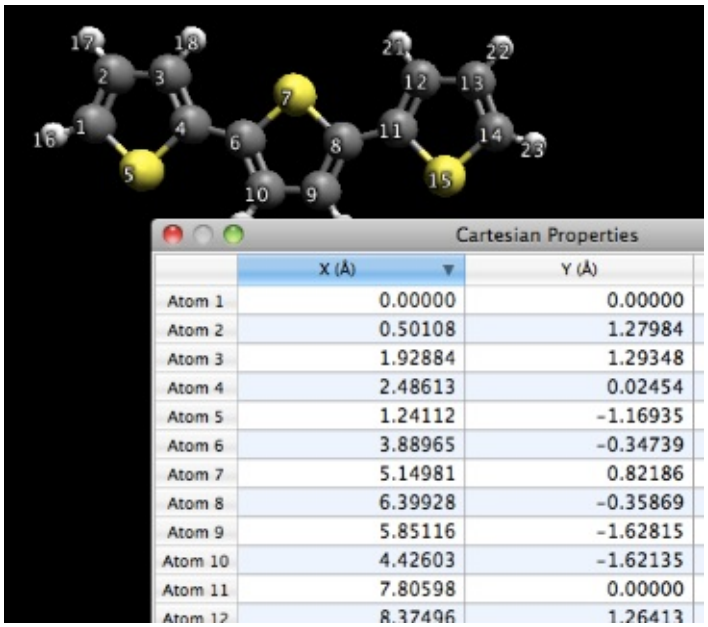
First click on the "start" atom of the polythiophene. This atom will be translated to the origin (0, 0, 0). Then click on the corresponding atom in the "next" unit cell. The distance between these two atoms will define one axis in the unit cell.



In the "Align Settings" window, define an axis for the unit cell. Then click the Align button. This will change the coordinate set to have atom #1 at the origin, and atom #2 (from the step above) projected onto the x-axis.

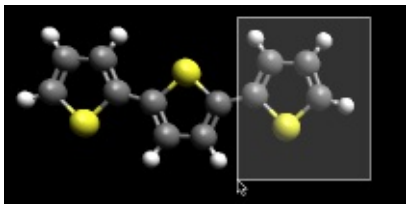


Open the Cartesian Editor window to verify the results of the Align operation.

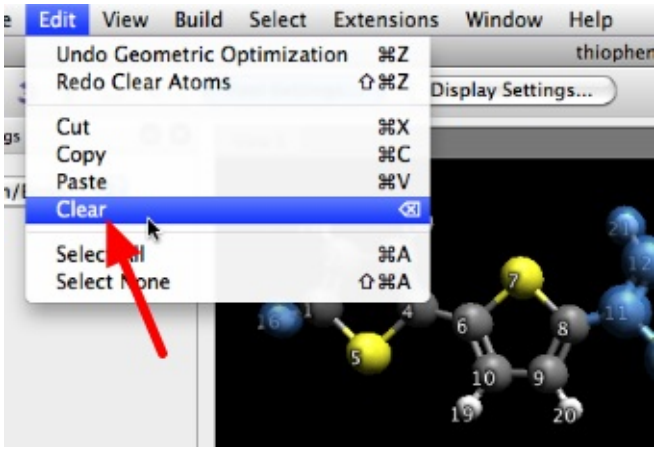


	X (Å)	Y (Å)
Atom 1	0.00000	0.00000
Atom 2	0.50108	1.27984
Atom 3	1.92884	1.29348
Atom 4	2.48613	0.02454
Atom 5	1.24112	-1.16935
Atom 6	3.88965	-0.34739
Atom 7	5.14981	0.82186
Atom 8	6.39928	-0.35869
Atom 9	5.85116	-1.62815
Atom 10	4.42603	-1.62135
Atom 11	7.80598	0.00000
Atom 12	8.37496	1.26413

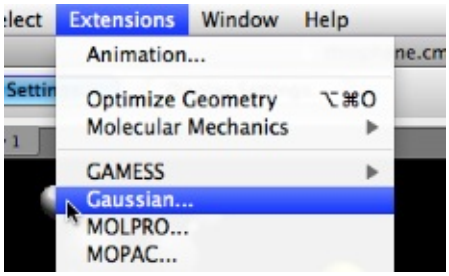
Notice that atom #1 is at the origin, and atom #11 is projected onto the X-axis. The size of the unit cell is 7.806Å -- the distance between atom #1 and atom #11.



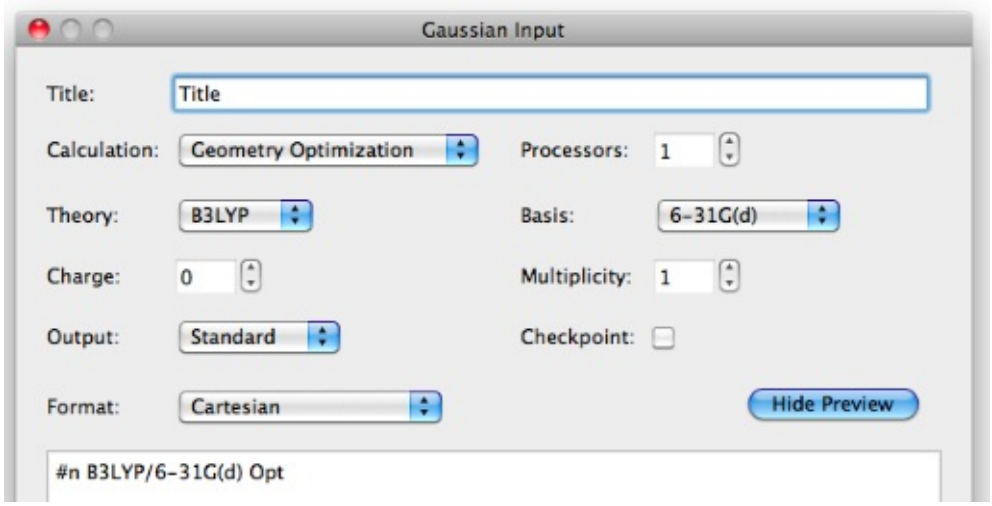
Now delete "extra" atoms which should not be included in the unit cell calculations. This includes the third ring (including atom 11) and the "end" hydrogen atoms. For example, you can use the select tool and drag over the atoms to be deleted to pick them.



Once selected, you can use the "Clear" menu command to delete the atoms.



If you wish to submit the unit cell to Gaussian, pick the Gaussian input extension.

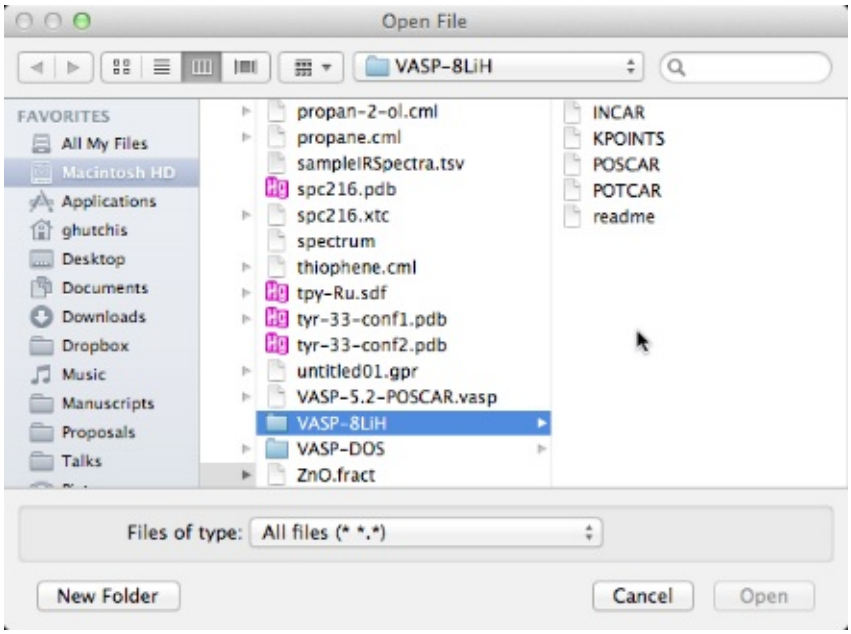


Set options as you desire. Make sure to add a "TV 7.806 0.0 0.0" line at the bottom of the preview text. This will enable the unit cell calculation by setting the translation vector for the unit cell.

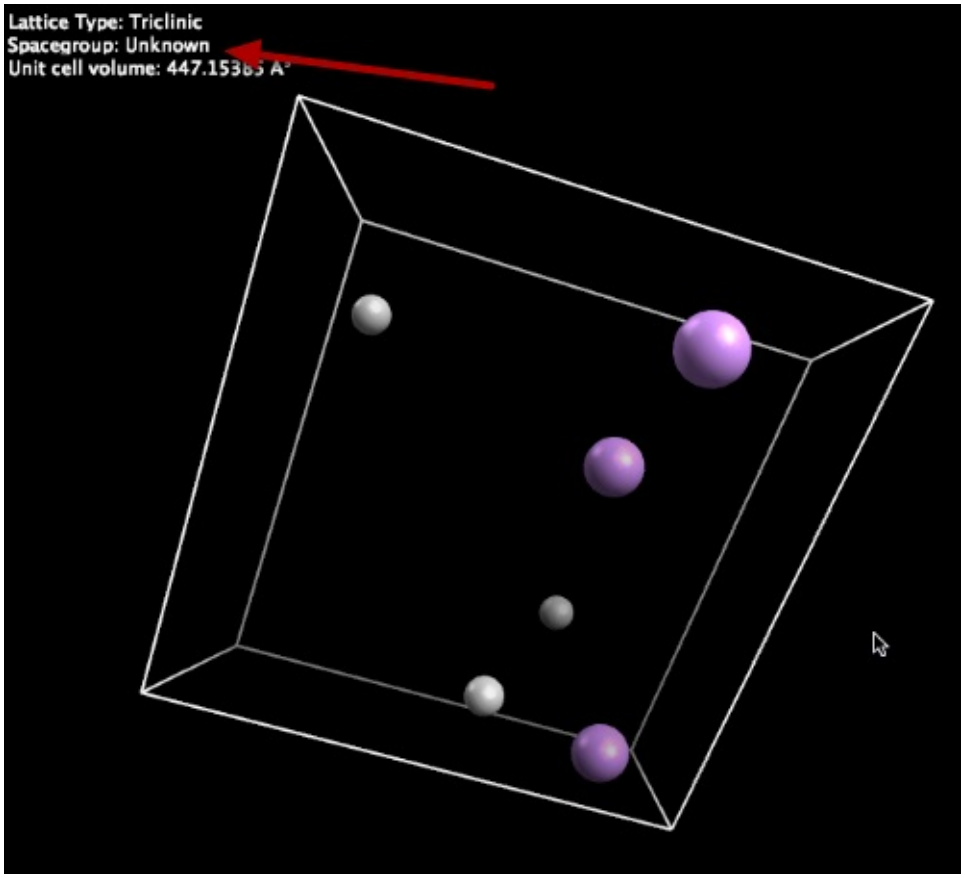
Crystal Symmetry Perception

Calculation results often specify all atoms and translation vectors, but not the space group. Here we see how to perceive the space group from a set of crystallographic coordinates.

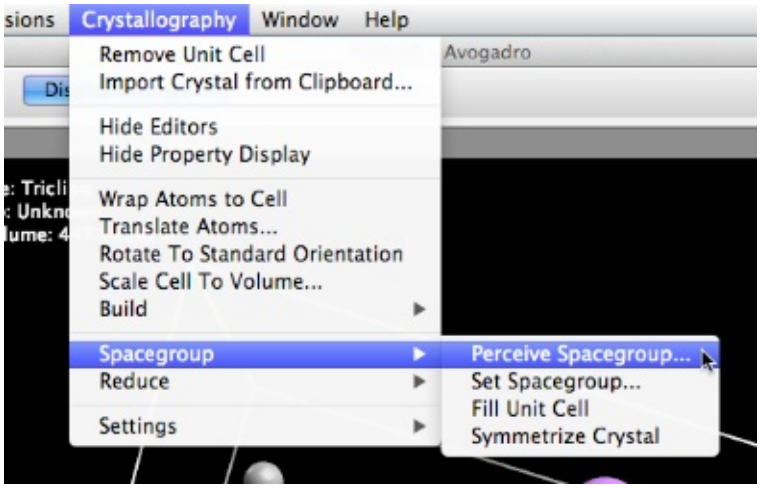
Open a Crystal File



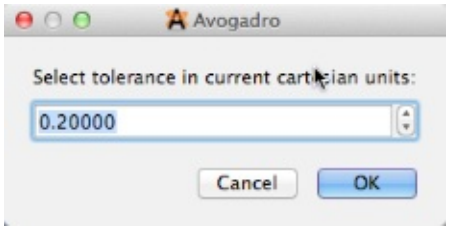
Here we open an example VASP calculation by opening the POSCAR file.



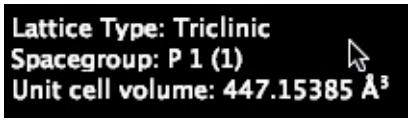
This example is triclinic, looking for Li / H structures. Note that VASP files do not specify a space group, so it is reported as "Unknown."



We can either set the spacegroup manually, or here, perceive the space group, using the open source spglib code.



We need to set the tolerance, since some atoms may be slightly out of place in Cartesian coordinates.

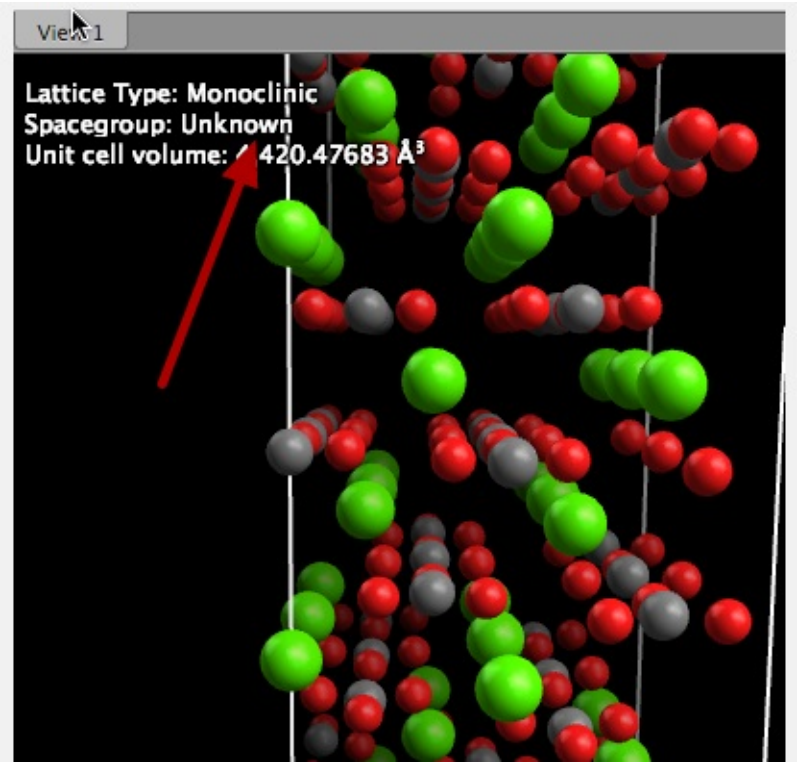


Our example VASP file isn't very interesting -- the space group is P1.

Here's another example, where the space group is P 1 21 1.

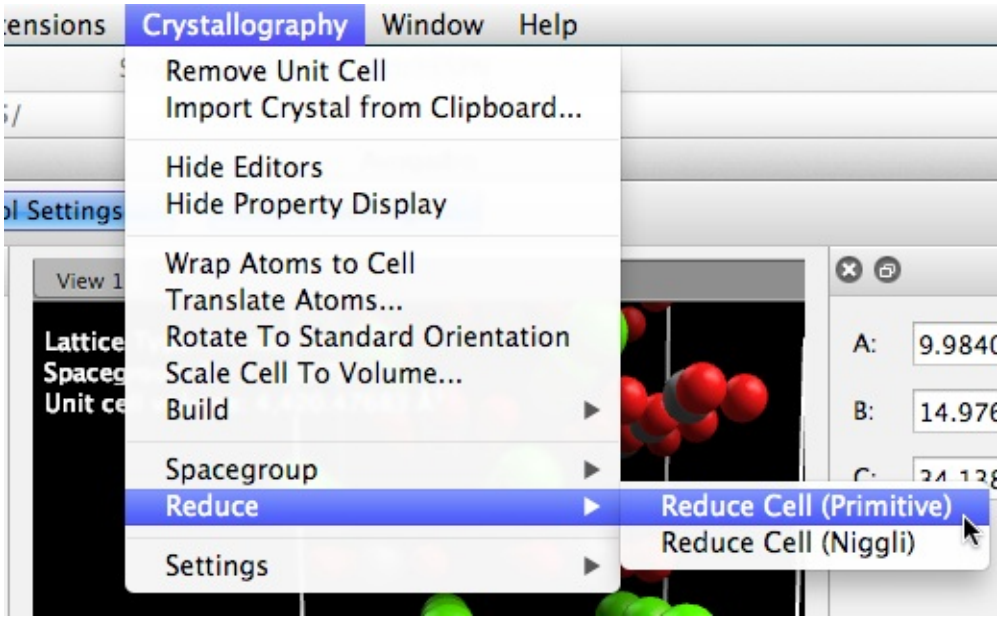
Reducing Crystals to Primitive Unit Cells

Some simulations use "supercells" -- larger periodic boundary systems than the primitive unit cell. Here is a walk-through on reducing a large supercell to the primitive unit cell.

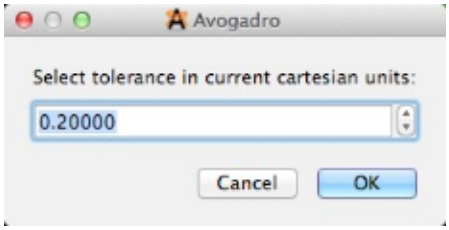


Open or import the file with the supercell -- here, CaCO3. Note that the space group is unknown, since the file came from VASP, which does not specify a space group with the coordinates.

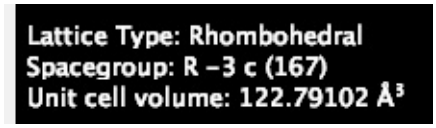
After perceiving the space group, we see correctly that the system is R -3 c. Now we can reduce the supercell to a primitive cell of CaCO3.



Avogadro provides two algorithms for reducing the unit cell to a primitive or Niggli cell. Here, pick "Primitive." Note that the volume of this supercell was over 4,000 Å3.



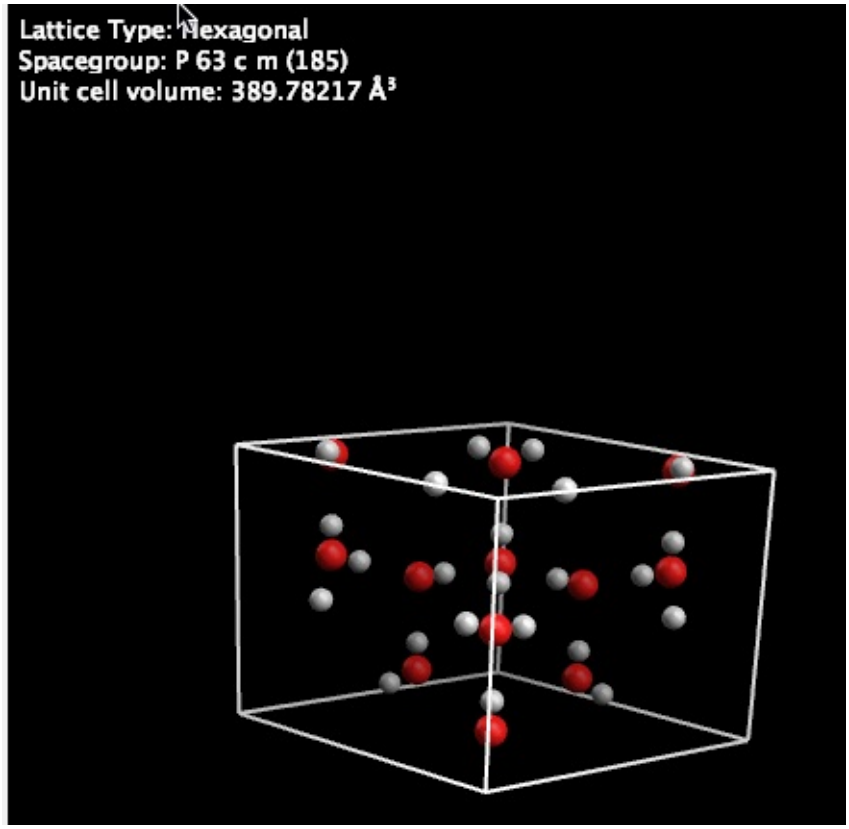
You will need to set a tolerance for the Cartesian coordinates (here, in Å).



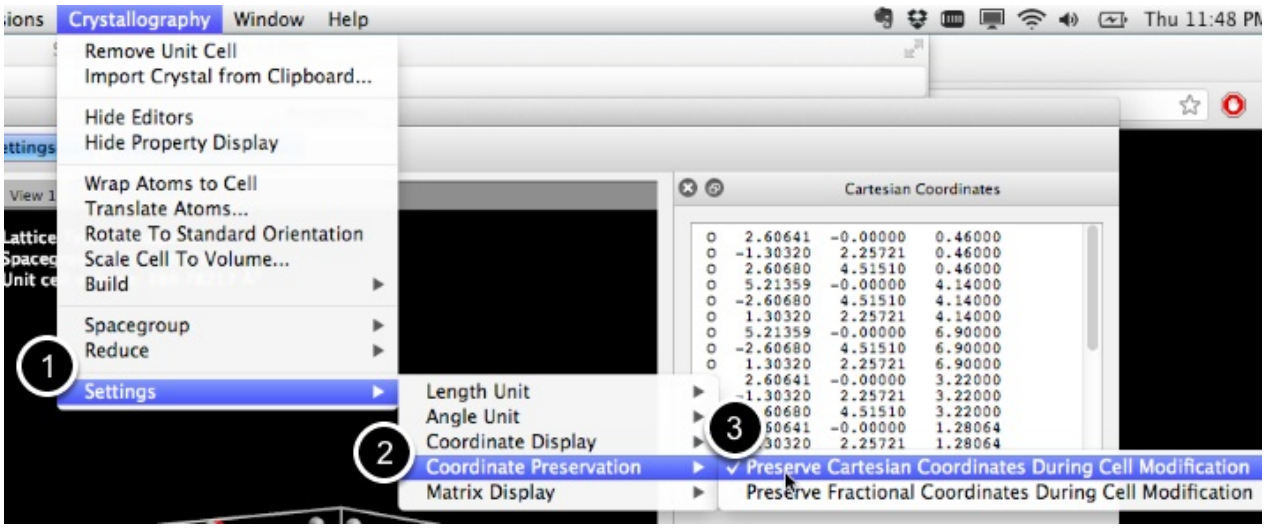
After reduction, note that the space group is retained, the lattice is properly Rhombohedral, and the unit cell volume is 36 times smaller.

Scaling Crystal Volumes

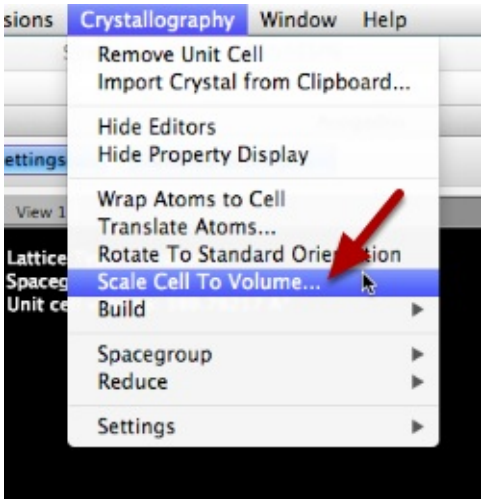
Avogadro 1.1 allows you to adjust the volume or spacing of a unit cell.



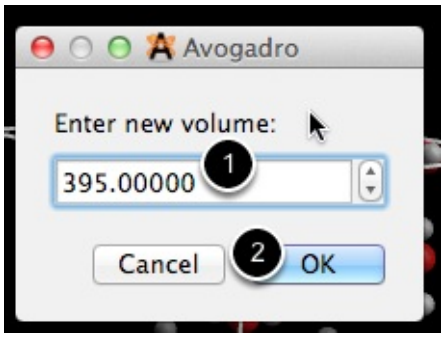
After creating or opening the crystal (here ice), we see the normal unit cell and lattice information. We will now adjust the cell volume.



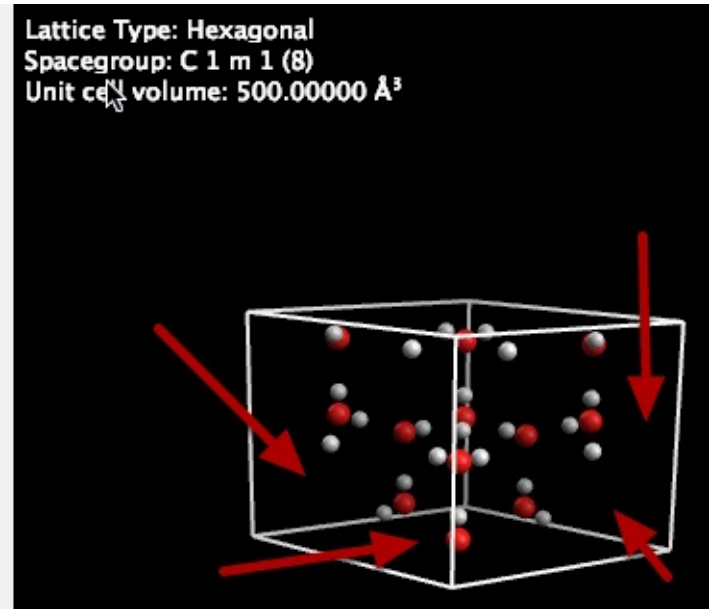
Before we scale volume, we can either choose to preseve Cartesian coordinates (which will add empty space to the edges of the unit cell) or preserve fractional coordinates (which will symmetrically scale the entire unit cell). This walk-through will show both.



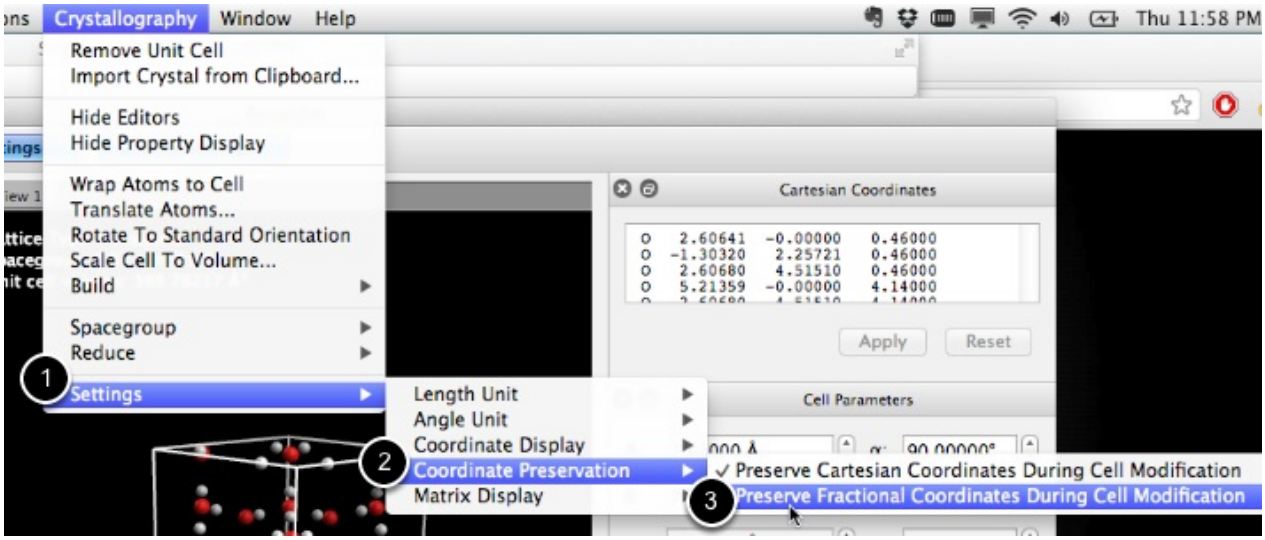
First we'll scale the cell while preserving Cartesian coordinates.



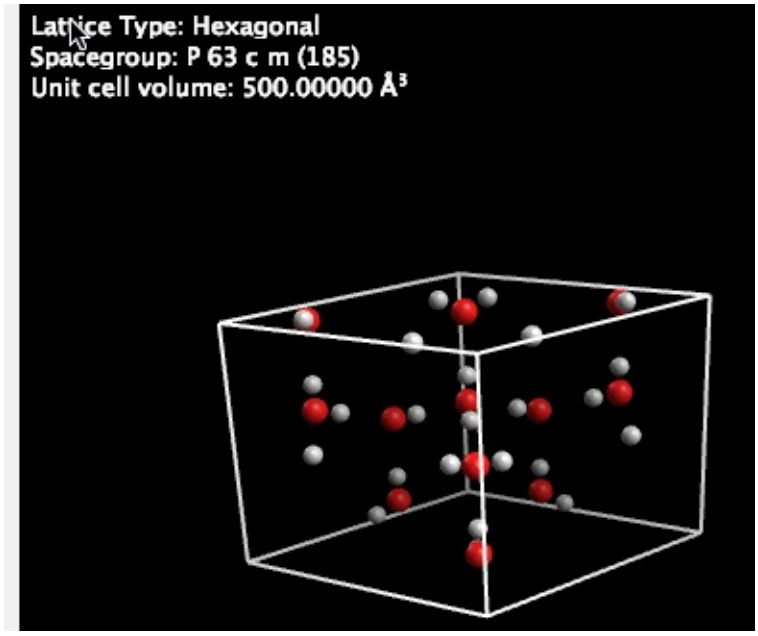
The units of the volume are determined by your settings (here Å). We adjust the volume from the original 389.78Å3, and click "OK."



Here, we've greatly exaggerated the volume, to show the empty space (arrows) around the outside of the unit cell boundaries, when preserving Cartesian coordinates. The space group has also changed (to C 1 m 1).



If you preserve fractional coordinates, you can scale the unit cell symmetrically.

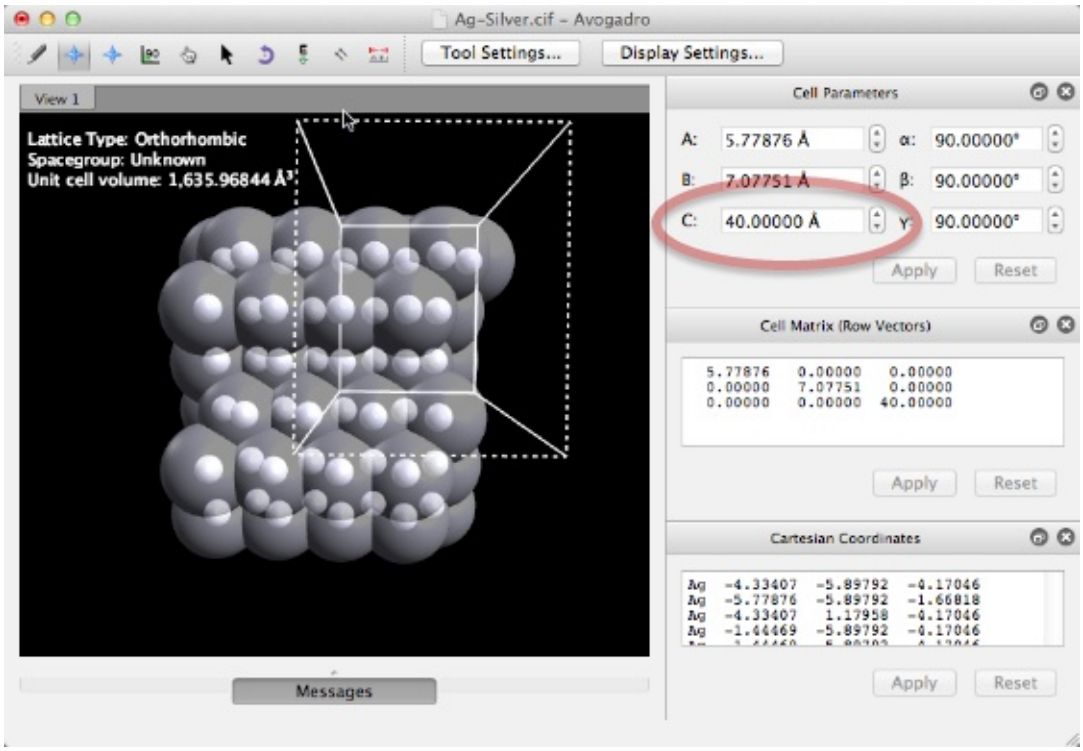


Note that while the volume is significantly expanded, the space group (and fractional coordinates) are retained.

Molecule-Surface Interactions

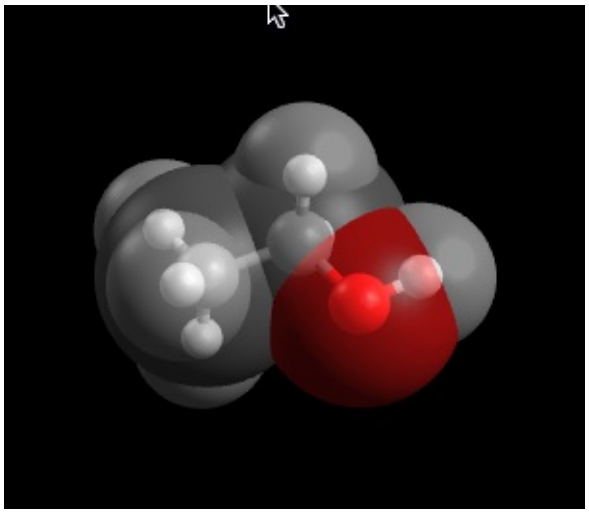
Beyond building a crystal surface, new features in Avogadro make it easy to consider molecule-surface interactions. The lesson picks up at the end of the "Building a Crystal Surface" lesson.

Start with a generated Crystal Surface

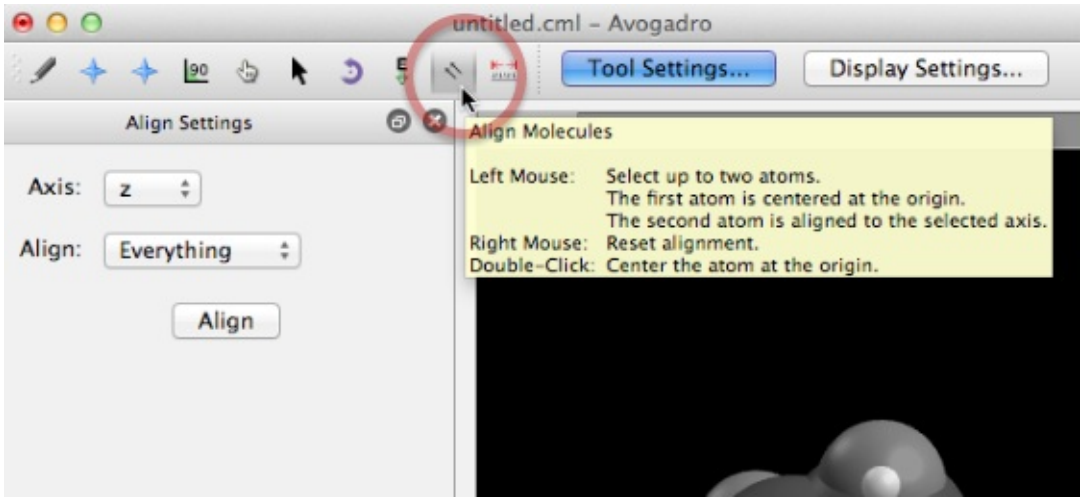


Generate the desired crystal surface. Avogadro will center the surface cell, aligned in the XY plane, with slab atoms defined below Z = 0. The Slab Builder also leaves a large space along the z-axis to allow insertion of molecules for surface interaction calculations. You can control this padding as indicated above.

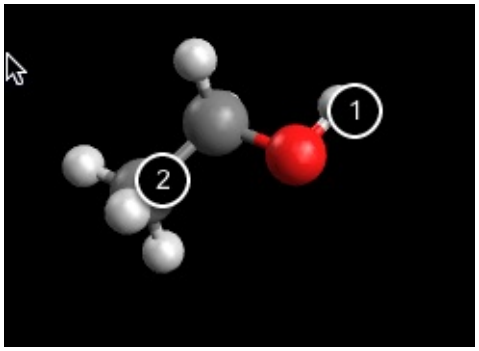
New Window: Create our Molecule



In a new window, draw the desired molecule, or open a file. Here we consider ethanol.

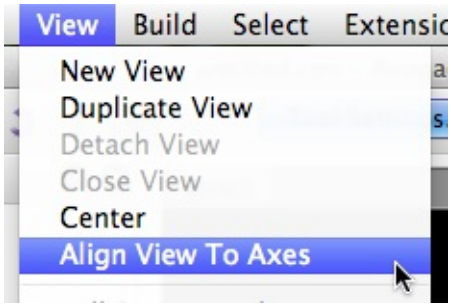


We will use the "Align Tool" to allow us to rotate and align the molecule with the OH group at the origin, and the molecule aligned along the z-axis.



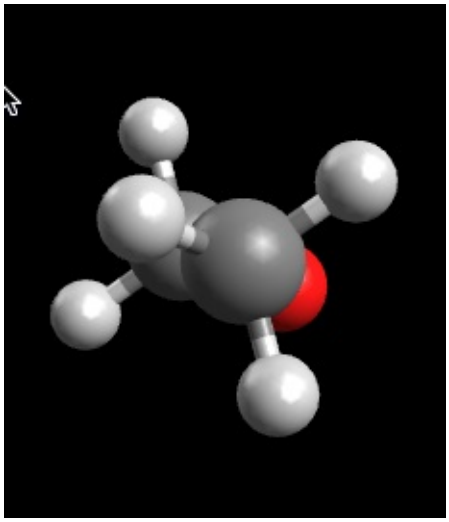
We will click on the terminal H atom (which will be translated to the origin) followed by the carbon atom (which will define the z-axis of the molecule).

After defining the atoms (they will show colored spheres and numbers once selected), click on the "Align" button to translate and rotate the molecule.

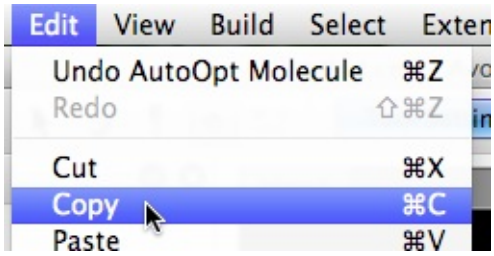


You may wish to alter the current camera view. Choosing View > Align View to Axes will reset the view to project the z-axis

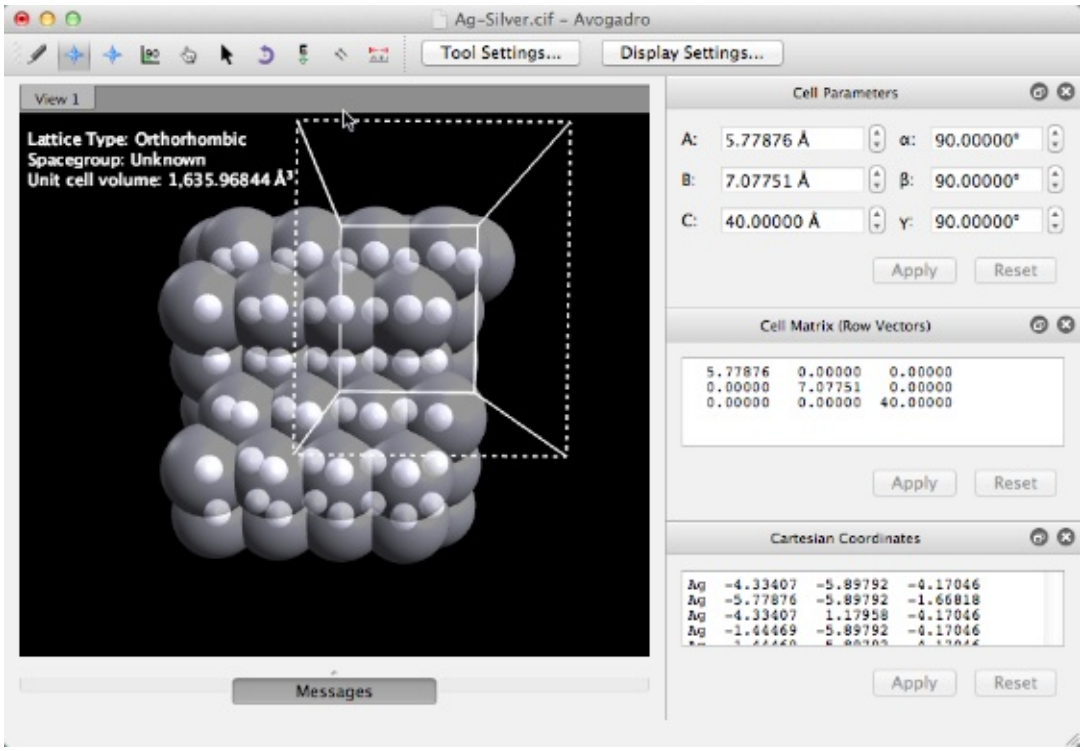
of the molecule to point towards you.



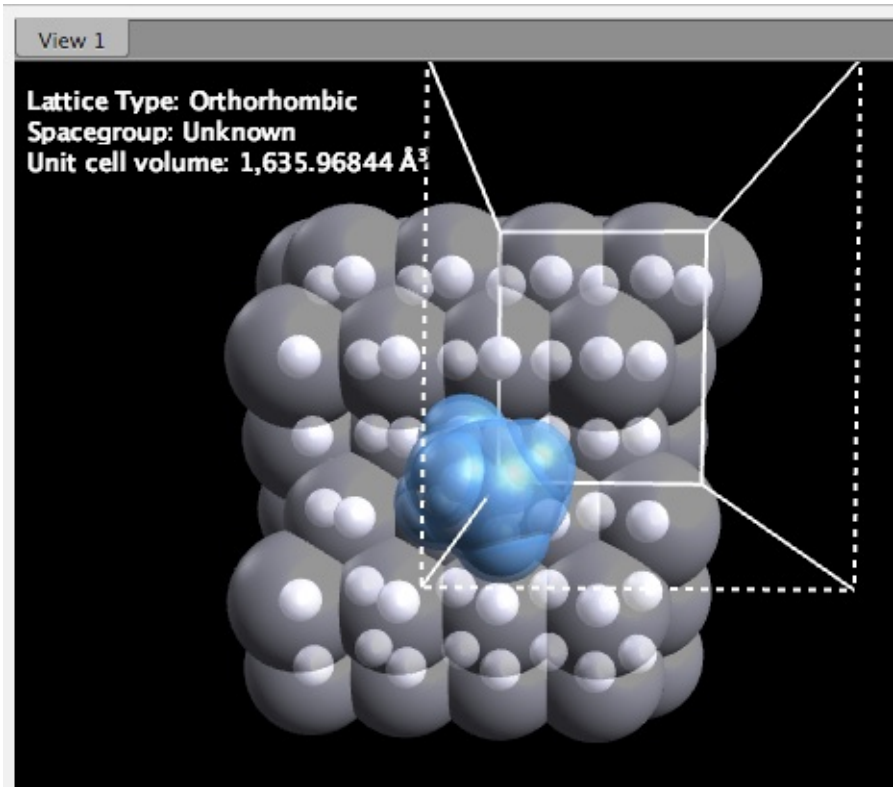
Perfect! Now we can copy our ethanol to the surface document.



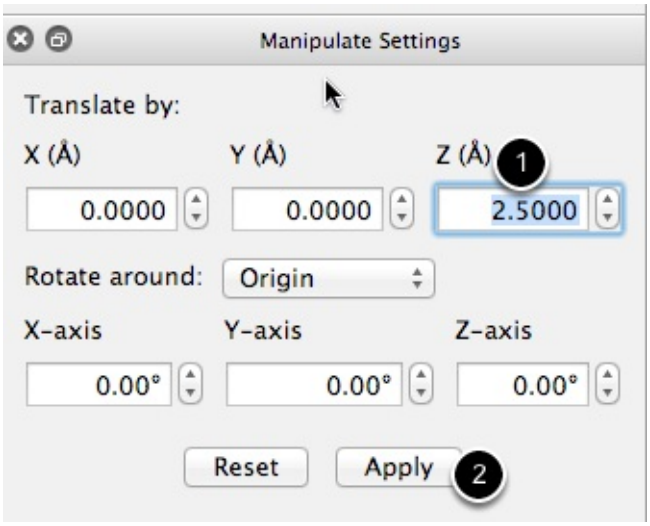
After copying, we can switch to our surface.



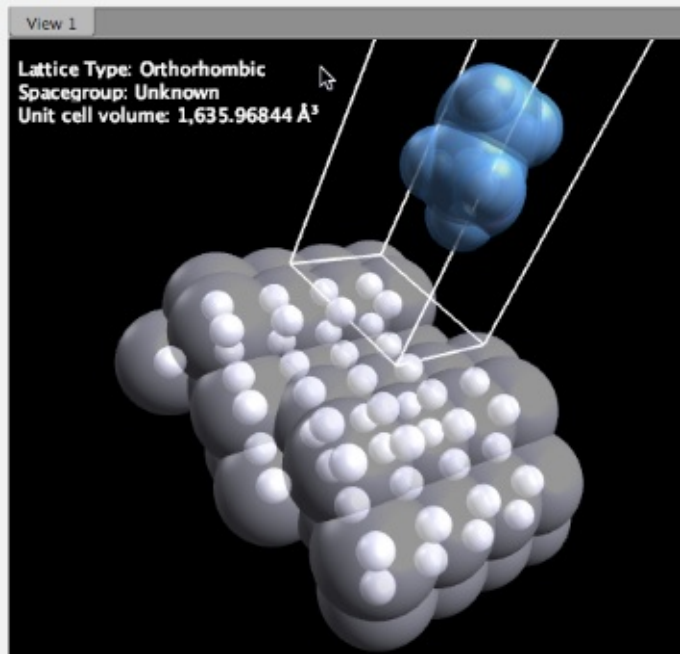
Now we'll paste in the ethanol molecule.



Note that the ethanol is now embedded in the surface, centered as desired. The Manipulate tool has been selected, allow us to translate the molecule as needed.



New in version 1.1 is an option to specify the exact amount to translate or rotate the selection (i.e., the molecule we just pasted). Here, we've specified that we want to move the molecule +2.5Å along the z-axis, above the surface, and then we click "Apply" to complete. We could also rotate around the z-axis if the positioning isn't as desired.

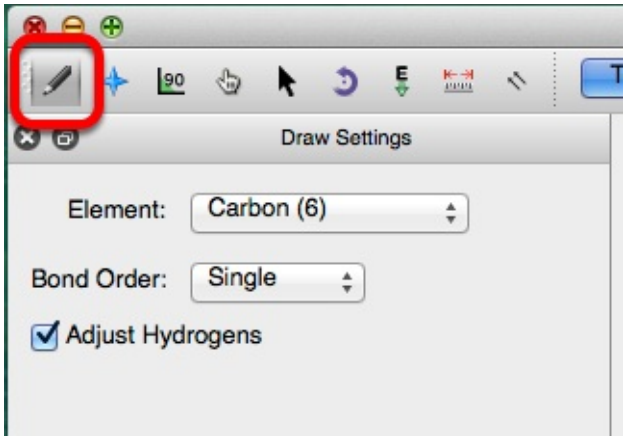


Here we have translated the ethanol 2.5 Å above the Ag <121> surface and are ready to submit for a calculation.

The Draw Tool

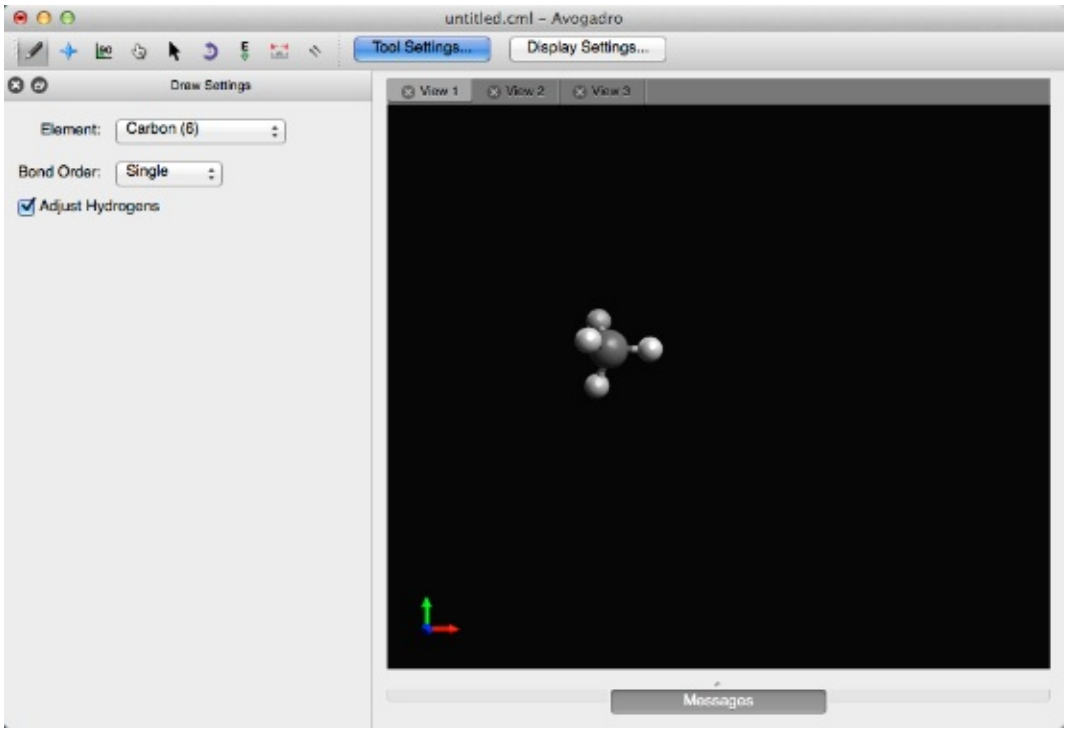
1. Creating a Molecule

Molecules can be built and edited with the draw tool.



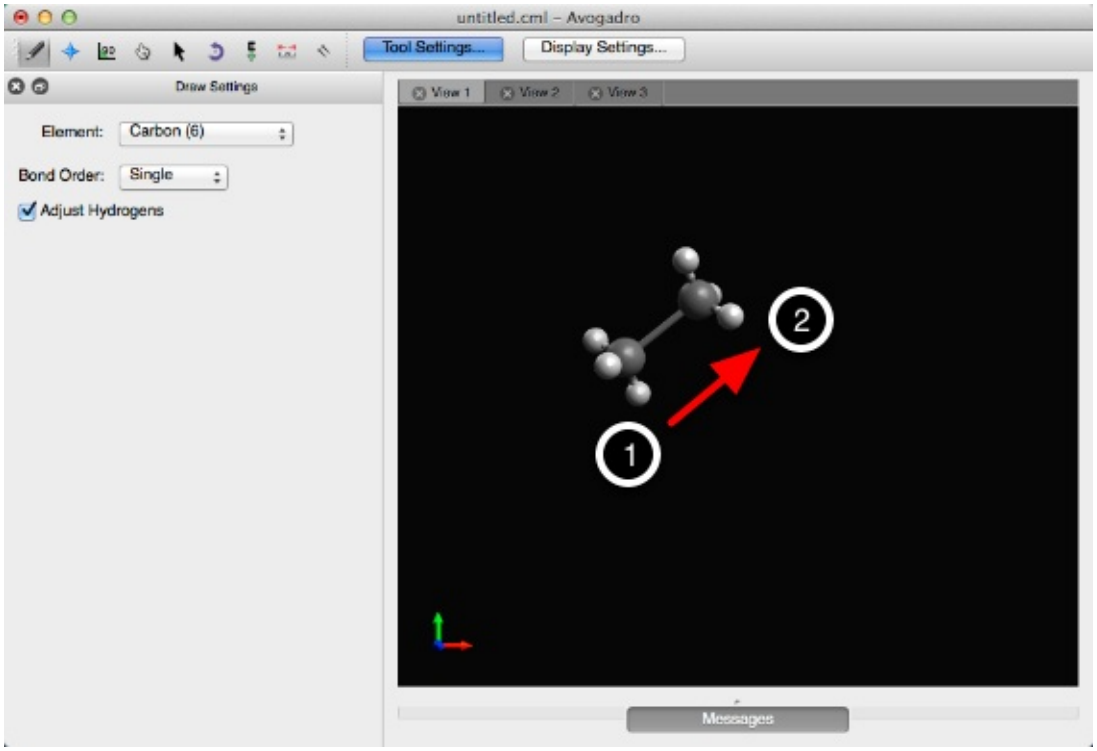
2.

You can begin creating a molecule by left clicking on the black display. This will generate a carbon atom. Right clicking on the atom will delete it.



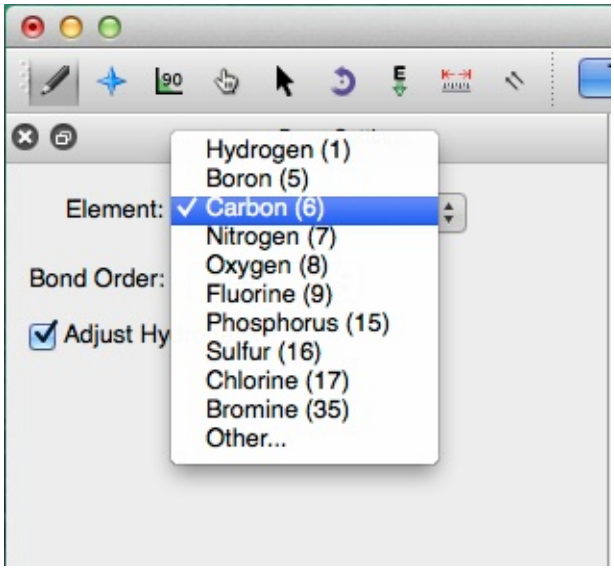
3.

Left clicking and dragging the mouse will generate a bond to another carbon atom.



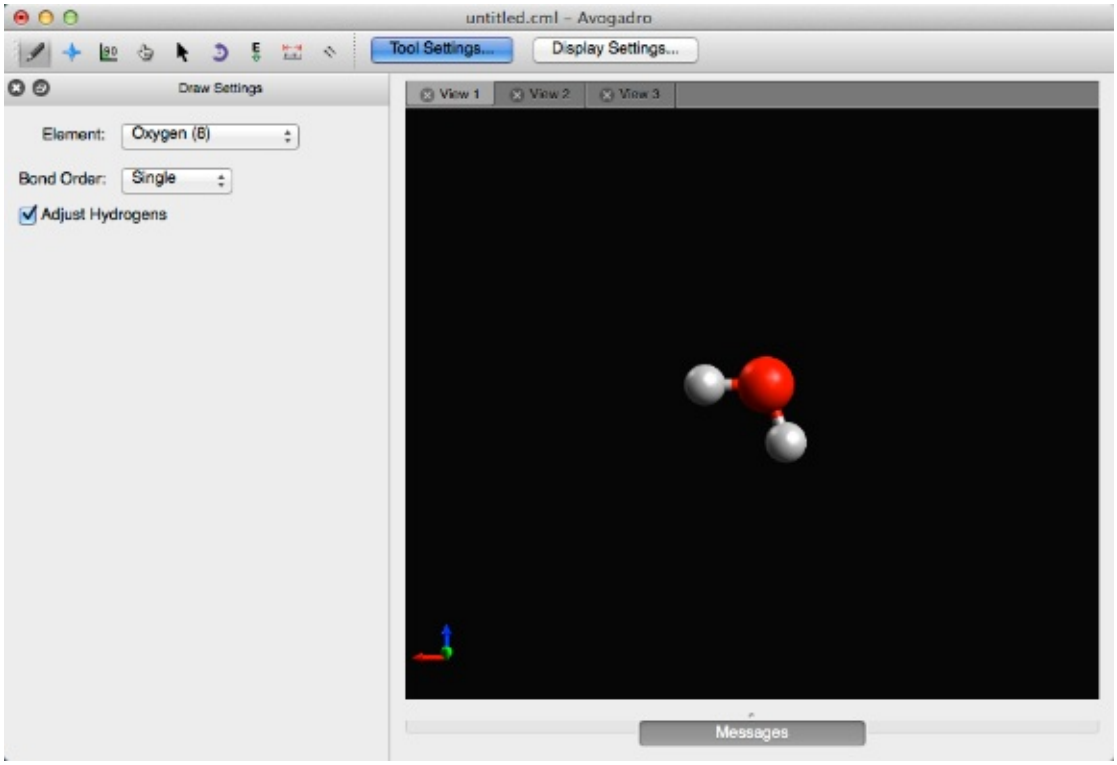
4.

Different elements can be selected from the Element drop down menu. Typing the atomic symbol (e.g., "A-s" for Arsenic) is a shortcut for changing the selected element.



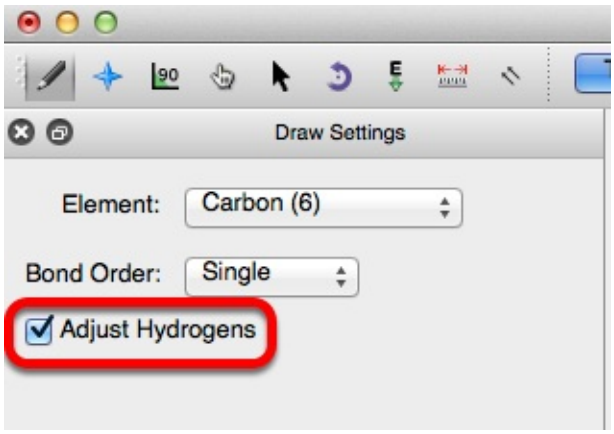
5.

For example, if you wanted to create water, you can type in "O", or select "Oxygen (8)" from the drop down menu and click on the black display.



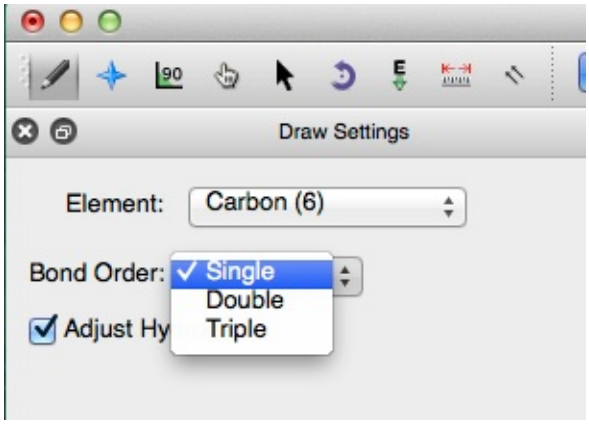
6.

If the "Adjust Hydrogens" box is checked, hydrogens in the molecule are automatically adjusted to satisfy valency (as shown above).



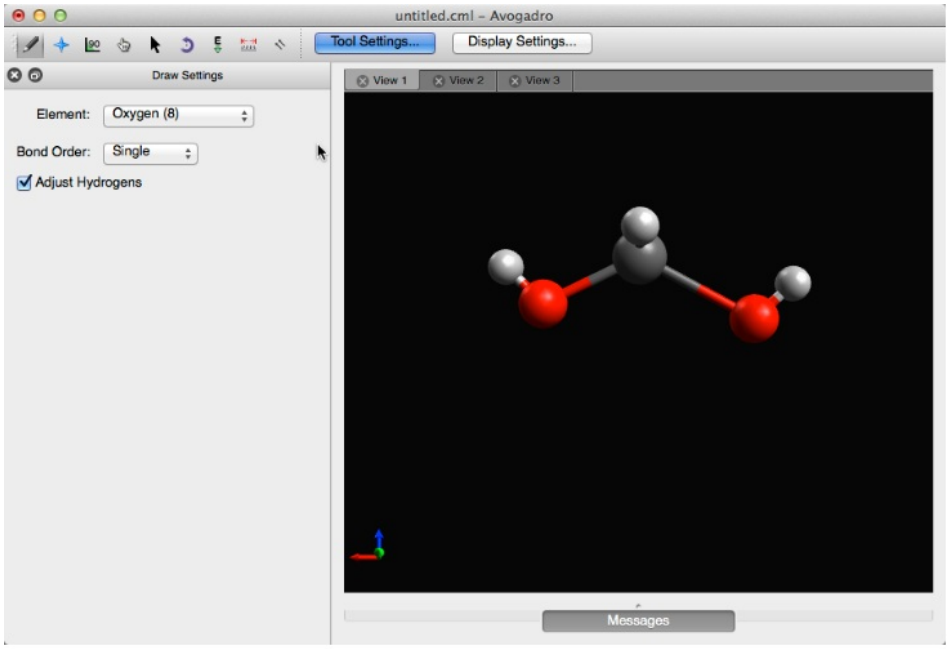
7.

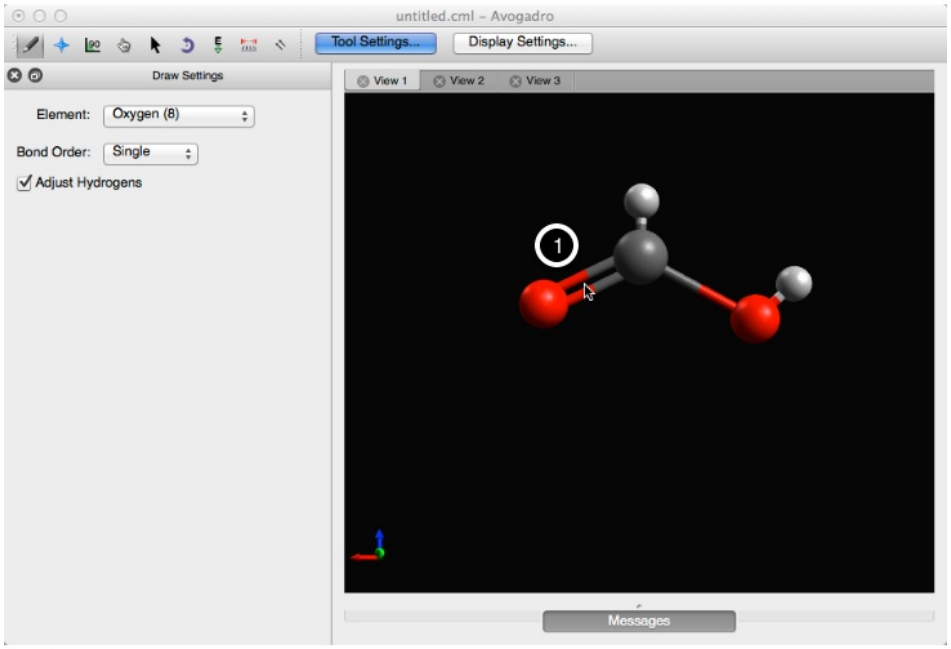
Bond order can be changed through the Bond Order drop down menu, or by typing the numbers "1", "2", or "3". Bonds can also be added to a molecule by left clicking on a bond that has already been created (this process cycles through single, double, and triple bonds). Right clicking on a bond will delete the bond, and the atom it's bonded to.

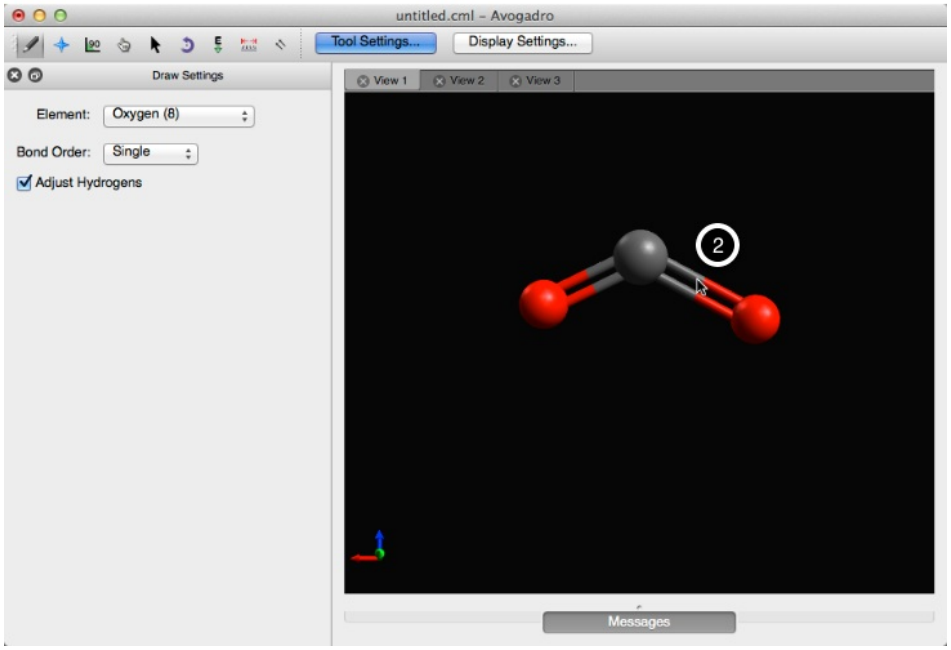


8.

For example, to create carbon dioxide, the general structure ("O-C-O") needs to be drawn, and then by left clicking the bonds in the molecule, double bonds will be created.

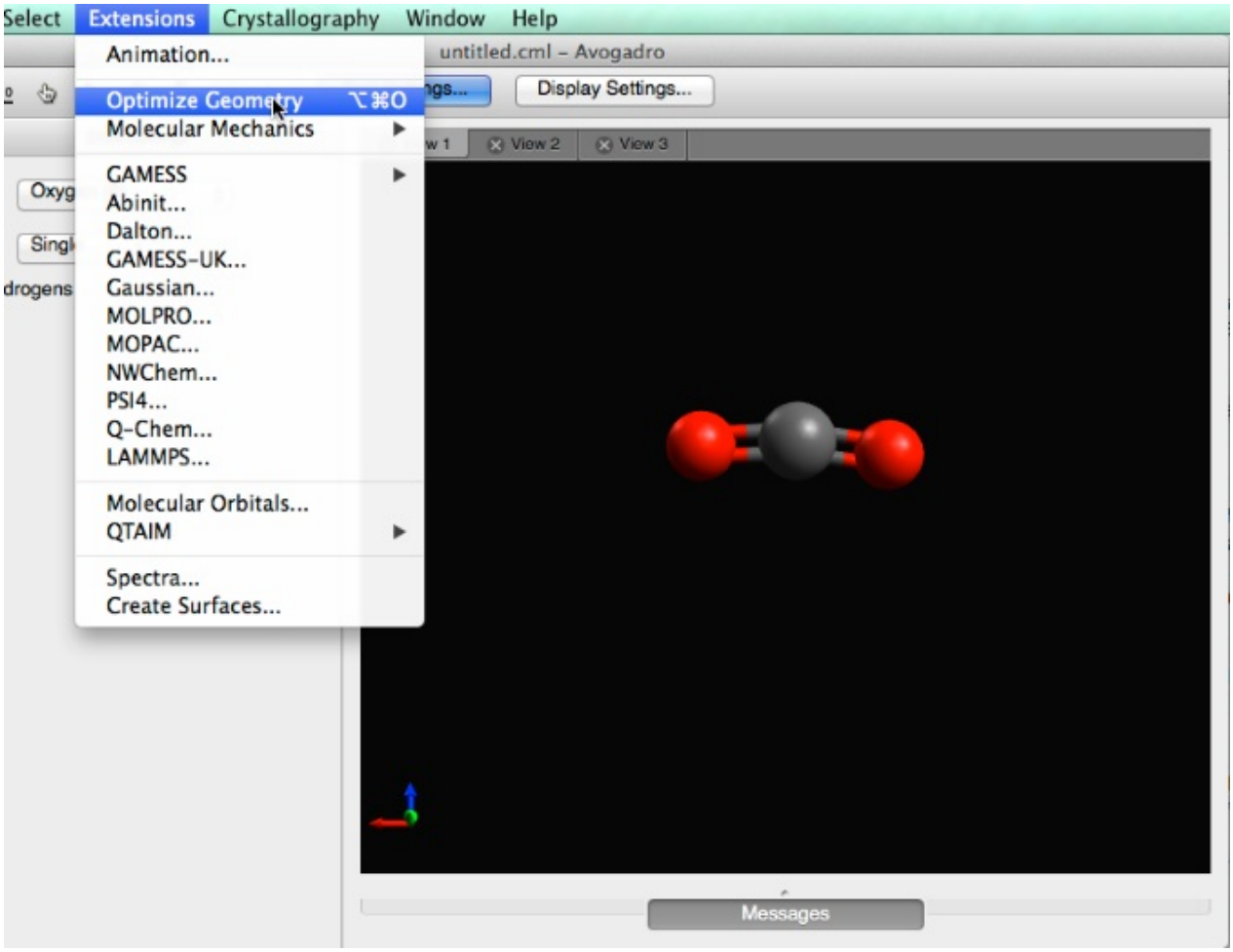

untitled.cml – Avogadro
Tool Settings...
Display Settings...
Draw Settings
Element: Oxygen (8)
Bond Order: Single
Adjust Hydrogens
View 1
View 2
View 3
Messages


untitled.cml – Avogadro
Tool Settings...
Display Settings...
Draw Settings
Element: Oxygen (8)
Bond Order: Single
Adjust Hydrogens
View 1
View 2
View 3
1
Messages


untitled.cml – Avogadro
Tool Settings...
Display Settings...
Draw Settings
Element: Oxygen (8)
Bond Order: Single
Adjust Hydrogens
View 1
View 2
View 3
2
Messages

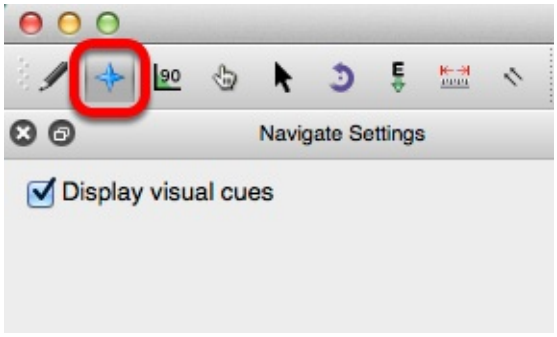
9.

Under the "Extensions" menu, the geometry of a molecule can be optimized by selecting "Optimize Geometry".

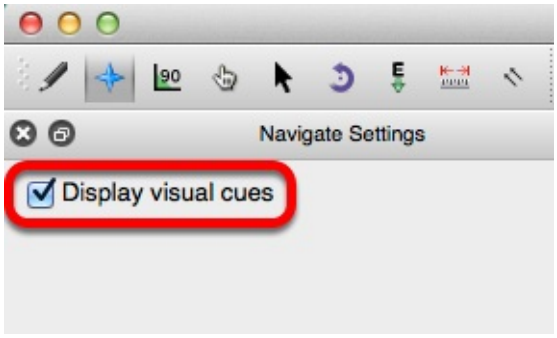


The Navigate Tool

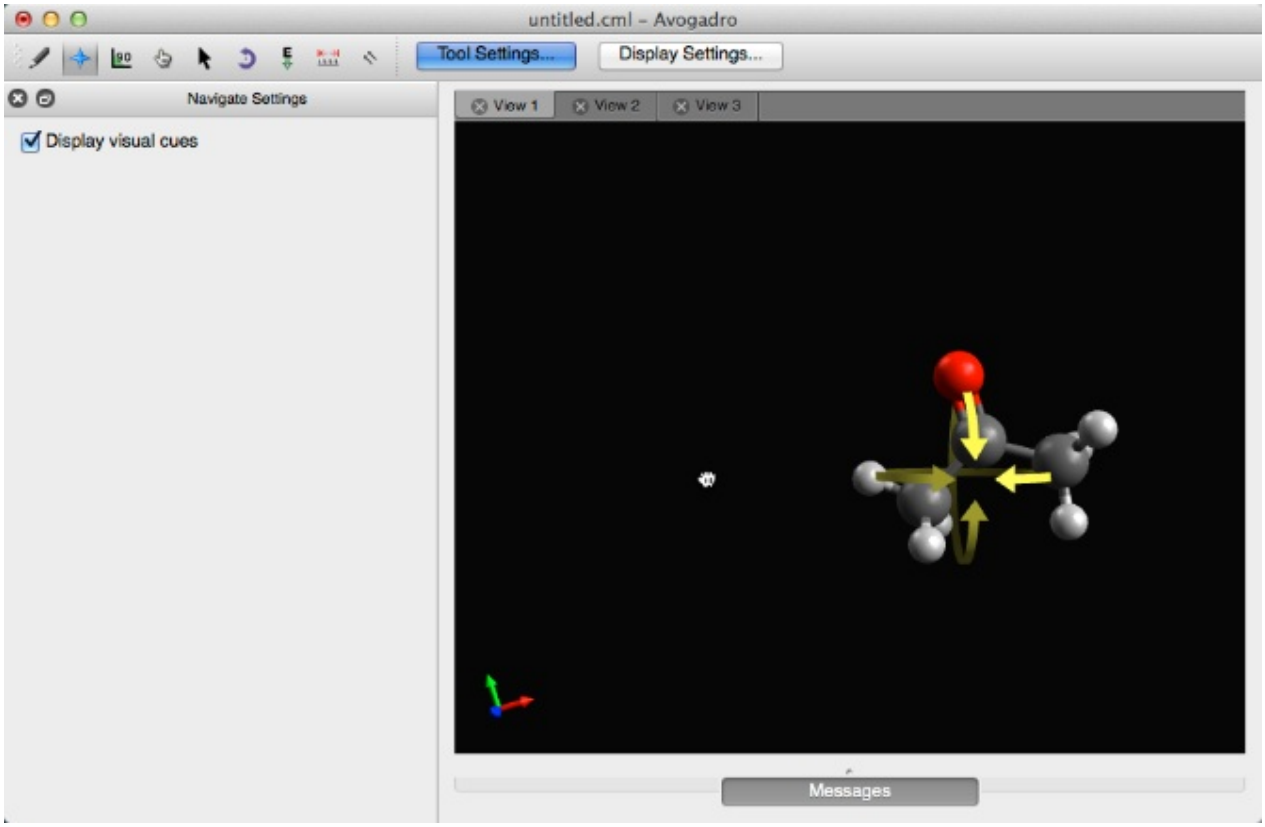
The navigation tool is used to pan, rotate, and scale the view of a molecule.



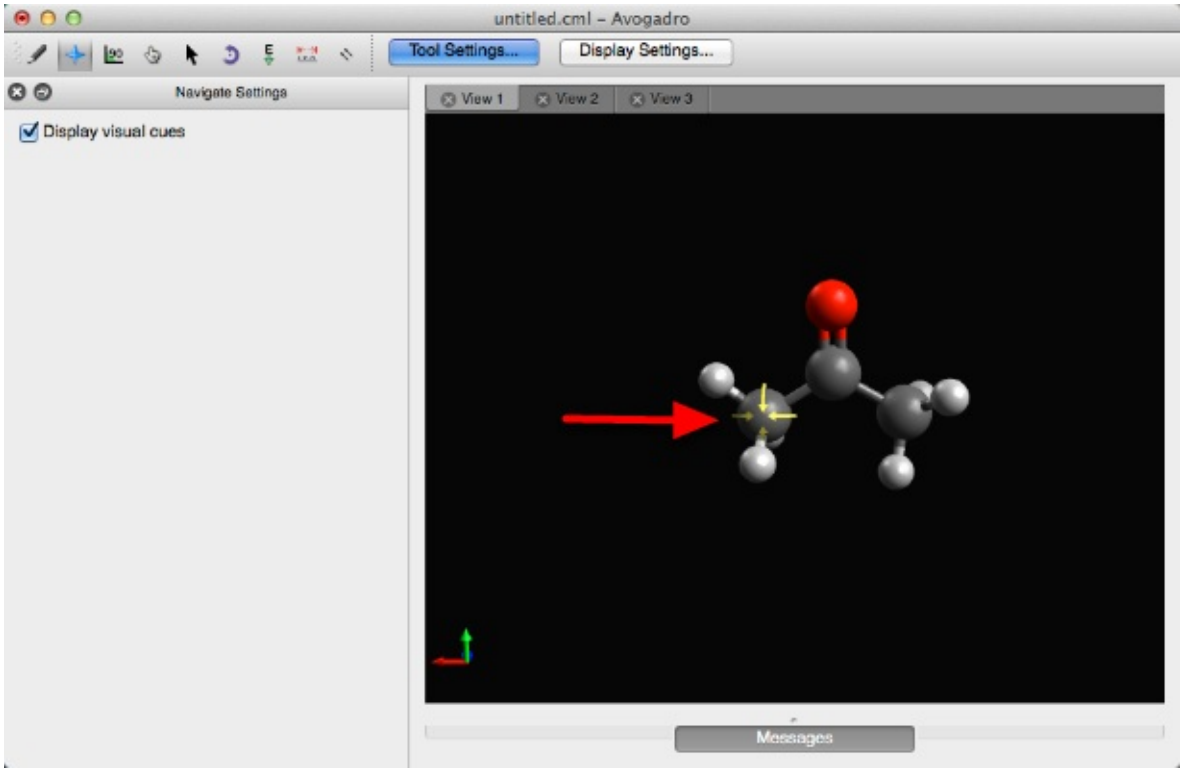
If the "Display visual cues" box is checked, yellow arrows will display what type of navigation is taking place.



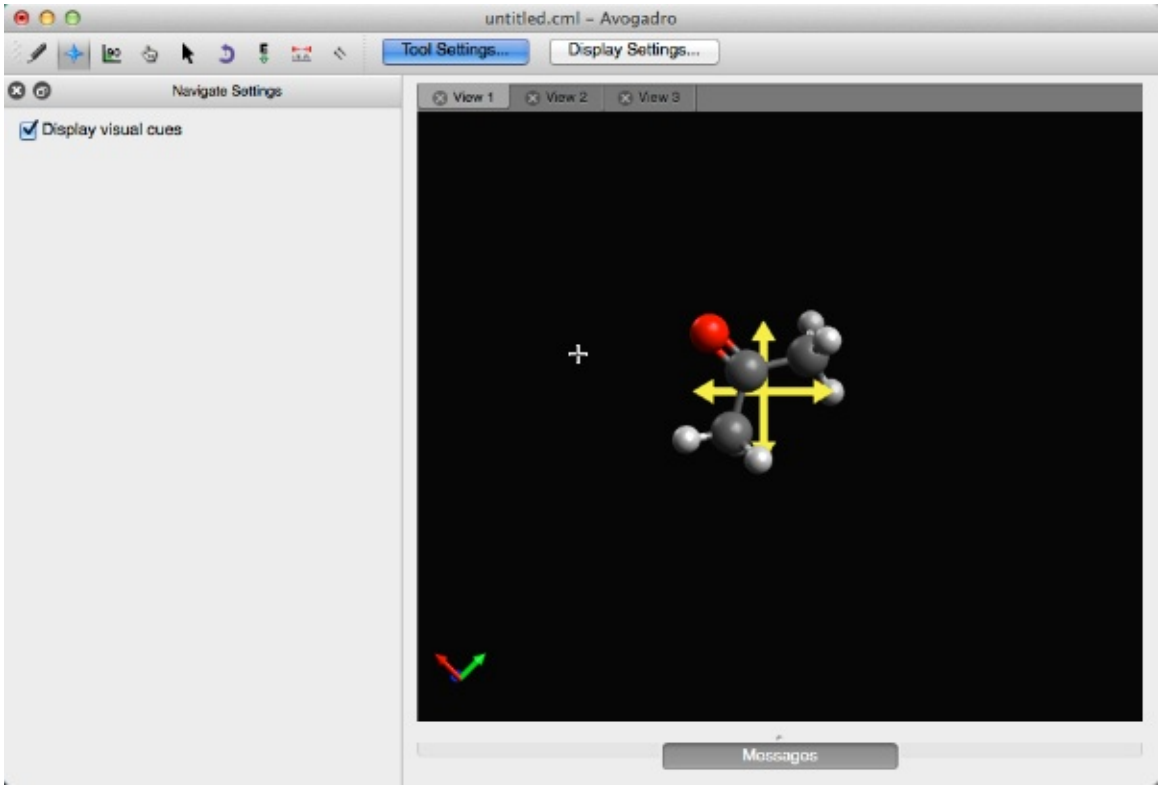
Clicking anywhere on the black display and dragging the mouse will tilt, and rotate the entire molecule (as shown below).



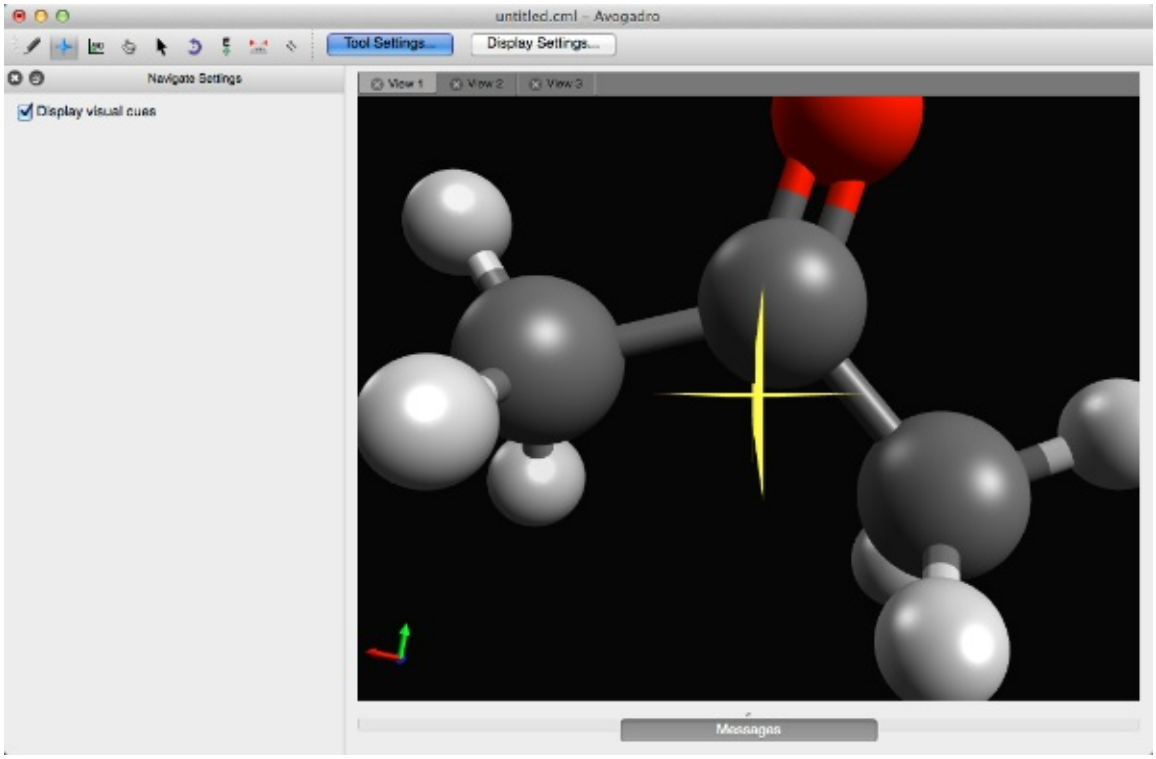
A molecule can also be rotated about an atom by clicking the atom and dragging the mouse. Depicted below, acetone is being rotated about it's initial carbon.



Right clicking allows you to change the molecules location on the display. Double clicking the molecule will reset the molecule's view.

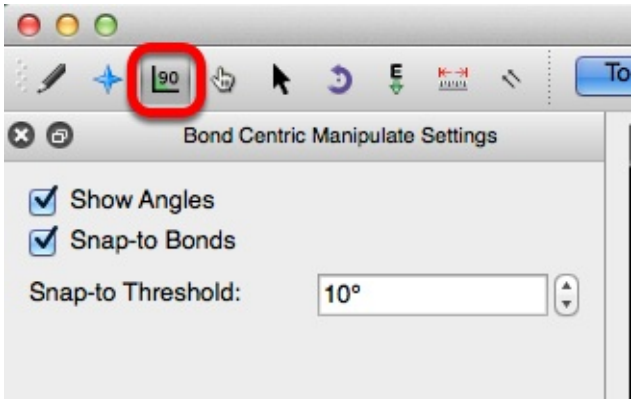


Using the middle scroll bar on a mouse will allow you to zoom in and out.

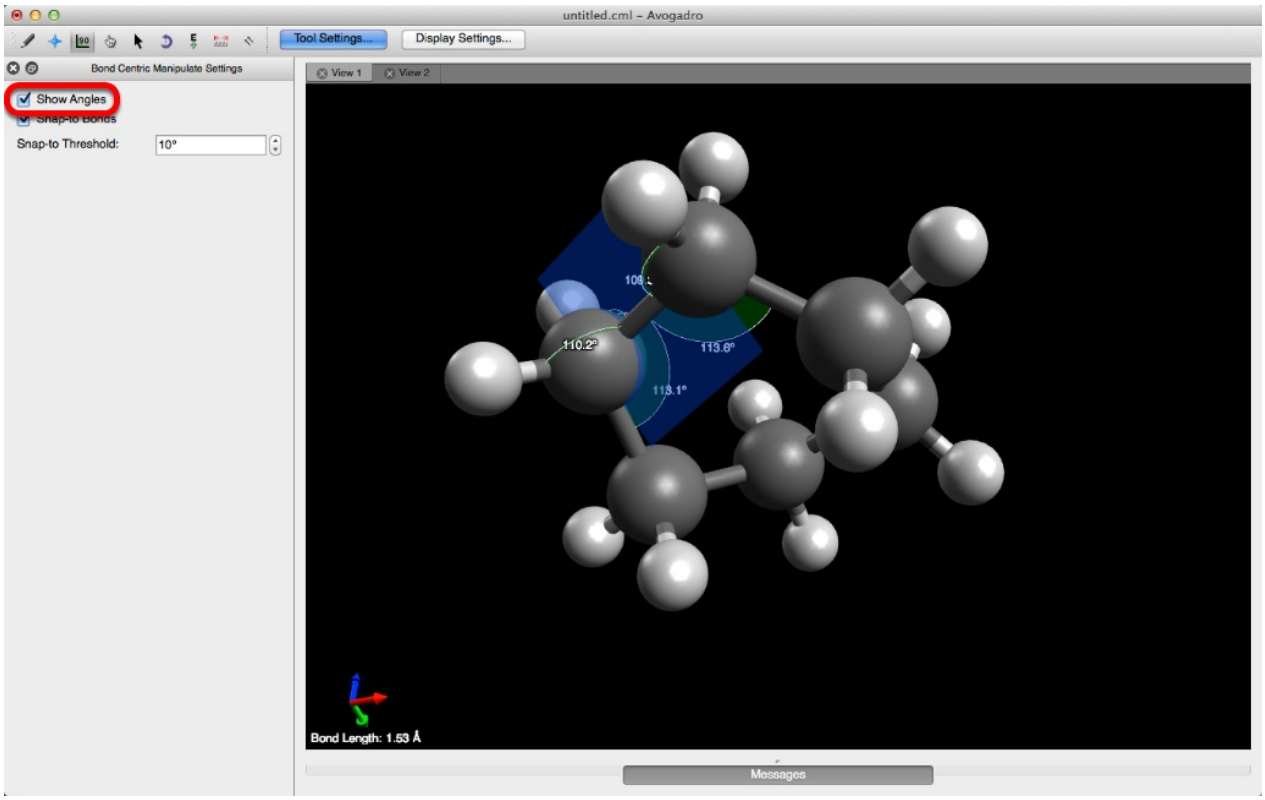

untitled.cml – Avogadro
Tool Settings...
Display Settings...
Navigate Settings
Display visual cues
View 1
View 2
View 3
Messages

The Bond-Centric Manipulate Tool

The Bond-Centric Manipulate tool alters angles, bonds, and torsions of a molecule.

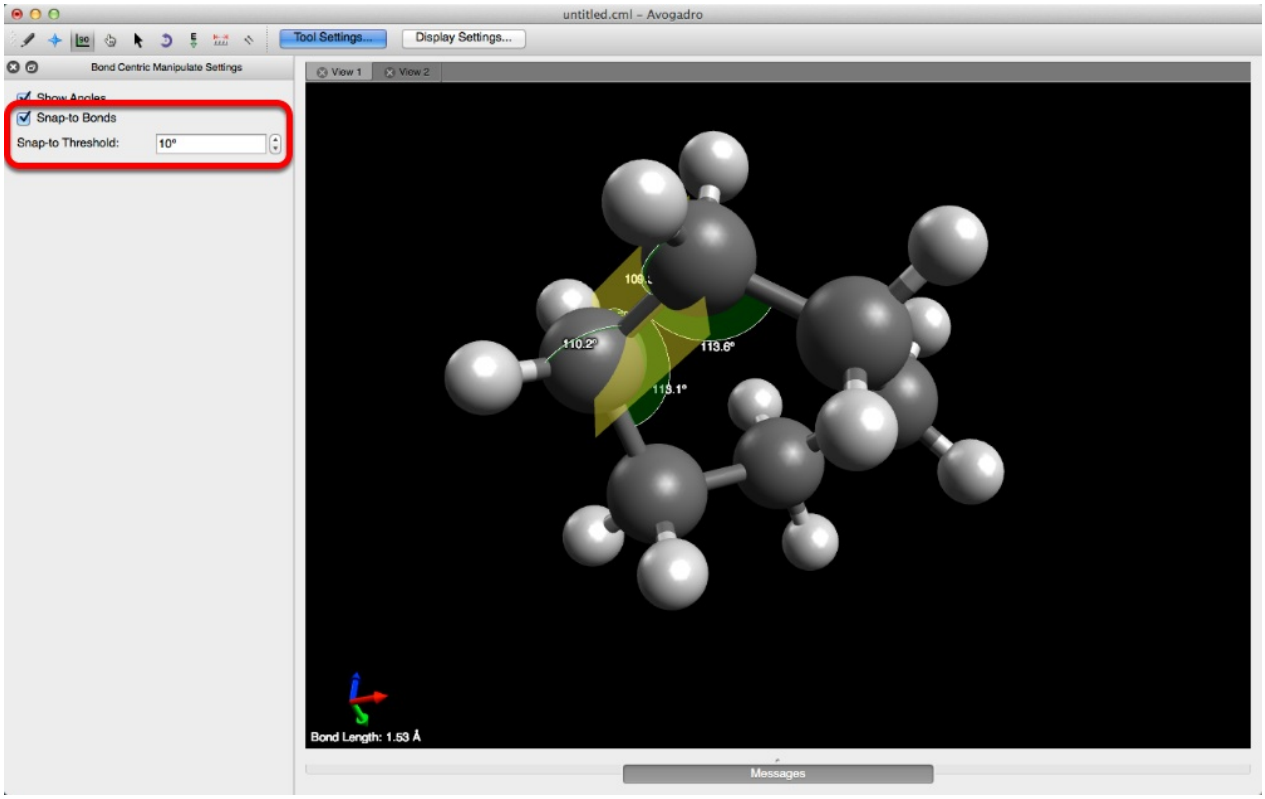


Left clicking on a bond and dragging your cursor allows you to adjust the plane. If the "Show Angles" box is checked, the angles from the selected bond to all adjacent bonds are displayed.

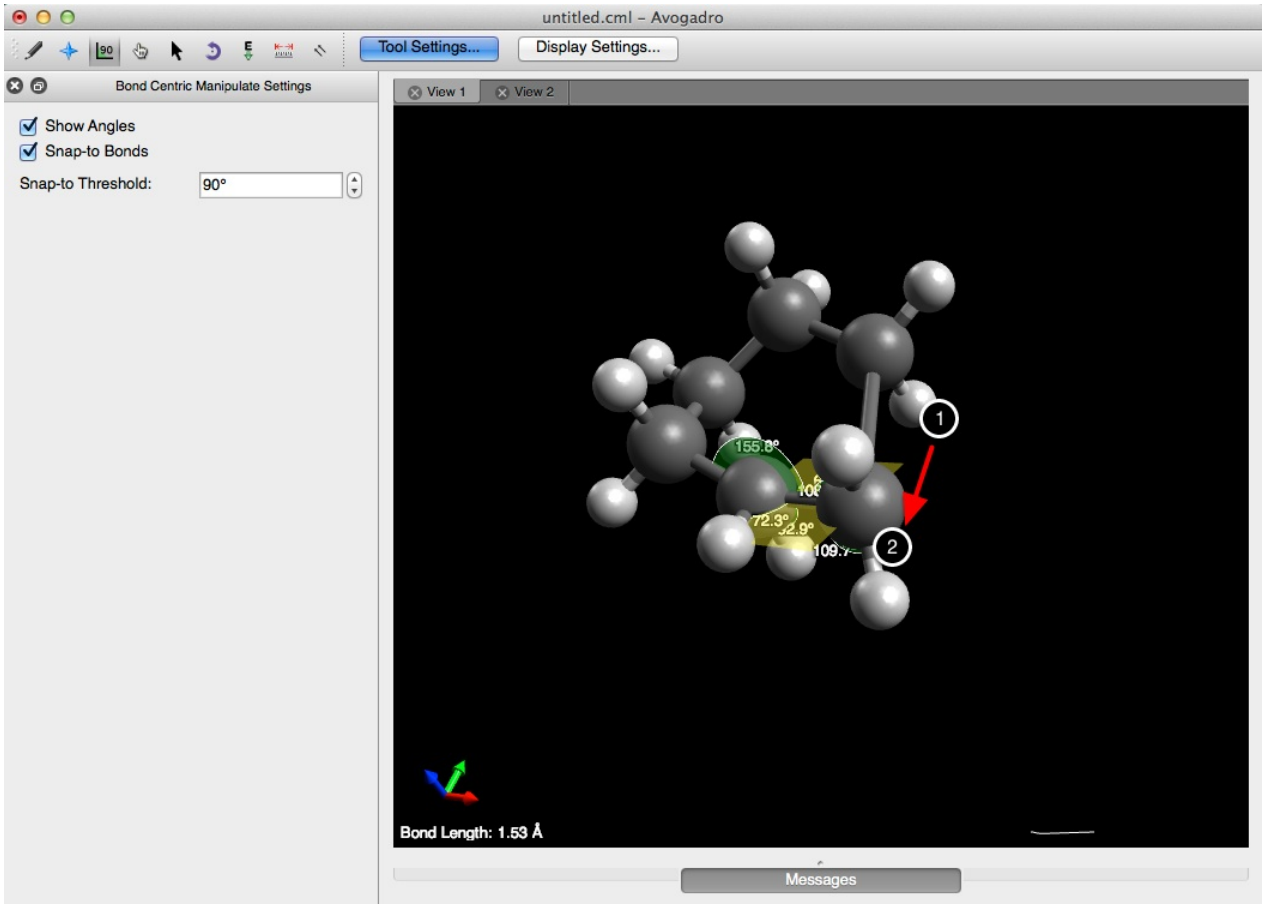


As you're rotating the plane you'll notice that if the "Snap-to Bonds" box is checked, the plane will change colors between yellow and blue. If the plane depicted is yellow then the plane *is* in line with an adjacent bond. If the plane depicted is blue the plane *is not* in line with any adjacent bonds.

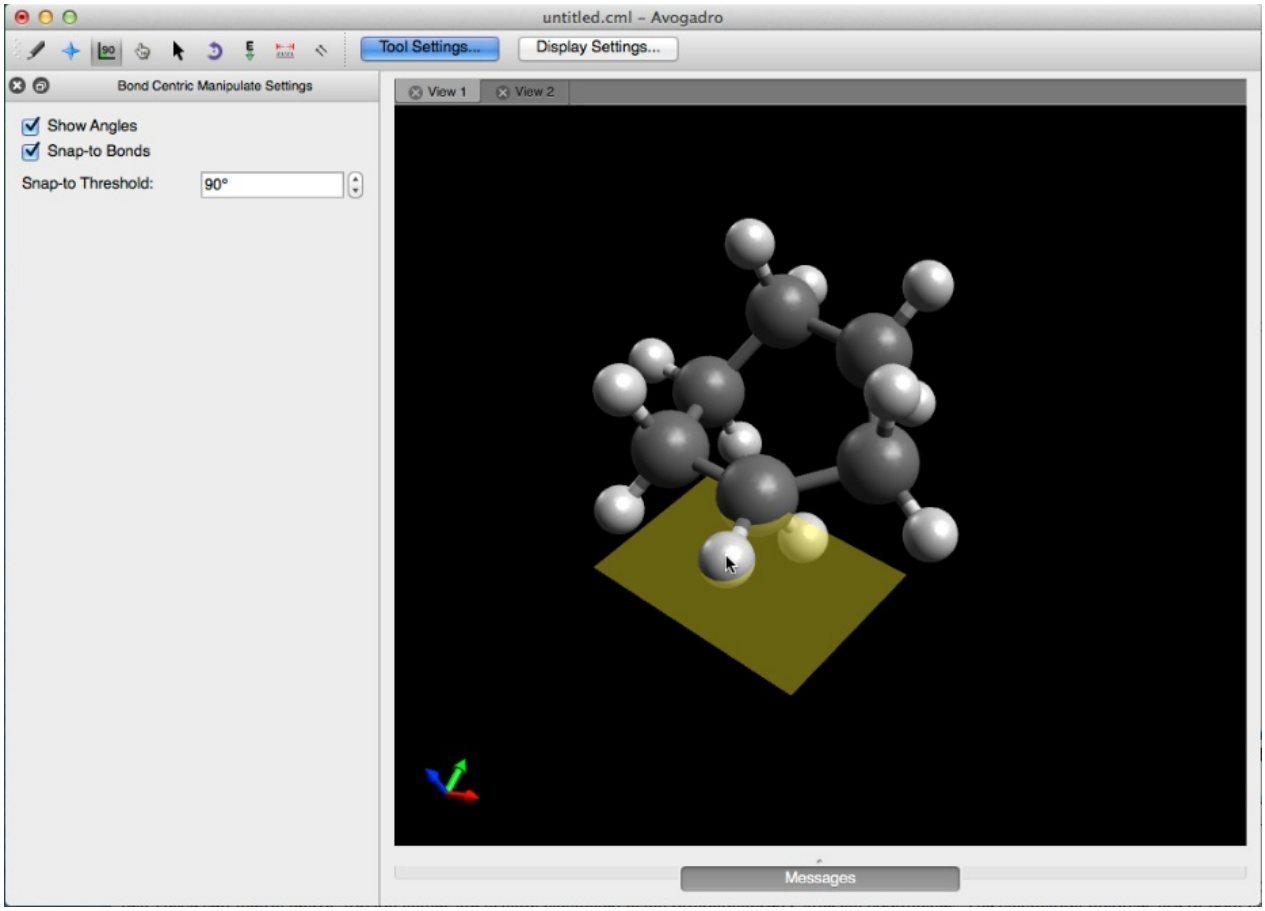
The "Snap-to Threshold" determines how far away a plane has to be to *snap* to an adjacent bond plane. For example, below the Snap-to Threshold is 10 degrees. If the plane being rotated comes within 10 degrees of an adjacent bond, that plane will snap to the adjacent bond plane. If the Snap-to Threshold is changed to 90 degrees, the rotating plane will only snap to adjacent bond planes.



Once a plane is selected the atoms on either end of the plane can be manipulated, by left clicking on the atom and dragging. The displayed angles will automatically adjust, and the selected bond will *not* change in length.

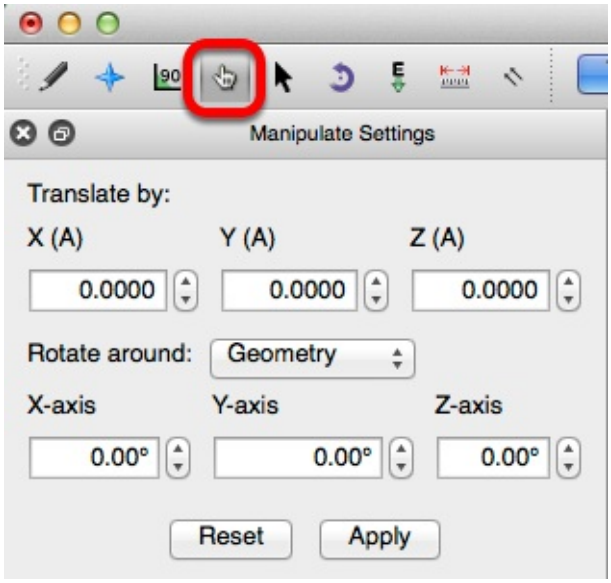


Left clicking on a substituent, or in this case a hydrogen bonded to one of the selected carbon atoms will allow you to adjust the torsion angle.


untitled.cml – Avogadro
Tool Settings...
Display Settings...
Bond Centric Manipulate Settings
Show Angles
Snap-to Bonds
Snap-to Threshold:
90°
View 1
View 2
Messages

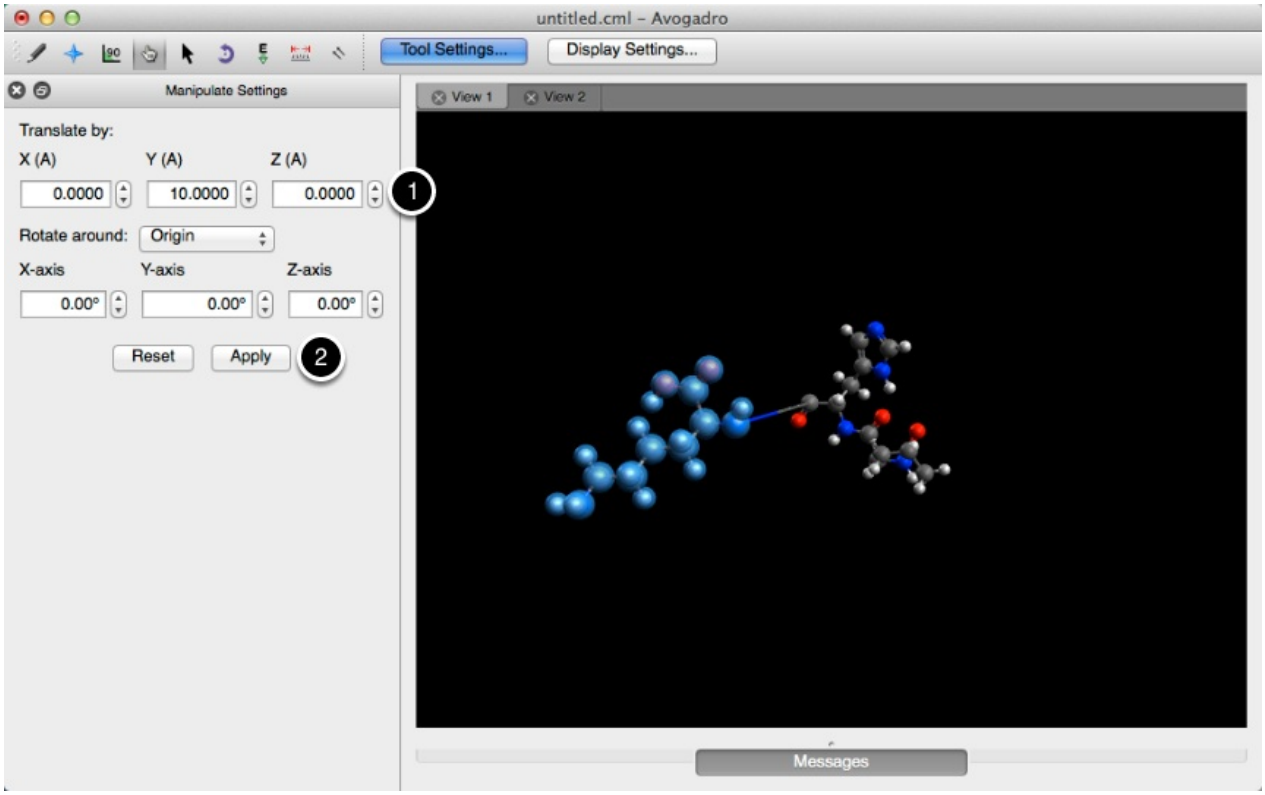
The Manipulate Tool

The manipulate tool allows you to move atoms and selected fragments.

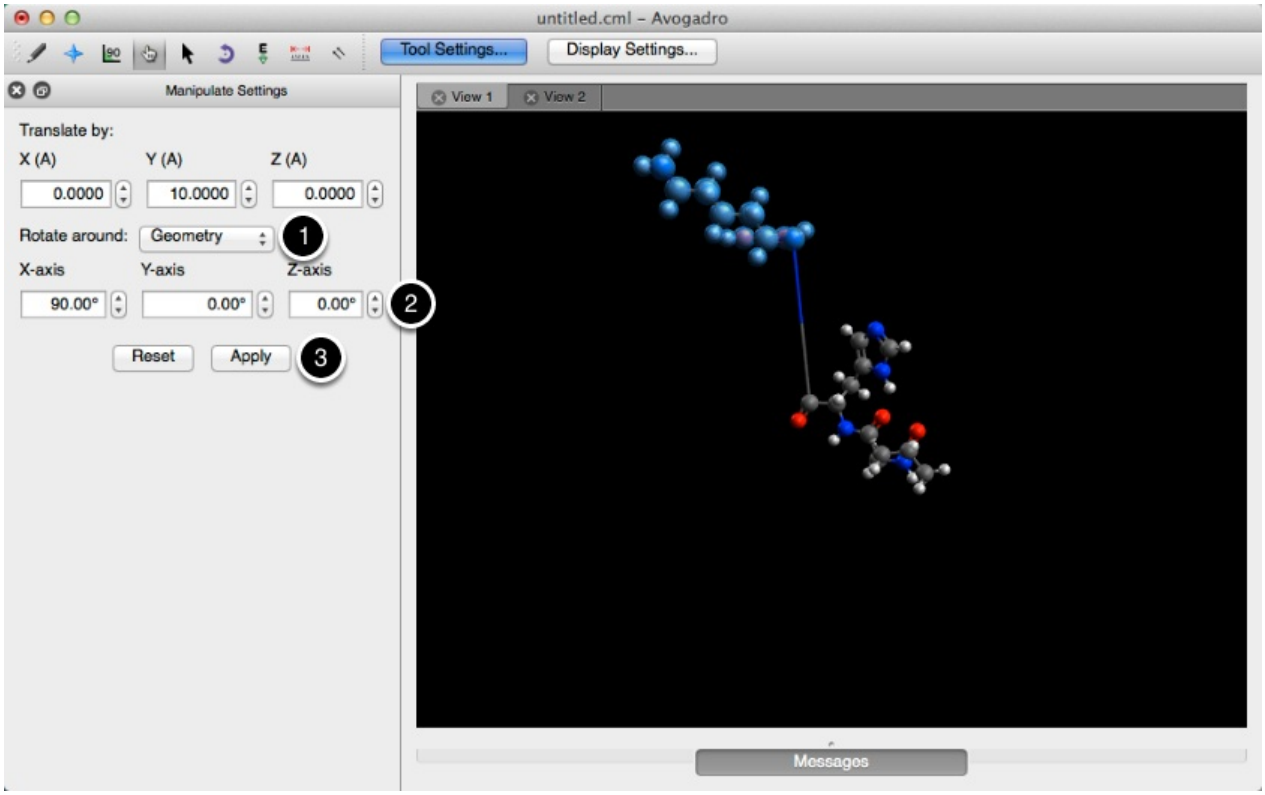


If inserting a fragment, the manipulate tool is automatically selected so that the fragment can easily be rotated into position.

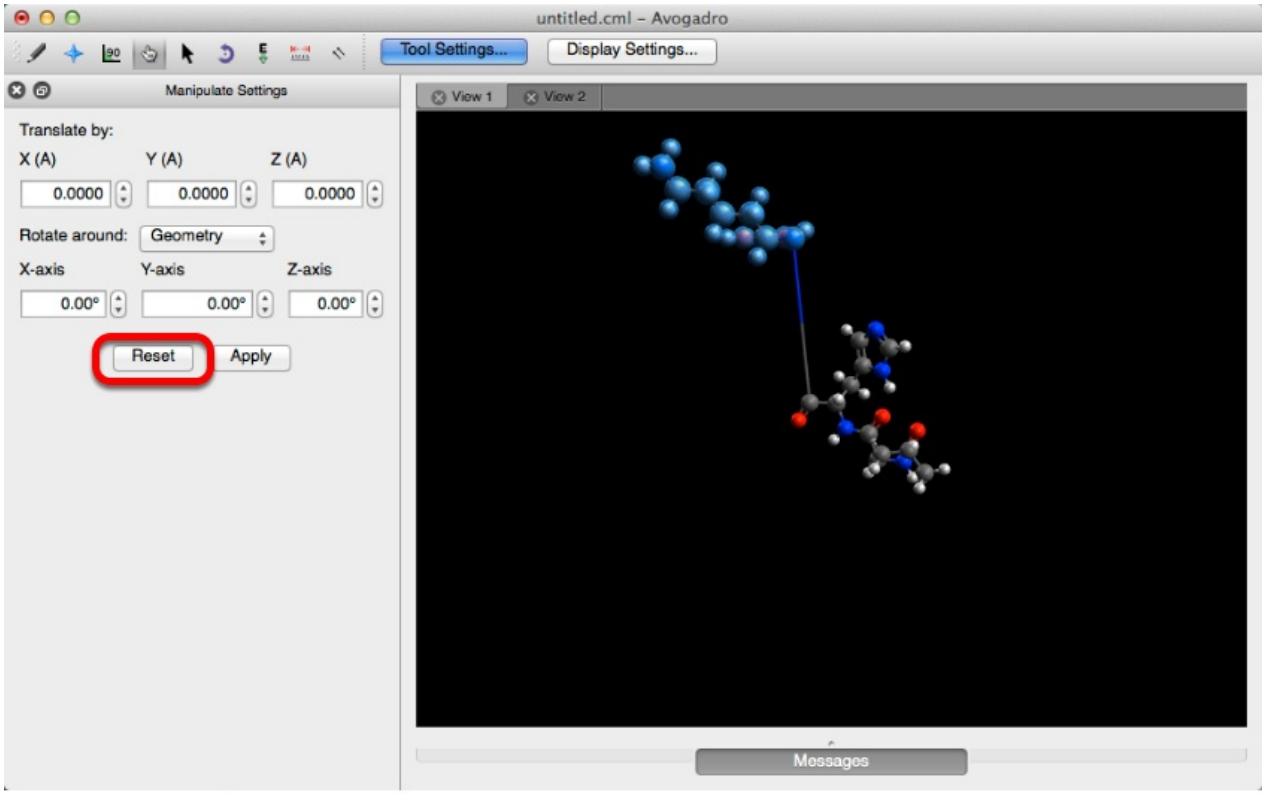
The "Translate by:" section allows you to easily translate the length of a bond (to a fragment or atom) into the desired positon. For a translation to take place, enter in the desired translation and then click "Apply".

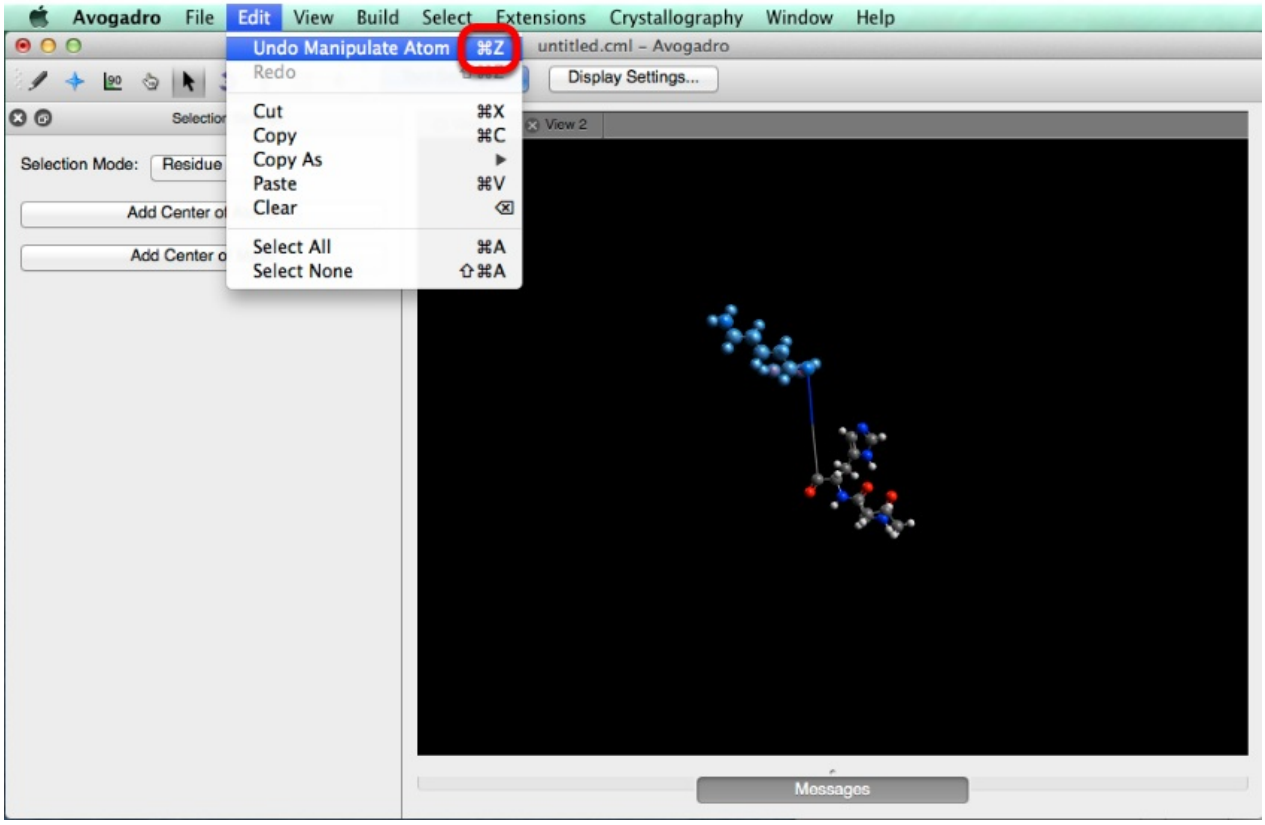


The "Rotate around:" section allows you to rotate your selection around the geometry, or the origin. This section then gives you the ability to choose how many degrees to rotate the fragment. Click "Apply" once you've made your selection.



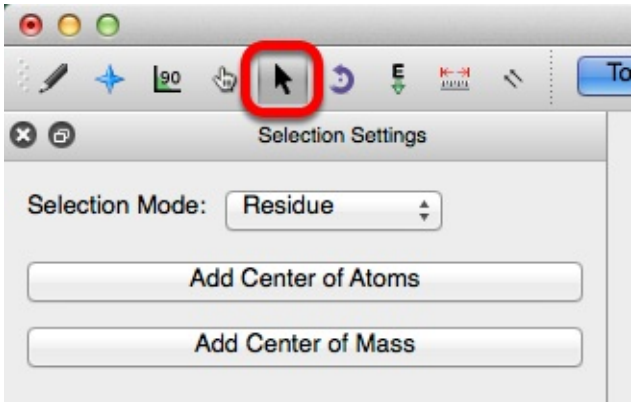
Clicking "Reset" will reset all of the information in the translation, and rotation boxes. This does not reset the molecule, if you want to undo your adjustments go to the "Edit" menu in the top bar and select "Undo Manipulate Atom".


untitled.cml – Avogadro
Tool Settings...
Display Settings...
Manipulate Settings
Translate by:
X (A)
Y (A)
Z (A)
0.0000
0.0000
0.0000
Rotate around:
Geometry
X-axis
Y-axis
Z-axis
0.00°
0.00°
0.00°
Reset
Apply
View 1
View 2
Messages


Avogadro
File
Edit
View
Build
Select
Extensions
Crystallography
Window
Help
Undo Manipulate Atom ⌘Z
Redo
Cut ⌘X
Copy ⌘C
Copy As
Paste ⌘V
Clear
Select All ⌘A
Select None ⇧⌘A
untitled.cml – Avogadro
Display Settings...
Selection Mode:
Residue
View 2
Messages

The Selection Tool

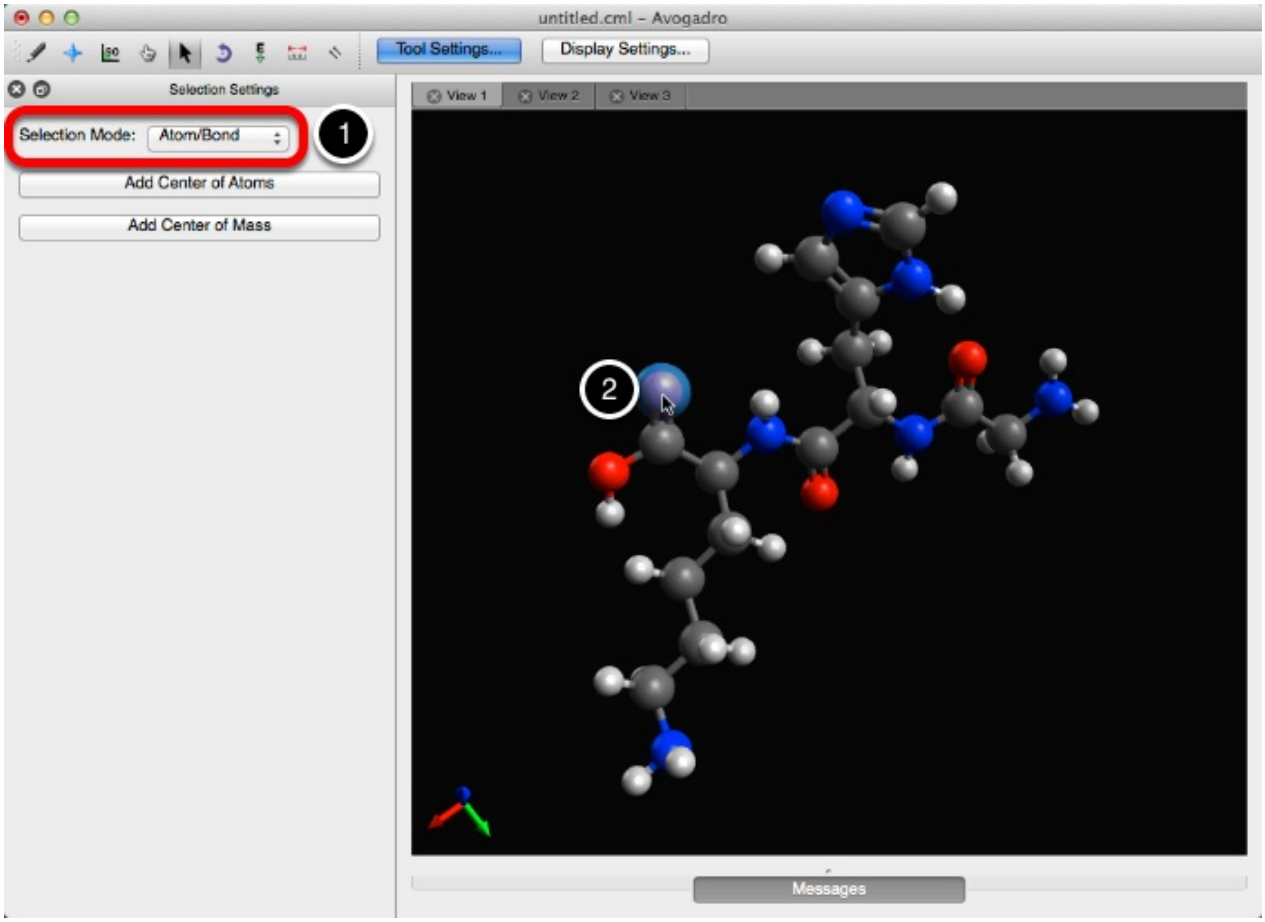
The selection tool allows the indiviual selection of atoms, bonds, or fragments.



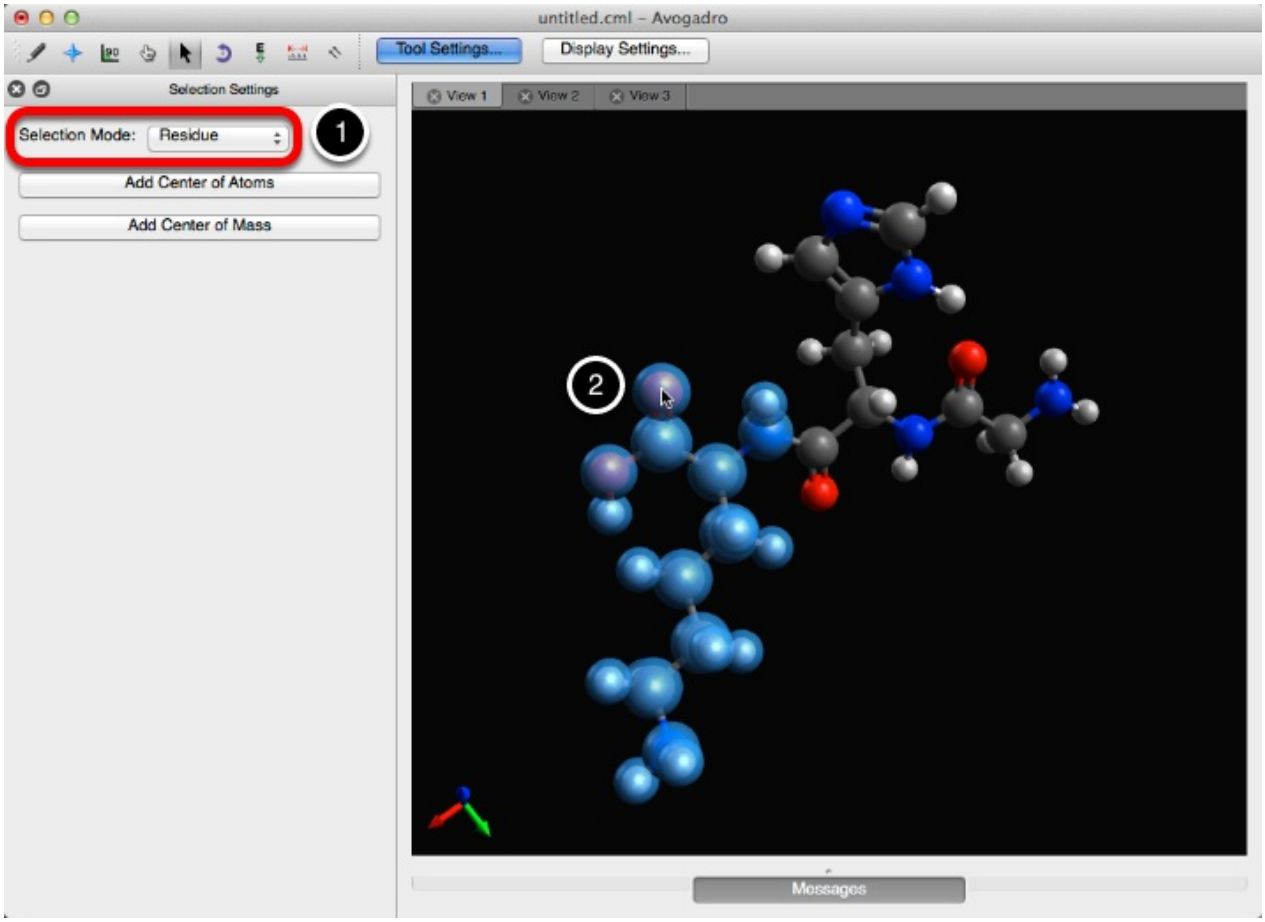
There are three types of selection modes: "Atom/Bond", "Residue", and "Molecule".

The "Atom/Bond" selection mode provides you with the ability to select a single atom within a molecule. This is achieved by left clicking the atom. Pressing down the "Shift" button on your keyboard allows the selection of multiple atoms.

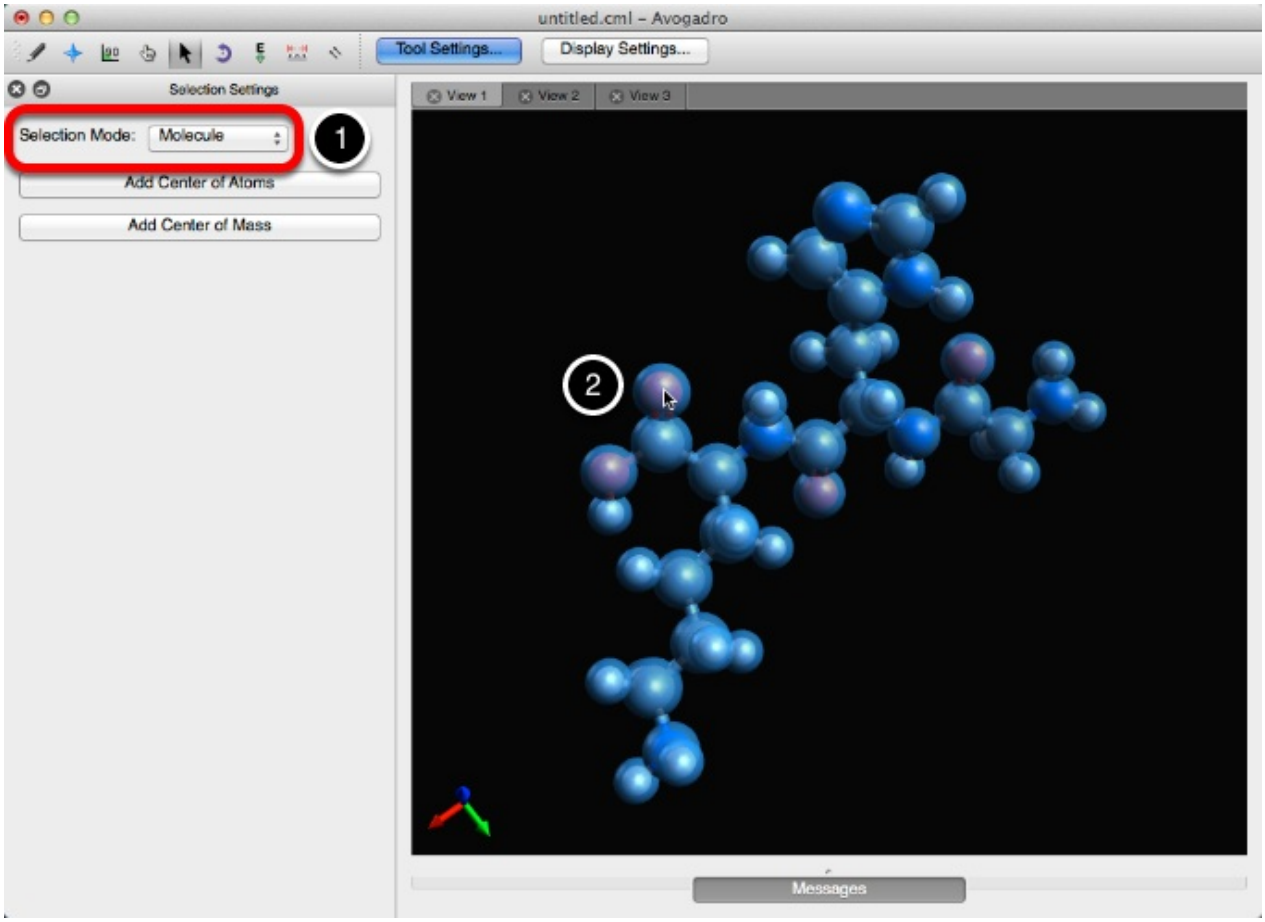
Right clicking on the black display will clear the selection made.



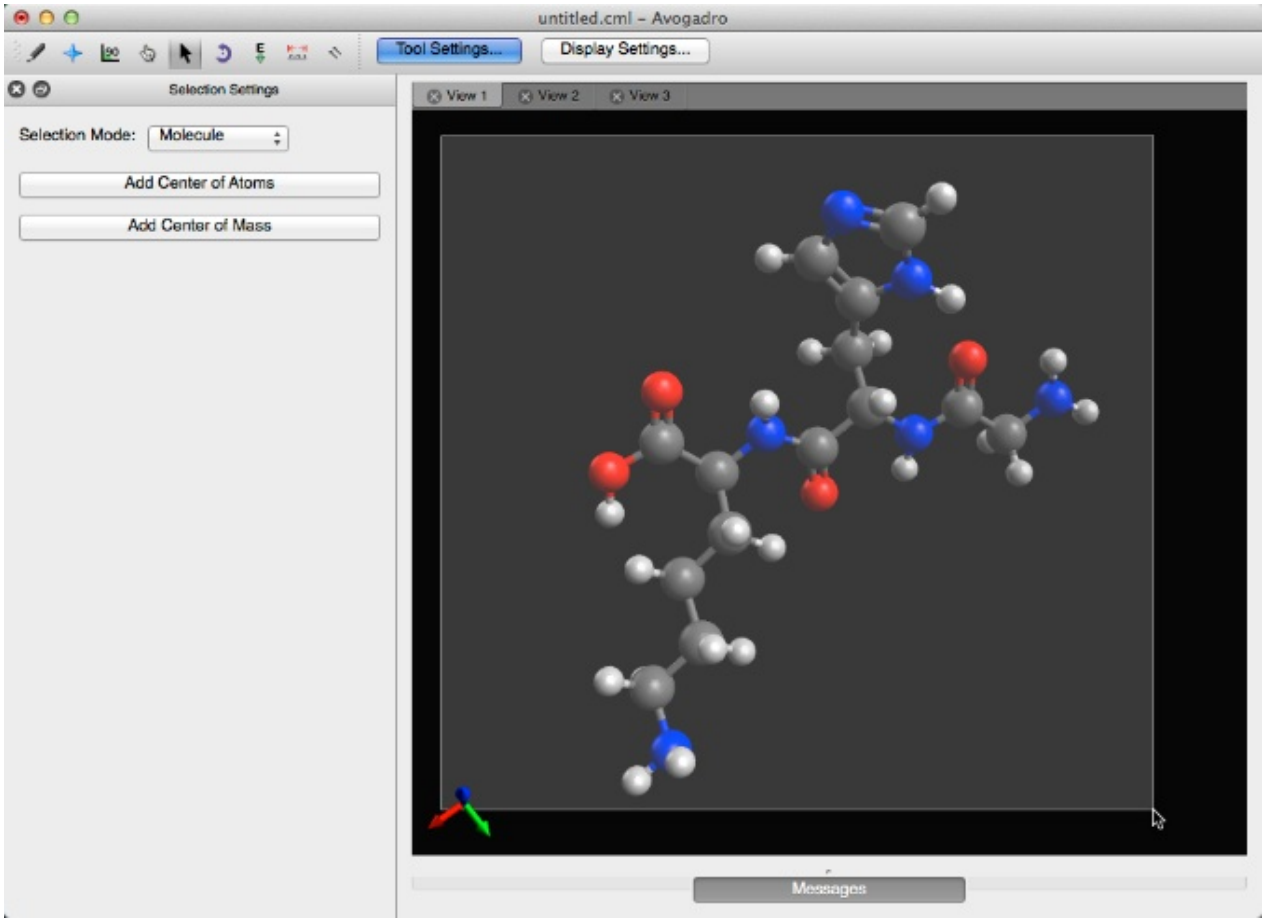
The "Residue" selection mode will select an entire residue within the molecule, by clicking on a single atom in the residue.



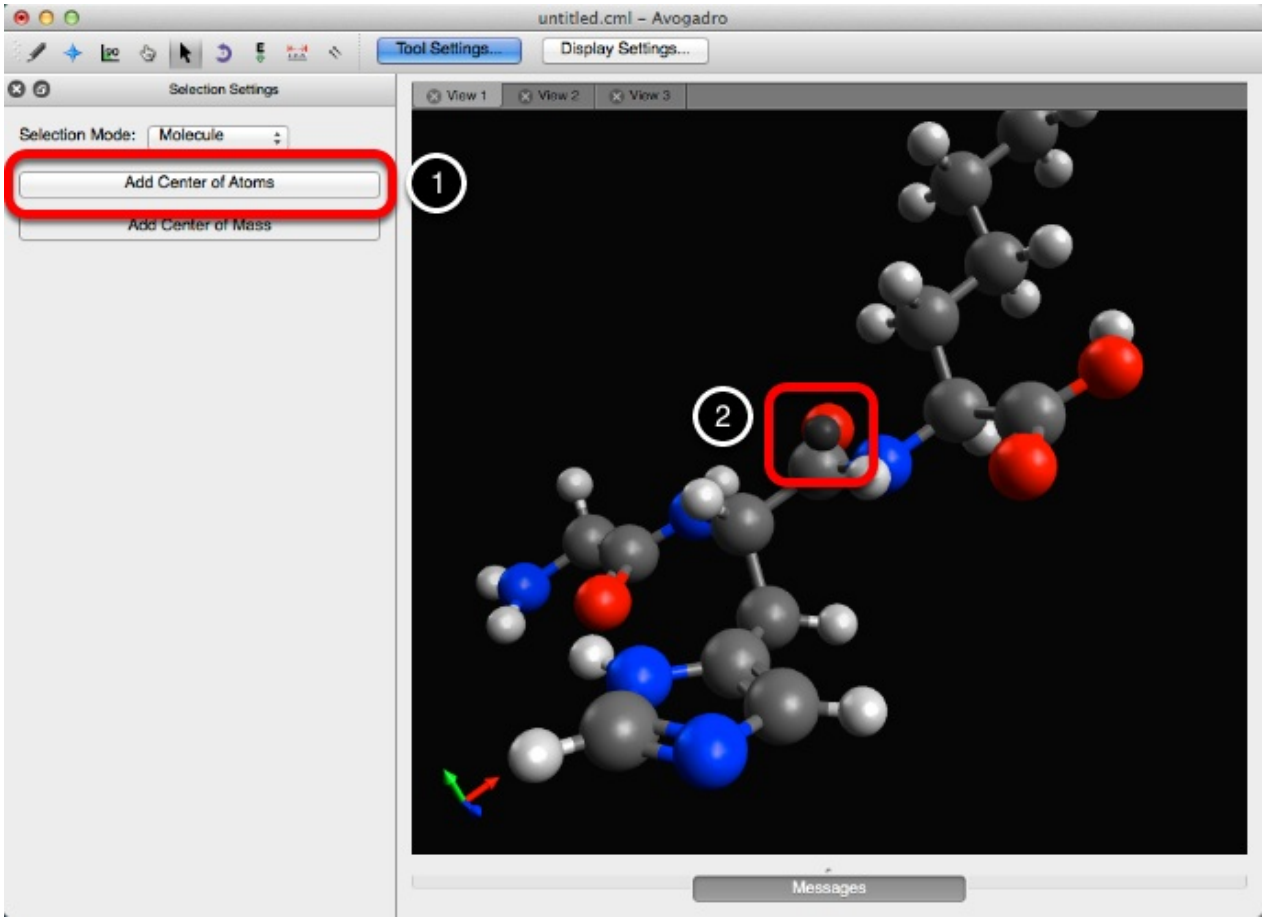
The "molecule" selection mode will select the entire molecule by clicking on an atom. Double clicking the molecule will also select the entire molecule.



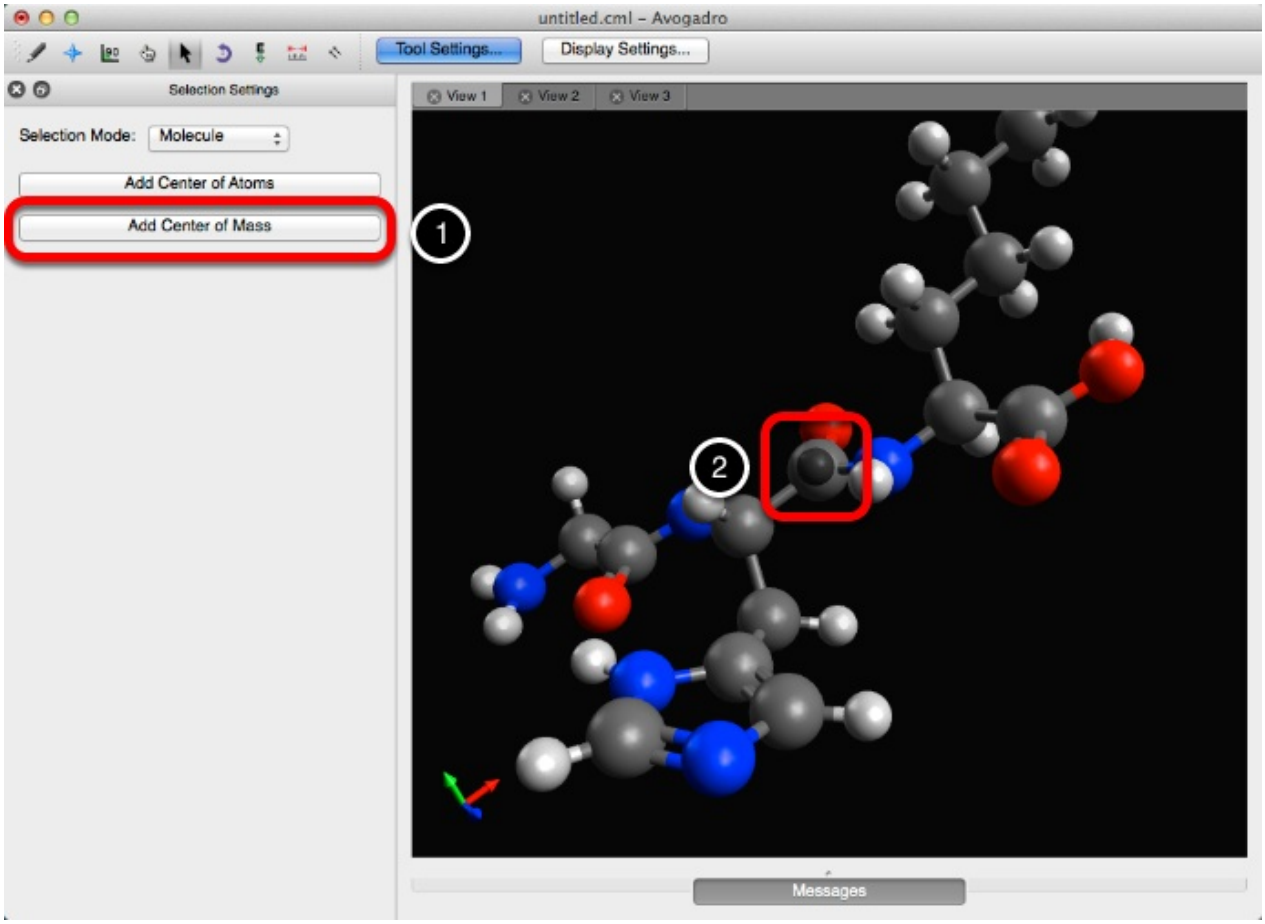
Molecules can also be selected by clicking and dragging your cursor across the display.



Clicking on "Add Center of Atoms" will display a black ball where the center of the atoms is found.

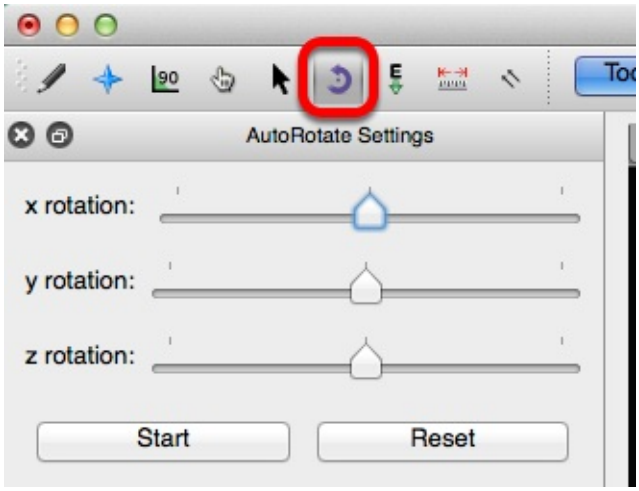


Clicking on the "Add Center of Mass" will display a black ball where the center of mass of the molecule is found.

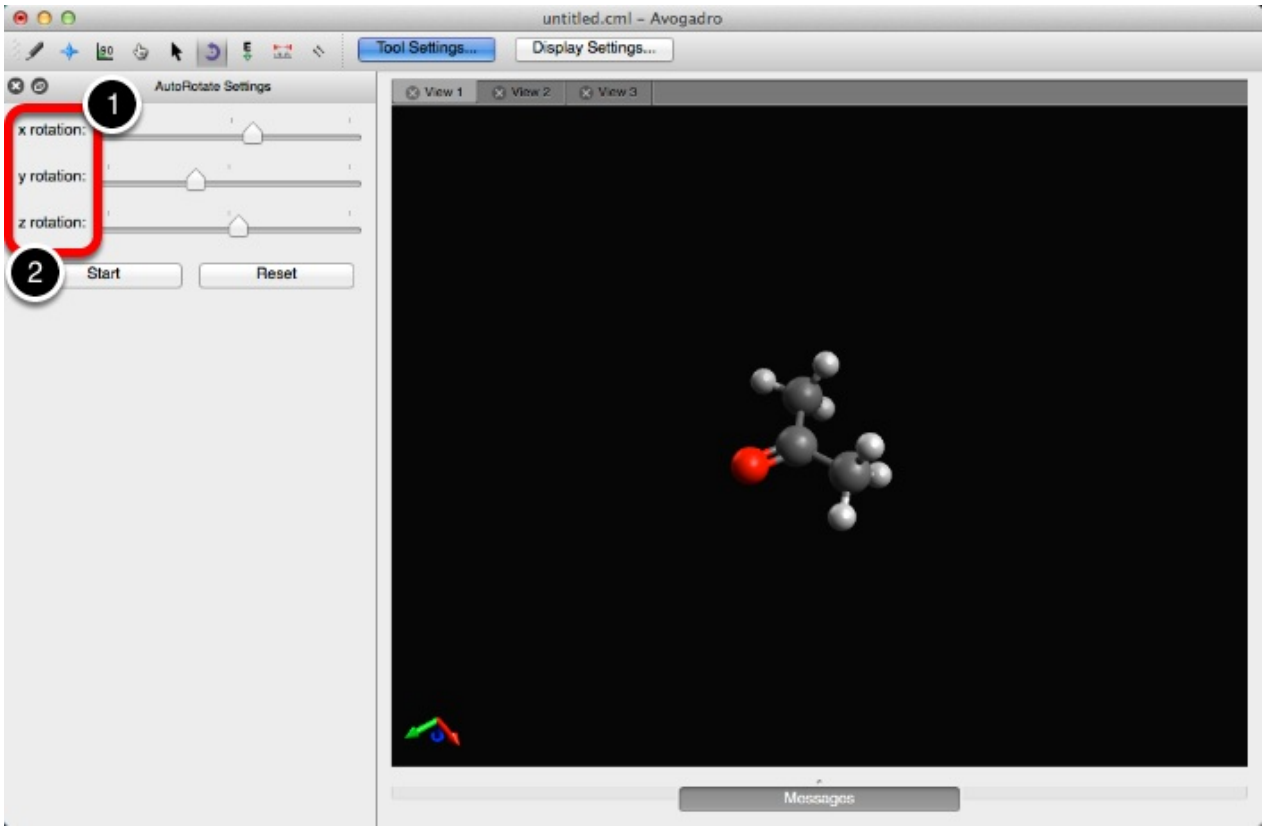

untitled.cml – Avogadro
Tool Settings...
Display Settings...
Selection Settings
Selection Mode:
Molecule
Add Center of Atoms
Add Center of Mass
View 1
View 2
View 3
1
2
Messages

The Auto-Rotate Tool

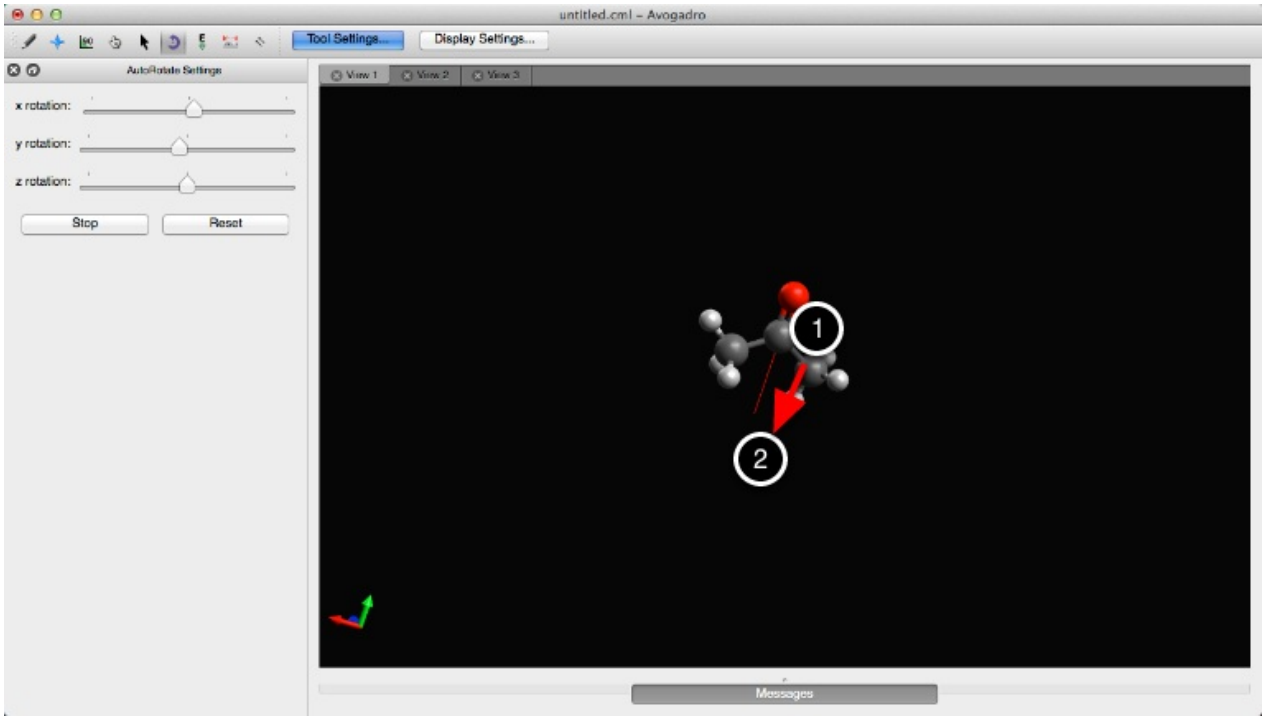
The auto rotate tool allows for the continuous rotation of a molecule.



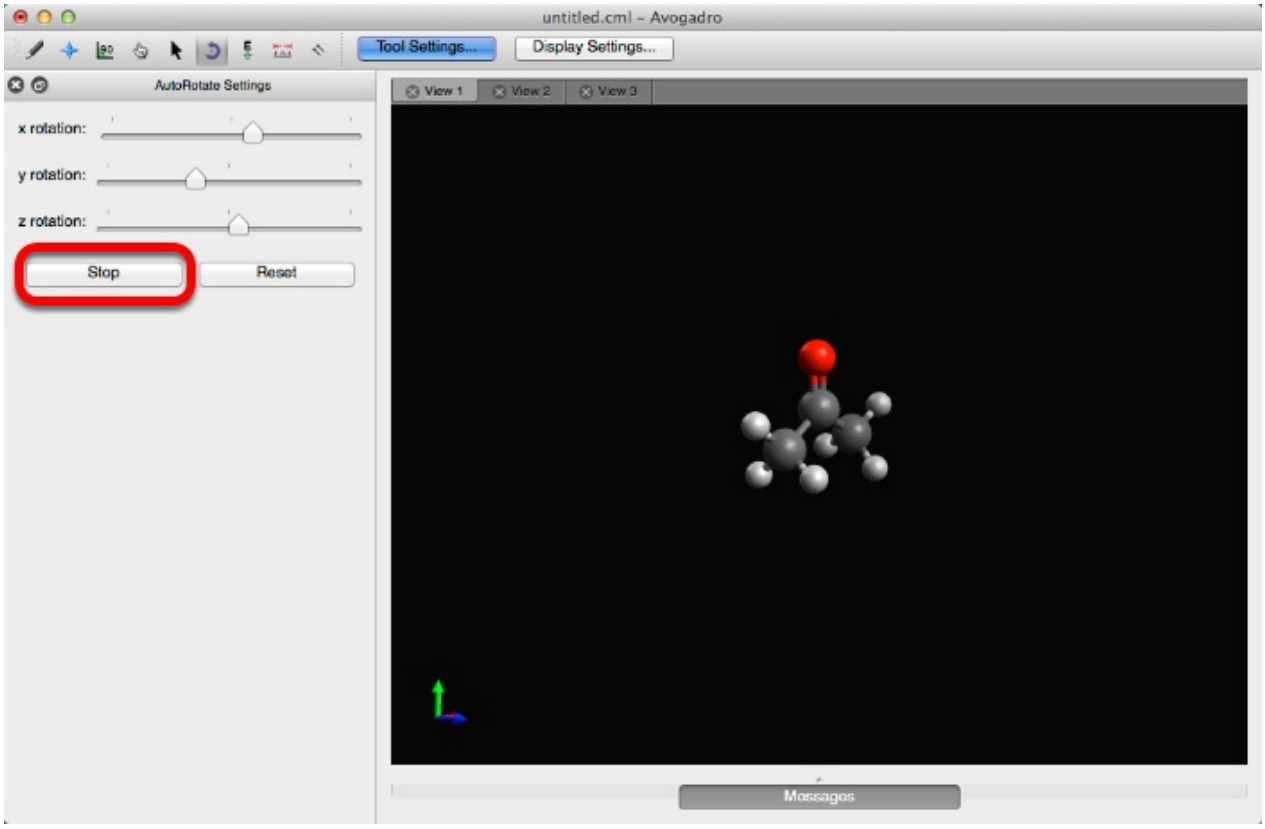
To rotate the molecule, adjust the x, y, and z rotation scales as desired. Then select "Start".



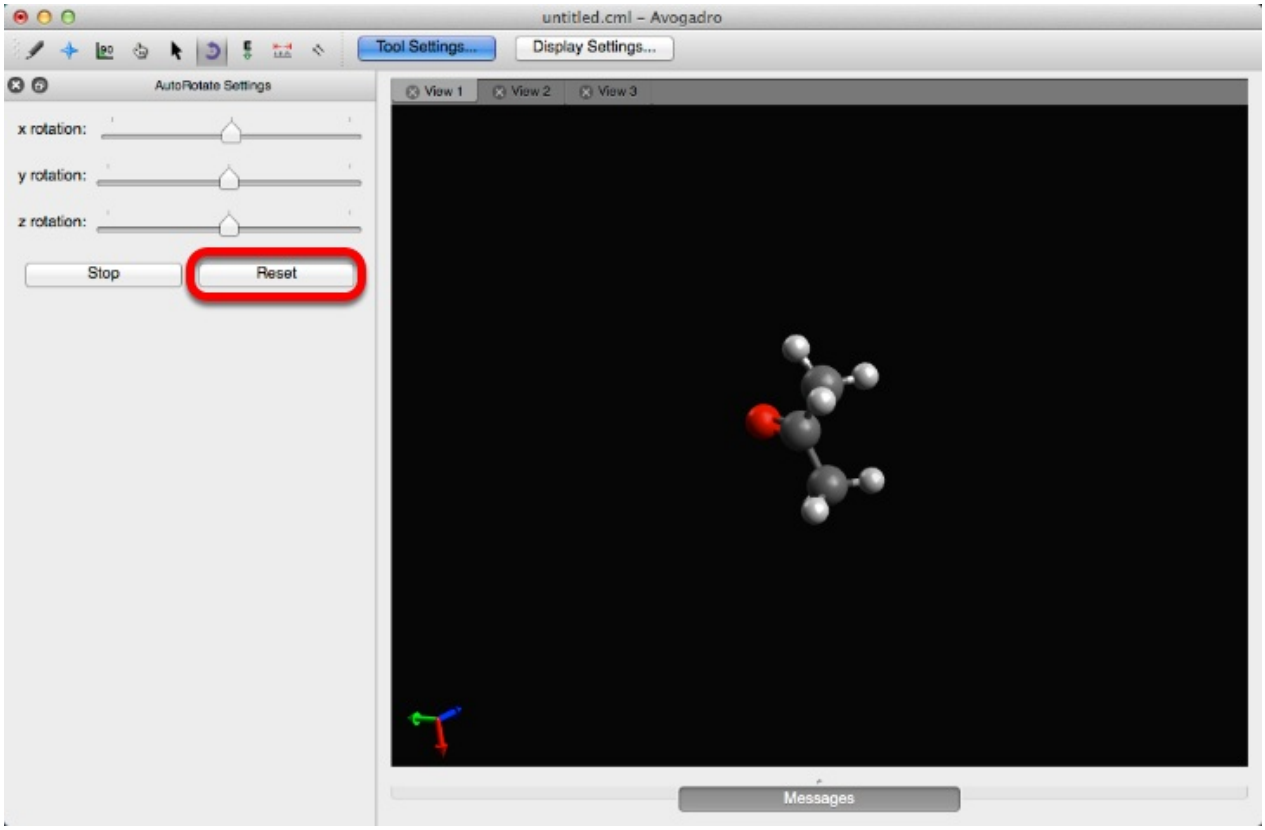
You can also click and drag from an atom to rotate the molecule in a specific direction.



Select "Stop" to end the molecule's rotation.

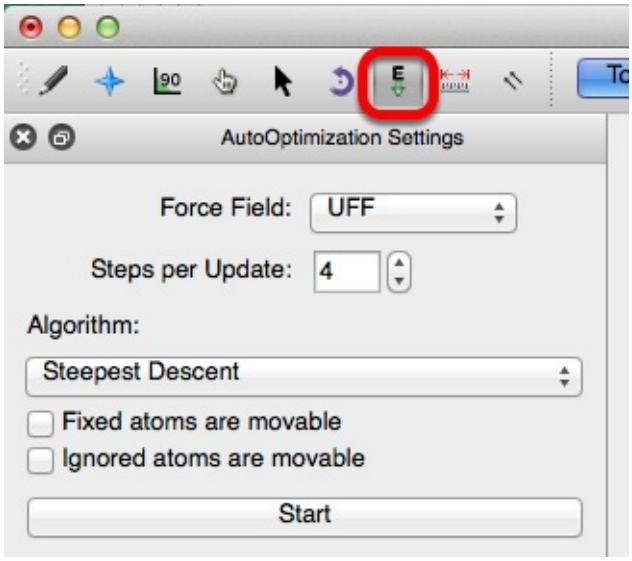


Clicking "Reset" will zero out the rotation scales and stop the rotation.

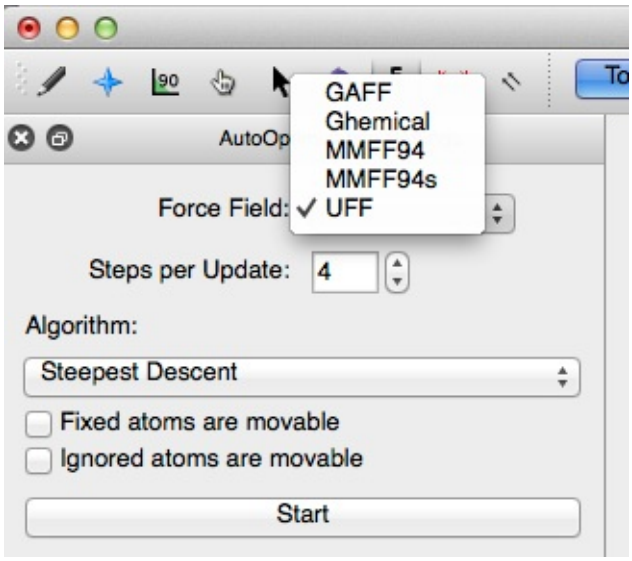

untitled.cml – Avogadro
Tool Settings...
Display Settings...
AutoRotate Settings
x rotation:
y rotation:
z rotation:
Stop
Reset
View 1
View 2
View 3
Messages

The Auto-Optimize Tool

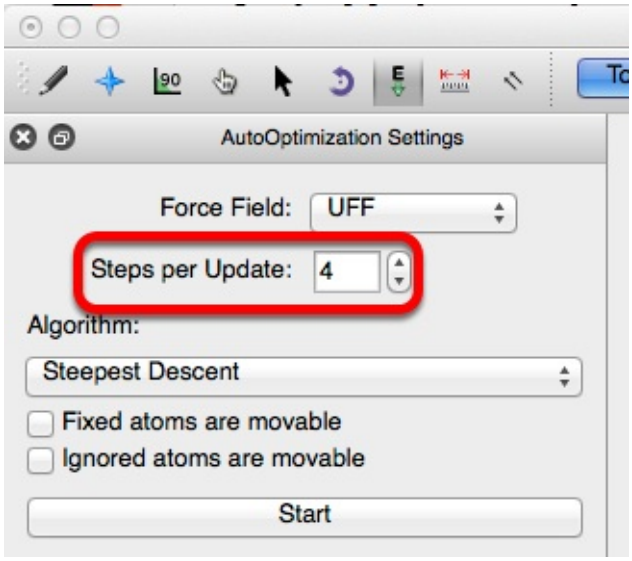
The Auto Optimize tool continuously optimizes molecular geometry through molecular mechanics. This tool also gives you the ability to manipulate the molecule while the molecular geometry is being minimized.



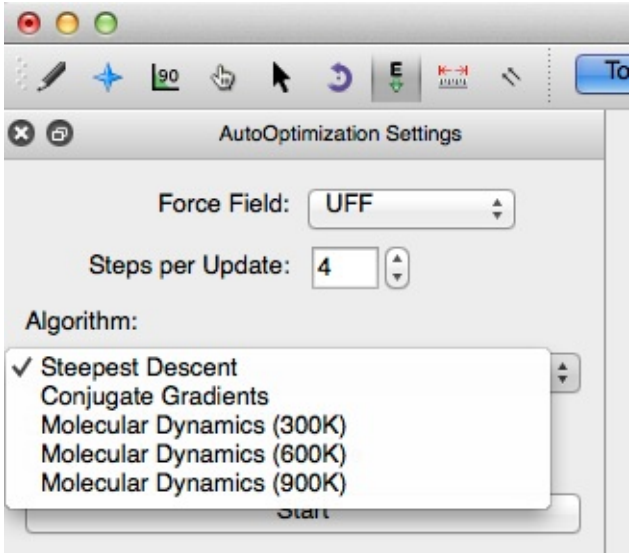
The Auto-Optimization settings provide several force field options. The default force field is UFF or the Universal Force Field. This force field is capable of reproducing the most structural features across the periodic table. However, depending on the molecule being tested, the other force fields may be better suited to optimize the molecular parameters. The force field options are shown below. For more information on force fields refer to the optimizing geometry section of this lab manual.



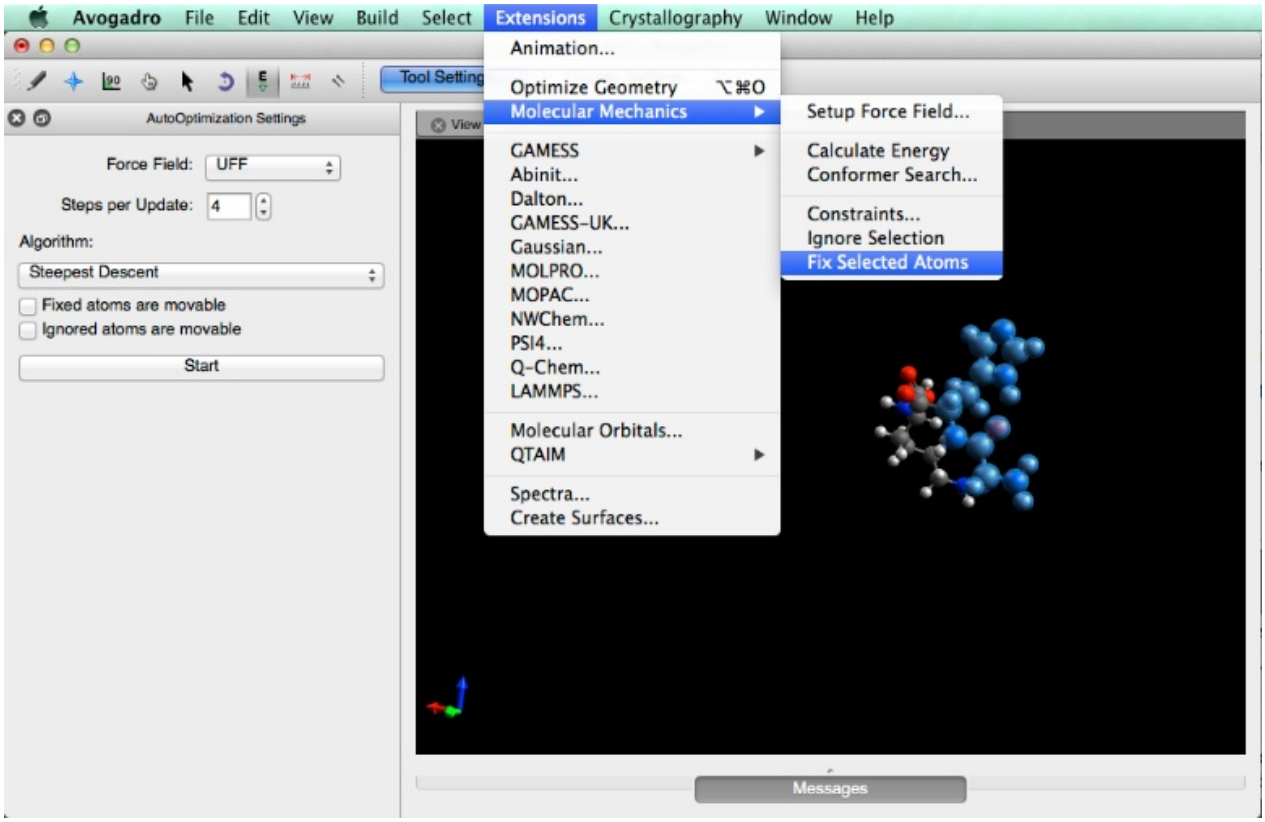
The default setting for "Steps per Update" is 4. This number can be increased or decreased, if you have a slower computer consider decreasing this number.



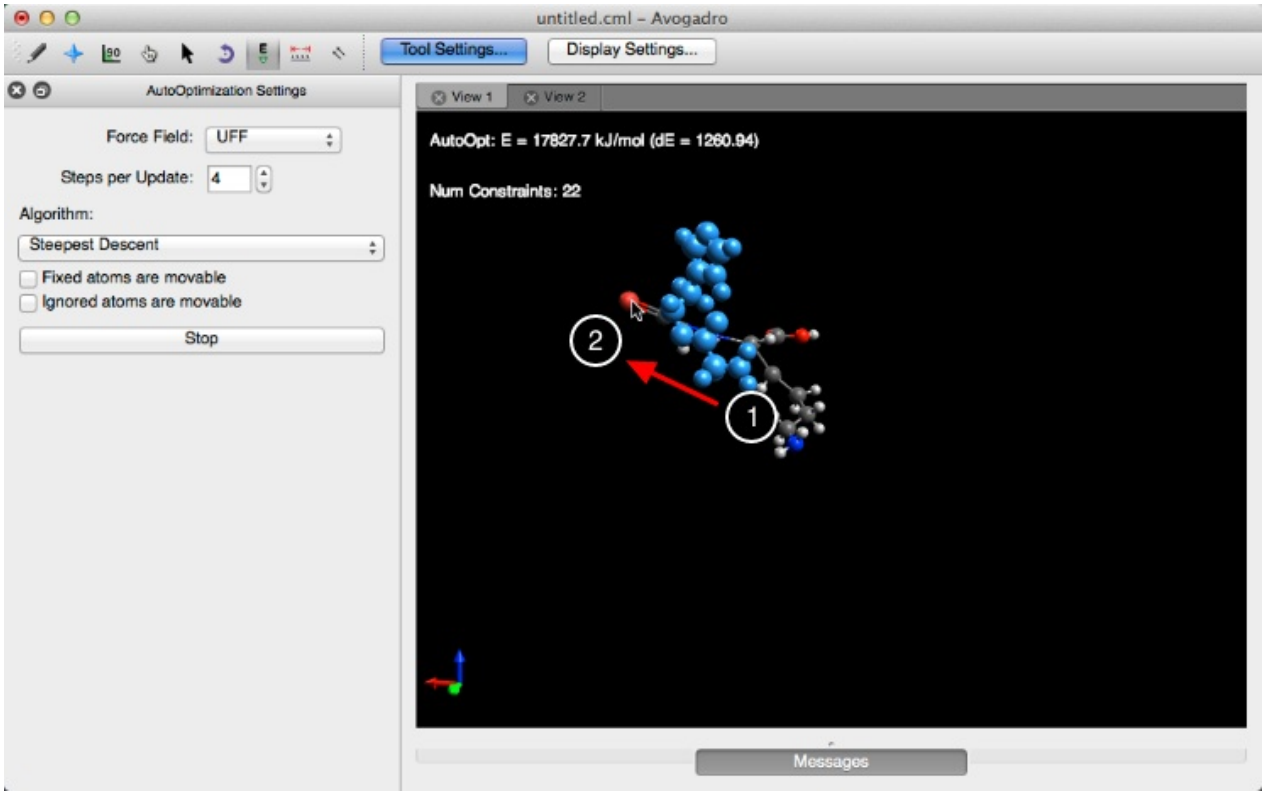
Avogadro can also apply specific algorithms dependent on your need. Steepest descent is the most fluid and interactive system, and is the default algorithm.



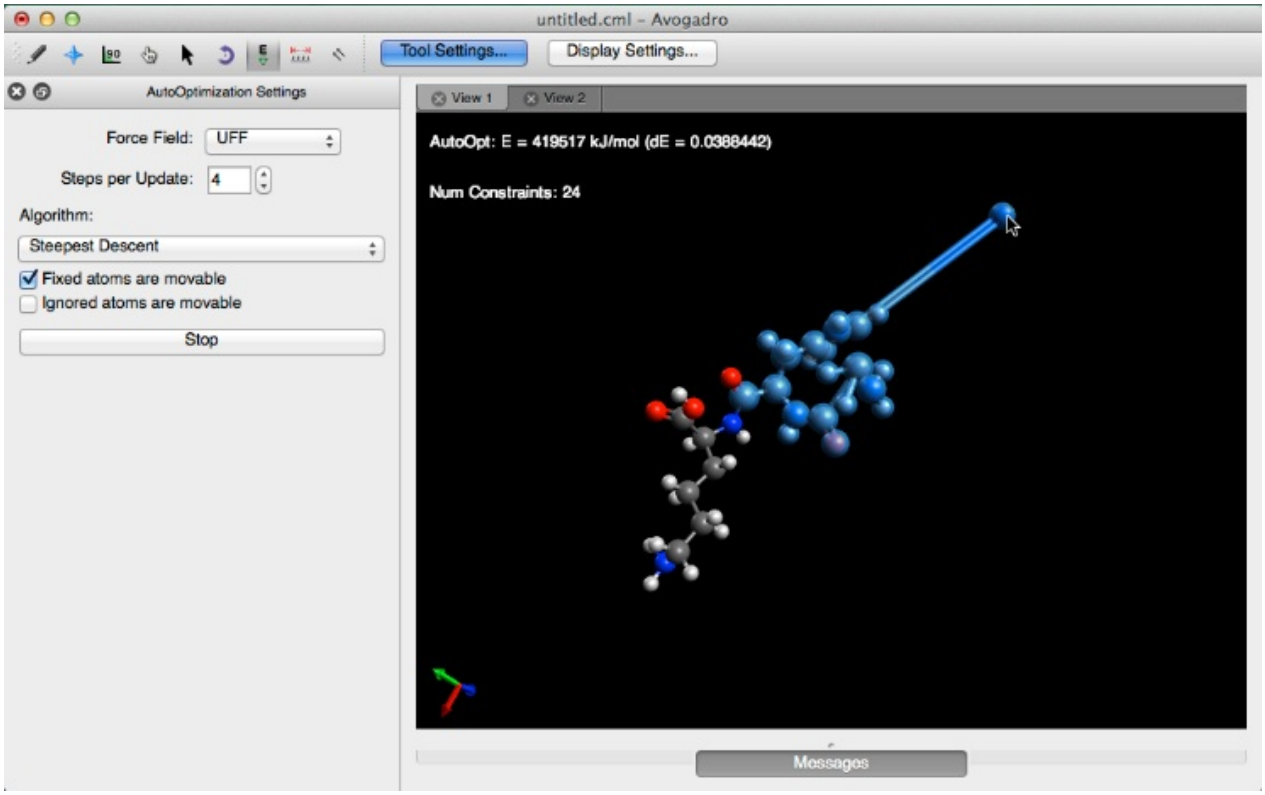
If necessary, atoms can be fixed into place before optimization so that they don't move. This is done by going to the "Extensions" menu, holding your cursor over "Molecular Mechanics" and selecting "Fix Selected Atoms".



Clicking on "Start" will allow you to manipulate the molecule by left clicking on an atom and dragging your cursor. Notice that the fixed atoms don't bend with the manipulation of the molecule.

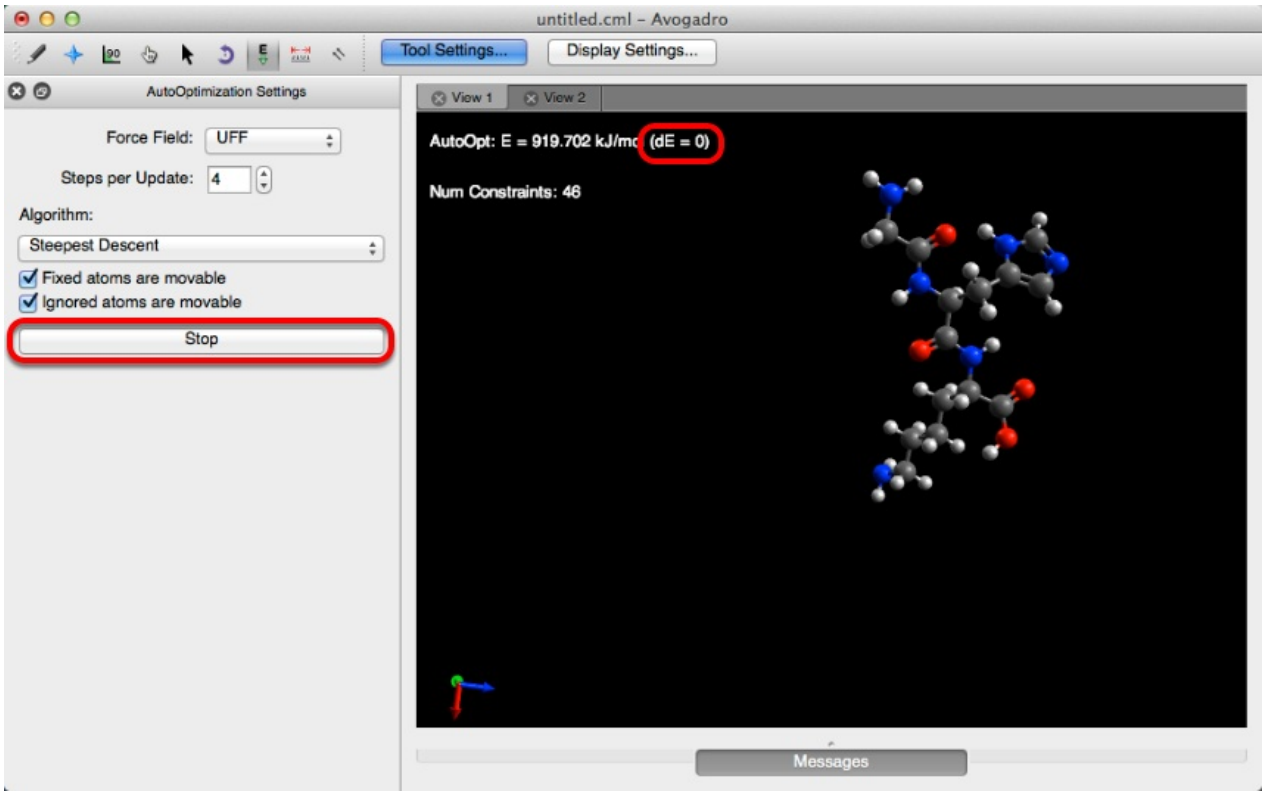


If the "Fixed atoms are movable" box is checked, the bonds between atoms can be manipulated but are constrained. In this instance the selected atom does not reoptimize once it's dragged.



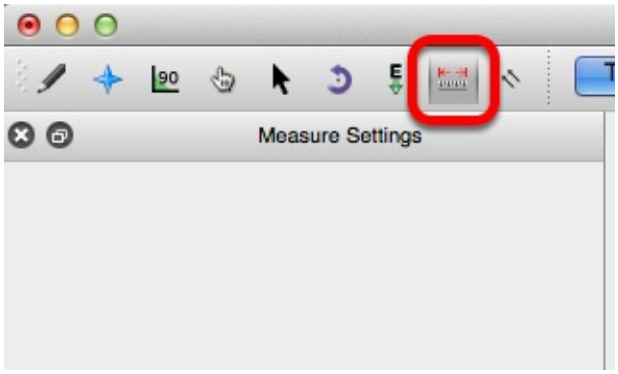
Essentially, the same thing takes place if the "Ignored atoms are movable" box is checked. However, ignored atoms (if the box is checked) *will* reoptimize once dragged. To ignore a selection select the "Extensions" drop down menu, hold your cursor over "Molecular Mechanics" option, and select "Ignore Selection".

The molecule will reoptimize until dE=0 or "Stop" is clicked.

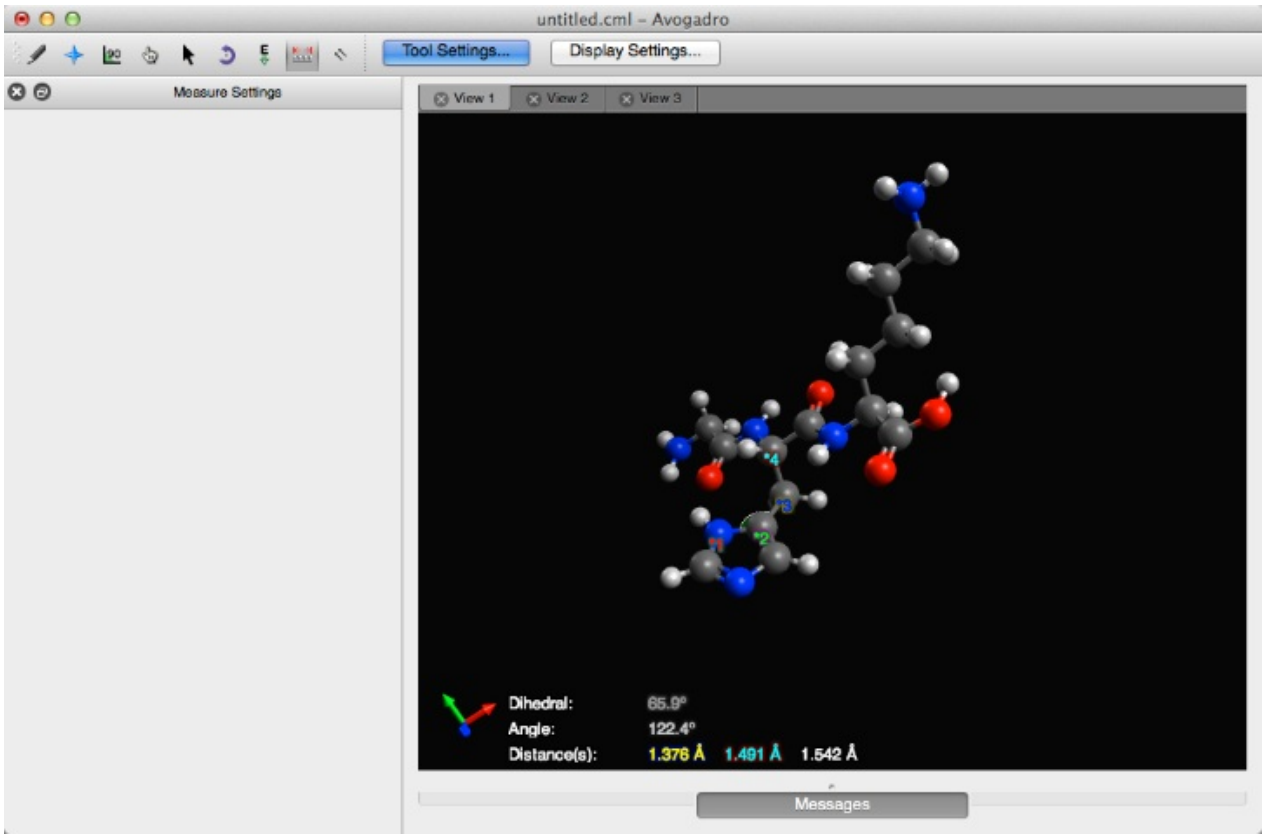


The Measure Tool

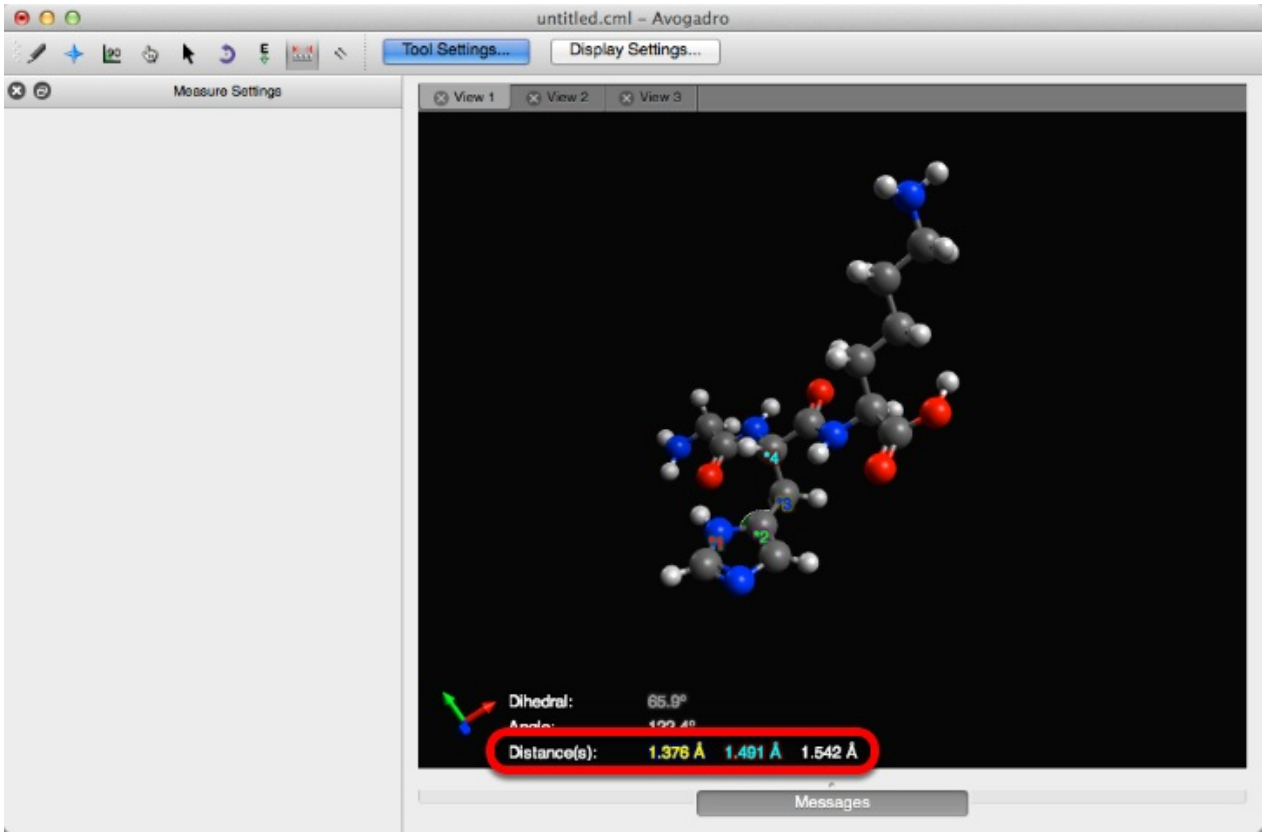
The measure tool determines bond lengths, angles, and dihedrals.



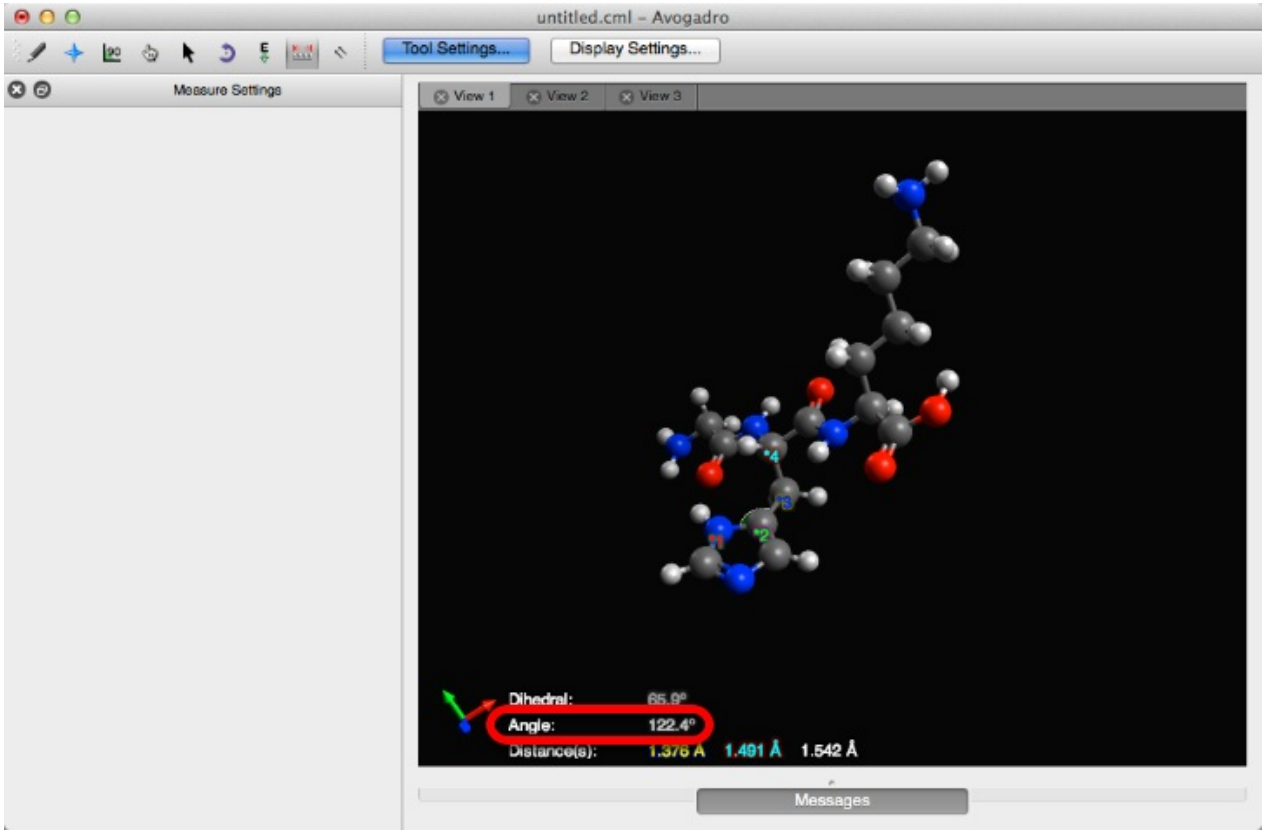
The measure tool allows you to select and assess up to four atoms.



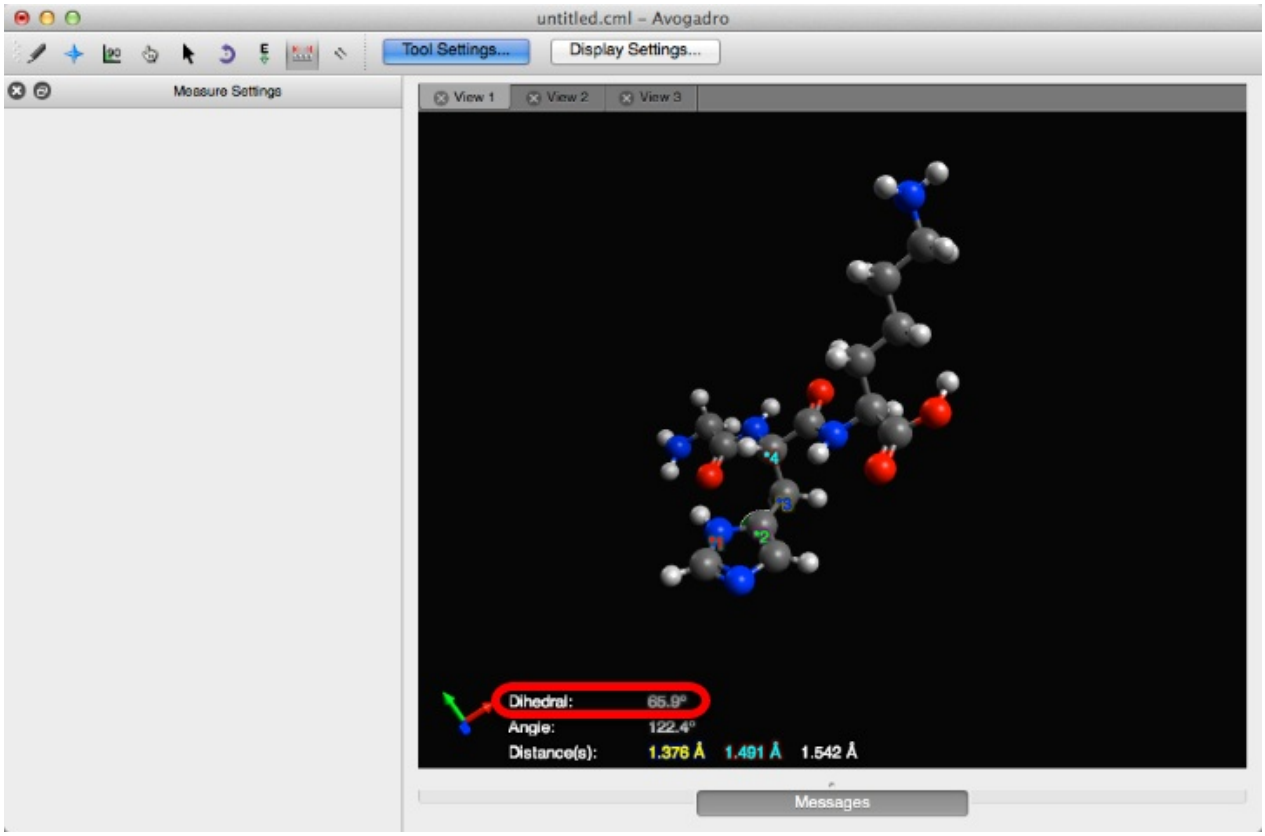
As you click on atoms Avogadro will automatically calculate the distances between atoms in a respective order. For example, the distance between atom 1 and 2 is 1.376 Å.



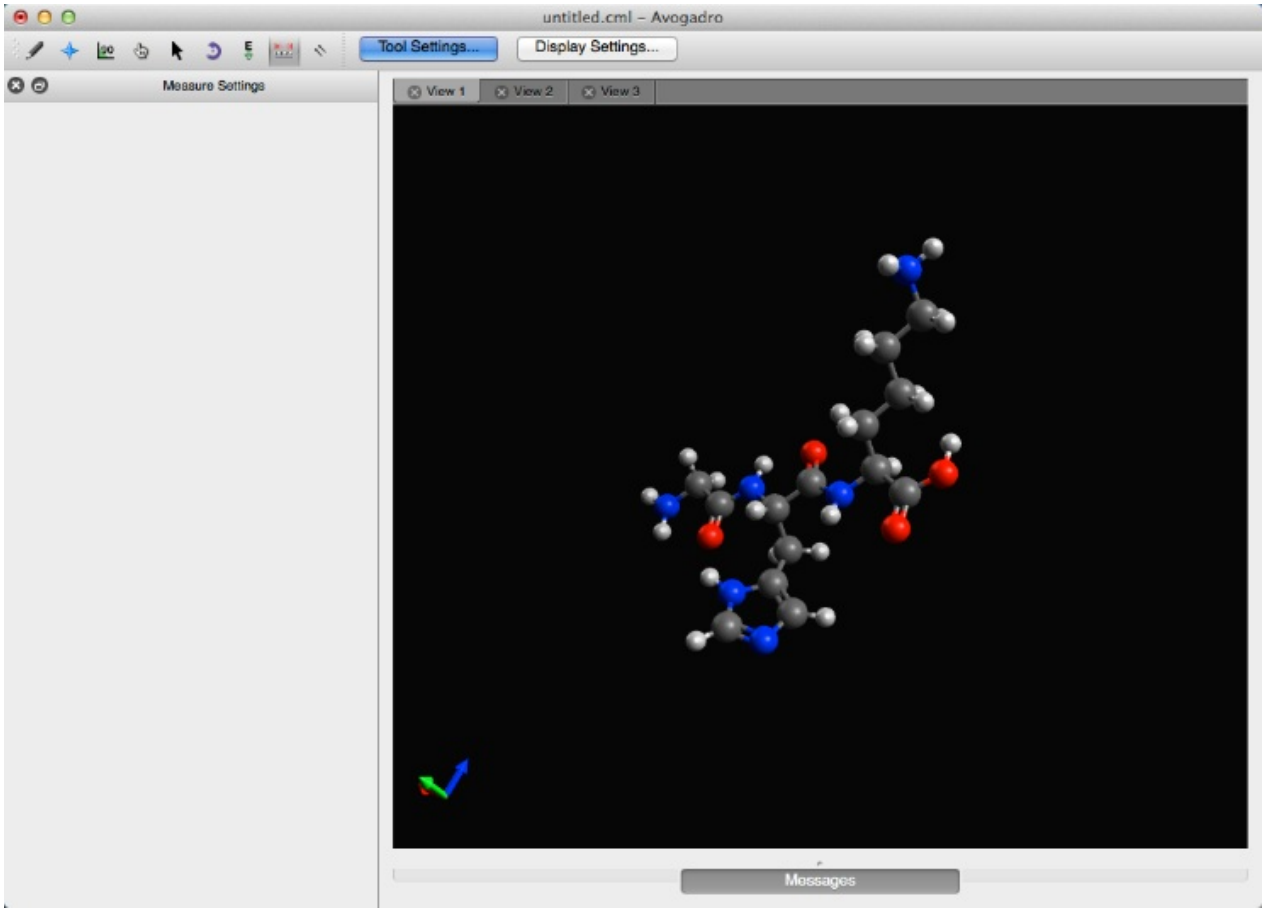
When three atoms are selected an angle is measured between the first and third atom, and the second atom is the vertex.



If four atoms are selected, a dihedral angle is determined.

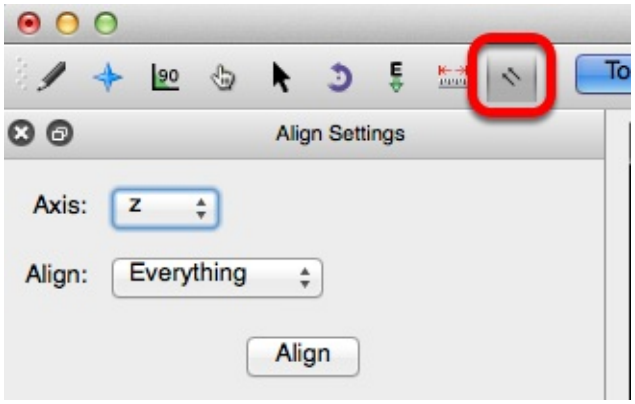


Right clicking the display will reset the atoms previously selected.

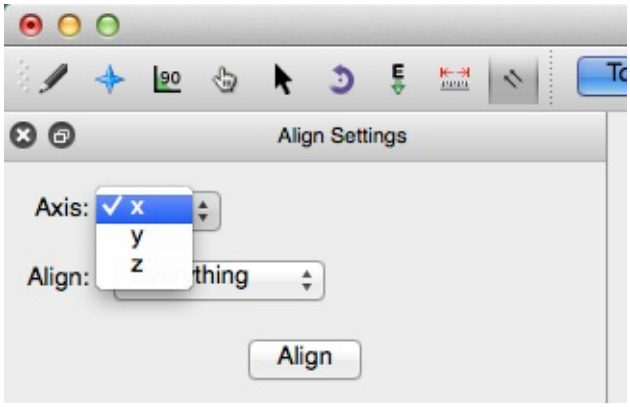


The Align Tool

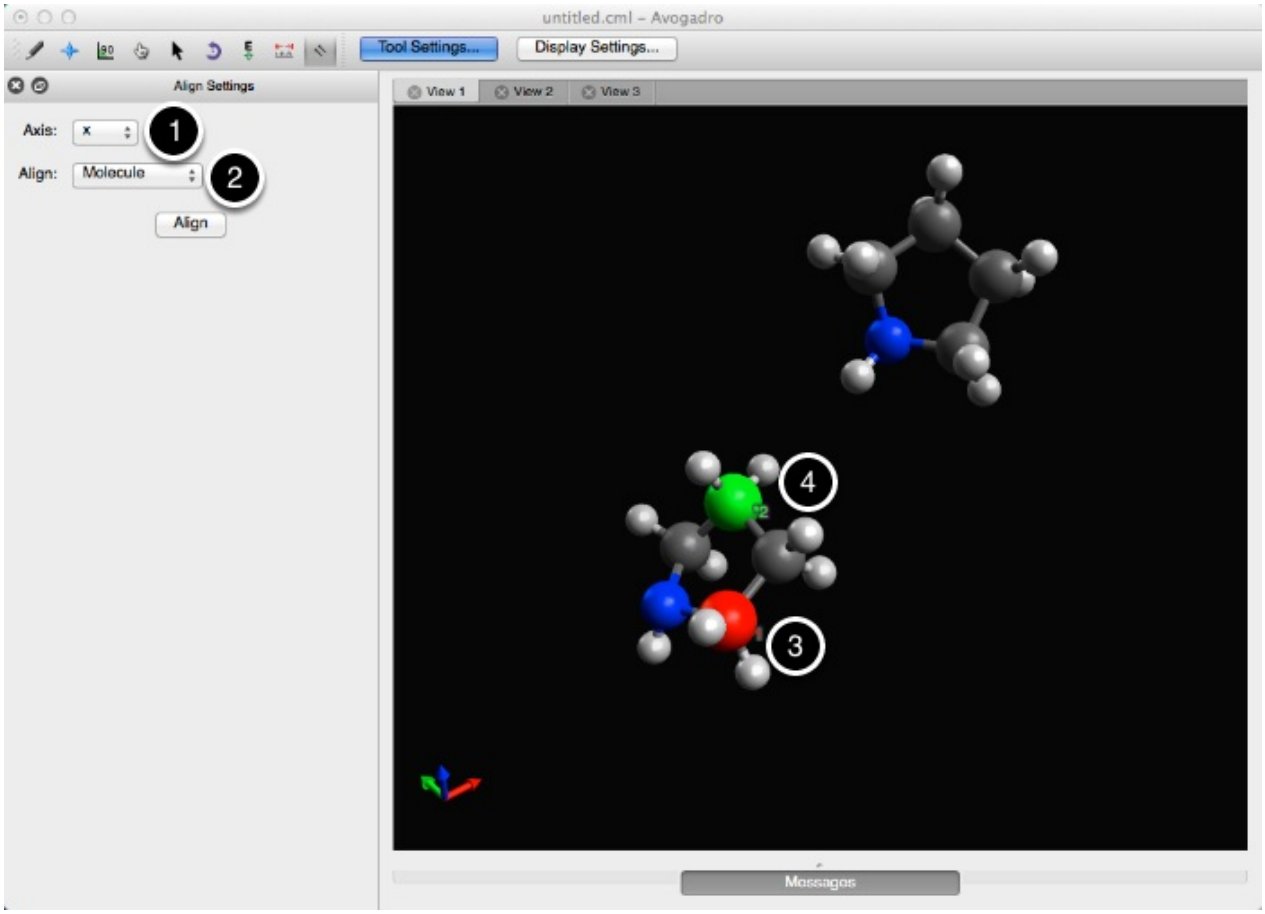
The align tool rotates, and translates a molecule(s) into a specific reference frame.



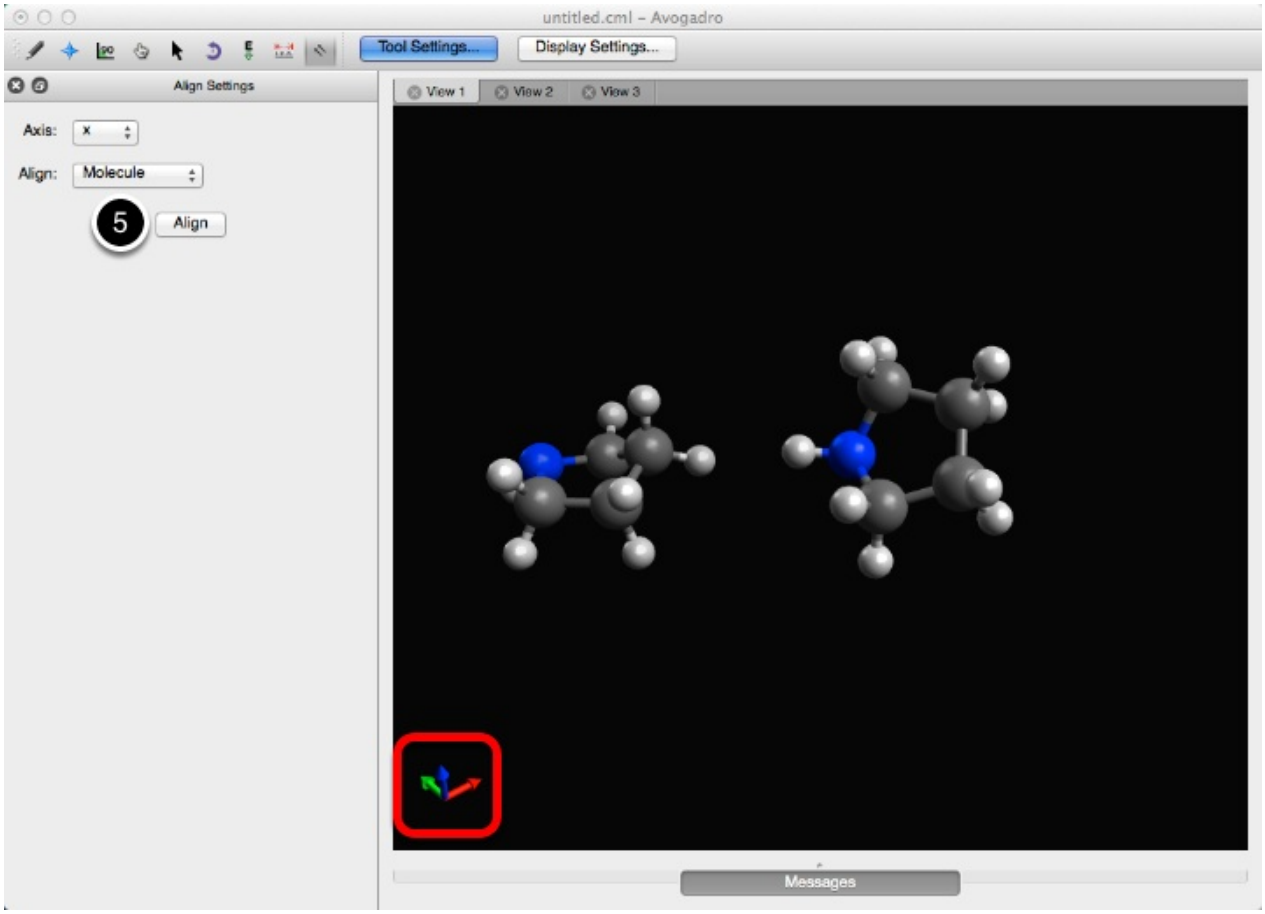
An alignment axis can be chosen from the "Axis" drop down menu. Typing "x", "y", or "z" is a shortcut for changing the alignment axis.



You can also choose to align everything in the frame, or a specific molecule with the respective option in the "Align" drop down menu. To align a molecule, or everthing in the frame you will then need to click two atoms as reference points.



Clicking "Align" will then reset the frame with the new alignment. The alignment axes are shown in the bottom left corner.

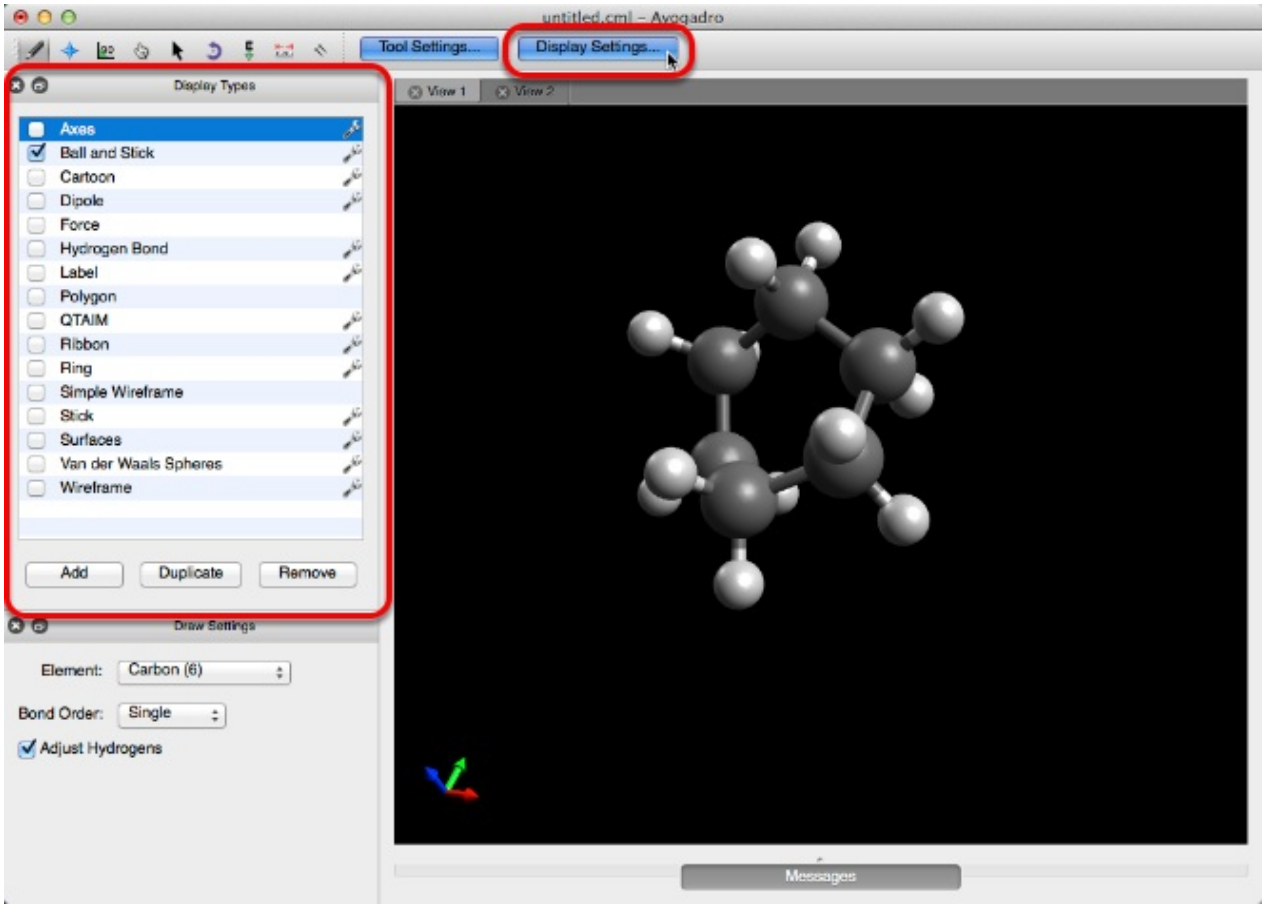


Different Display Types in Avogadro

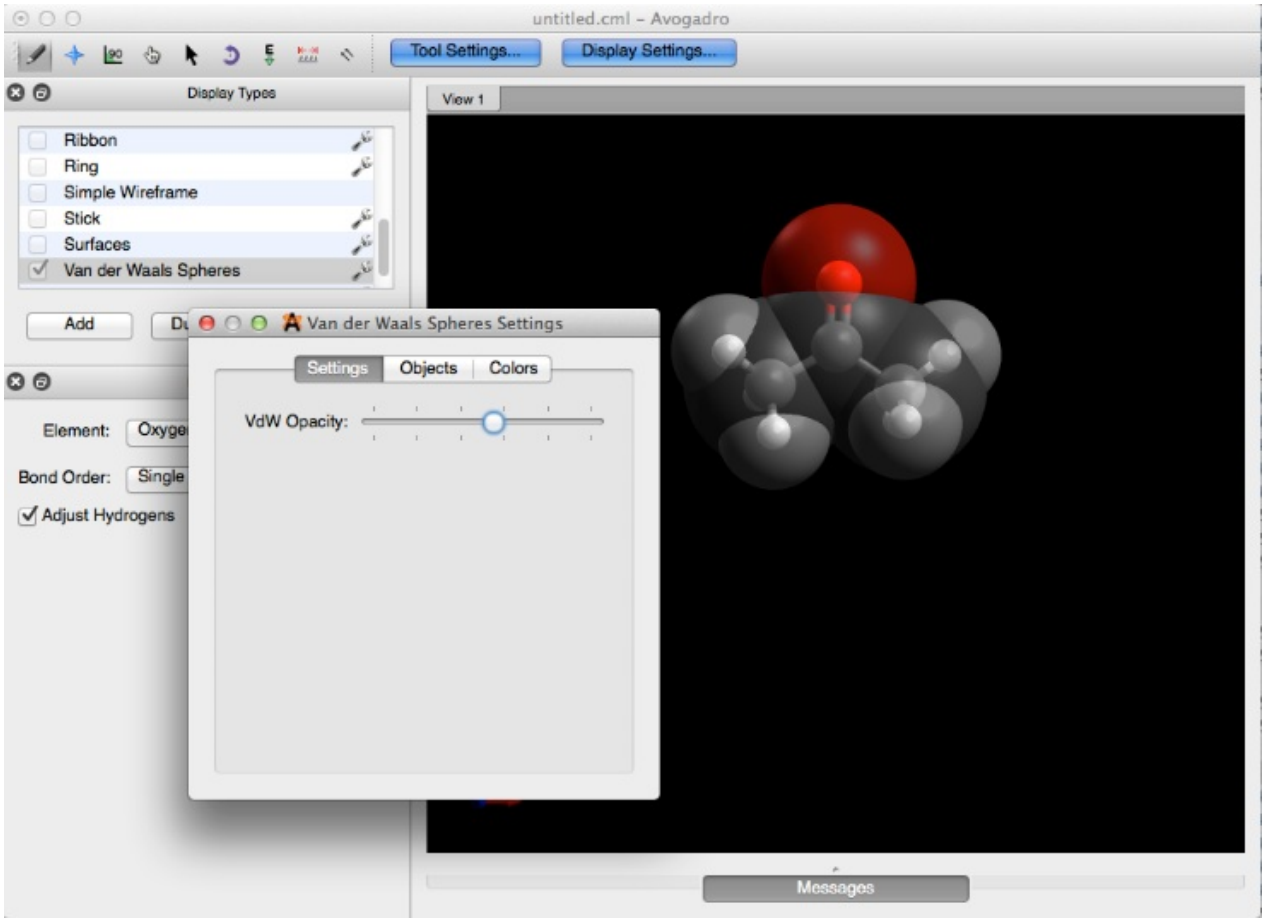
Avogadro comes equipped with various display types to aid in molecular interpretation. The default engine plugins include Axes, Ball and Stick, Cartoon, Dipole, Force, Hydrogen Bond, Label, Polygon, QTAIM, Ribbon, Ring, Simple Wireframe, Stick, Surface, Van der Waals Spheres, and Wireframe.

Locating Display Types

The different display types can be accessed by clicking "Display Settings..." in the top middle of the open Avogadro window. The display types toolbar will be added above the "Tool Settings..." toolbar that is currently opened. All of the plugins featured below can be used in conjunction with one another.

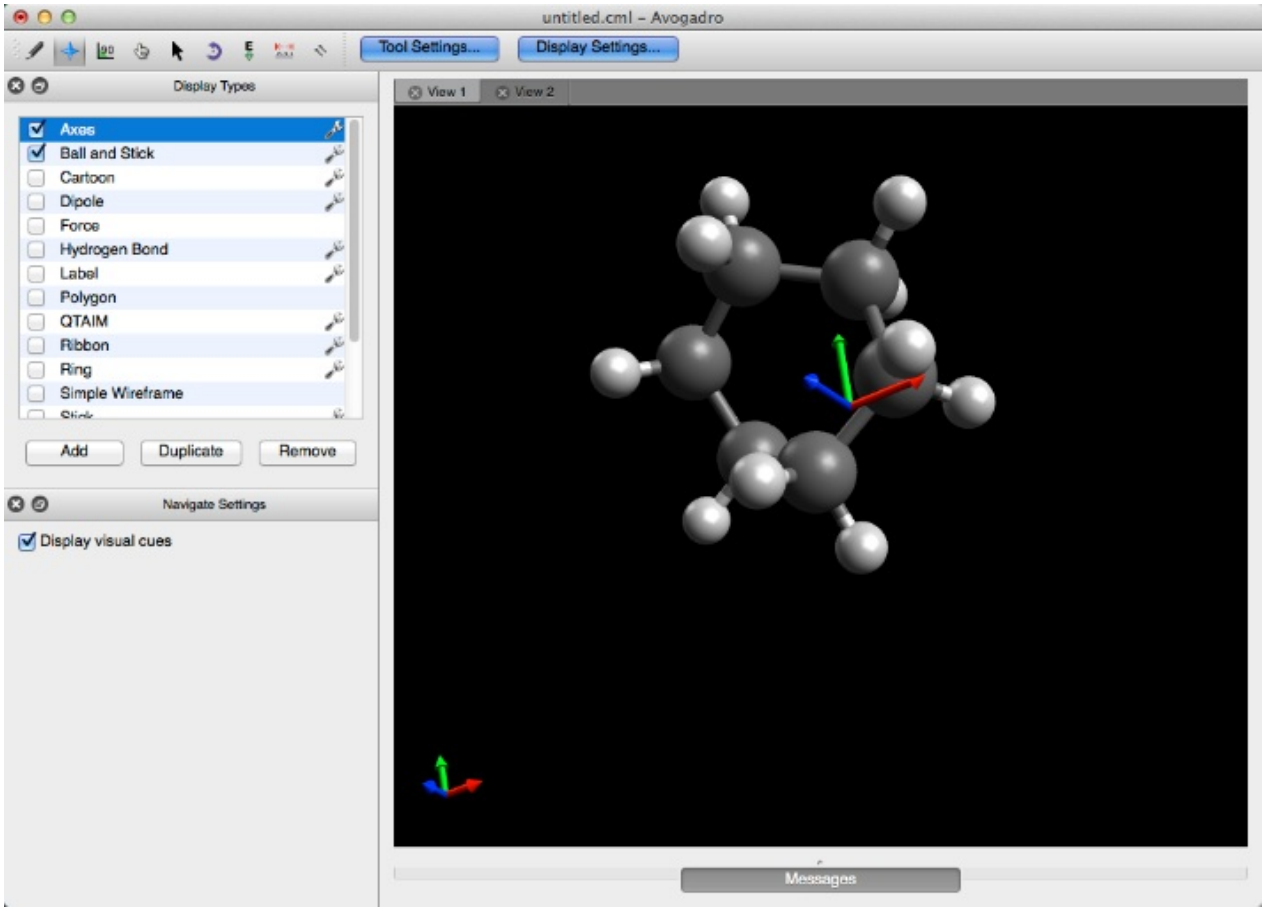


Clicking on the wrench located on the right of some display types will allow various adjustments to be made to the display. For example, you can choose to edit the opacity of the Van der Waals Spheres feature so that you can still view the ball and stick model underneath.



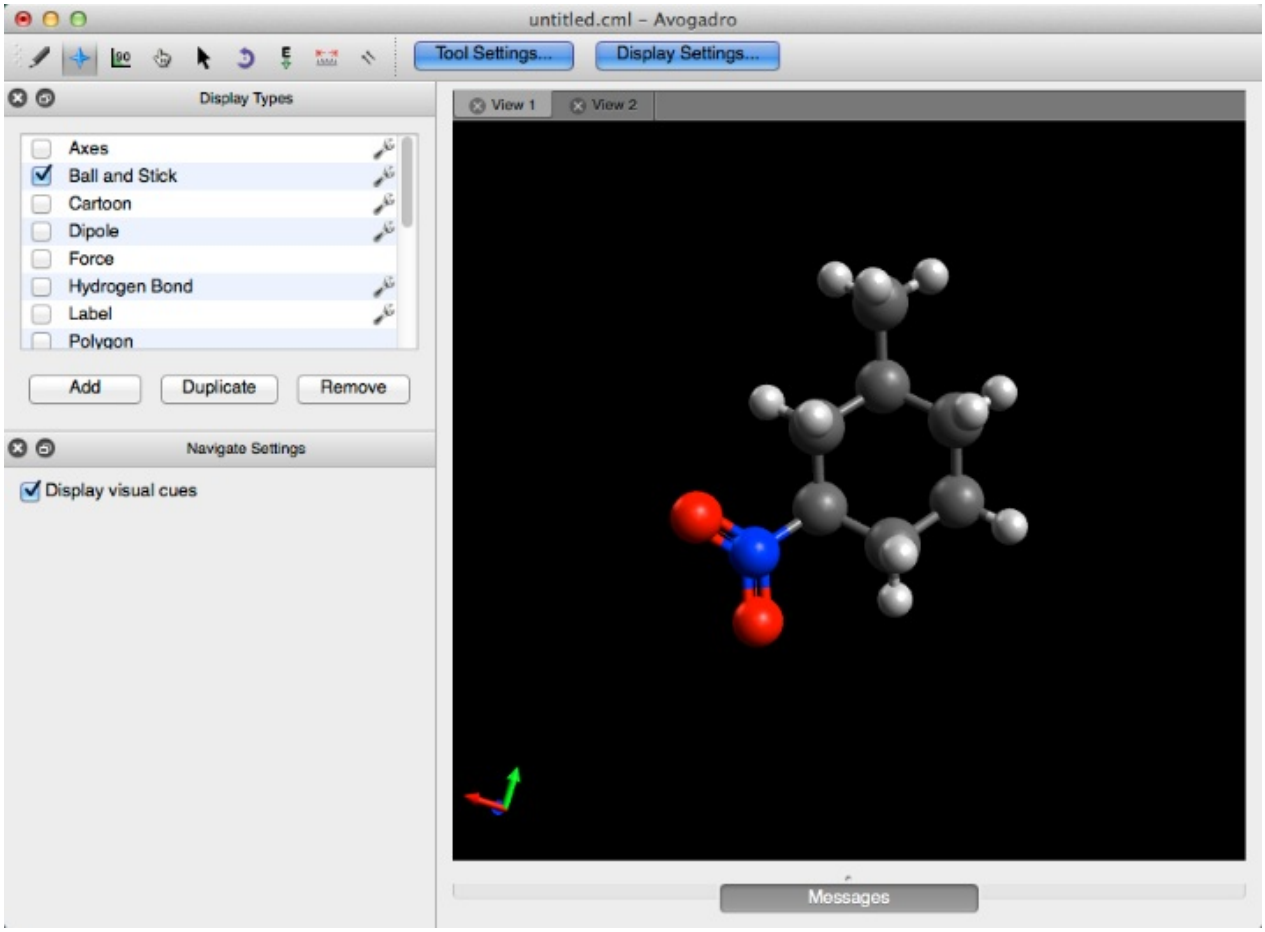
Axes

Clicking on the Axes plugin will provide the cartesian axes of the molecule from the origin. Note that the red, green, and blue arrows represent the x, y, and z axes respectively.



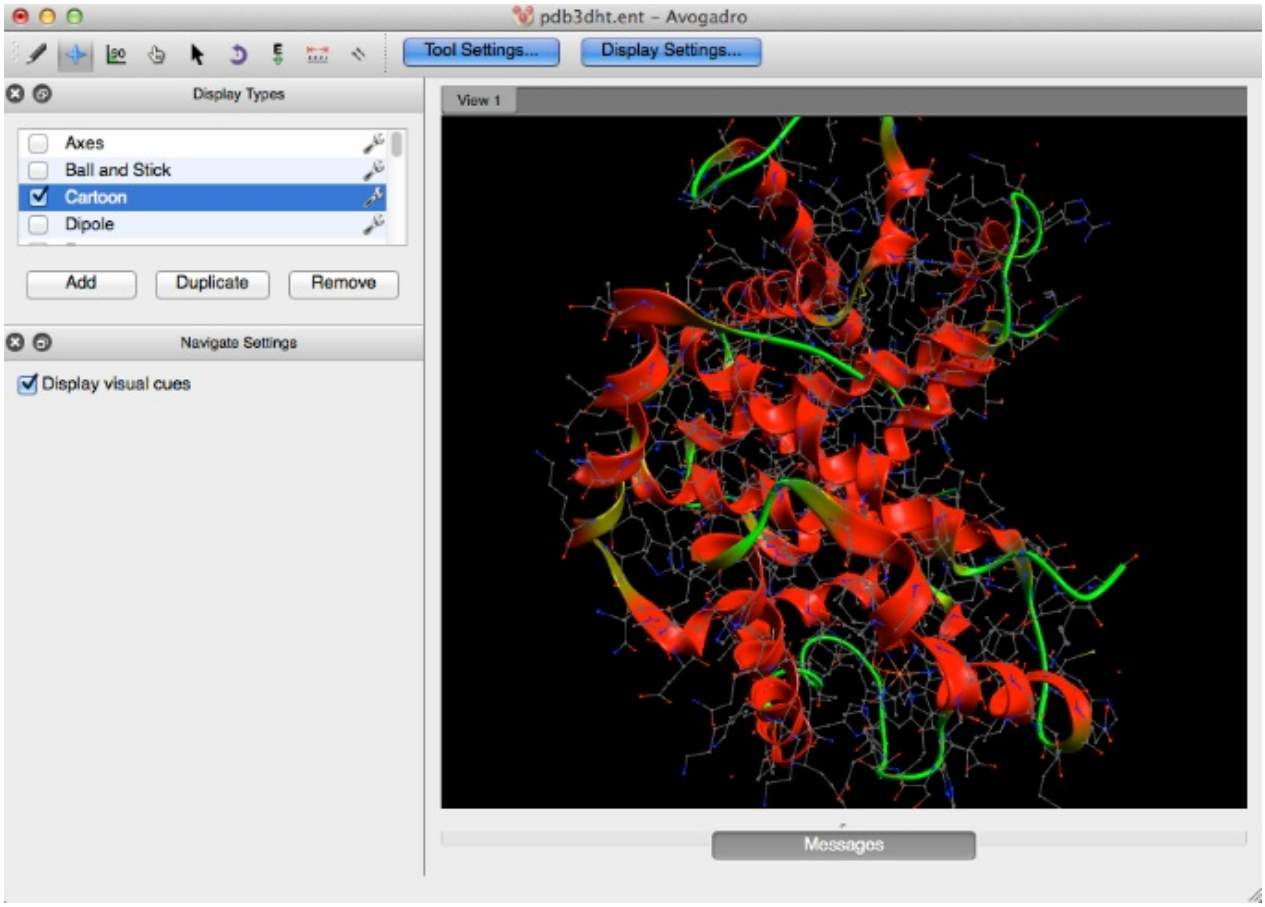
Ball and Stick

Ball and Stick is the default plugin when Avogadro is opened. This plugin provides the standard ball and stick representation of a molecule.



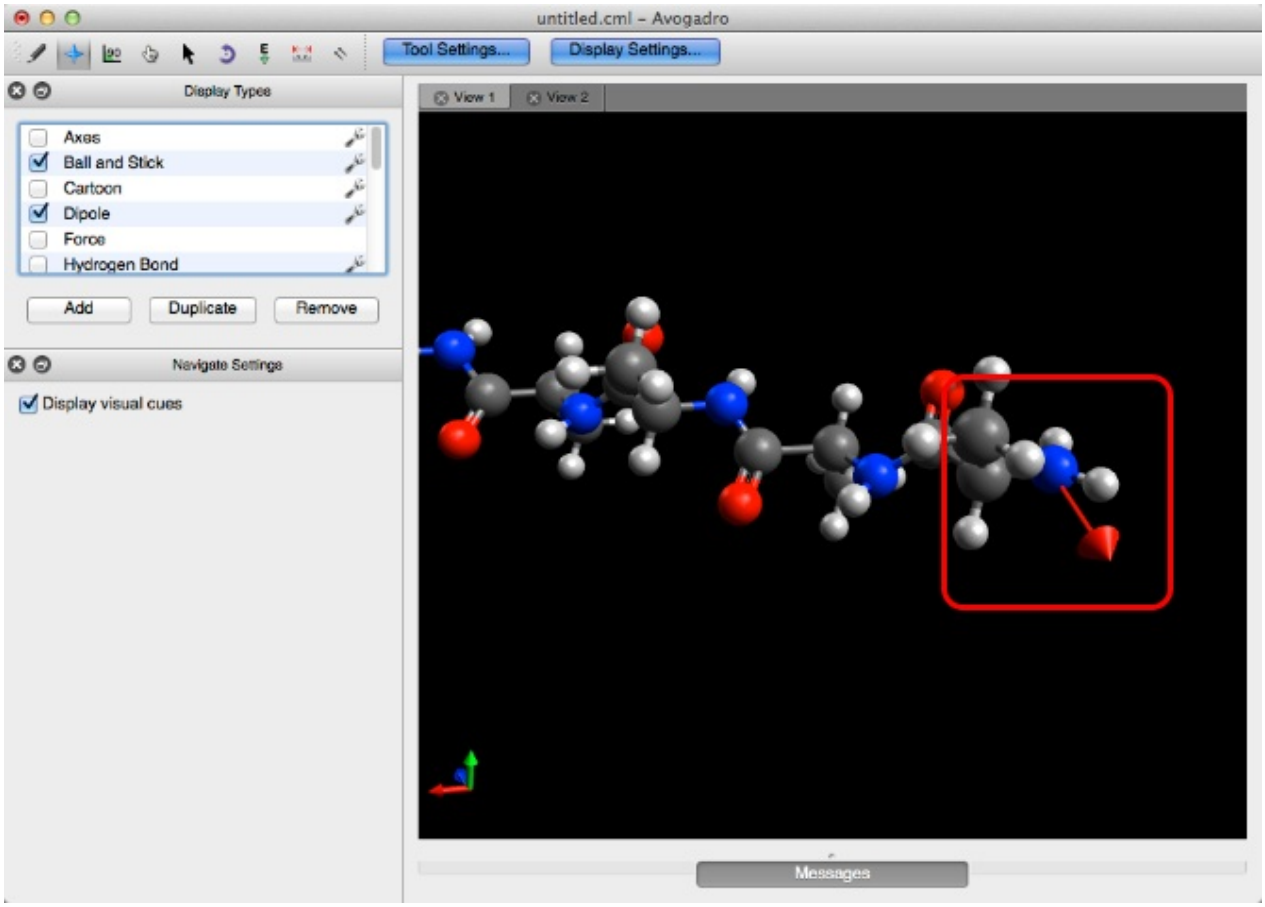
Cartoon

The cartoon feature only applies to secondary biological structures (α helix and β sheet). Below is the cartoon for hemoglobin.



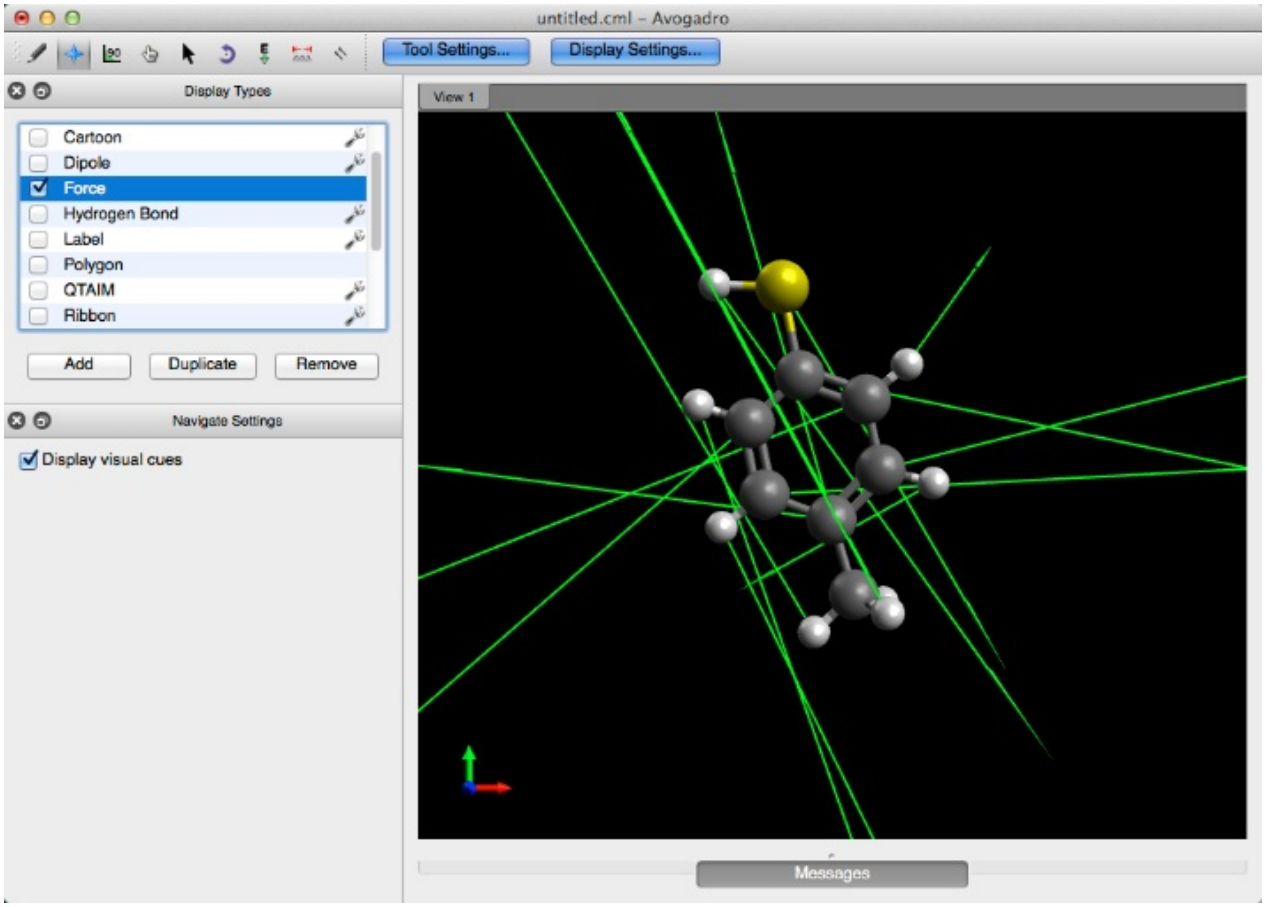
Dipole

The Dipole plugin will display an overall net dipole if one is present.



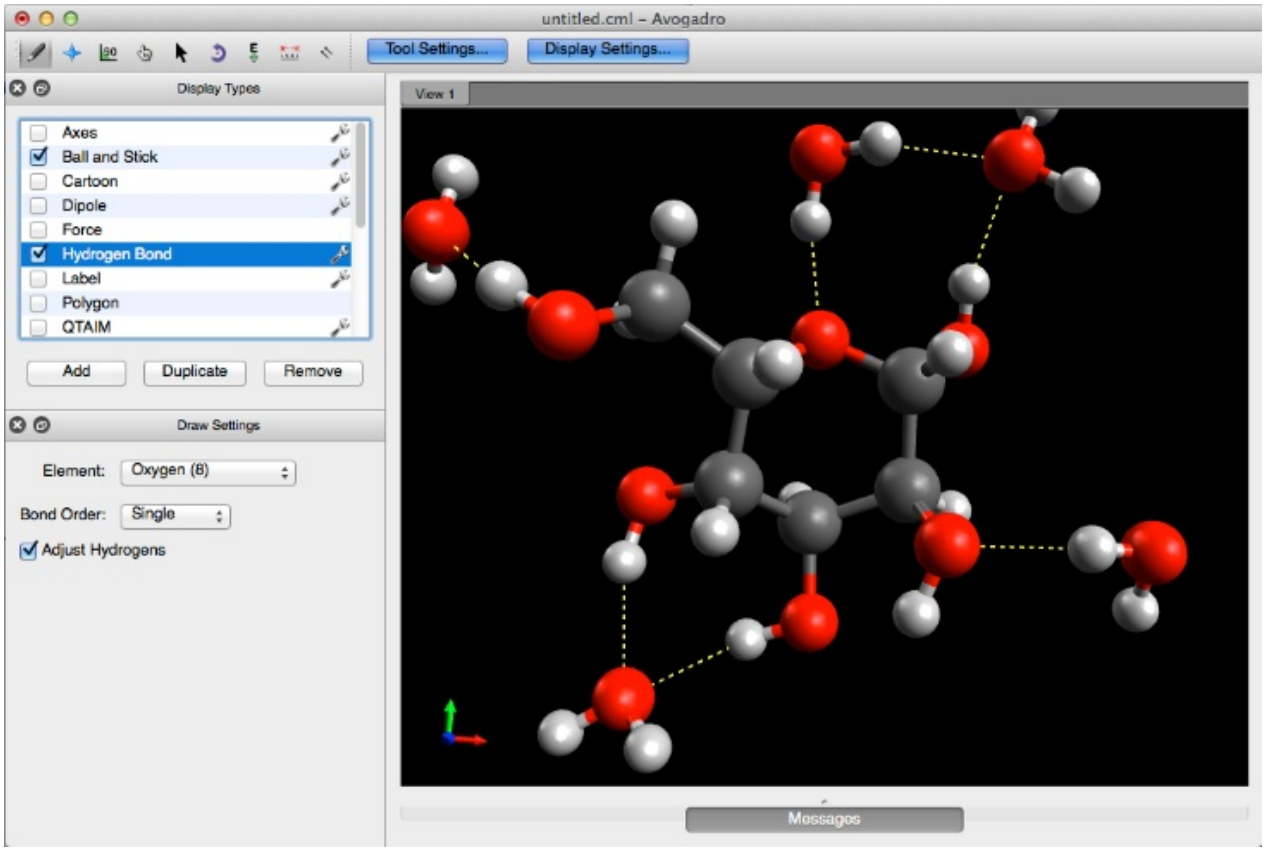
Force

The Force plugin displays green arrows on atoms (as shown below), to qualitatively demonstrate the forces being applied to the atoms.



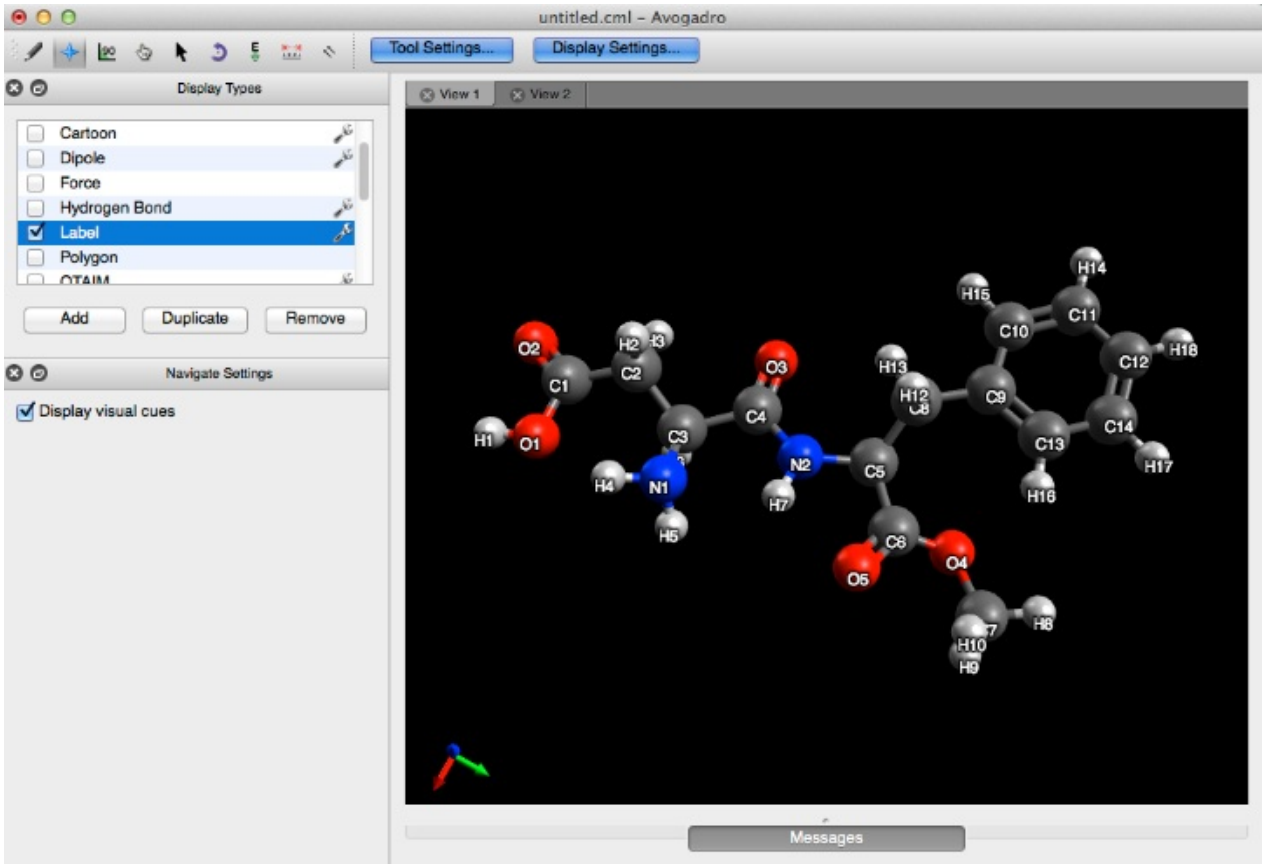
Hydrogen Bond

The Hydrogen Bond plugin demonstrates implicit hydrogen bonding that can occur between atoms.



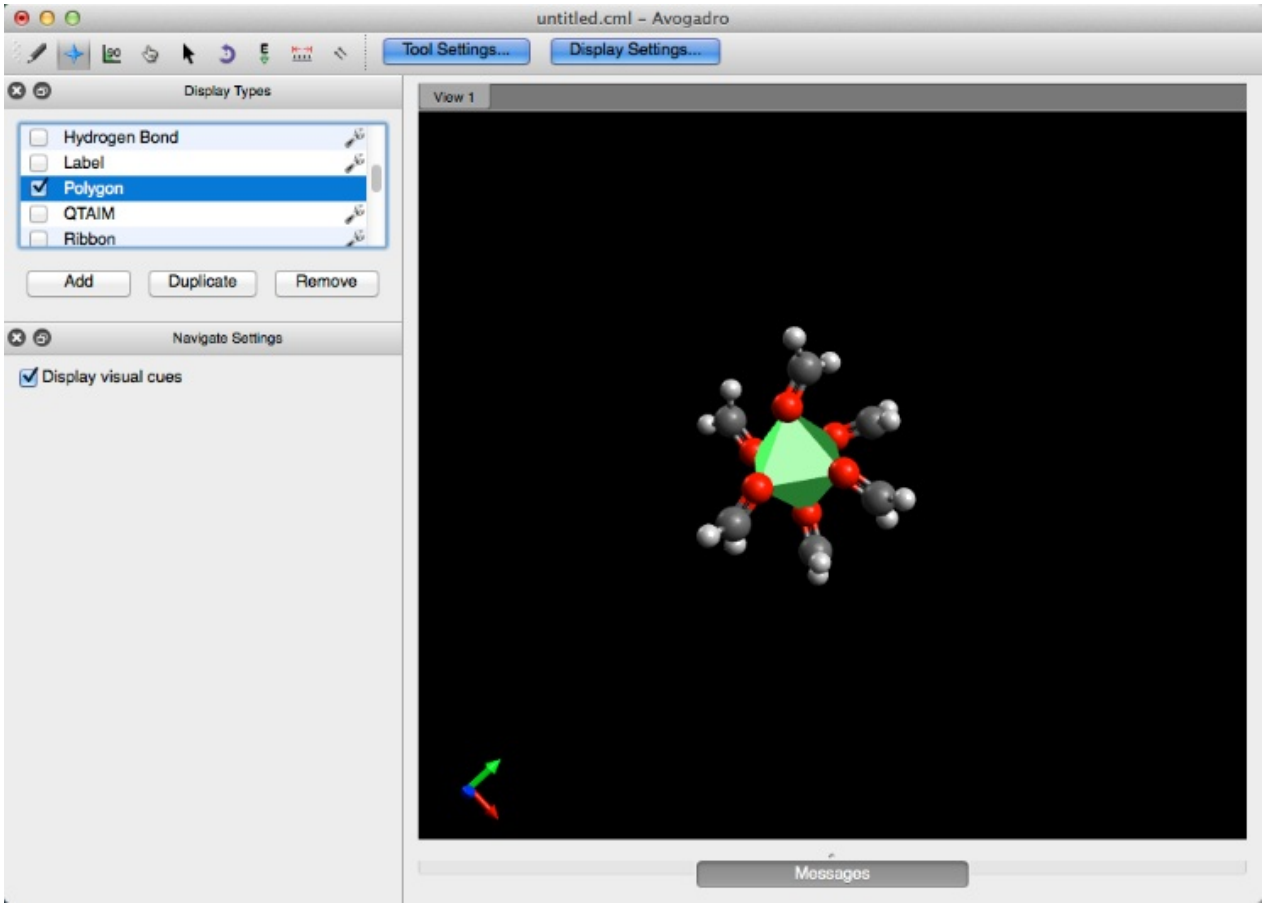
Label

The label plugin numbers and labels all atoms present in a molecule.



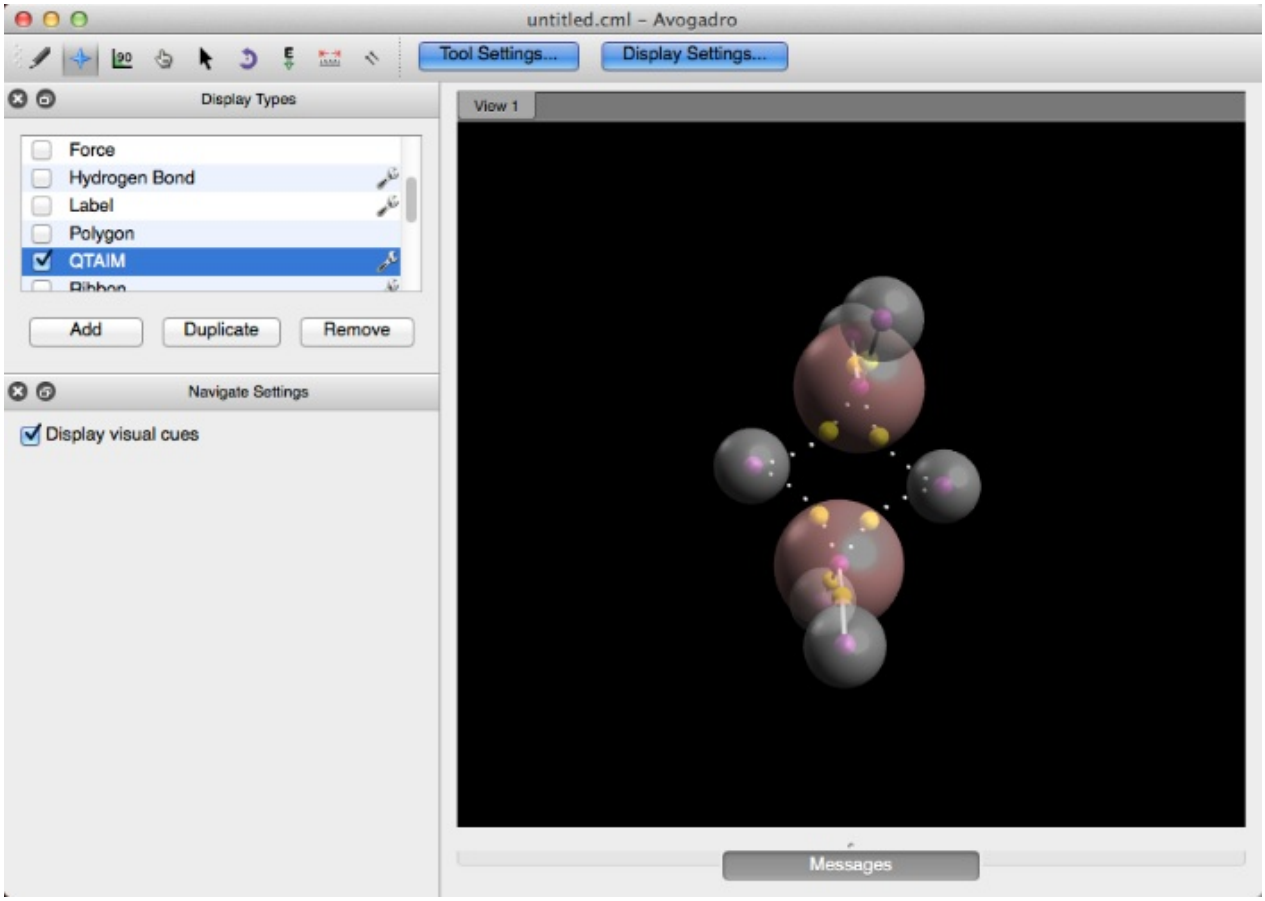
Polygon

The Polygon feature takes metallic centers with three or more atoms bonded to them, and draws a polygon around them.



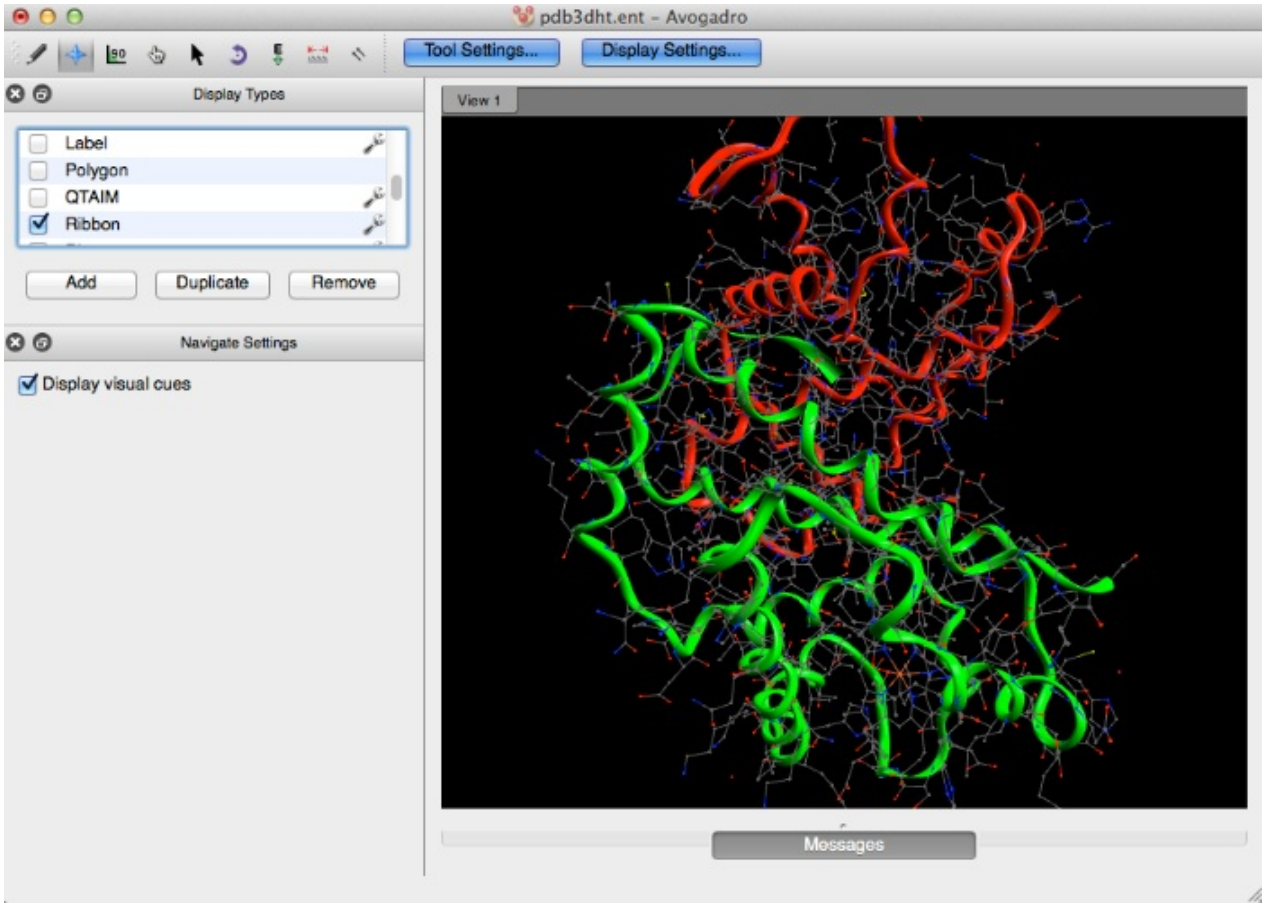
QTAIM (Quantum Theory of Atoms in Molecules)

QTAIM displays the implicit bonding that is theorized to take place between the hydrogens of organic crystals (the implicit bonding is conveyed through dots). This display type is utilized by importing a .wfn file from the "QTAIM", "Molecular Graph" selection under the "Extensions" menu. More information can be found on this process in the Tutorial section of this manual.



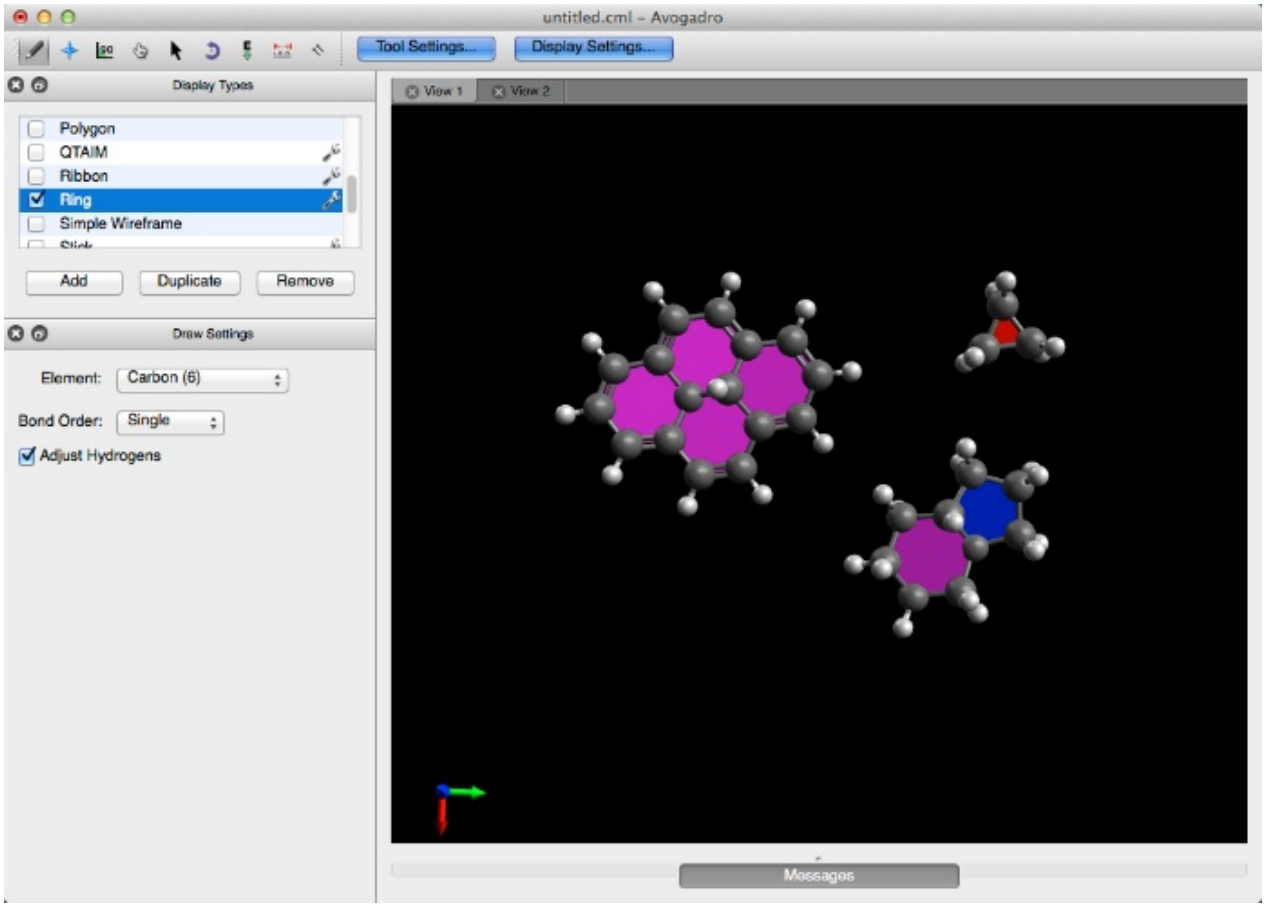
Ribbon

Similar to the Cartoon plugin, the Ribbon plugin conveys secondary biological structures as a simple ribbon rendering.



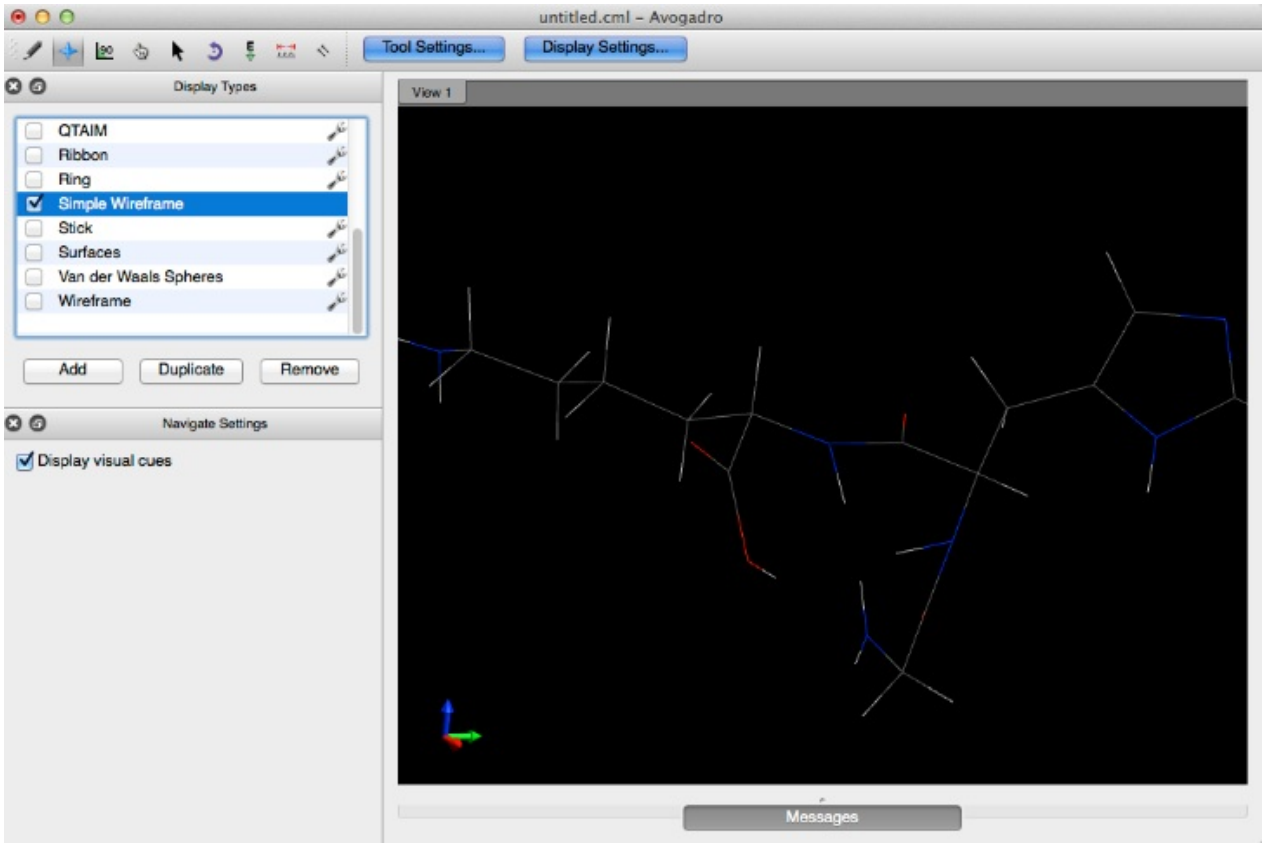
Ring

This feature distinguishes rings with different colors dependent on their size. As shown below a six-membered ring is purple, and five membered ring is blue, etc.



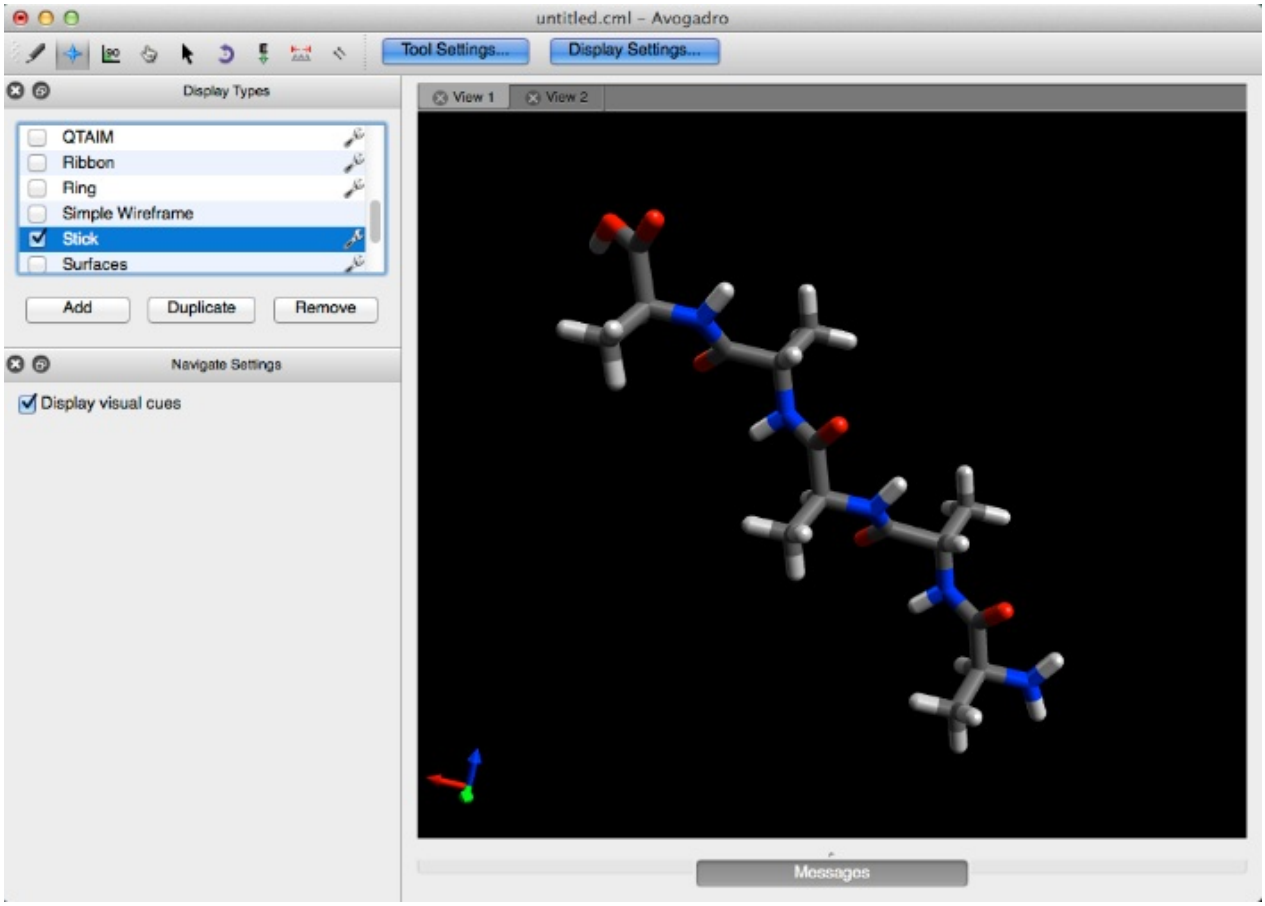
Simple Wireframe

This feature provides a basic wireframe display of a molecule.



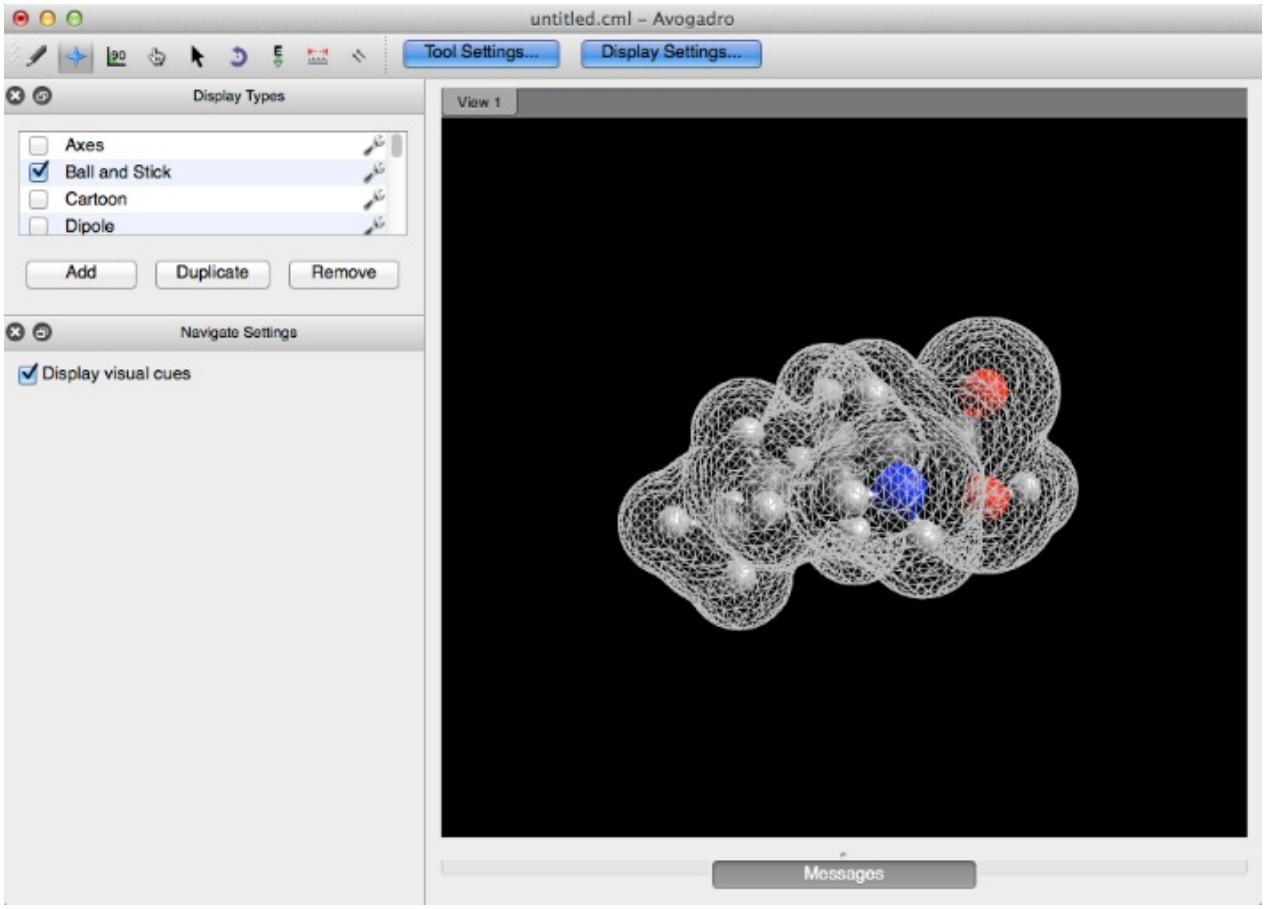
Stick

Stick is another molecular visual display type, that renders a stick representation of a molecule.



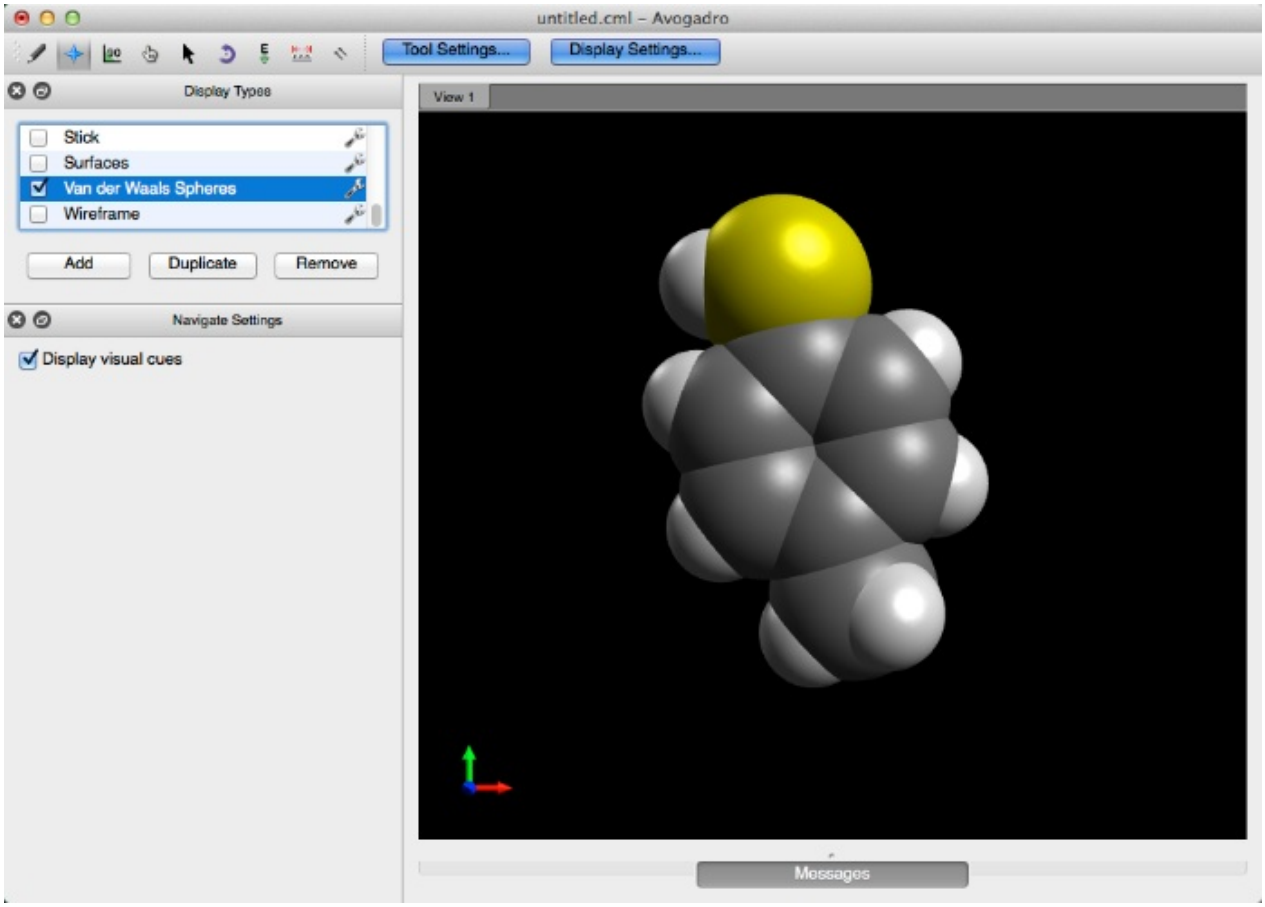
Surfaces

Once a surface has been created (Extensions Menu -> Create Surfaces...), the Surface display type can be used. This display type allows adjustments to the orbital, opacity, rendering, style, and color.



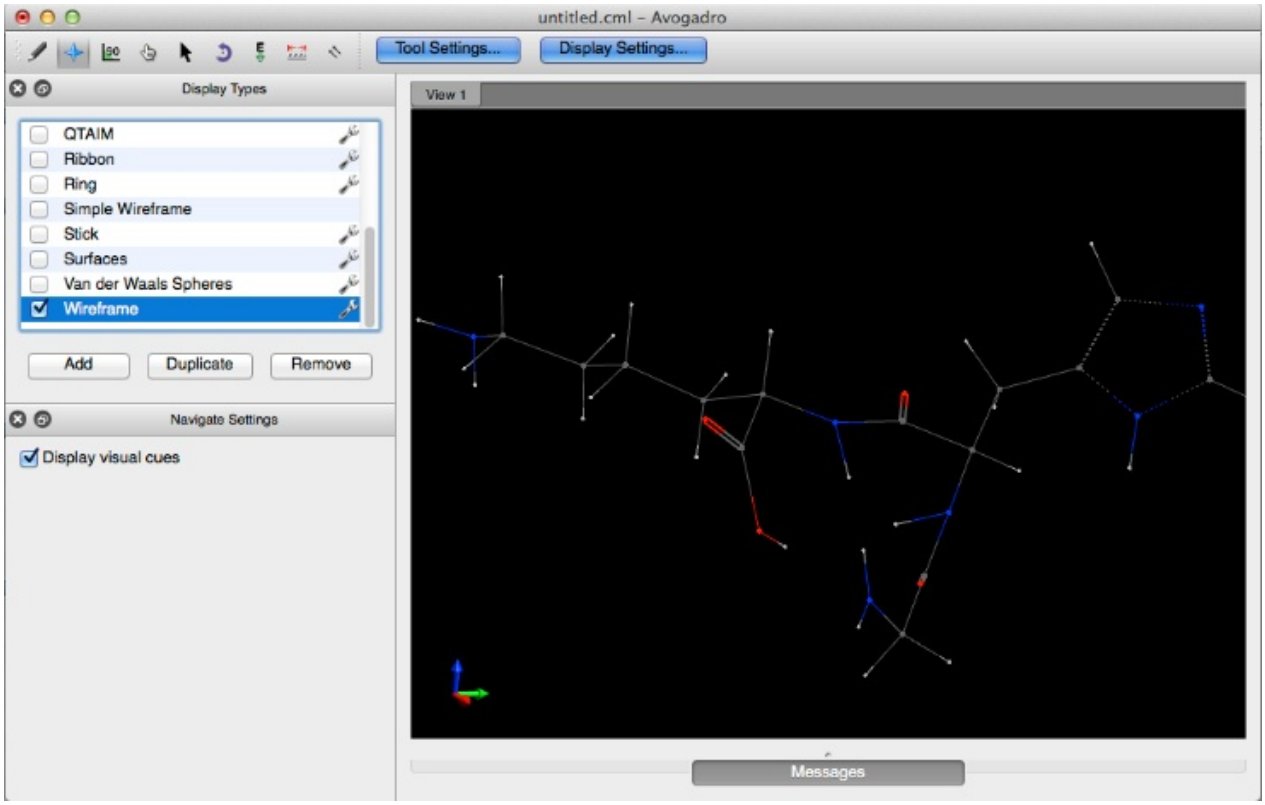
Van der Waals Spheres

The Van der Waals plugin provides the classic sphere rendered Van der Waals image.



Wireframe

Unlike Simple Wireframe, Wireframe draws atoms and bond order into the molecule.

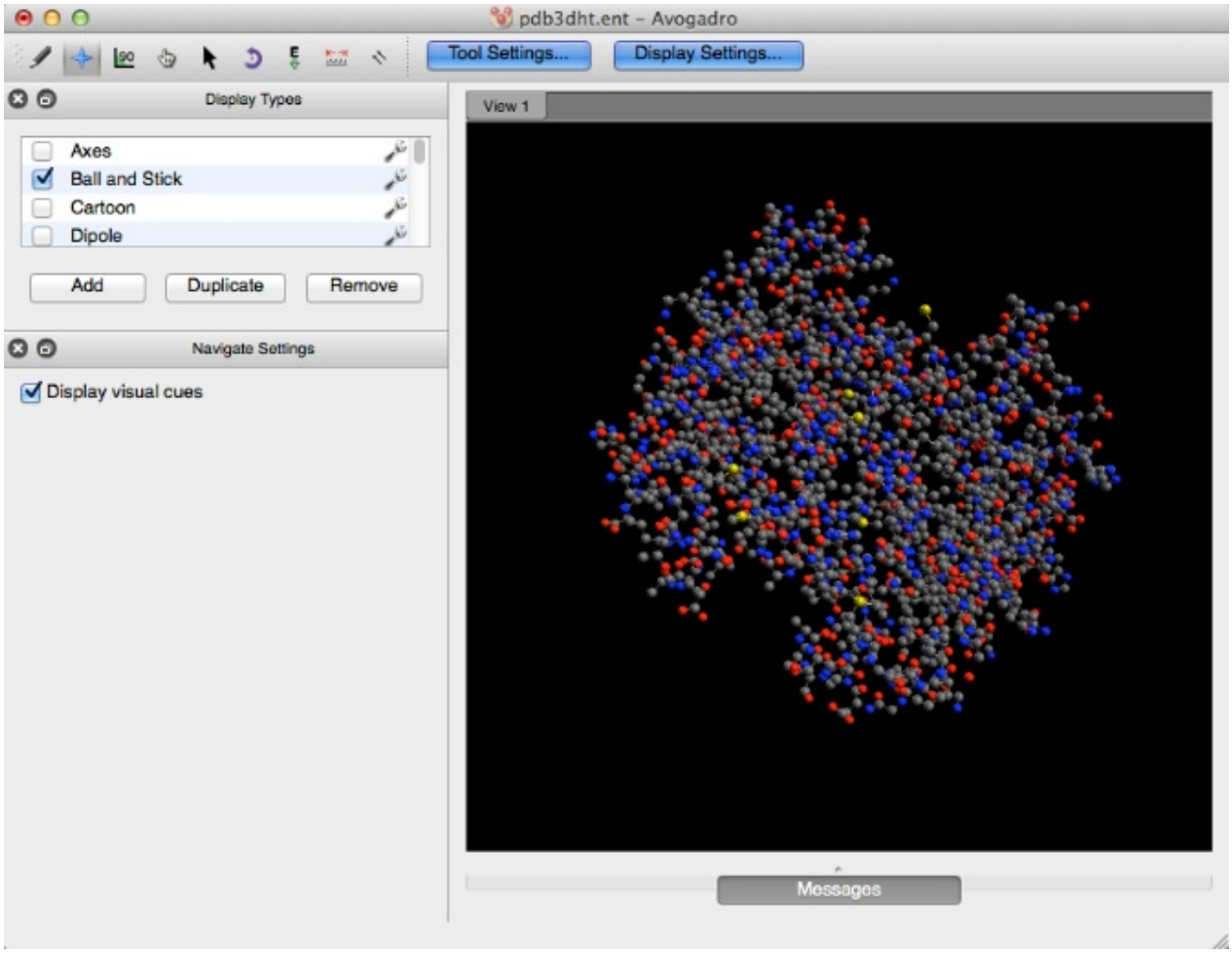


Coloring Part of a Molecule

Coloring various parts of a molecule can provide a more visually stimulating way to display qualitative information.

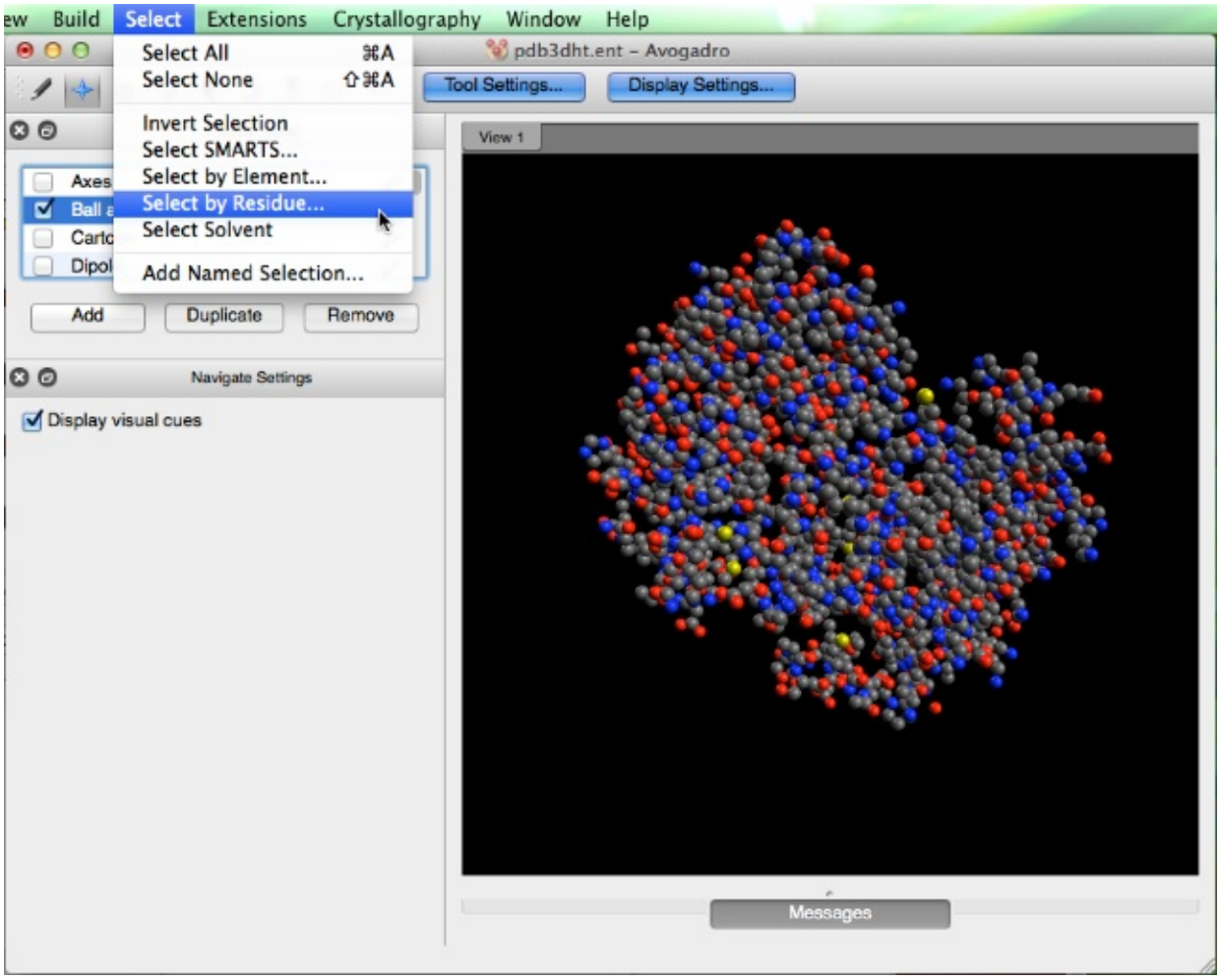
Hemoglobin

Below hemoglobin is depicted in its ball and stick form (file imported from PDB).

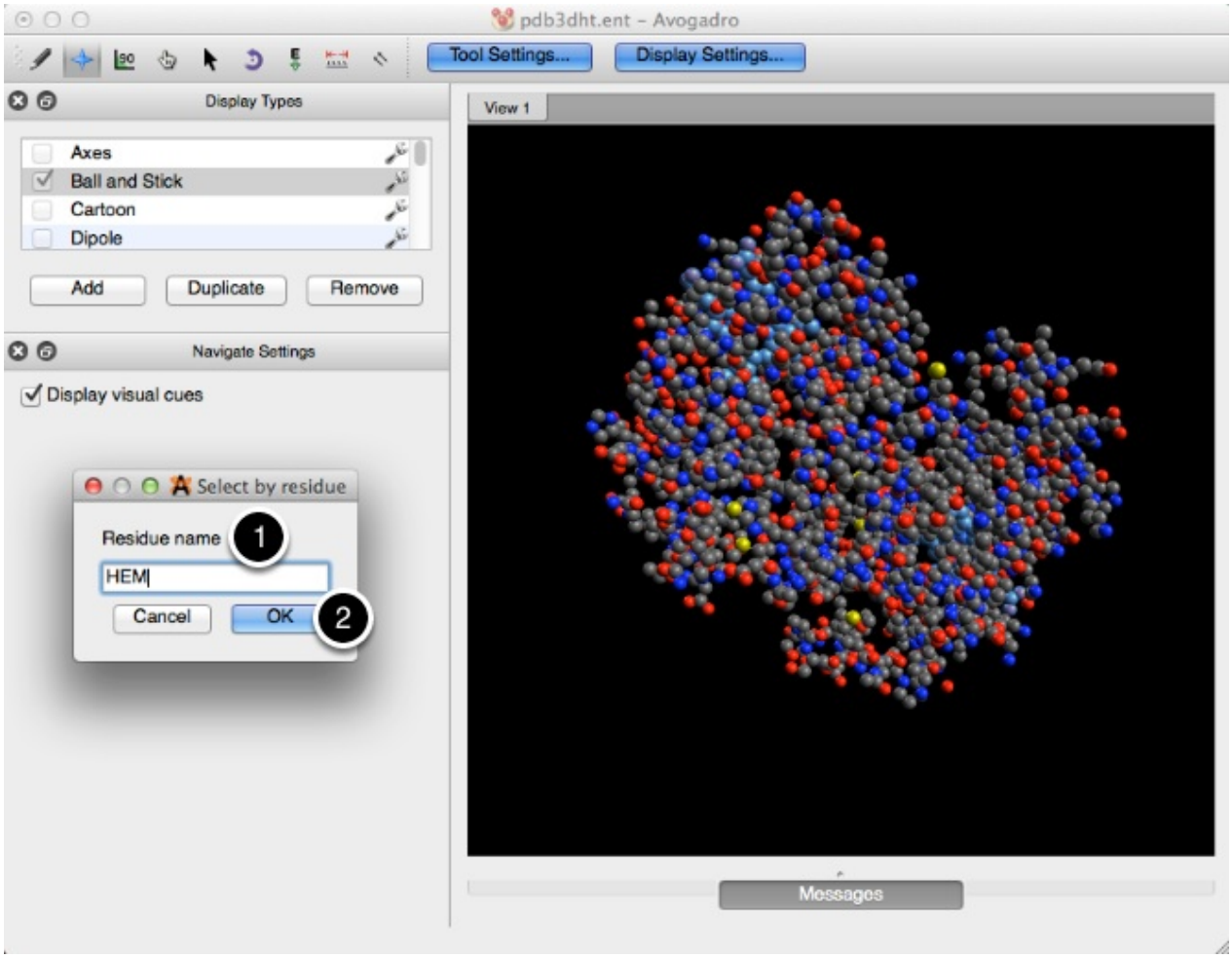


Select by Residue

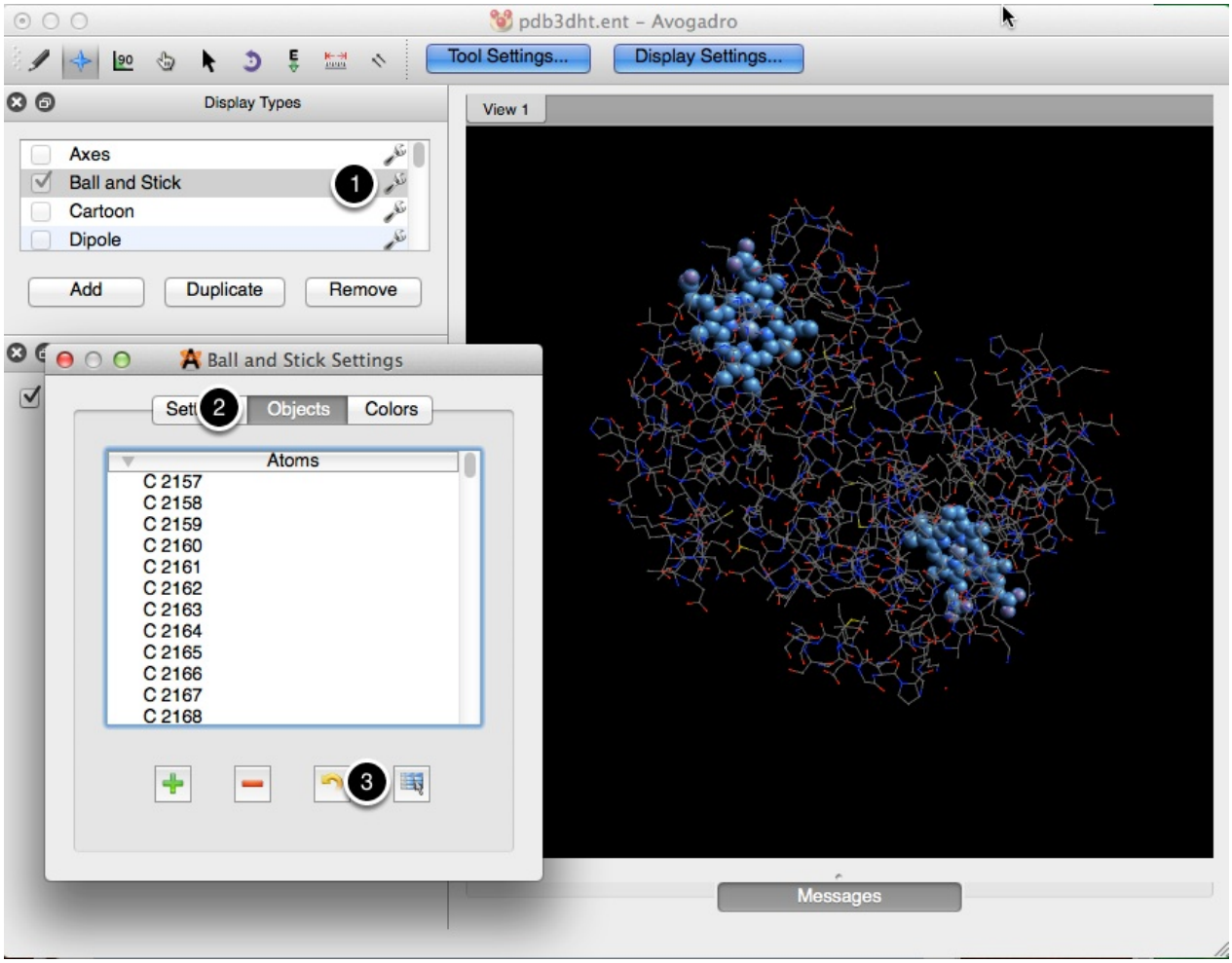
We can select specific residues in the molecule through the "Select" menu.



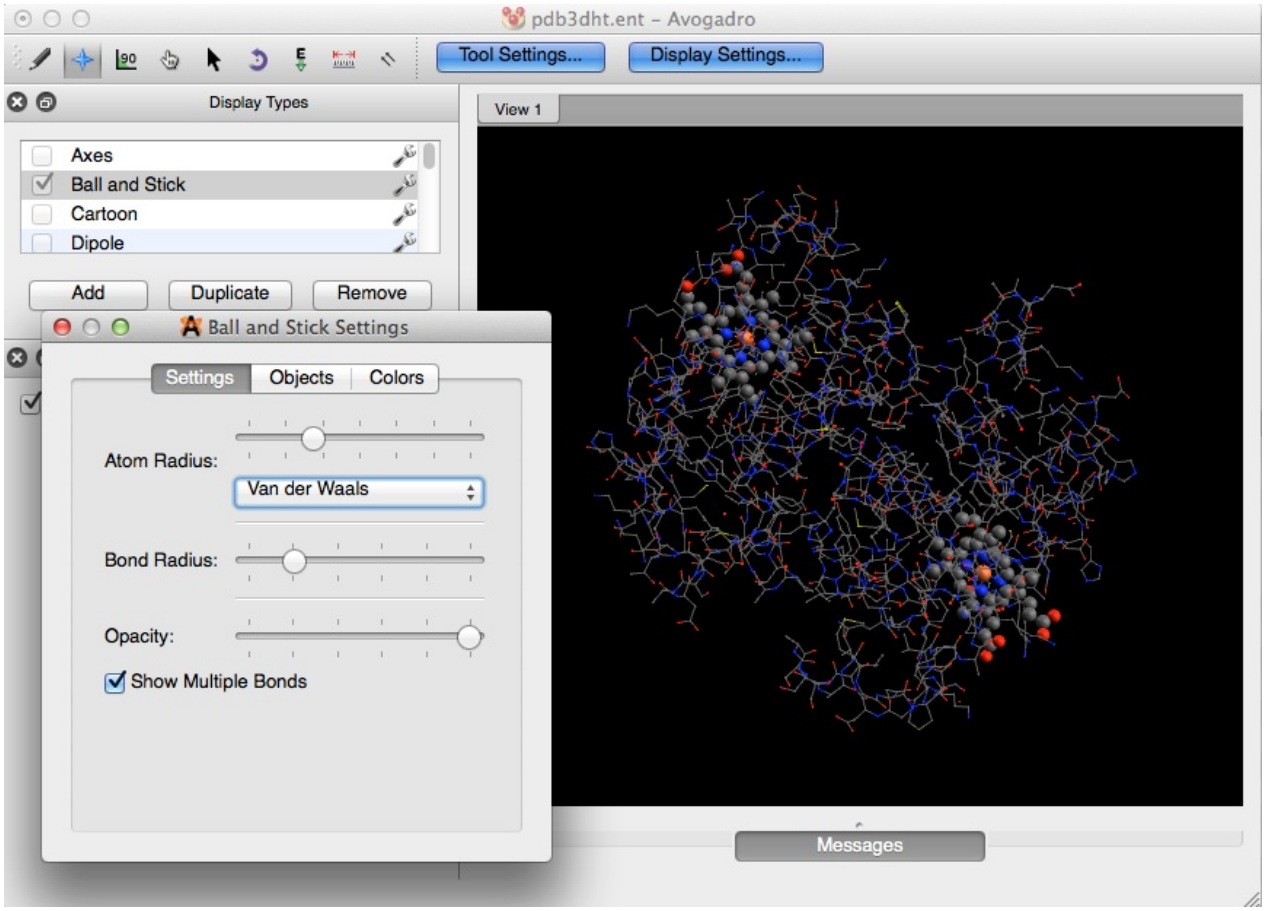
After typing in the residue name (this feature is case sensitive), and clicking "OK", adjustments can be made to emphasize the selection.



After making a selection, click the wrench next to the display type you're choosing to edit (in this instance the Ball and Stick display). When the dialog box pops up select "Objects", and then click the blue table button in the bottom right hand corner. This feature adjusts what was initally considered an object (Hemoglobin), and edits the selection so that the display type will only encompass the heme residues.

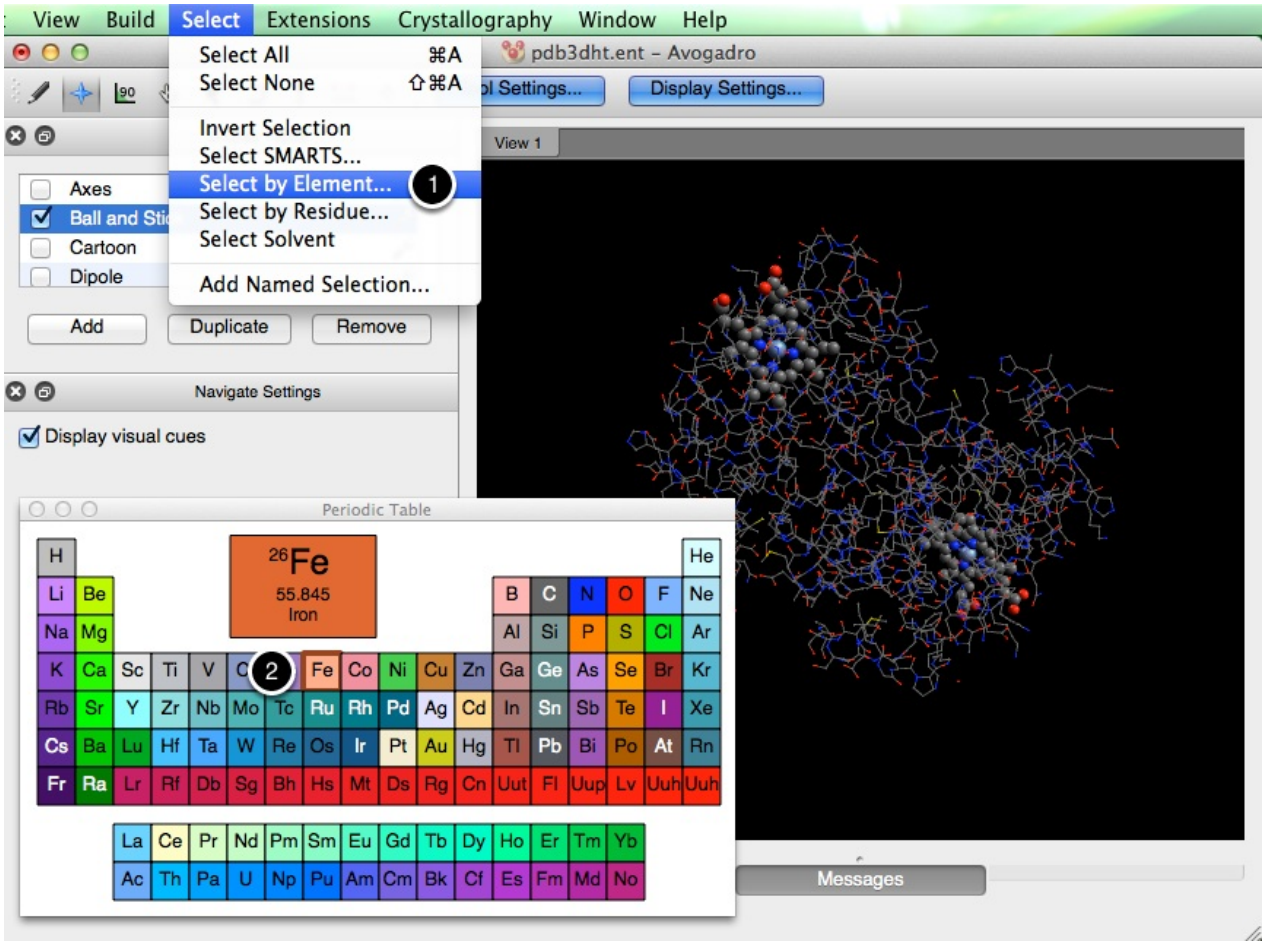


From there you can edit other settings of the display type by clicking on "Settings" or "Colors".

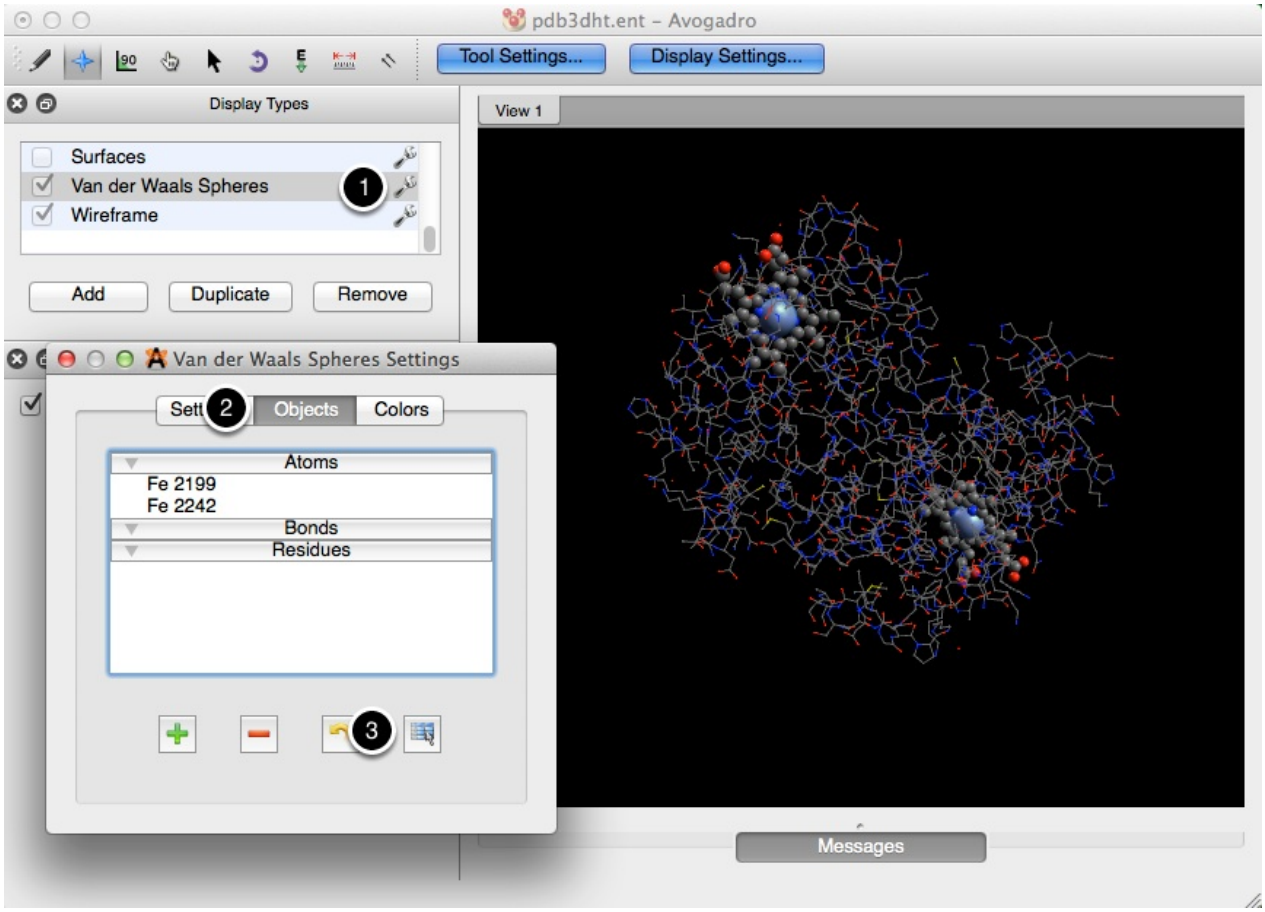


Select by Element

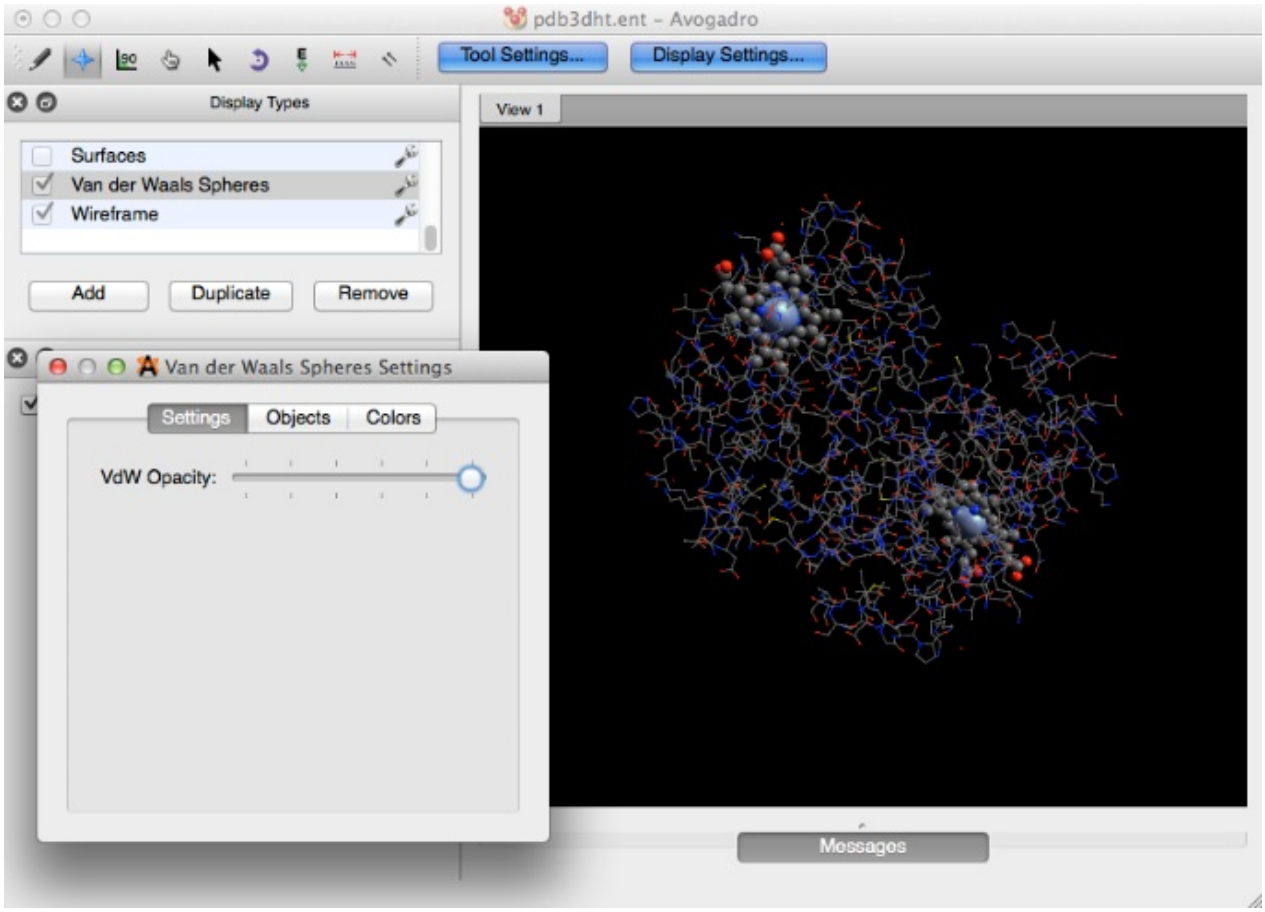
Coloring parts of a molecule doesn't have to end after a single adjustment. Say we want to stress that iron is at the center of the heme residue. We can go to the "Select" menu, "Select by Element...", and choose to select all of the iron atoms in the molecule.



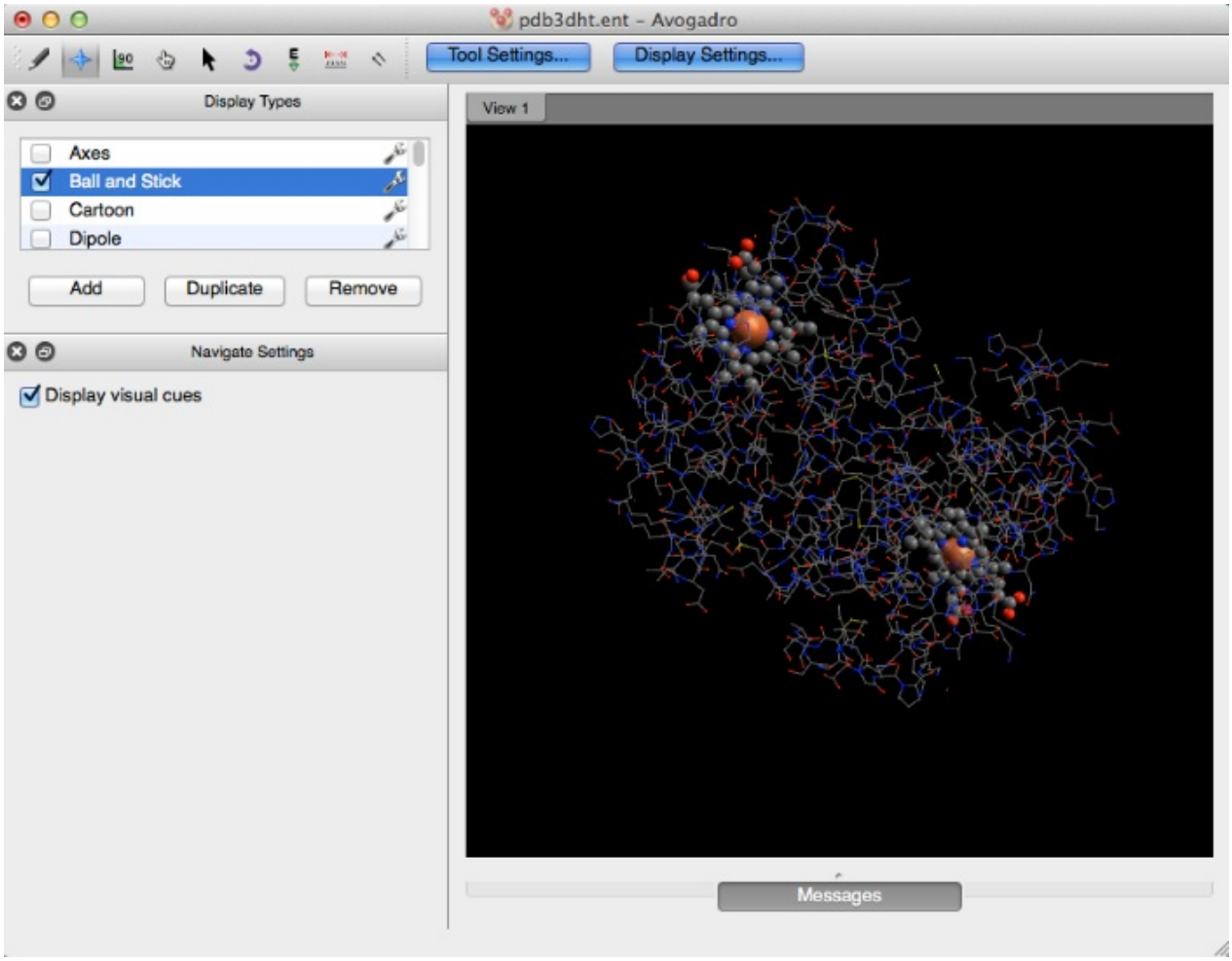
After the selection has been made, with the same procedure as before, we can choose a display type and edit the selection so that it only encompasses the iron atoms.



Then adjustments can be made to the settings.

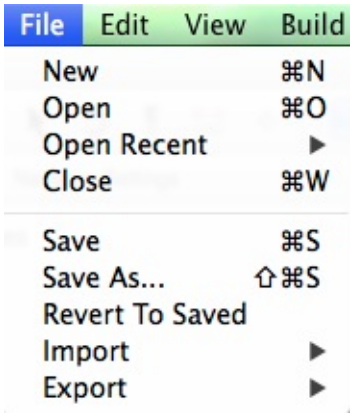


The final product is an intuitive view of qualitative information about the molecule.



The File Menu

The file menu provides the standard abilities of creating a new file, opening & closing documents, as well as saving documents. It also yields the capability to import files from various databases.



New

The "New" selection will open a new file in Avogadro.

Open

After selecting "Open", a file that has previously been saved is accessible through the pop up browser.

Open Recent

"Open Recent" displays a list of documents recently launched.

Close

"Close" dismisses the window currently open.

Save

"Save" will maintain your progress.

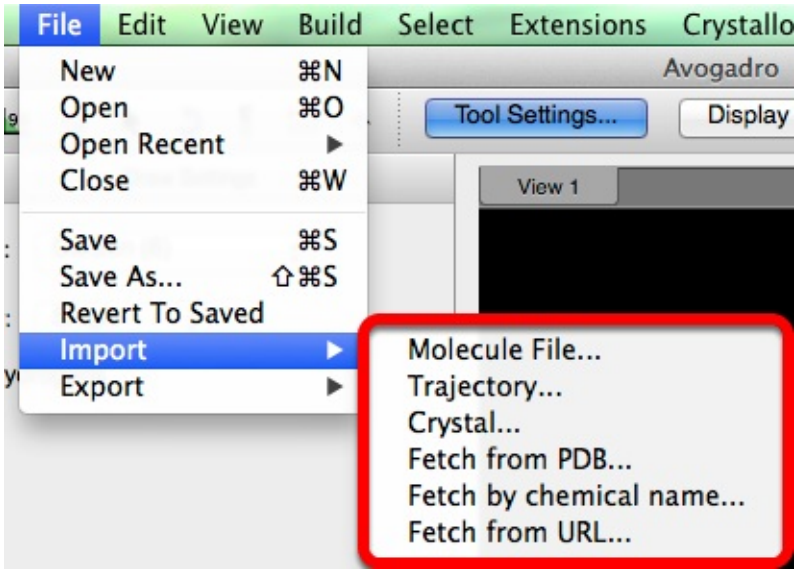
Save As...

"Save As..." allows you to save progress without overwriting the original file.

Revert to Saved

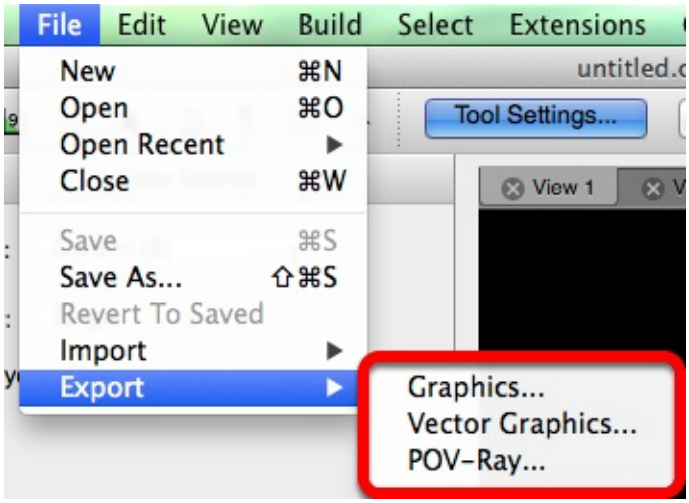
"Revert to Saved" will revert any changes made to the previously saved file.

Import



"Import" will open chemical files that have already been created, from a database.

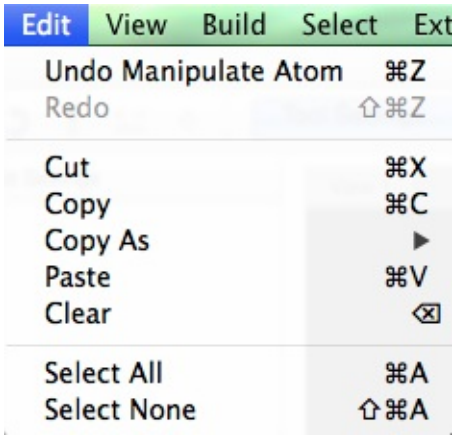
Export



"Export" will make files created in Avogadro suitable for other programs.

The Edit Menu

The edit menu administers basic file revisions.



Undo

"Undo" will negate the last change to the document.

Redo

"Redo" will recover the last change to the document.

Cut

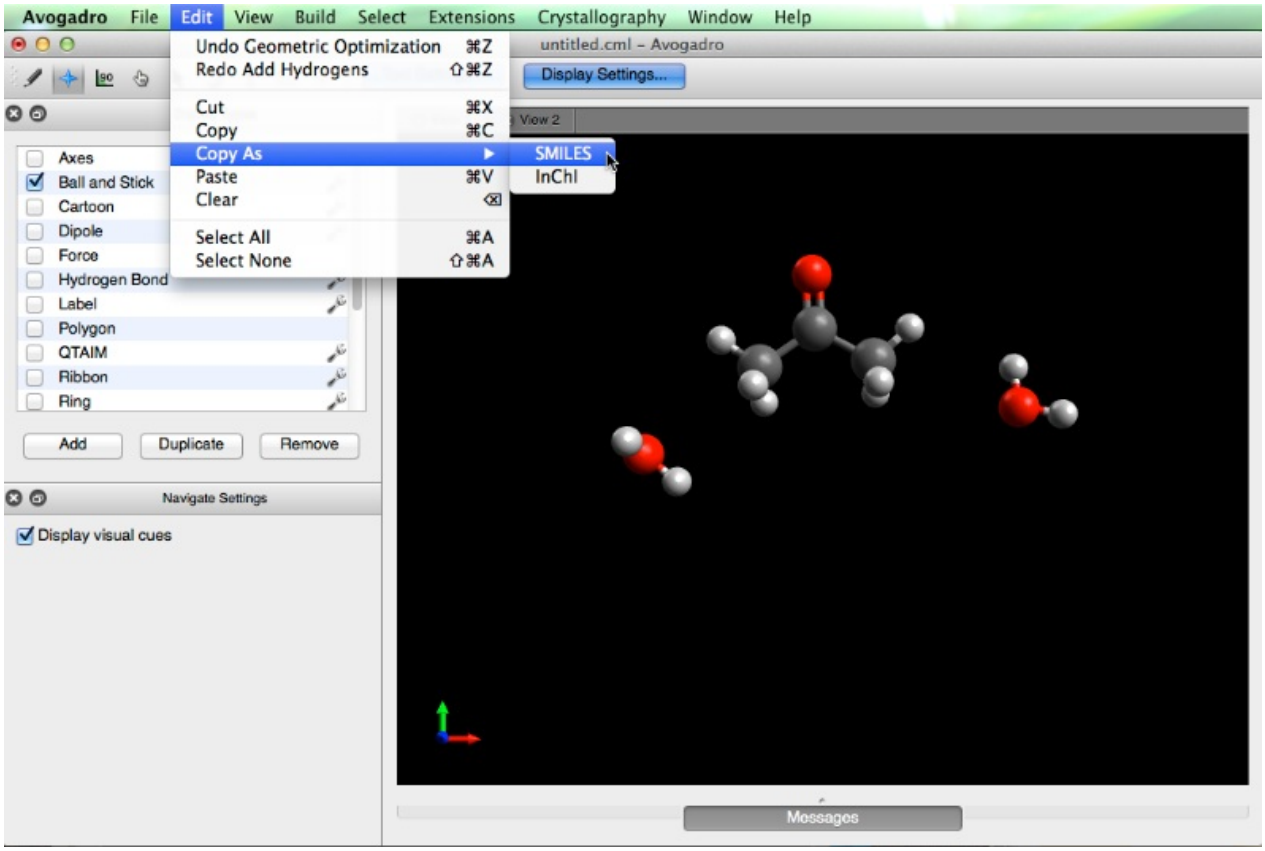
"Cut" will remove and copy the whole molecule or a selection.

Copy

"Copy" will create a duplicate of the entire molecule or a selection, and place it on a clipboard.

Copy As

"Copy As" provides text representations of the molecules present in the viewing screen. For example, selecting "Copy As" and "SMILES", renders "C(=O)(C)C.O.O" as the output for the viewing screen below. This selection can then be pasted in a text document for external projects.



Paste

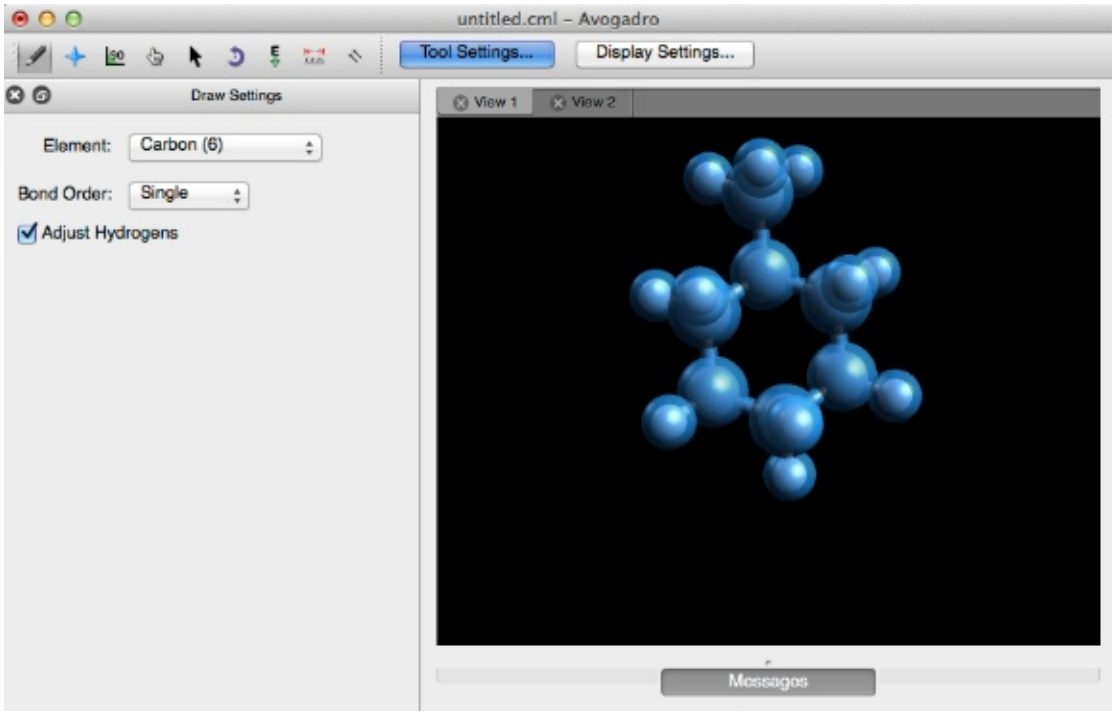
"Paste" recalls the last data copied onto the clipboard.

Clear

"Clear" removes all chemical structures from the viewing window.

Select All

"Select All" highlights everything in the screen (this feature can also be found under the "Select" menu).

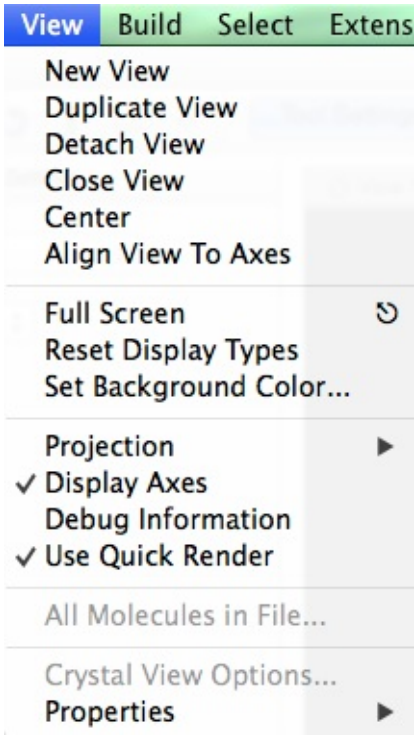


Select None

"Select None" will dismiss everything in the display (this feature is also found under the "Select" menu).

The View Menu

The view menu gives the user the ability to add, and adjust the display views currently in use.

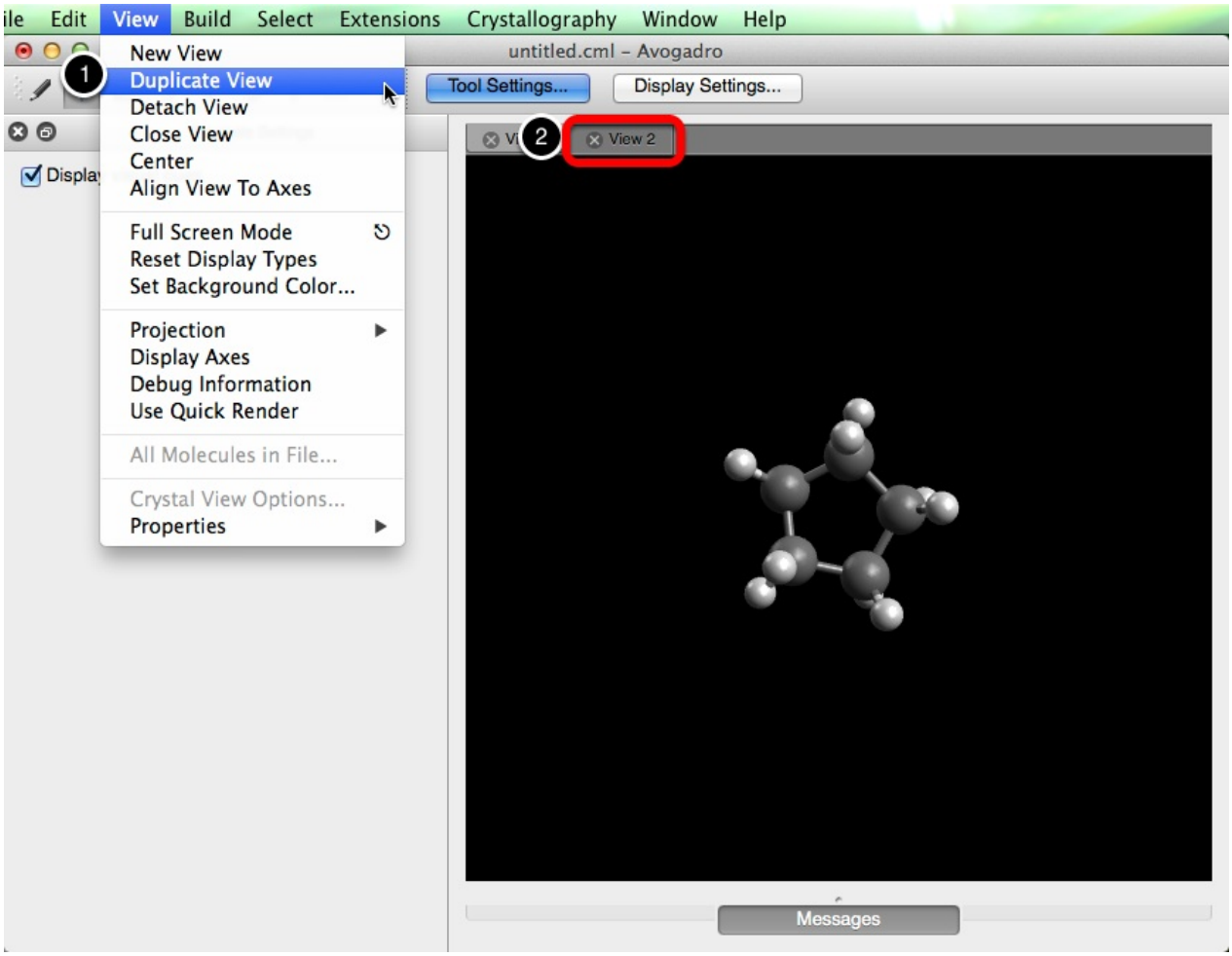


New View

"New View" creates a new, blank viewing window.

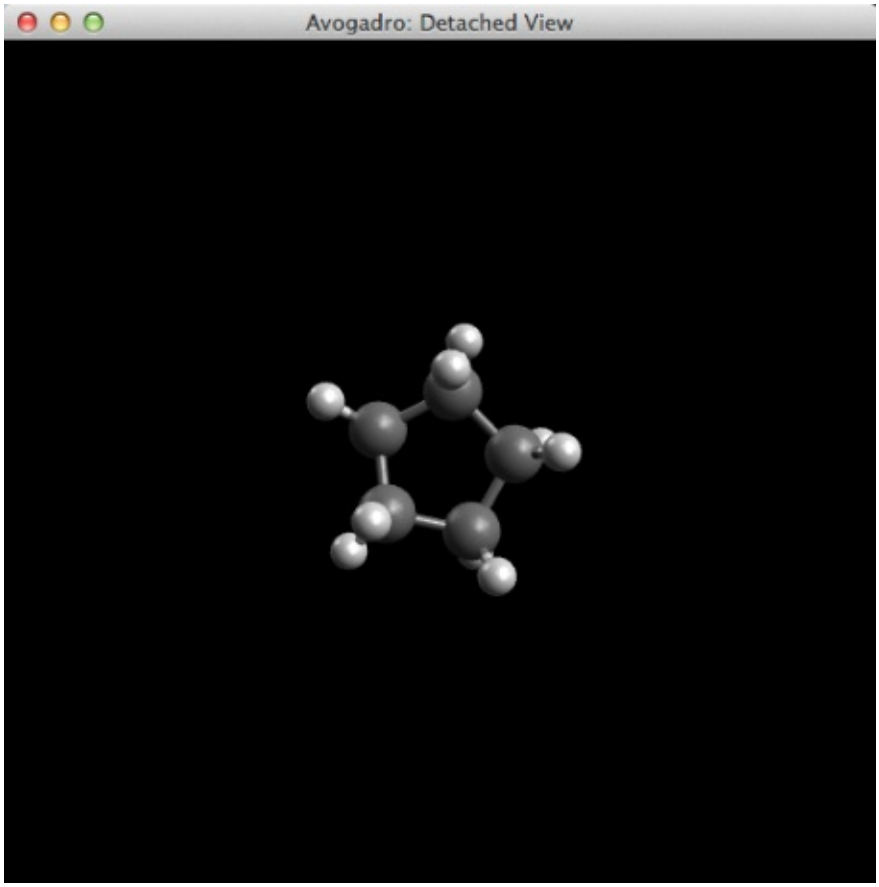
Duplicate View

By selecting "Duplicate View" from the drop down bar, a duplicate of the current view will be created. Any changes made to the display window will automatically update in all of the views.



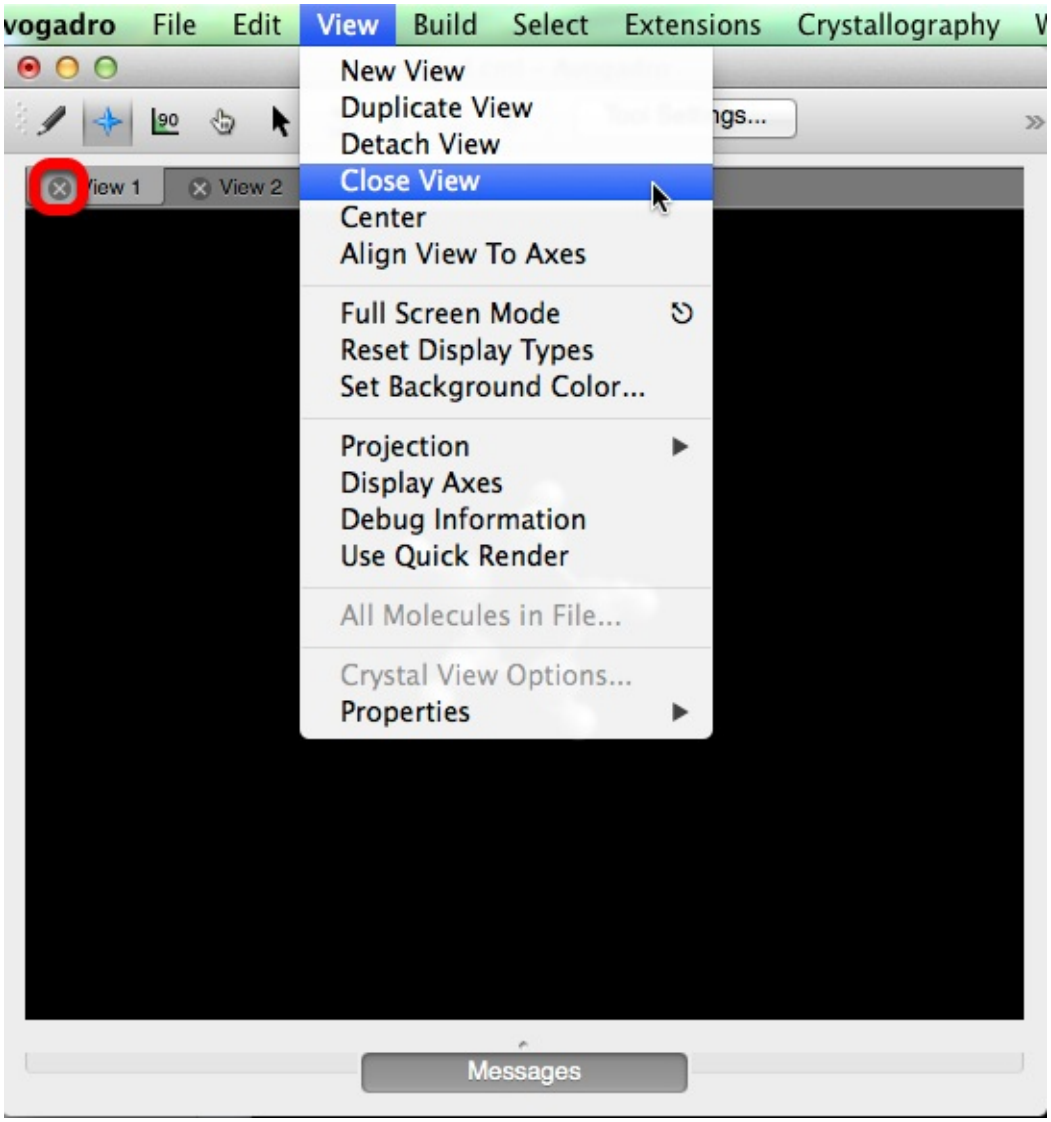
Detach View

The "Detach View" selection will display the current view in a new window.



Close View

"Close View" deletes the display that's open. A view can also be closed by clicking the x on the left of the view tab.

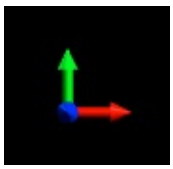


Center

"Center" will align the molecule(s) to the middle of the viewing screen.

Align View to Axes

"Align View to Axes" adjusts the display view to be in the x, y plane with the positive z-axis pointing toward you.

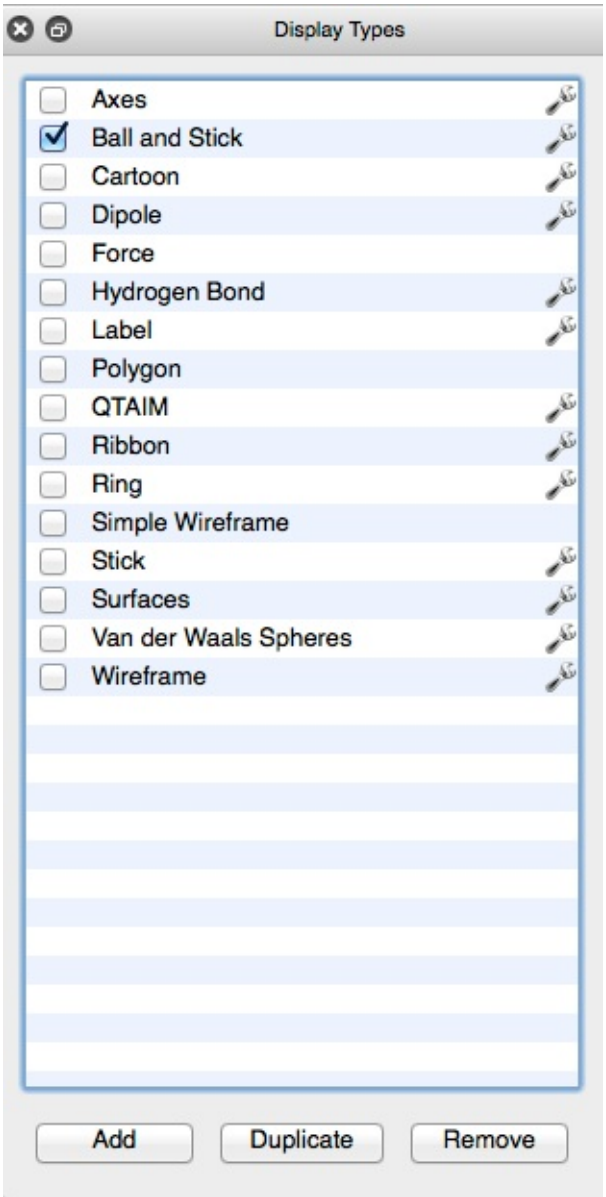


Full Screen

"Full Screen" expands the window to fill the computer screen.

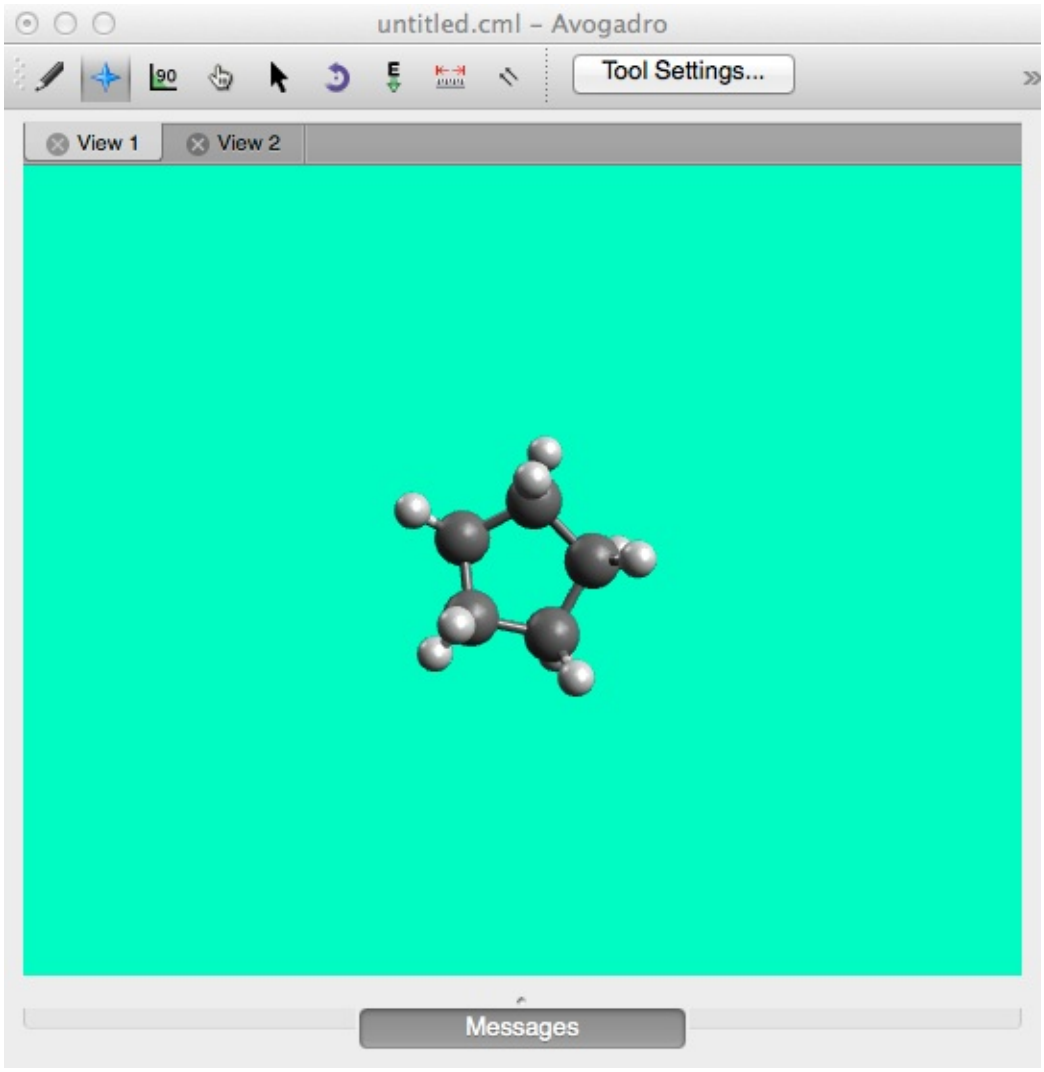
Reset Display Types

"Reset Display Types" will deselect all display types checked, and revert back to the default "Ball and Stick" display type.



Set Background Color...

The "Set Background Color..." feature will allow you to change the background color of the viewing window.

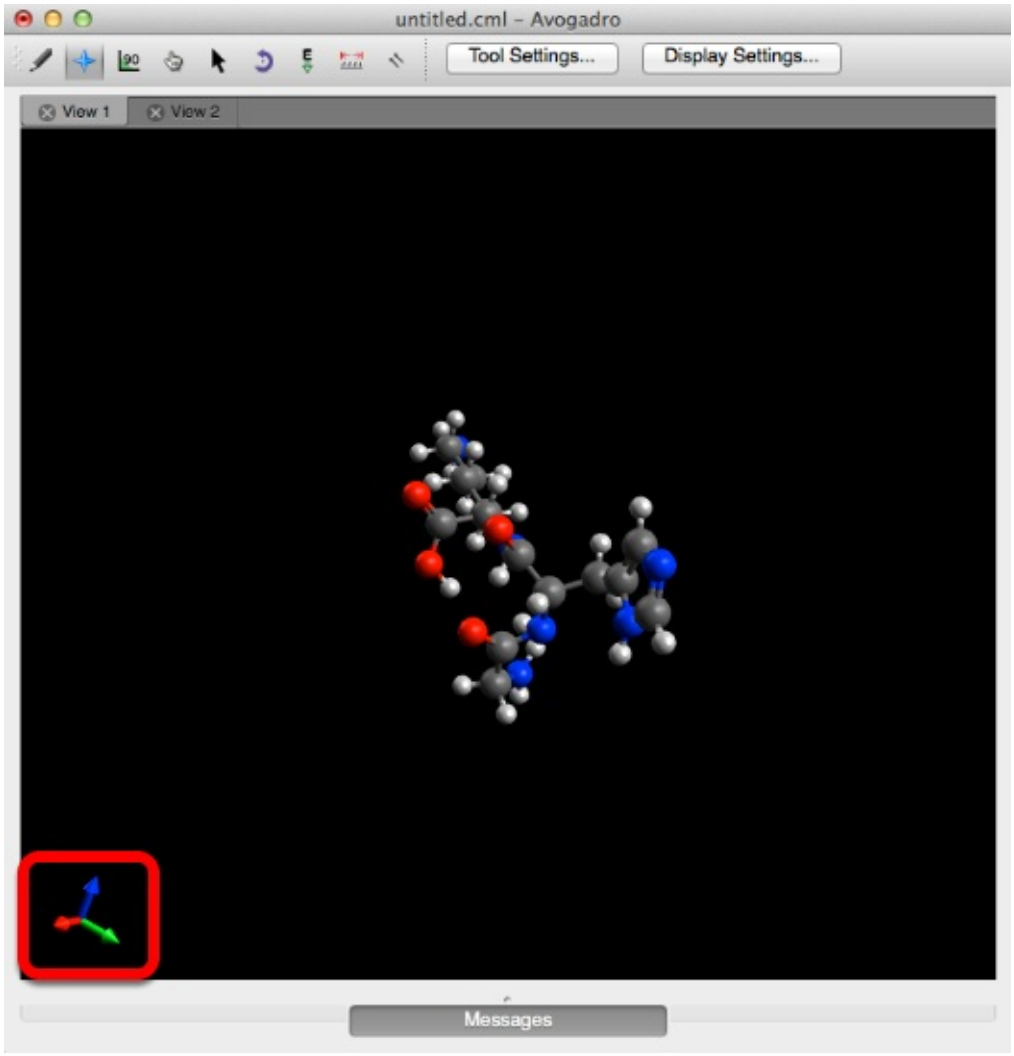


Projection

There are two types of projection features (prospective, and orthographic projection), the default projection is perspective projection. Perspective projection provides a more realistic (3D) view of a molecule in space. Orthographic projection provides, and adjusts the molecule into a planar (2D) view, where all like atoms are adjusted to stay the same size. The projection views are most evident when drawing molecules.

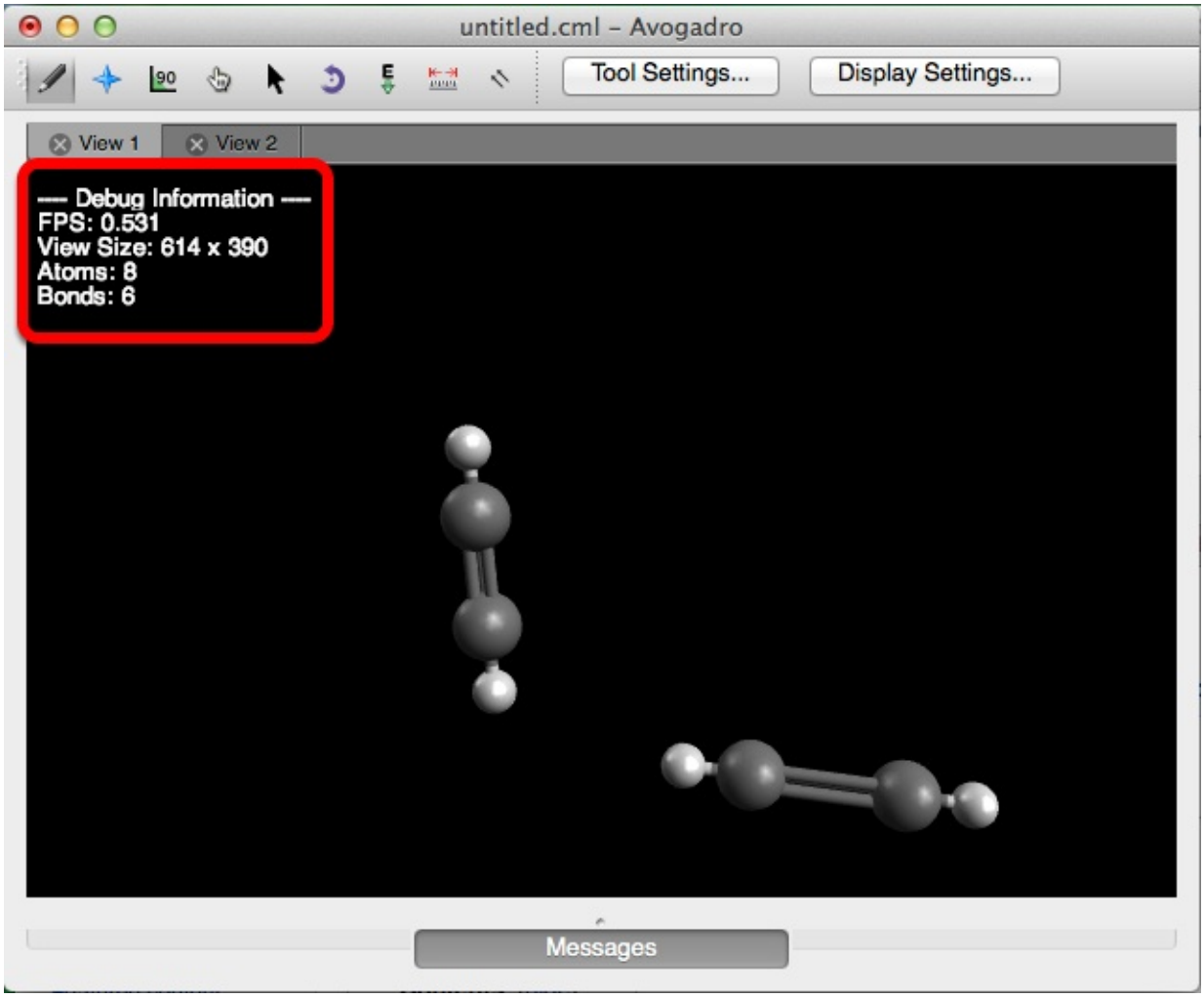
Display Axes

"Display Axes" will render an axes display in the lower left hand corner.



Debug Information

"Debug Information" provides additional information about the view, and what's currently taking place on your screen.

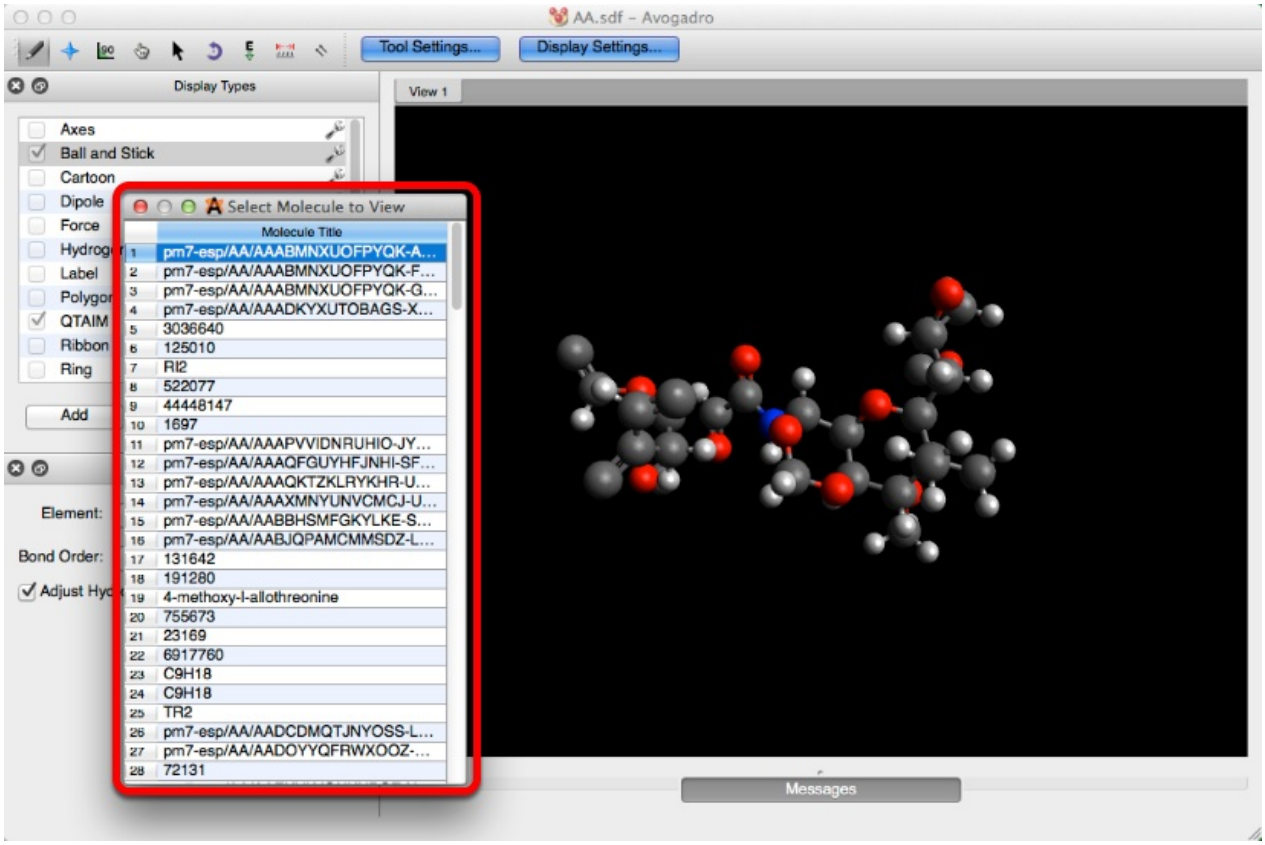


Use Quick Render

Adjusts the 3D molecular image in the viewing screen to achieve a faster image rendering on slow computers. **On most modern (2012 or later) computers, this is not necessary.**

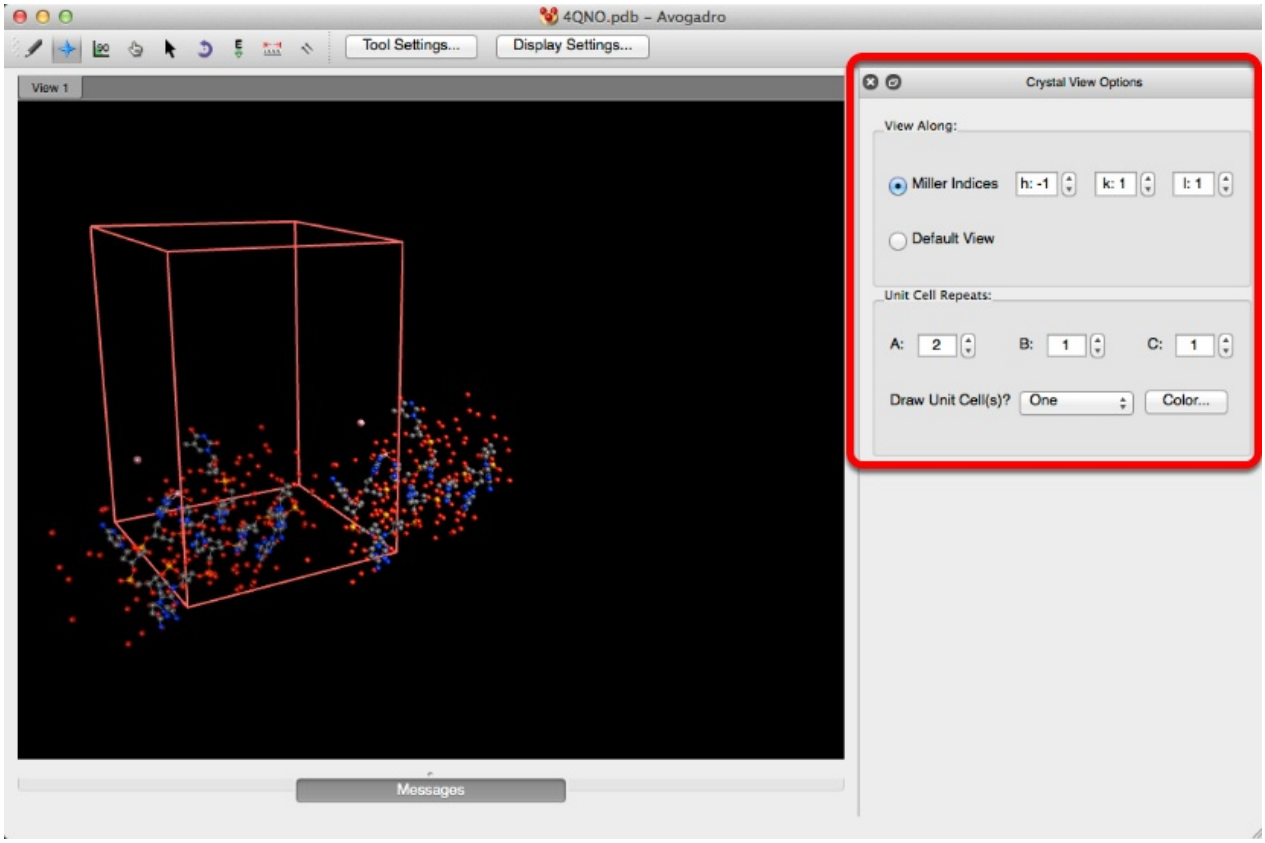
All Molecules in File...

"All Molecules in File..." allows you to look at all of the molecules that have previously been created and embedded into one file. From the dialog box that pops up, you can select and edit a molecule by clicking on the molecule's title.



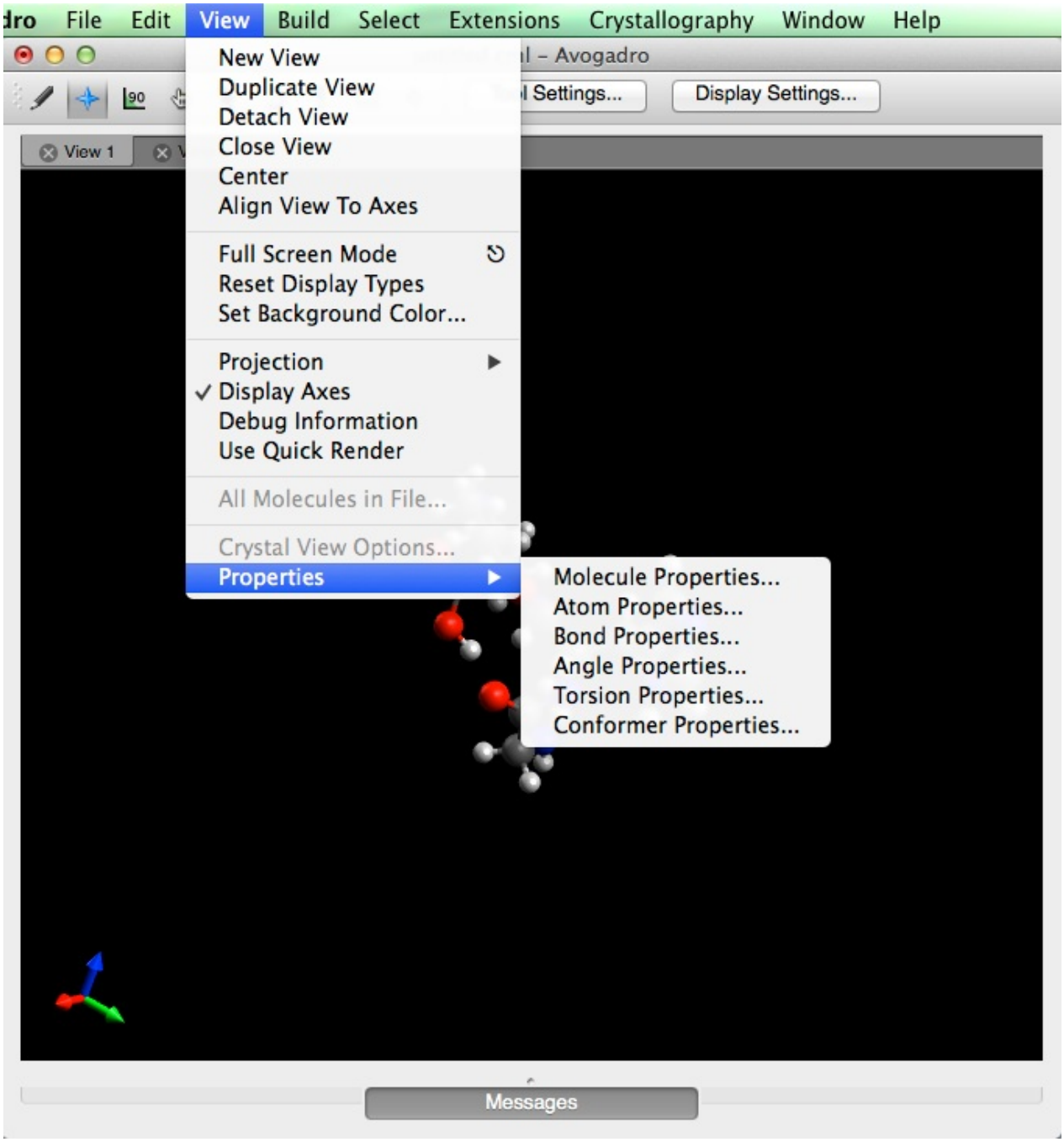
Crystal View Options...

"Crystal View Options..." when selected will open the toolbar shown below. This toolbar allows you to edit the Miller indices, and the Unit Cell for any crystal structure.

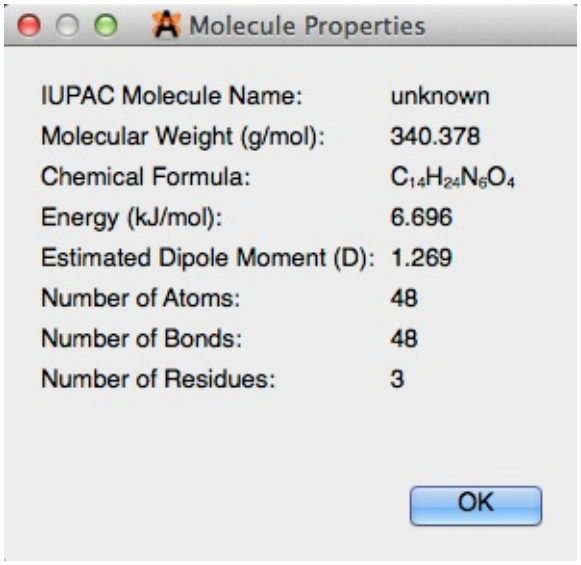


Properties

The "Properties" selection will provides you with molecule, atom, bond, angle, torsion, and conformer properties. These settings display general compository information about the molecule and atoms present.

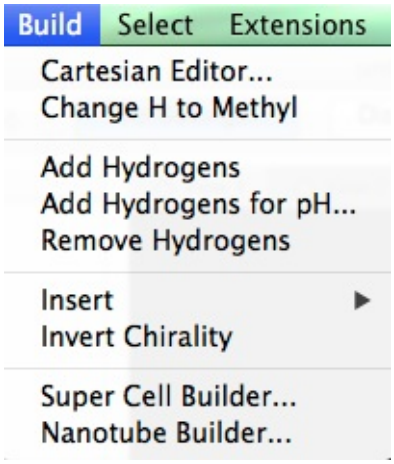


For example, clicking on "Molecule Properties" will display general molecular information.


Molecule Properties
IUPAC Molecule Name: unknown
Molecular Weight (g/mol): 340.378
Chemical Formula: $C_{14}H_{24}N_6O_4$
Energy (kJ/mol): 6.696
Estimated Dipole Moment (D): 1.269
Number of Atoms: 48
Number of Bonds: 48
Number of Residues: 3
OK

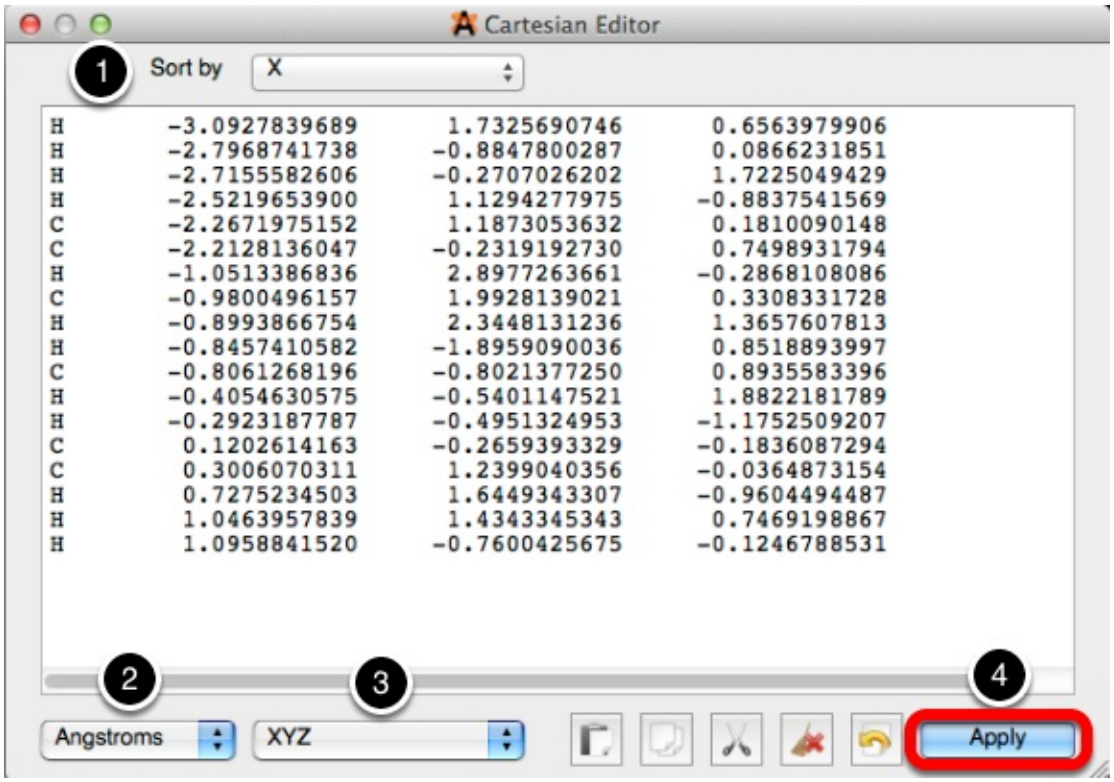
The Build Menu

The build menu helps to ease the process of constructing molecules.



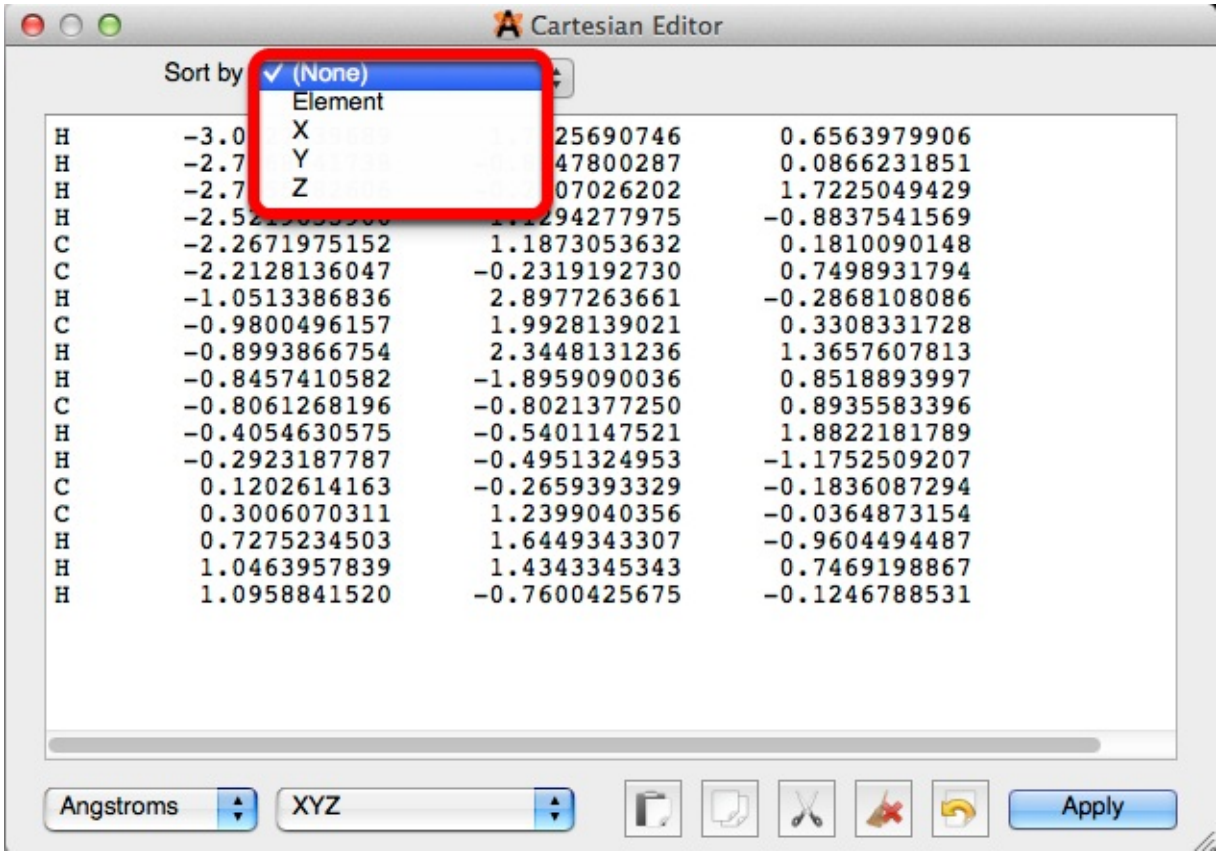
Cartesian Editor...

"Cartesian Editor..." when selected provides you with the capability to manually adjust bond lengths. The dialog box for the cartesian editor is displayed below.



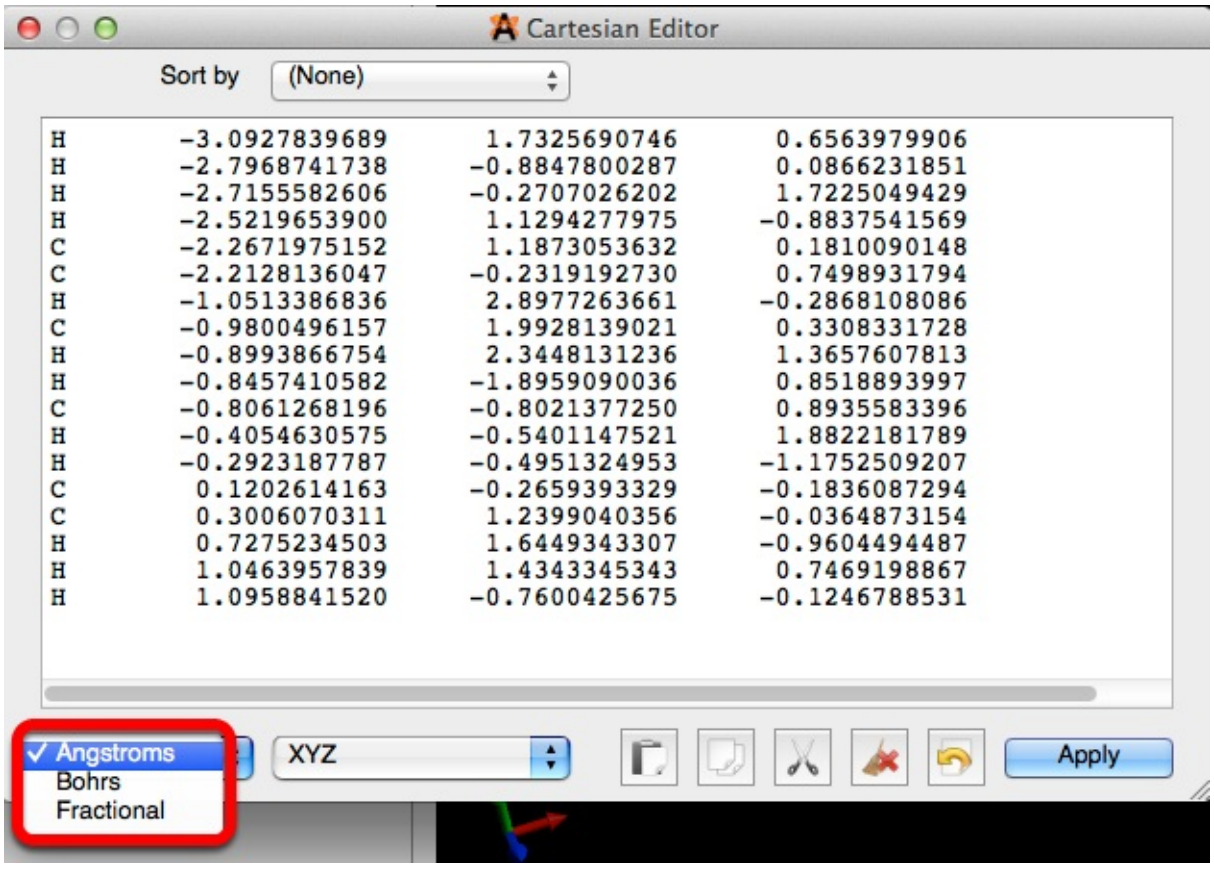
1. Sort by...

The sort by drop down menu will rearrange the data in the dialog box for your convenience. Sort by can arrange the data by element, or by location of the atom. All of the data for sorting by X, Y, and Z coordinates will start reading at the atom to the furthest left in the molecule, and continue until it reaches the atom at the right most point.



2. Unit of Measure

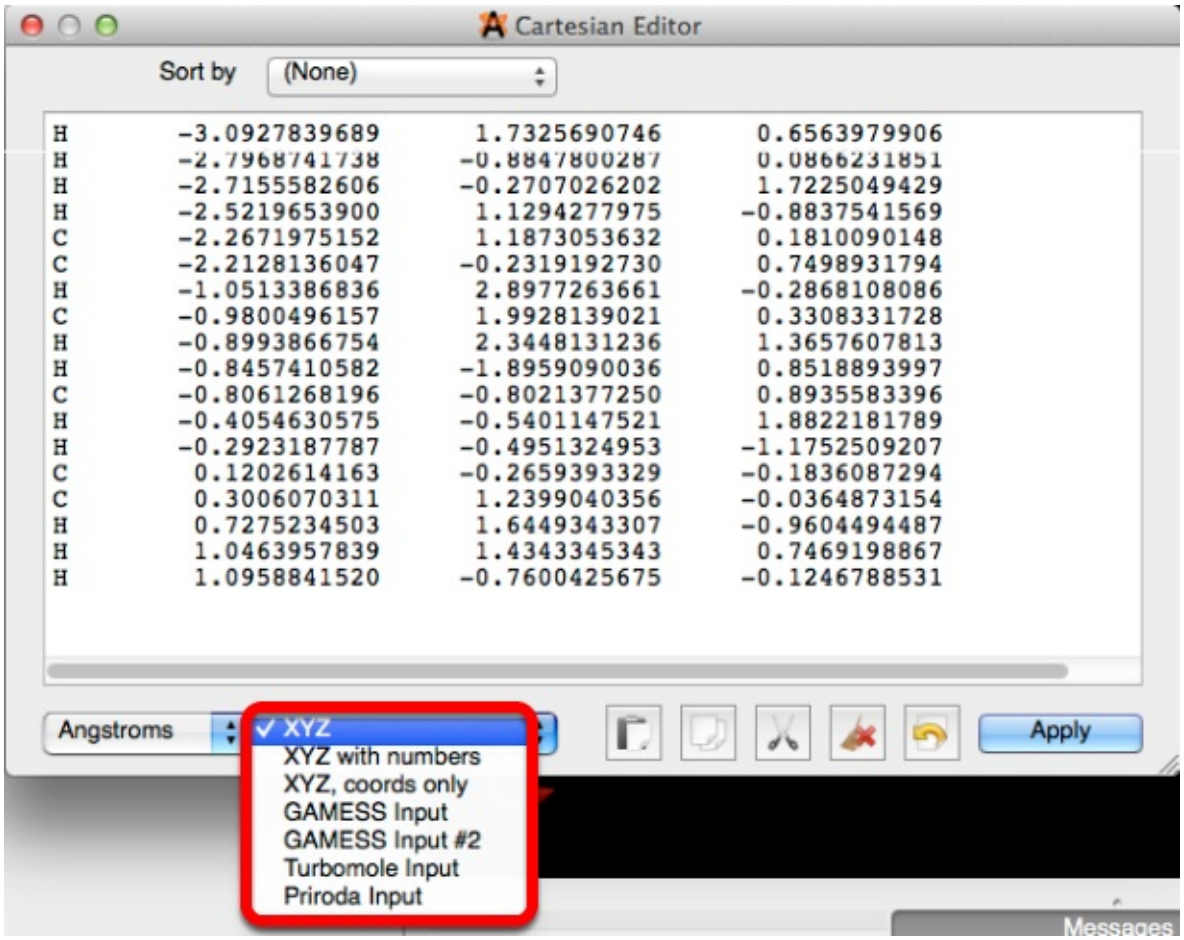
Avogadro provides three units of measure to adjust bond lengths, Angstroms, Bohrs, and Fractional coordinates. A unit cell must be defined to use fractional coordinates.



3. Editing & Modifying Data

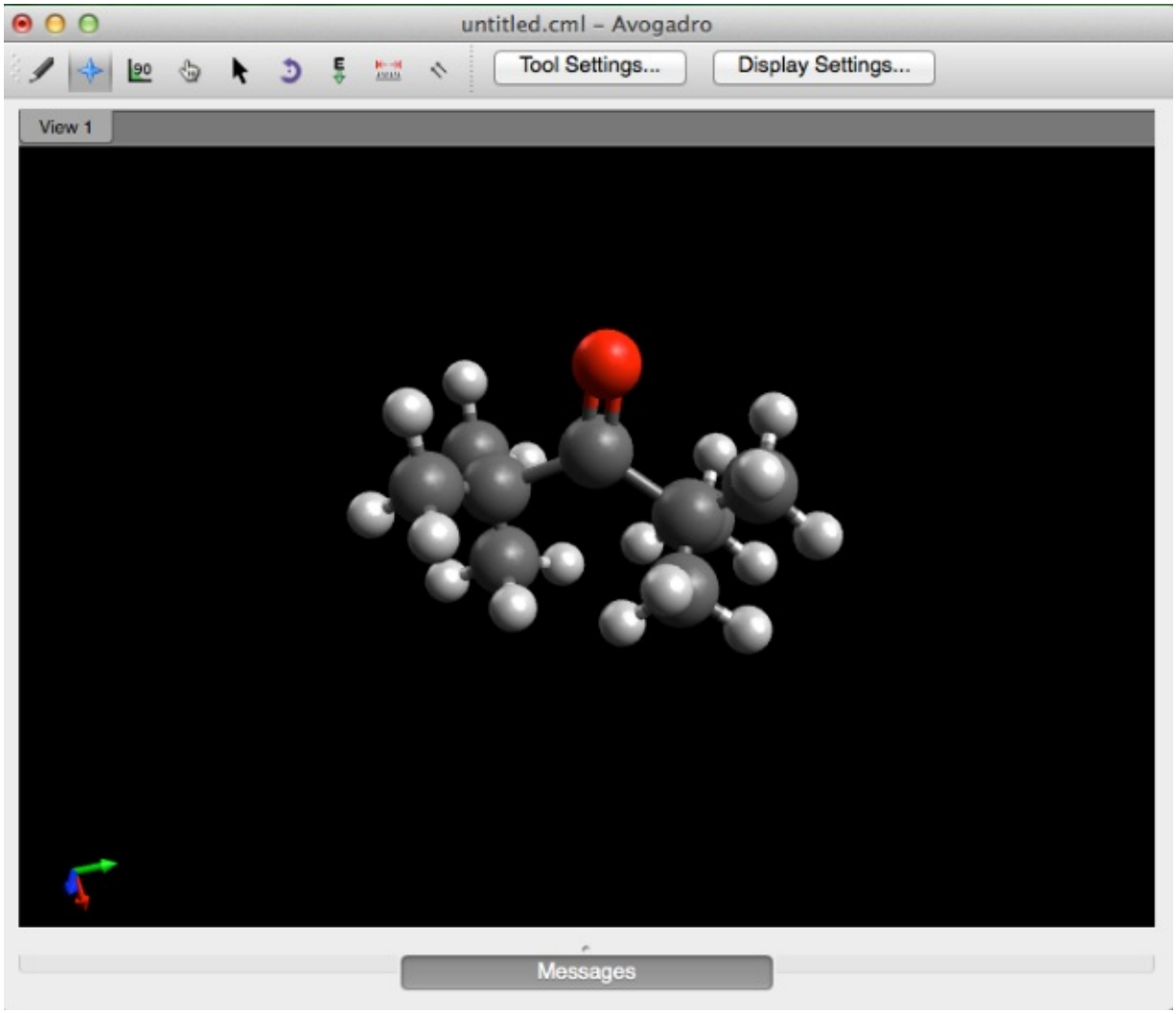
Editing the data is as simple as clicking on the number you wish to edit, and typing in a new coordinate. After clicking "Apply" and returning back to the Avogadro display screen, you should notice that the atom has changed position.

The displayed data can also be modified according to your personal preference, or for the use of additional plugins.



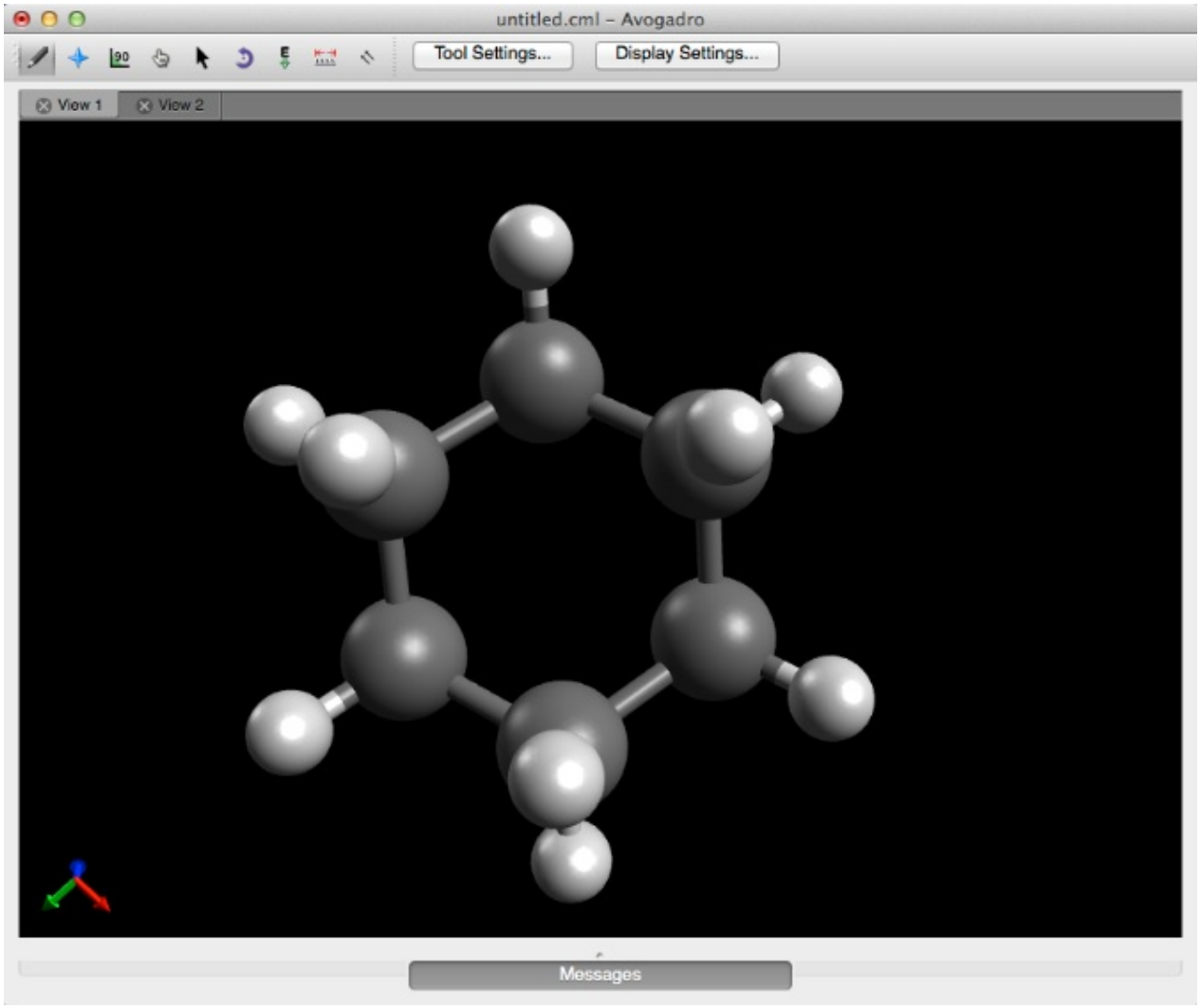
Change H to Methyl

"Change H to Methyl" will replace any Hydrogens present in the display window with methyl groups. Depicted below is acetone with all of its hydrogens replaced by methyl groups.



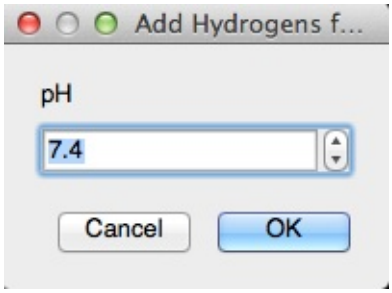
Add Hydrogens

"Add Hydrogens" will satisfy the valency of the atoms present with hydrogens.



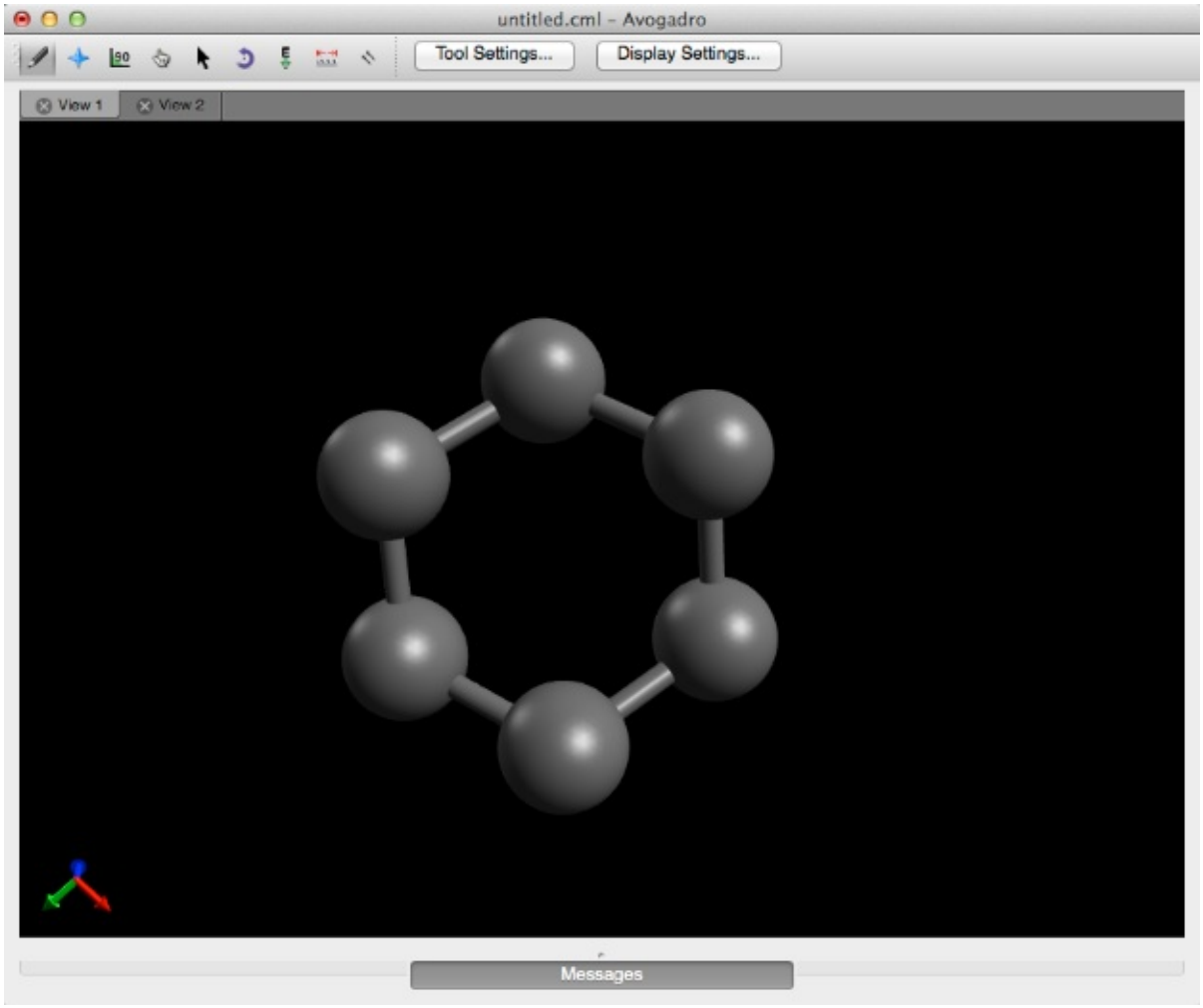
Add Hydrogens for pH...

"Add Hydrogens for pH..." will create a dialog box (displayed below) that allows you to adjust the pH of the molelcular environment. This feature will add (or subtract) acidic hydrogens to ionizable groups in peptides, according to the desired pH.



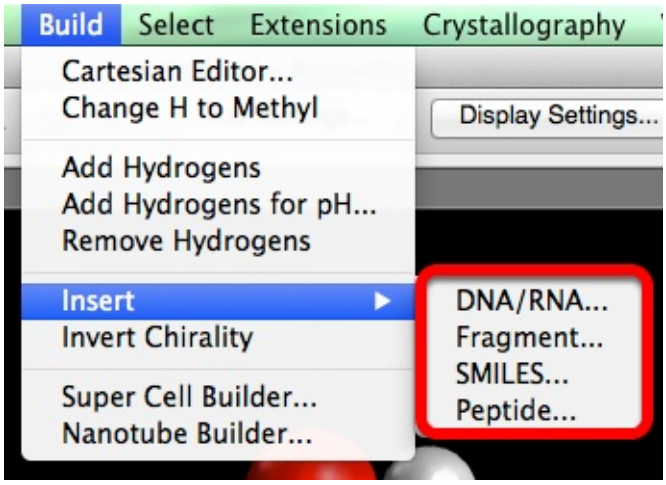
Remove Hydrogens

"Remove Hyrogens" will delete all hydrogens in the display screen.



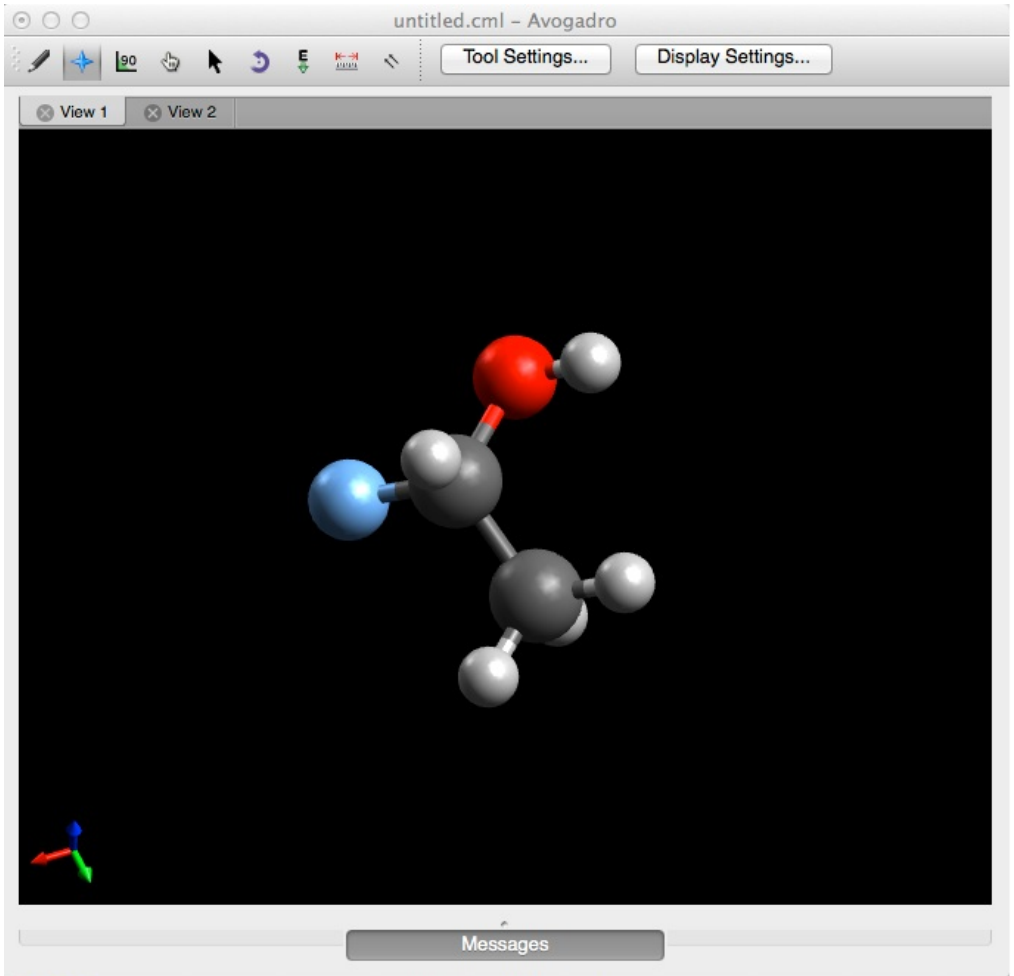
Insert

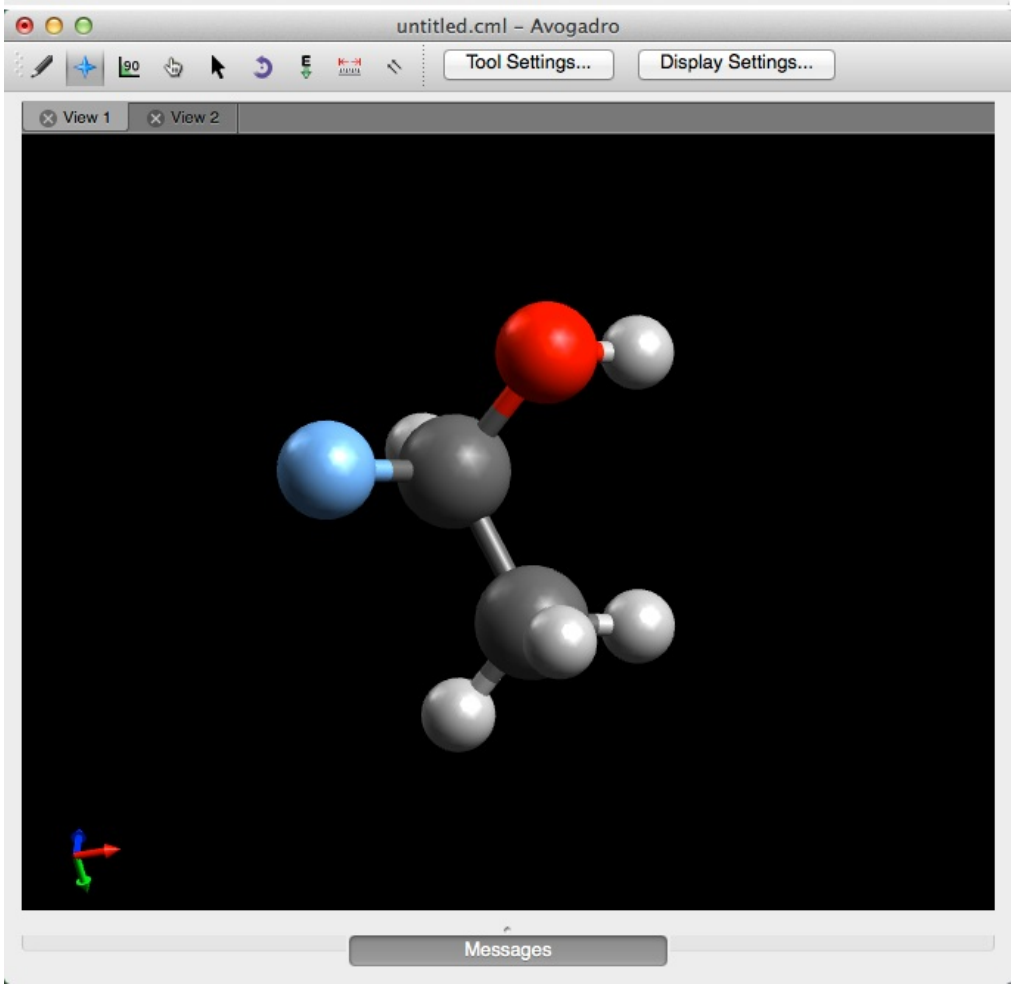
"Insert" provides a faster, simpler way of building molecules. A depicted below, you can insert DNA/RNA, a Fragment, a Peptide, and can also insert a molecule based on SMILES text.



Invert Chirality

"Invert Chirality" will reverse (invert) the initial configuration to the opposite R/S configuration.


untitled.cml – Avogadro
Tool Settings...
Display Settings...
View 1
View 2
Messages


untitled.cml – Avogadro
Tool Settings...
Display Settings...
View 1
View 2
Messages

Super Cell Builder...

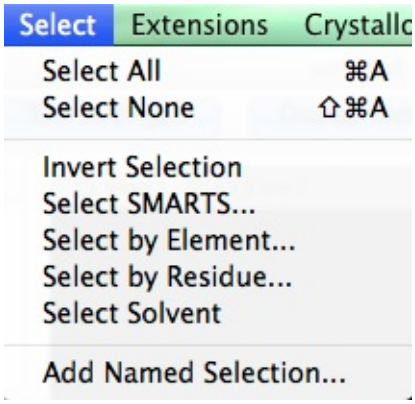
Information on the Super Cell Builder can be found in "Building and Editing Crystals and Materials" section.

Nanotube Builder...

Information on building Carbon Nanotubes in Avogadro can be found in the "Building Molecules" section.

The Select Menu

The select menu makes chemical alterations more efficient through various modes of selection.



Select All

"Select All" highlights everything in the display (this feature can also be found under the "Edit" menu).

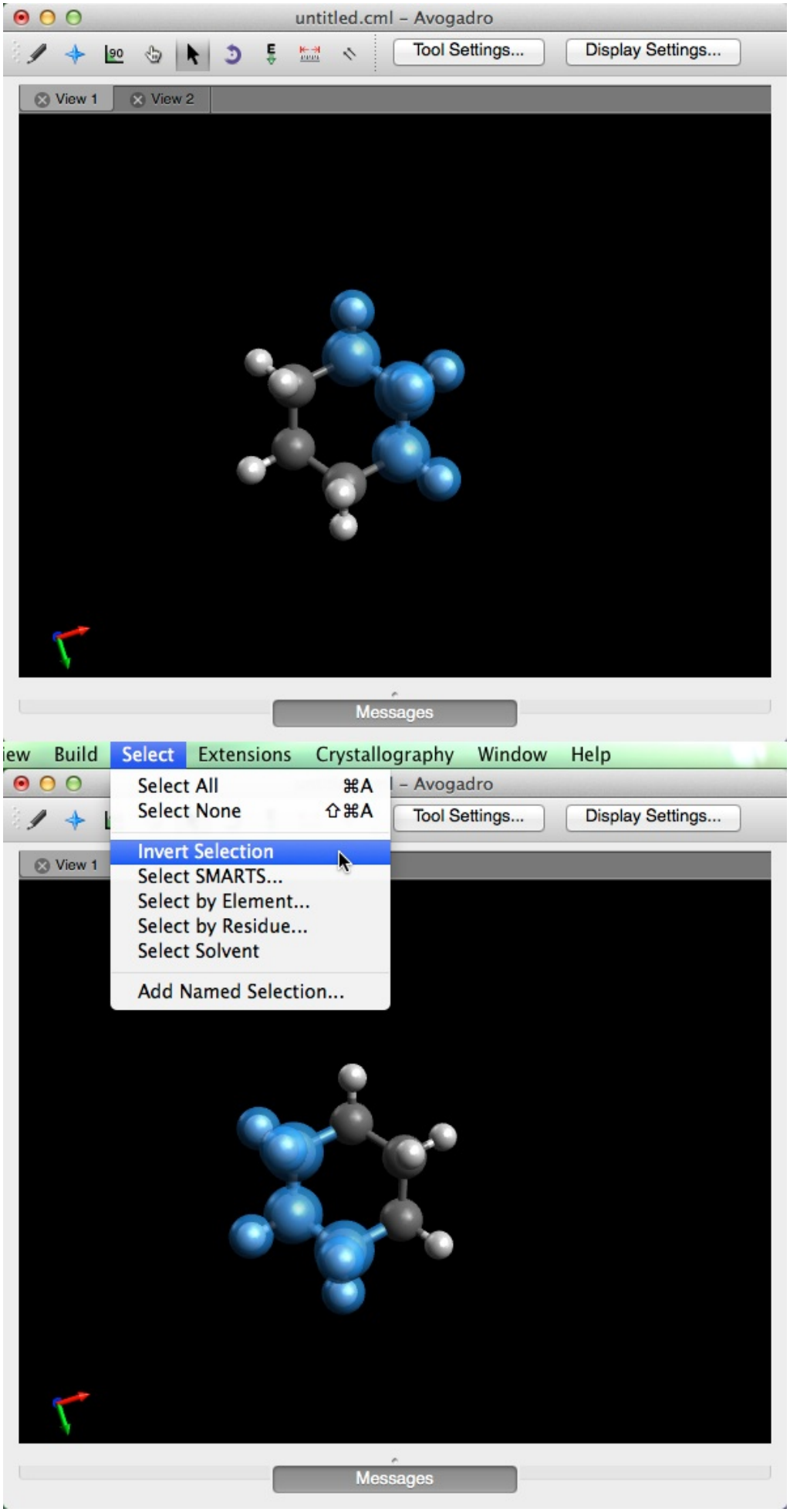
Select None

"Select None" will dismiss everything in the display (this feature is also found under the "Edit" menu).

Invert Selection

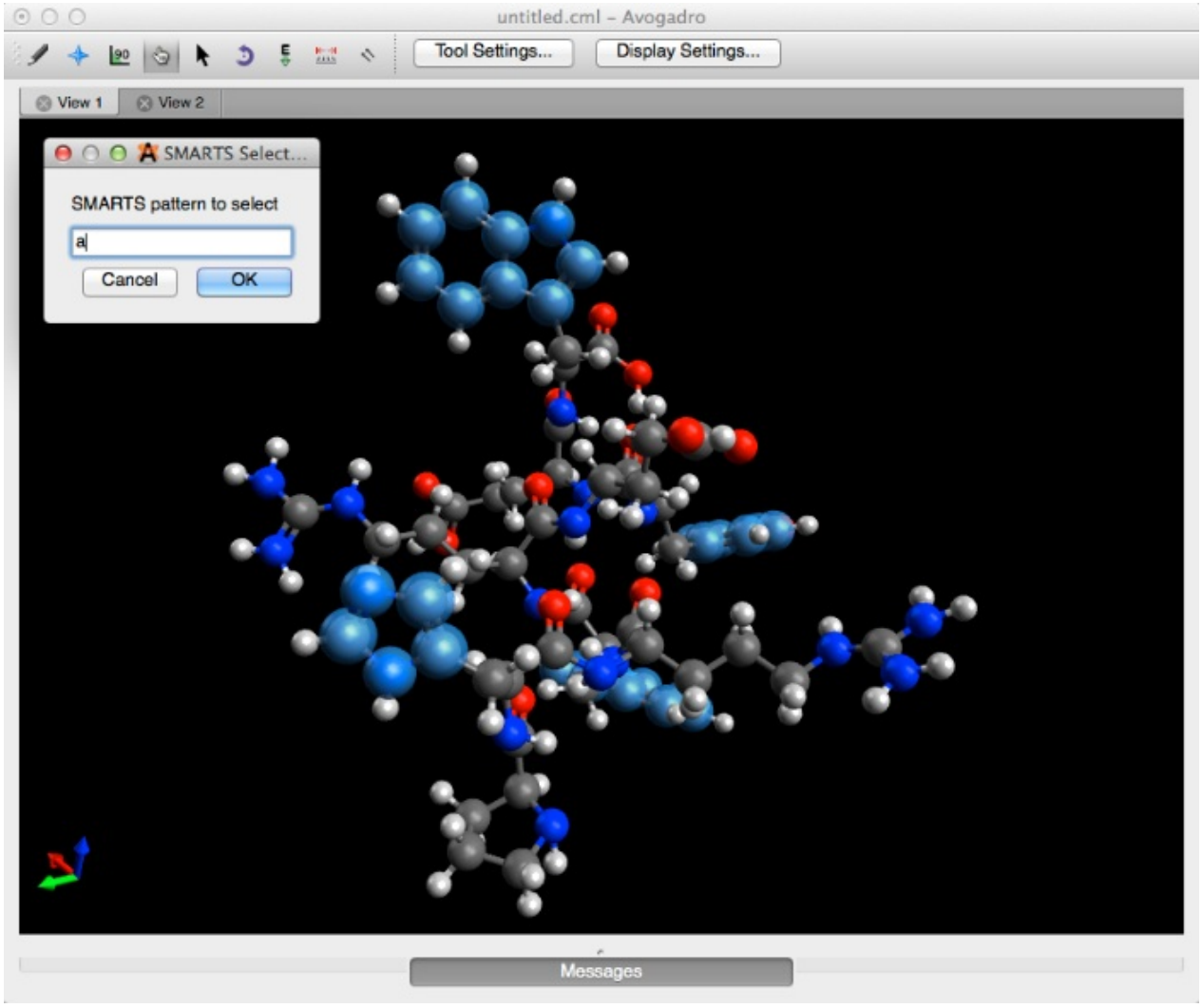
"Invert Selection" reverses the selection made.

The first image displayed below is the orginal selection, and the second image demonstrates the inverted selection.


untitled.cml – Avogadro
Tool Settings...
Display Settings...
View 1
View 2
Messages
Build
Select
Extensions
Crystallography
Window
Help
Select All ⌘A
Select None ⇧⌘A
Invert Selection
Select SMARTS...
Select by Element...
Select by Residue...
Select Solvent
Add Named Selection...
– Avogadro
Tool Settings...
Display Settings...
View 1
Messages

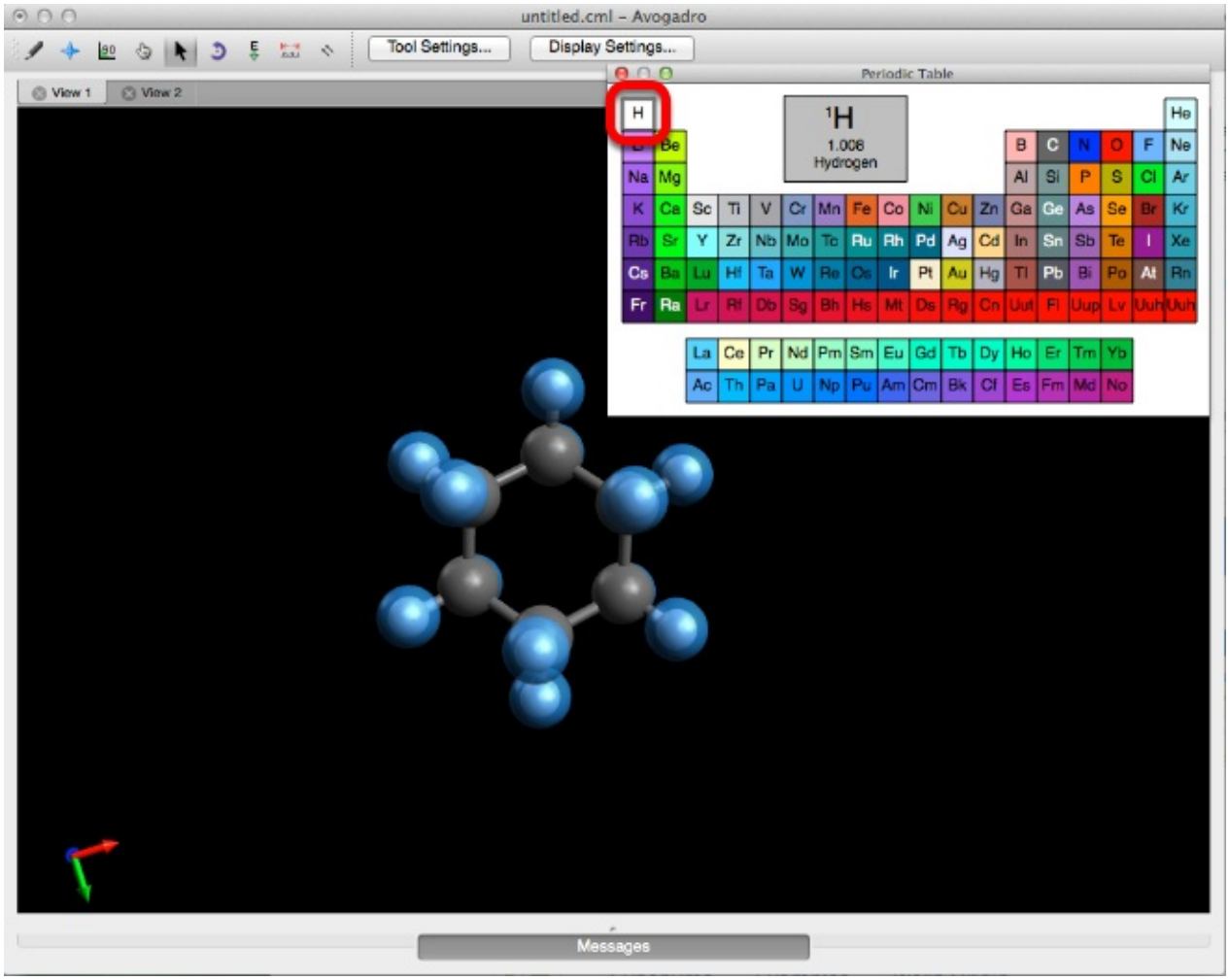
Select SMARTS...

SMARTS **(****SMiles ARbitrary Target Specification)** is a more general chemical language extension of SMILES. "Select SMARTS..." allows you to use this chemical language to select various atoms, or groups of atoms within the molecule. For example, typing "a" into the dialog box and clicking ok will select all atoms with aromaticity. More information can be found at the Daylight SMARTS webpage.



Select by Element...

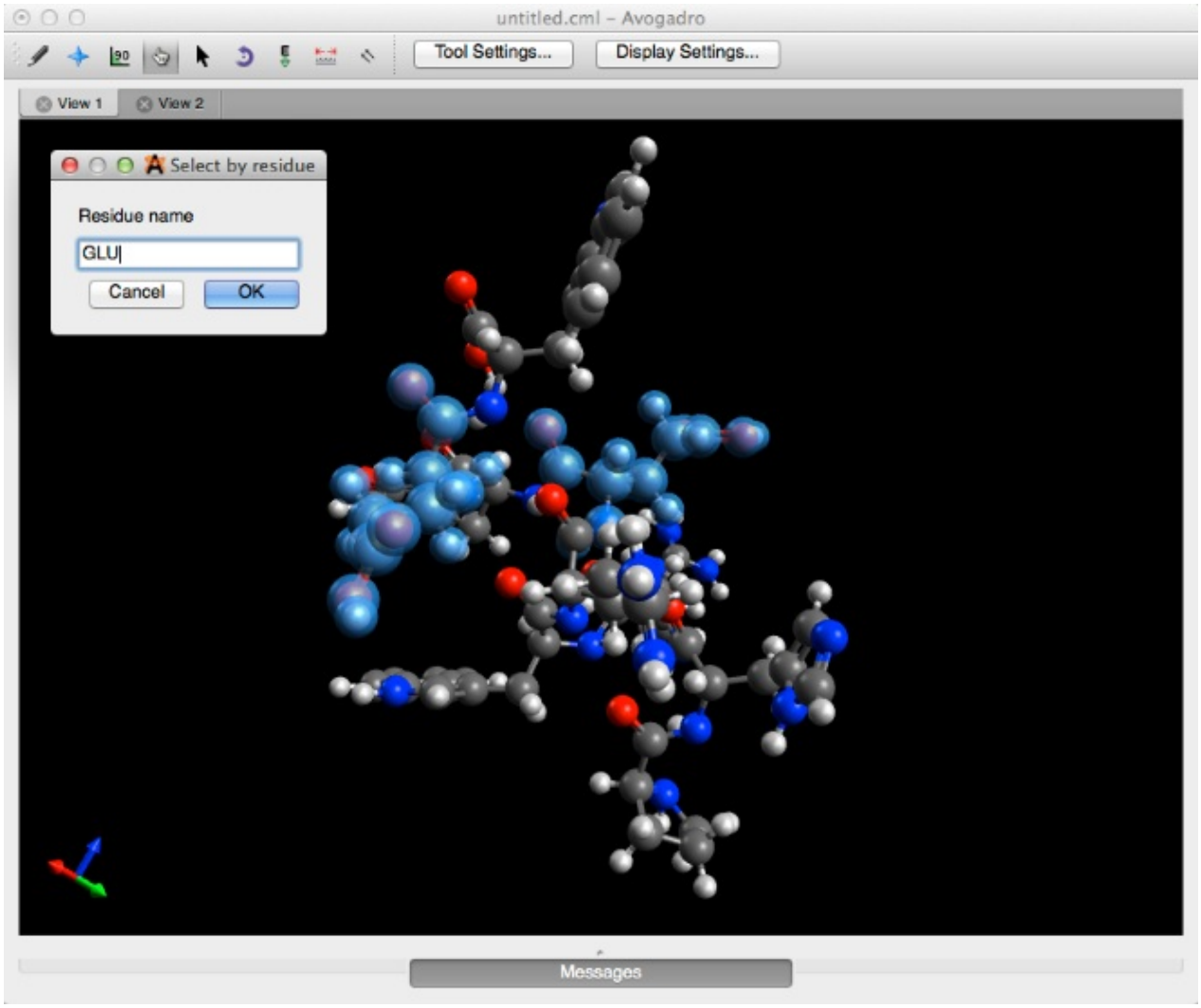
"Select by Element..." generates a periodic table pop up screen that allows you to select an element throughout the viewing display.



Select by Residue...

"Select by Residue..." generates a pop up screen that allows you to select residues with specified names. For example, typing in "ALA" (this feature is case sensitive) to select an alanine residue.

This feauture only works with residues that were made using the peptide builder.



Select Solvent

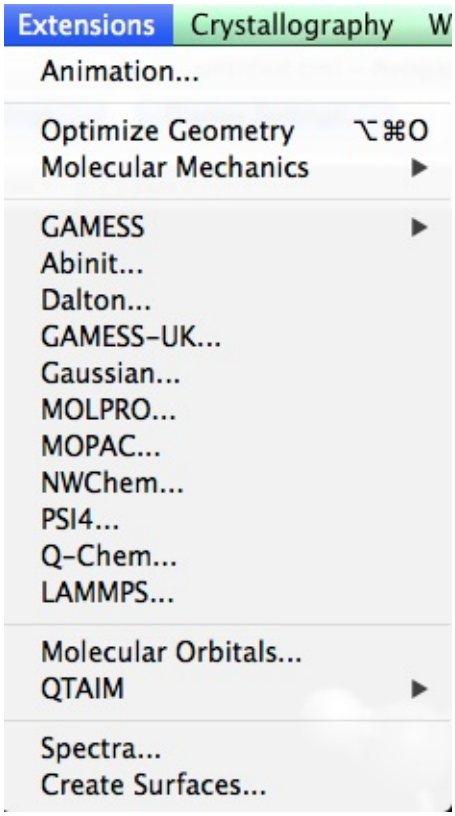
This feature will select "HOH" residues in PDB (protein data bank) files.

Add Name Selection...

"Add Name Selection..." allows you to add a new selection to the current data base, which you can then recall at your convenience.

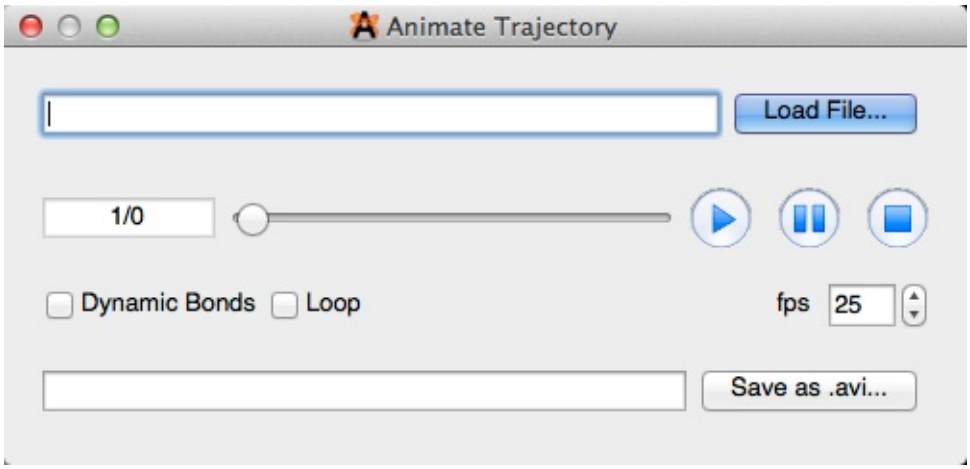
The Extensions Menu

The Extensions Menu is a list of plugins to Avogadro, including molecular mechanics geometry optimizations and interfaces to other computational chemistry packages.



Animation

Selecting "Animation" will open the animate trajectory dialog box shown below. From here you can load a file, view and edit the animation, as well as save the file in a PC compatible format.

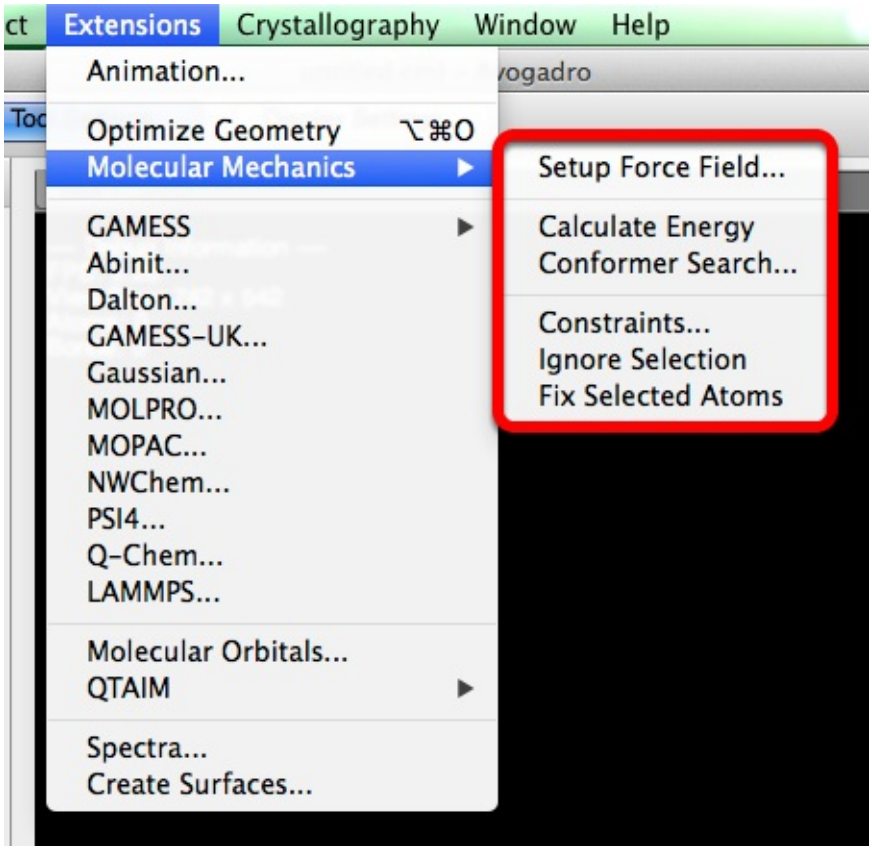


Optimize Geometry

"Optimize Geometry" provides a quick, realistic rendition of a molecule using molecular mechanics.

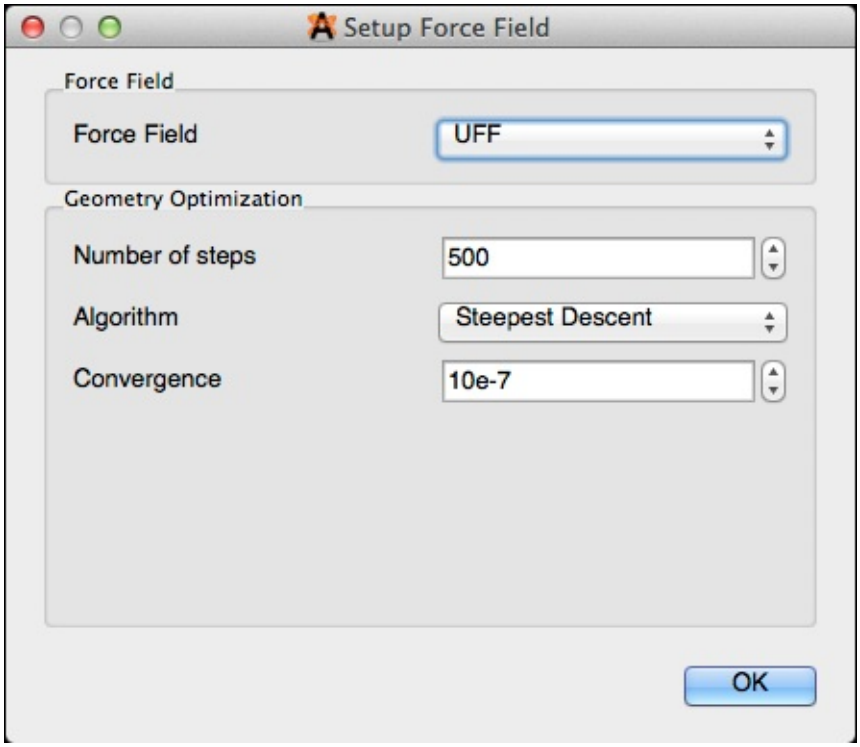
Molecular Mechanics

"Molecular Mechanics" allows you to edit the geometry optimization of a molecule, so that it best suits your purposes.



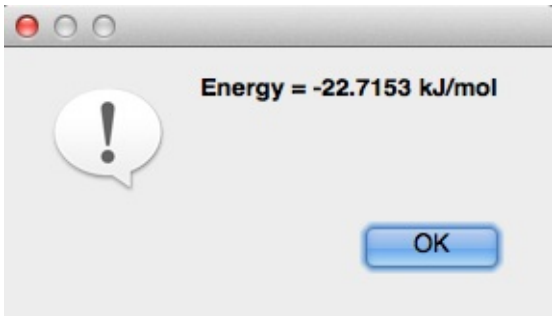
Setup Force Field...

A dialog box will open when "Setup Force Field..." is selected. This dialog box provides you with the ability to choose the type of force field that would best optimize your molecular parameters.



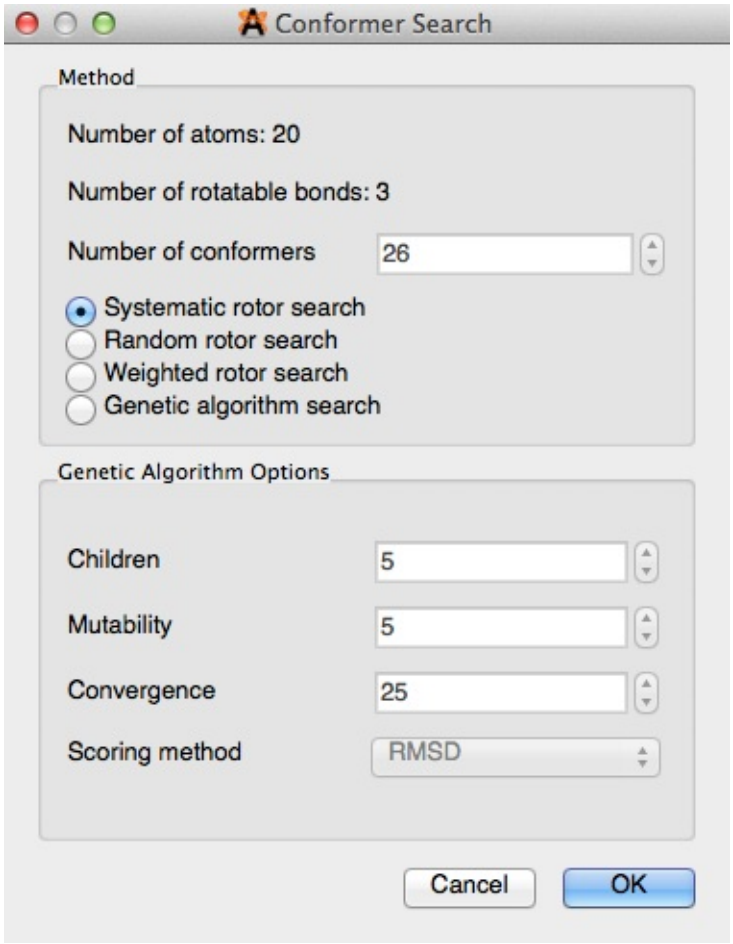
Calculate Energy

"Calculate Energy" determines the amount of energy per the amount of material (kJ/mol), and displays this number in a pop up dialog box.



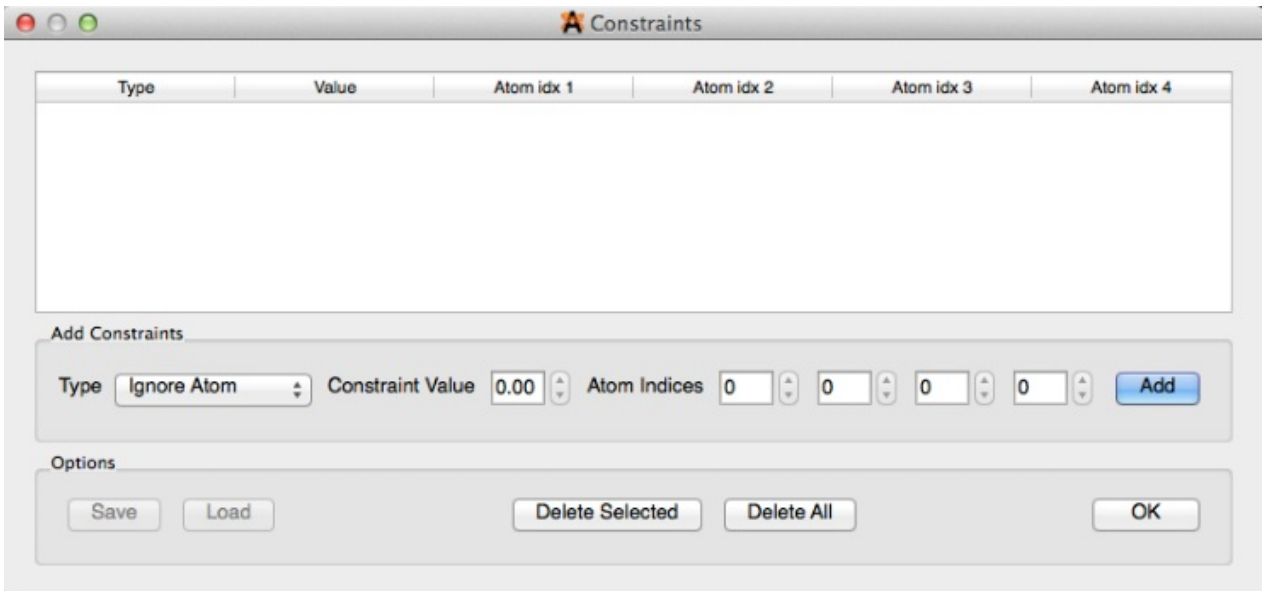
Conformer Search

"Conformer Search" is a way to easily search for conformers within a molecule (dialog box shown below). A more detailed outline on how to perform a conformer search is found in the "Optimizing Geometry" section of this manual. Avogadro only renders staggered conformations, and does not calculate ring conformers.



Constraints

"Constraints" is a way to ensure atom stability in various selections (dialog box depicted below). The constraints that can be applied to a molecule include Ignore Atom, Fix Atom, Fix Atom X, Fix Atom Y, Fix Atom Z, Distance, Angle, and Torsion Angle. A detailed outline on how to use the constraints feature is found in the "Optimizing Geometry" section of this manual.



Ignore Selection

"Ignore Selection" allows you to select a specific part of a molecule to omit during a geometry optimization.

Fix Selected Atoms

"Fix Selected Atoms" also allows you to set a certain part of a molecule to fix during optimization.

Avogadro Extensions--Plugins

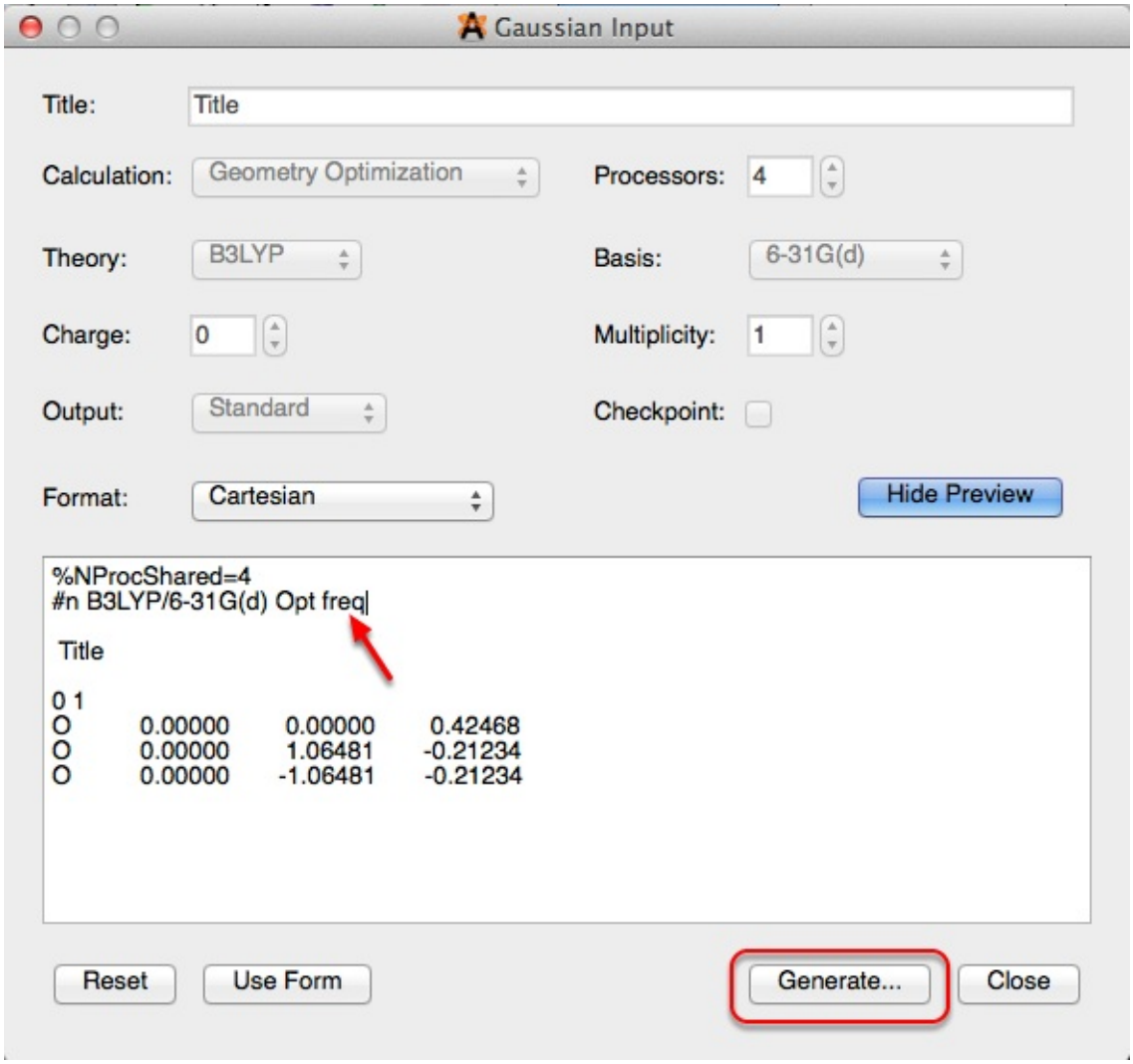
Avogadro provides you with the ability to interface your molecules with other dialog based plugins. These extensions interact with a molecule to provide further molecular information, and additional computation abilities. These plugins include but aren't limited to GAMESS, Abinit, Dalton, GAMESS-UK, Gaussian, MOLPRO, MOPAC. NWChem, PSI4, Q-Chem, and LAMMPS.

General "How To" for Plugins

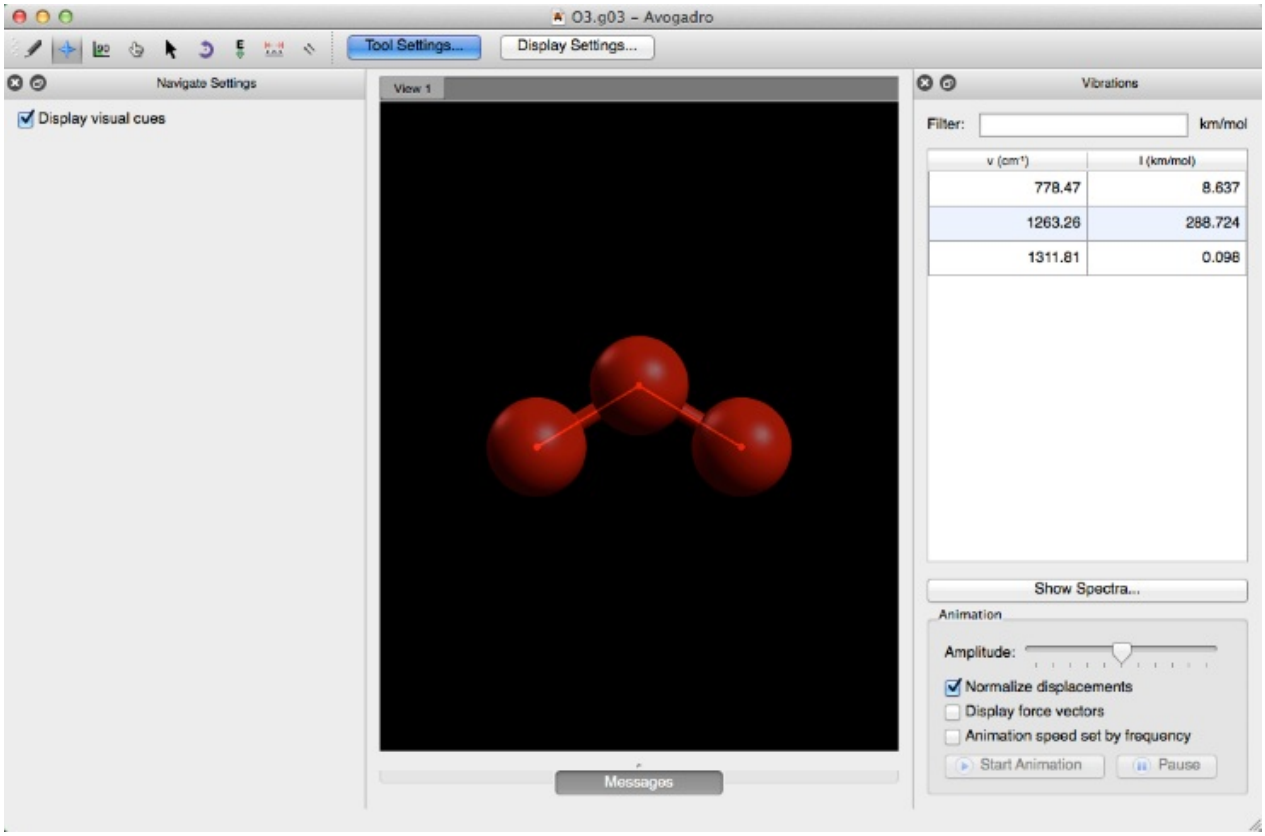
Avogadro (as you will see below) can be used to display molecular orbitals, QTAIM, spectra, as well as create various surfaces. However, many of these features can not be used to their full potential without first running one of the plugins listed in the section above. Gaussian is one of the most common plugins used, due to it's wide range of basis sets/functions.

Running Gaussian

After selecting "Gaussian" from the Extensions menu, the dialog box depicted below will appear. You can edit the dialog box and add specific keywords to utilize these features in Avogadro. For example, typing "freq" in the dialog box will compute force constants and vibrational frequencies. More information on keywords for Gaussian can be found at the Gaussian website (http://www.gaussian.com/g_tech/g_ur/l_keywords09.htm). Then clicking generate will let you save the file to your computer, so you can run the file in external software.

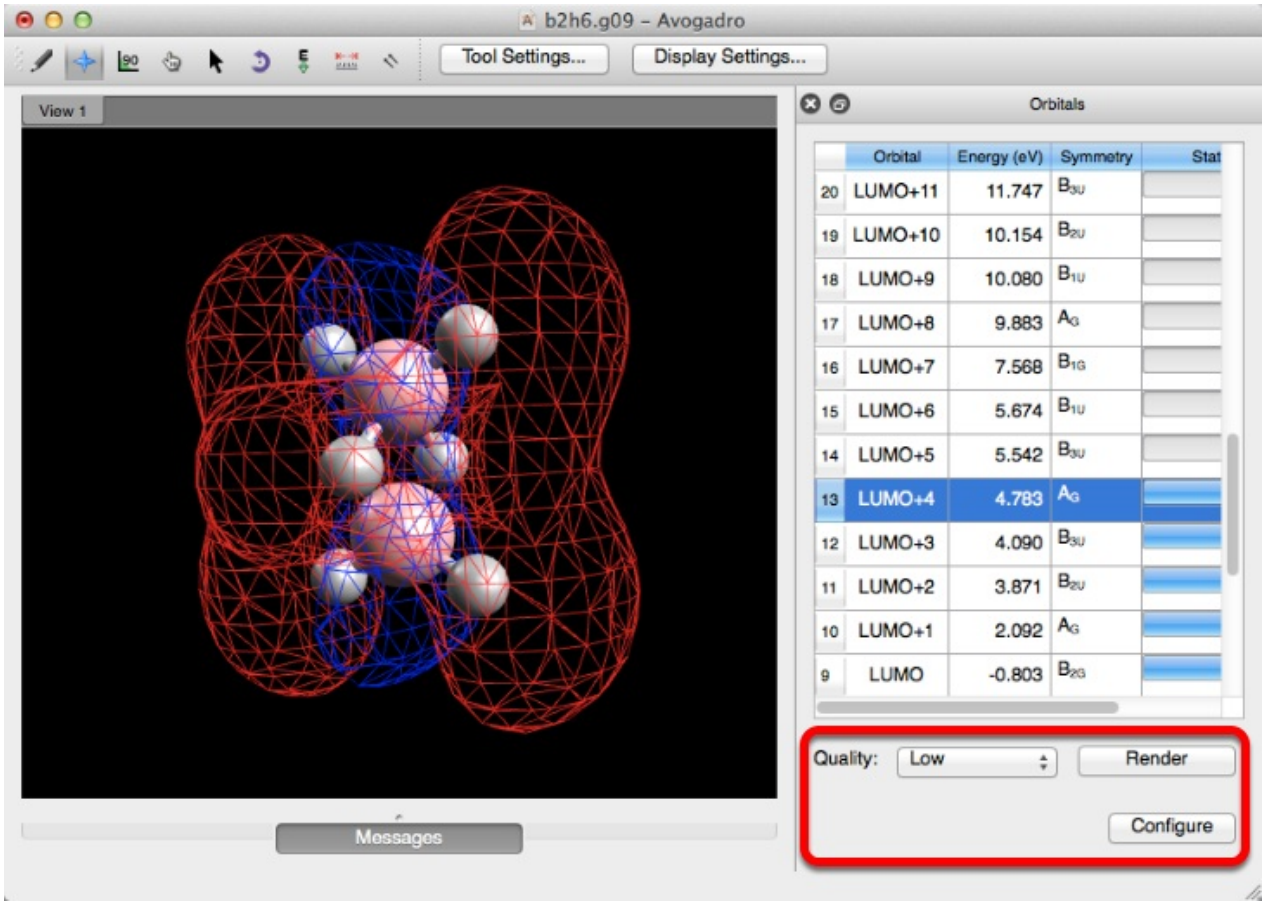


Once the file has been run through the external software, you will have a .g03 or .g09 file that will open the keyword selection in a toolbar on the right hand side of the screen. "Freq" will open the vibrations toolbar shown below.



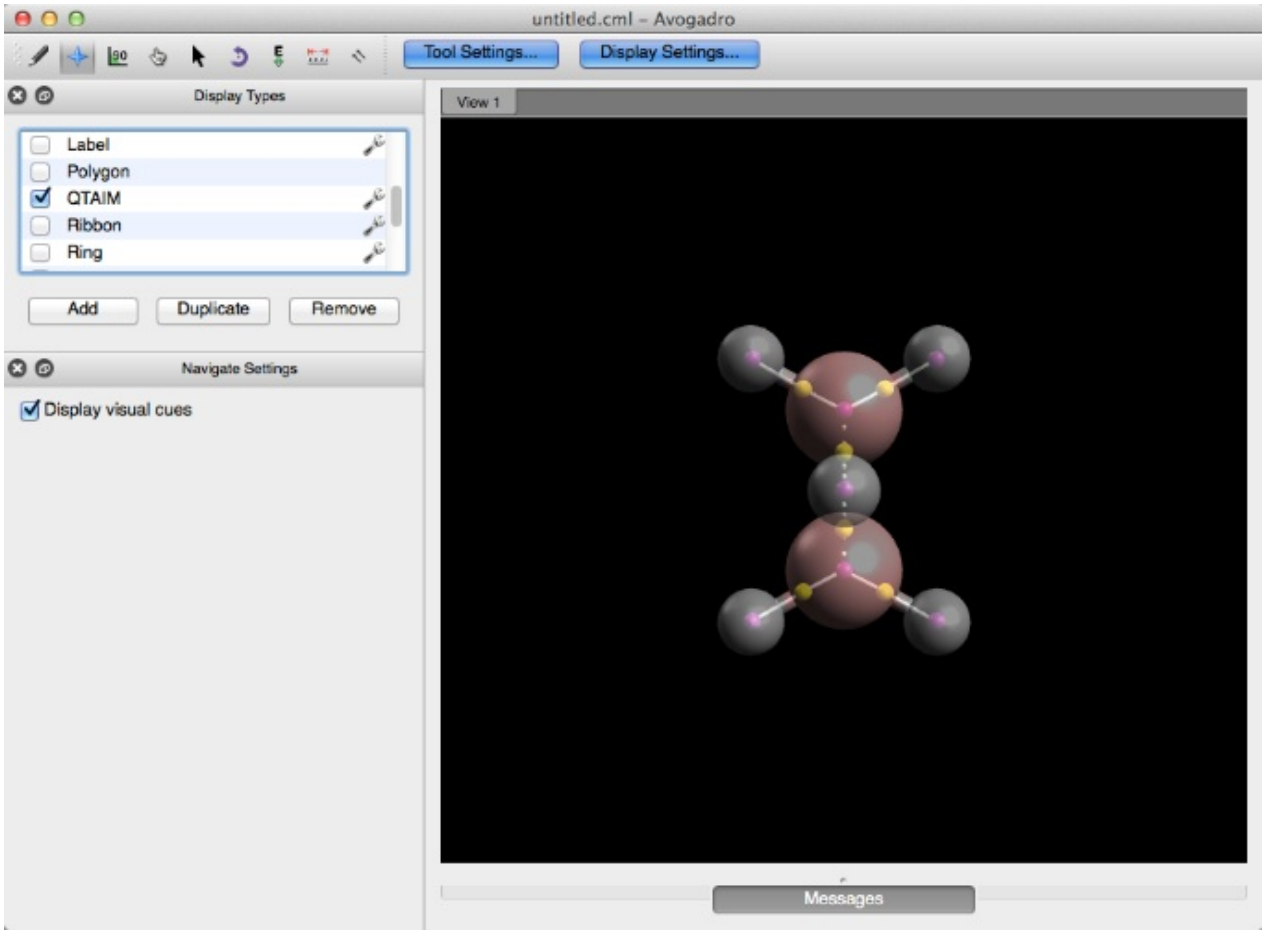
Molecular Orbitals

The "Molecular Orbitals" selection will display the molecular orbitals for orbitals with full status bars. The quality of the orbitals can be adjusted an reconfigured if need be. This feature only works by running gaussian extension files (.fchk, .g03, .g09, etc.).



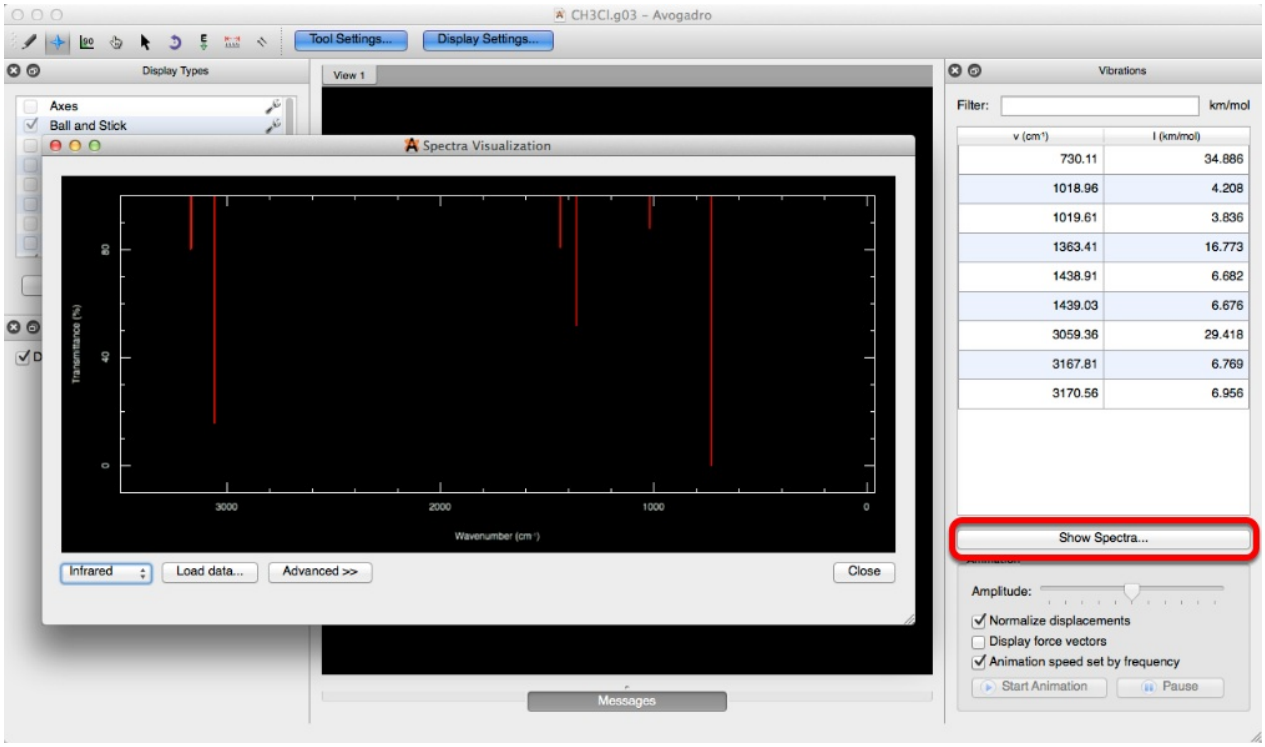
QTAIM (Quantum Theory of Atoms in Molecules)

QTAIM displays the implicit bonding that is theorized to take place between the hydrogens of organic crystals (the implicit bonding is conveyed through dots). This display type is utilized by importing a .wfn file from the "QTAIM", "Molecular Graph" selection under the "Extensions" menu. Selecting "Molecular Graph with Lone Pairs" or "Atomic Charge" will provide concurrent information about the molecule. More information can be found on this process in the Tutorial section of this manual.



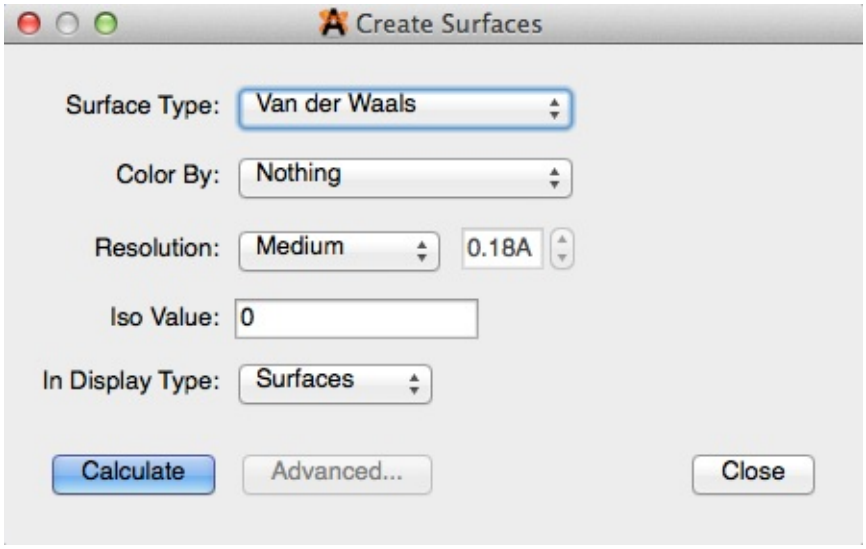
Spectra...

Clicking on "Spectra..." will create a spectra visualization of a .g03, or .g09 file that has been run with the keyword "freq". A spectral visualization can also be created through the vibrations toolbar by selecting "Show Spectra...".



Create Surfaces...

"Create Surfaces..." allows you to view the Van der Waals, Electrostatic Potential, Electron Density, and Molecular Orbital Surfaces. The surface type options for viewing depend on what type of calculations have previously been run on the molecule. The type of file you open/create allows for more or less surface viewing options (generally discussed under Avogadro Extensions--Plugins). This feature also allows you to edit the color, resolution, and iso value to further enhance your surface.



Molecular Mechanics & Force Fields

Avogadro comes equipped with multiple different force fields. Below is general information regarding the force fields to help you select the best optimization method.

UFF

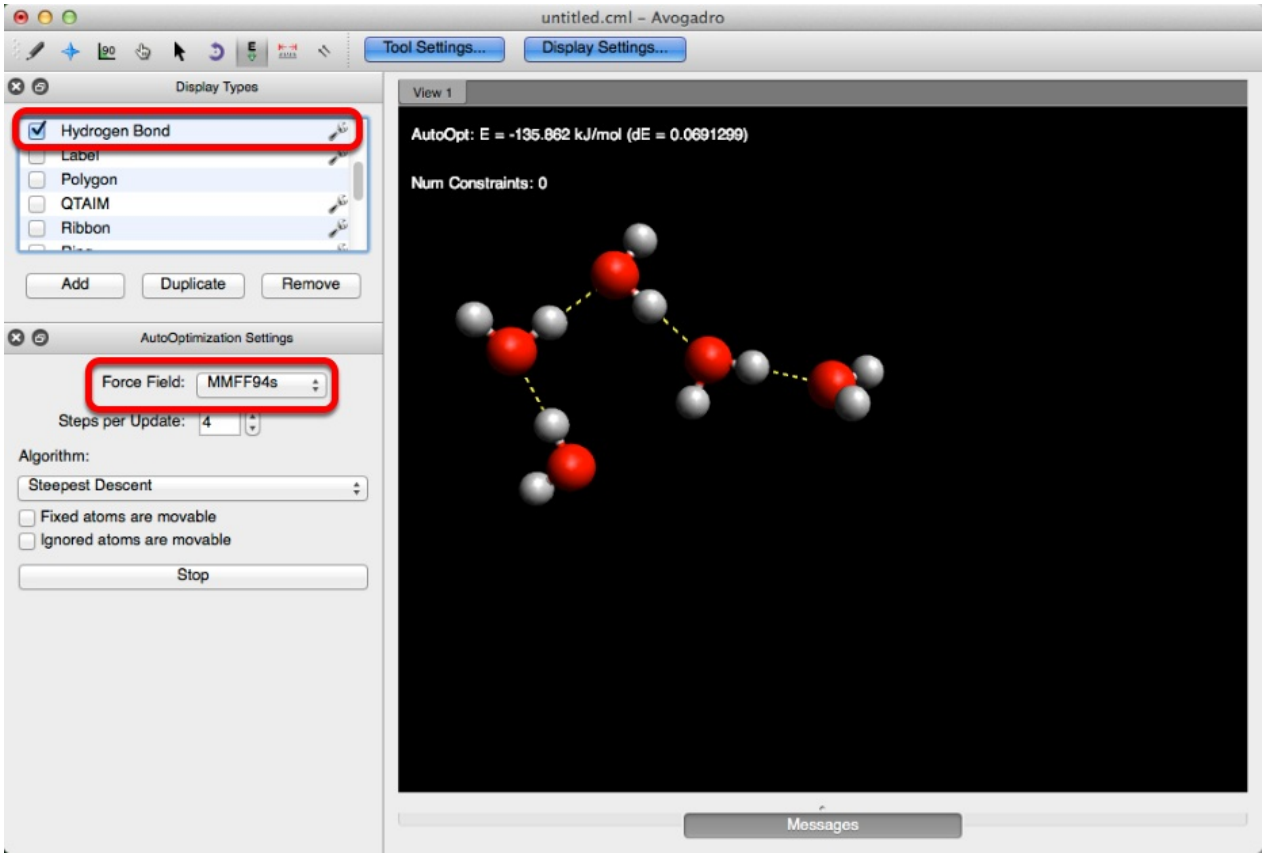
UFF (Universal Force Field) is capable of reproducing the most structural feature across the periodic table. This force field can optimize the geometry for all elements, and does well with inorganic materials, and organometallic materials.

MMFF94(s)

MMFF94 & MMFF94s (designed by Merck), is particularly good with organic compounds. MMFF94 has specifically been parameterized for alkanes, alkenes, alcohols, phenols, ethers, aldehydes, ketones, ketals, acetals, hemiketals, hemiacetals, amines, amides, peptide analogs, ureas, imides, carboxylic acids, esters, carboxylate anions, ammonium cations, thiols, mercaptans, disulfides, halides (chlorides and fluorides), imines, iminium cations, amine N-oxides, hydroxylamines, hydroxamic acids, amidines, guanidines, amidinium cations, guanidinium cations, imidazolium cations, aromatic hydrocarbons, and heteroaromatic compounds.

MMFF94 and MMFF94s use the same functional form to calculate the potential energy. They only differ in the Torsion and Out-Of-Plane bending parameters used. The 's' in MMFF94s stands for static and this set of parameters is more suited for tasks where the output is static.

These force fields also add electrostatic charges, and hydrogen bonds (displayed below).



GAFF

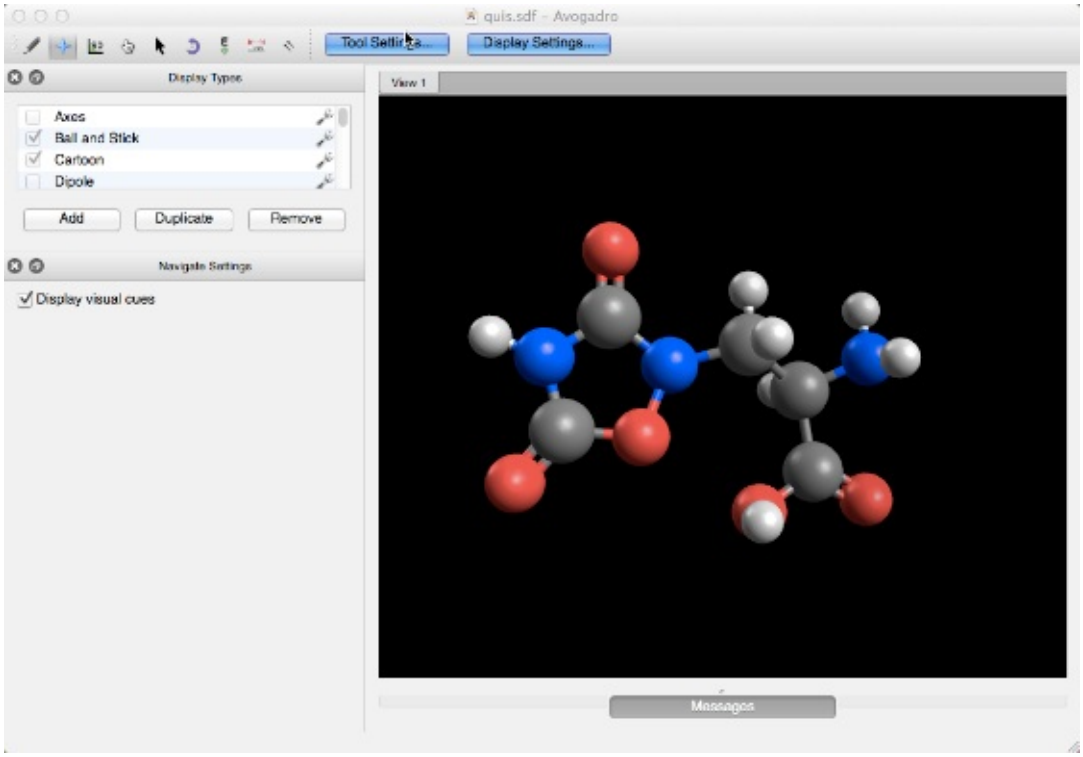
GAFF (General AMBER Force Field) is often used for optimizing the geometries of drugs. AMBER (Assisted Model Building with Energy Refinement) is a common protein force field.

GAFF has specifically been parameterized for organic molecules made of C, N, O, H, S, P, F, Cl, Br, and I.

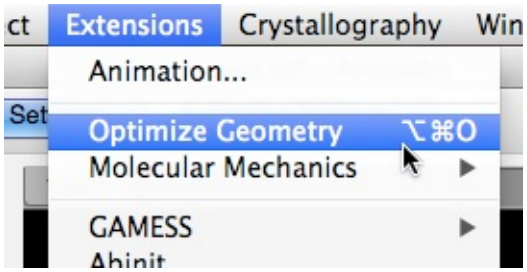
Conformers

How to search for low-energy conformations

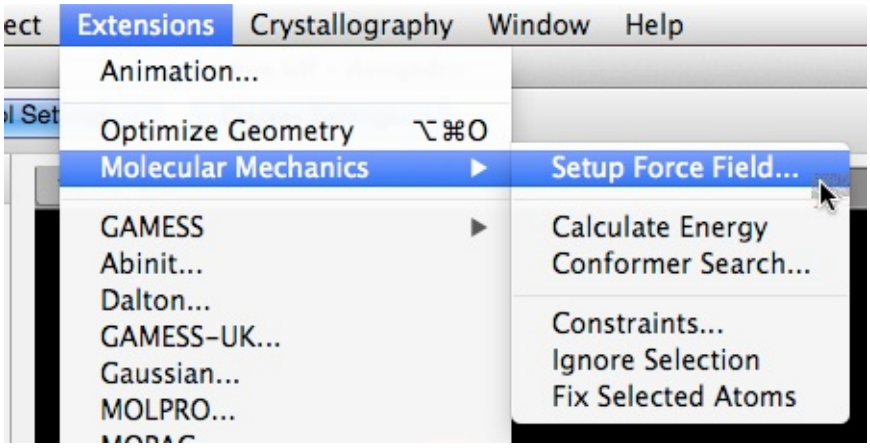
Start with your molecule of interest



Optimize the geometry

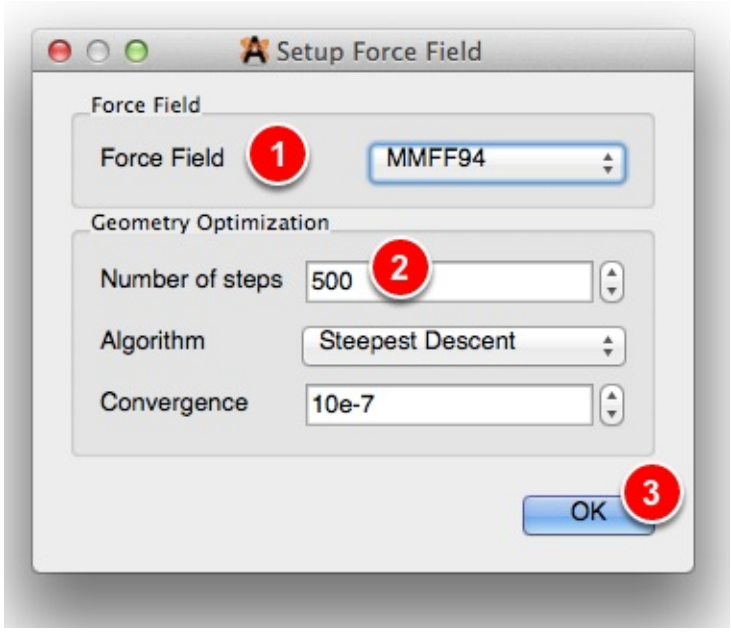


Before finding a low-energy conformer, we should make sure the current geometry is at least a near-optimal geometry. Perform an "Optimize Geometry" for a quick clean-up.



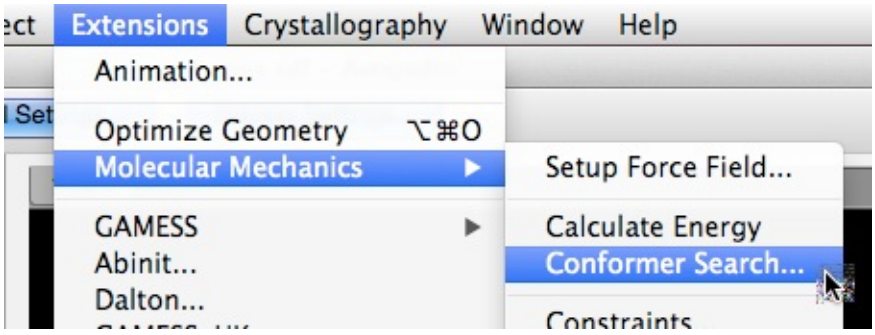
Now we will want to change the force field and/or the number of optimization steps.

Change the force field options

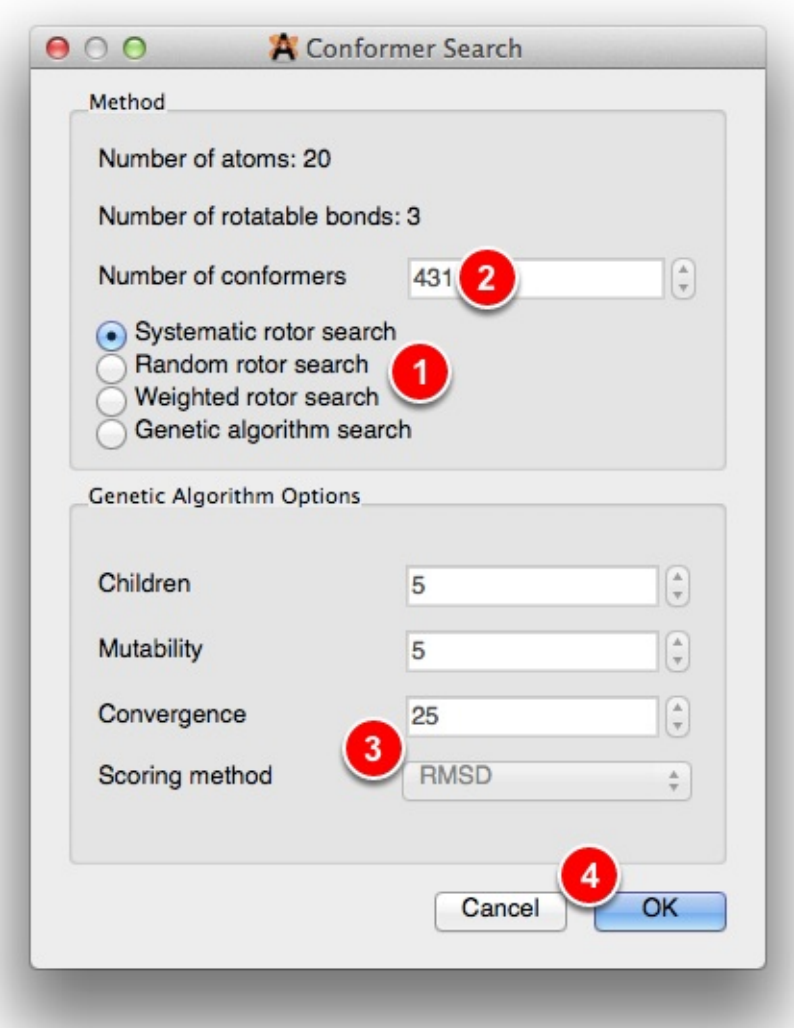


You may want to change the force field used. MMFF94 is a good default for organic-like molecules. If the molecule contains metals or is otherwise unusual, UFF is a better choice. Next, change the number of geometry optimization steps — for each conformer tested, it will be optimized. Switch to a small number like 20 or 50 for a quick clean-up to prevent "clashing" atoms when bonds are rotated.

Set the conformer search options



Pick a search method and start the search



1) Pick a search method. Systematic searches are exhaustive, but will always find the global minimum. A Weighted rotor search or Genetic Algorithm search are preferred. 2) If you pick a Weighted Search, set the number of conformers to test (e.g., 200). 3) If you pick the Genetic Algorithm search, set the options, including the Energy scoring method. 4) Click "OK" to start the search.

Constraints & Optimizations

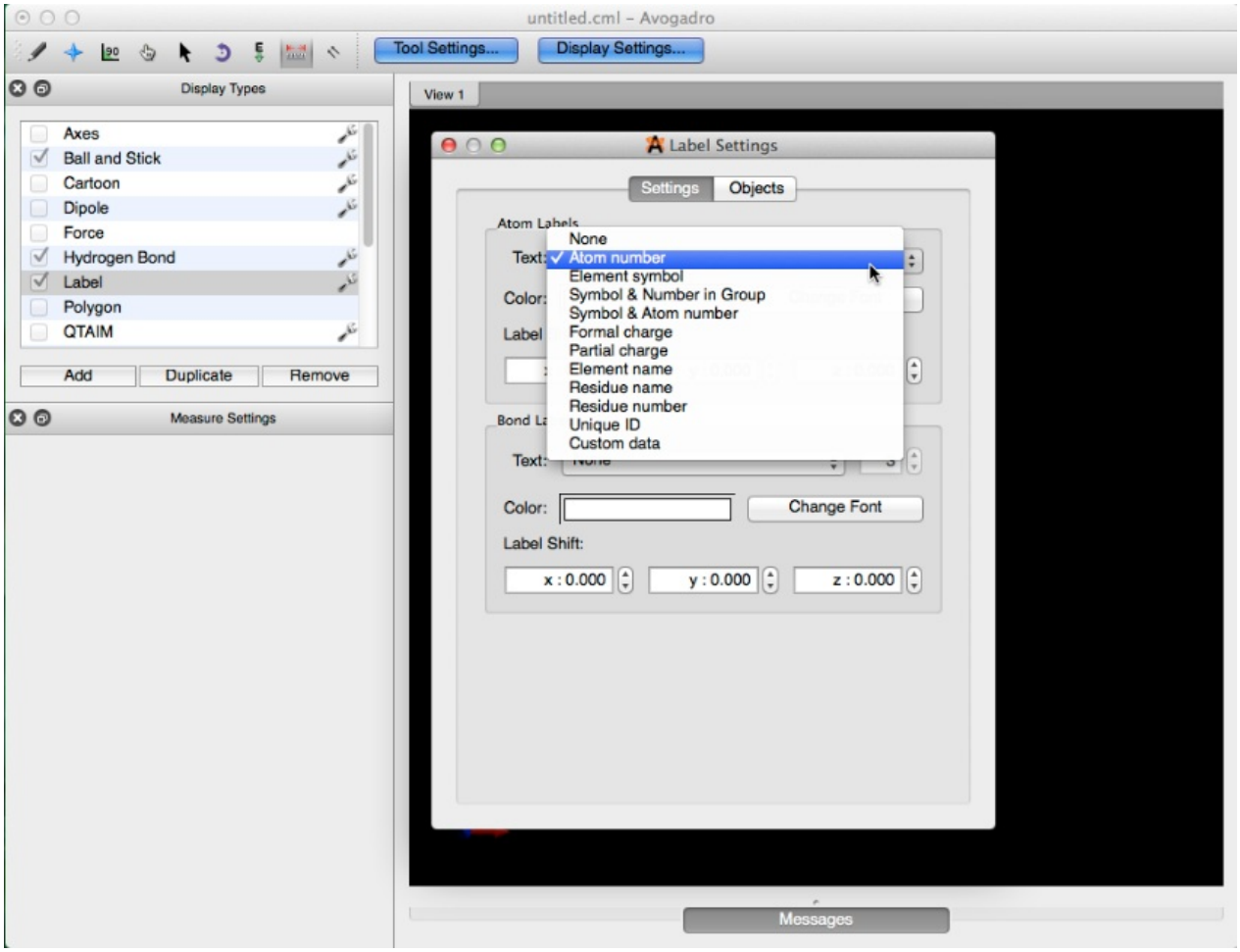
Avogadro allows for the optimization of an object, with respect to a variable(s). Below is one example of how constraints can be applied while optimizing a molecule.

Constraints

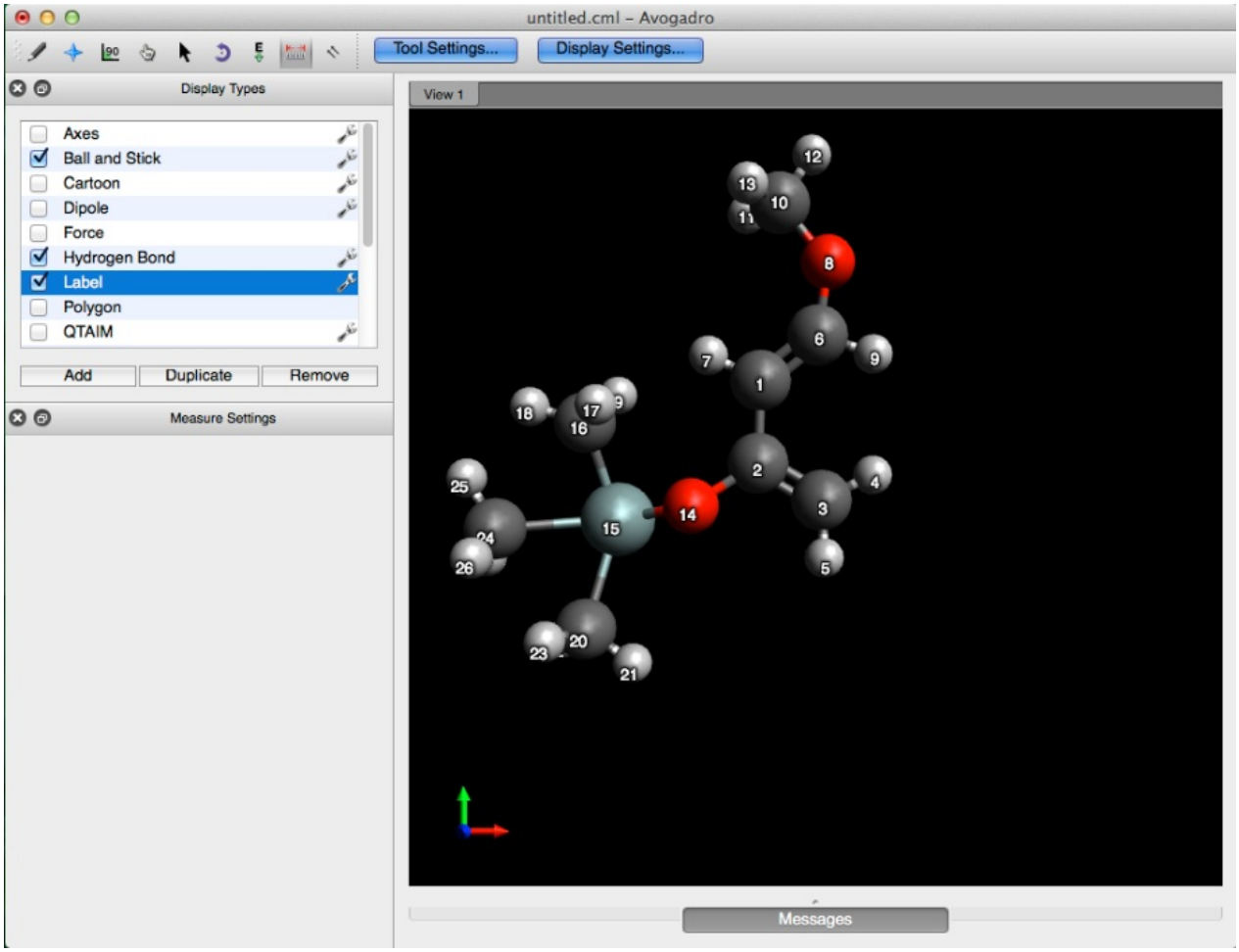
Constraints can be applied to fix or ignore a specific selection of atoms in a molecule, as well as to fix distances, and angles. For additional information review the "Auto-Optimization Tool" and "The Extensions Menu" sections of this manual.

Example

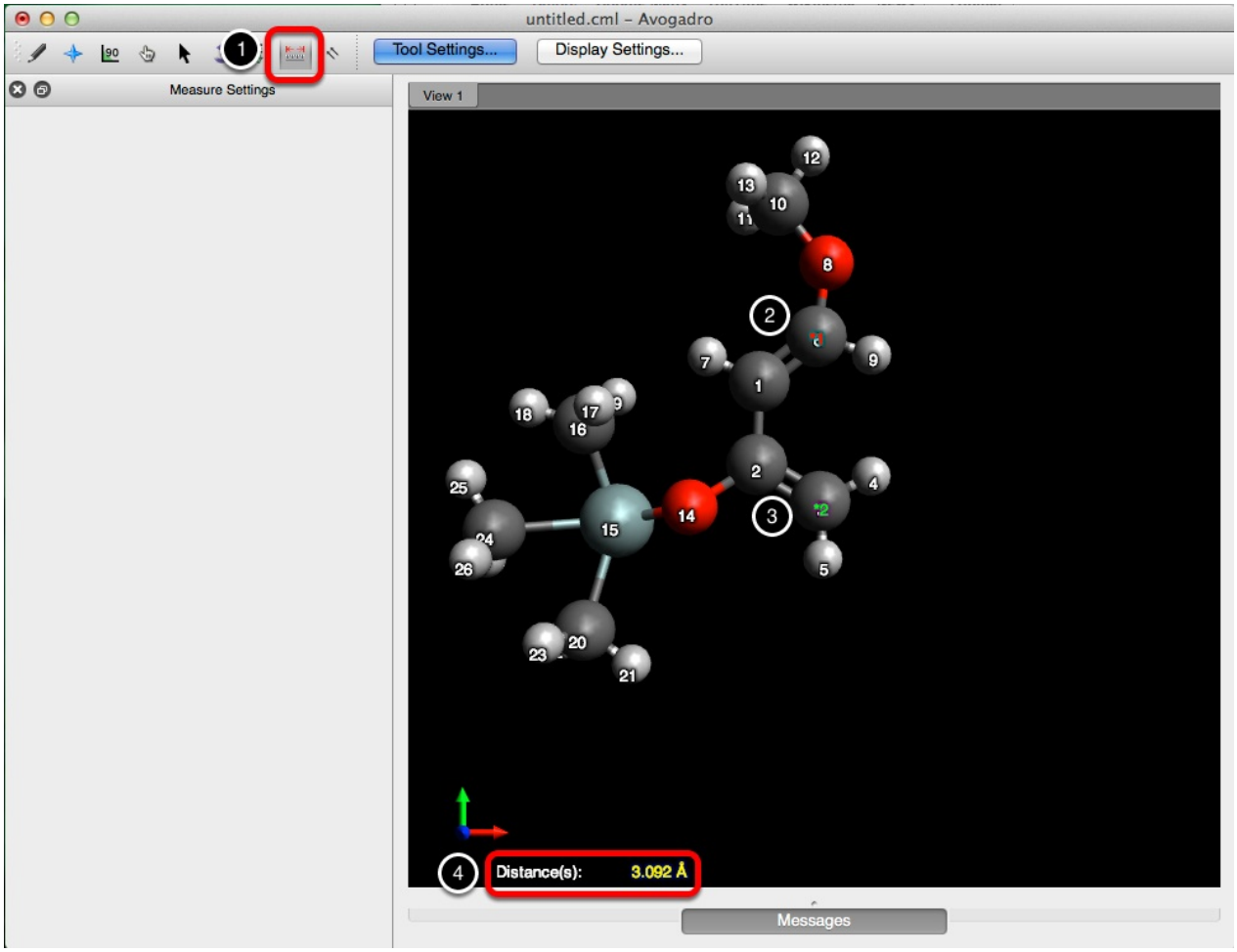
Let's say we have a diene, that we want to fix in a cisoid conformation before optimizing the geometry of the rest of the molecule (example shown below). After drawing your molecule, check the label display type, and click the wrench to the right of the name. Select the "Atom number" label form and close the dialog box.



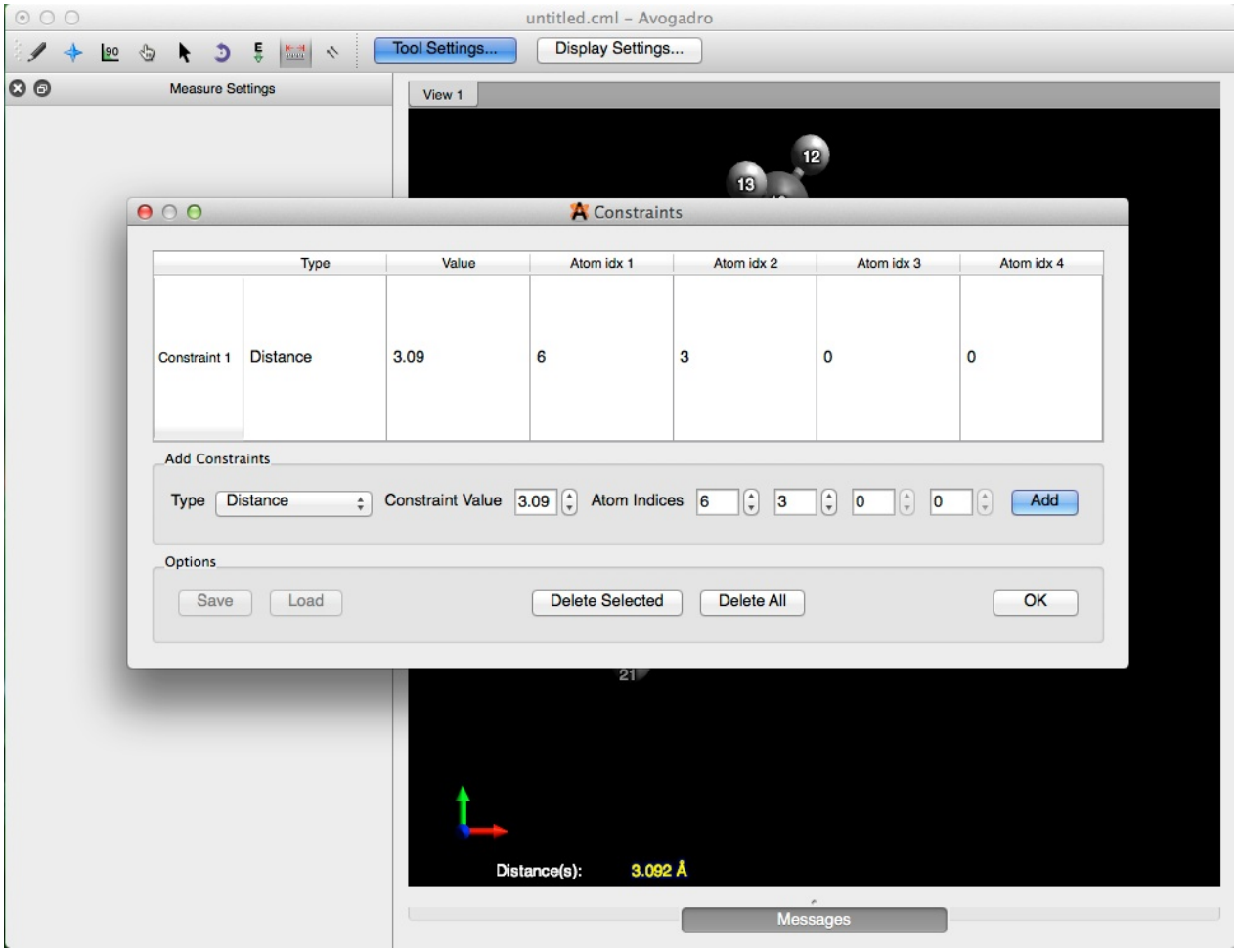
This will label all of the atom indices.



Before we can apply the constraint, we'll need to figure out the distance between atom 3 & 6. Following the procedure displayed below, select the measure tool, and then choose the two atoms that you want to apply a constraint to. This will output a distance in angstroms at the bottom of the screen.



From here go to the "Extensions" menu, and under "Molecular Mechanics", select "Constraints...". Then choose "Distance", as the type of constraint, enter in the length (3.092 Å), and the atom indices. Select "Add", and then click "OK", to add the constraint and close the dialog box.

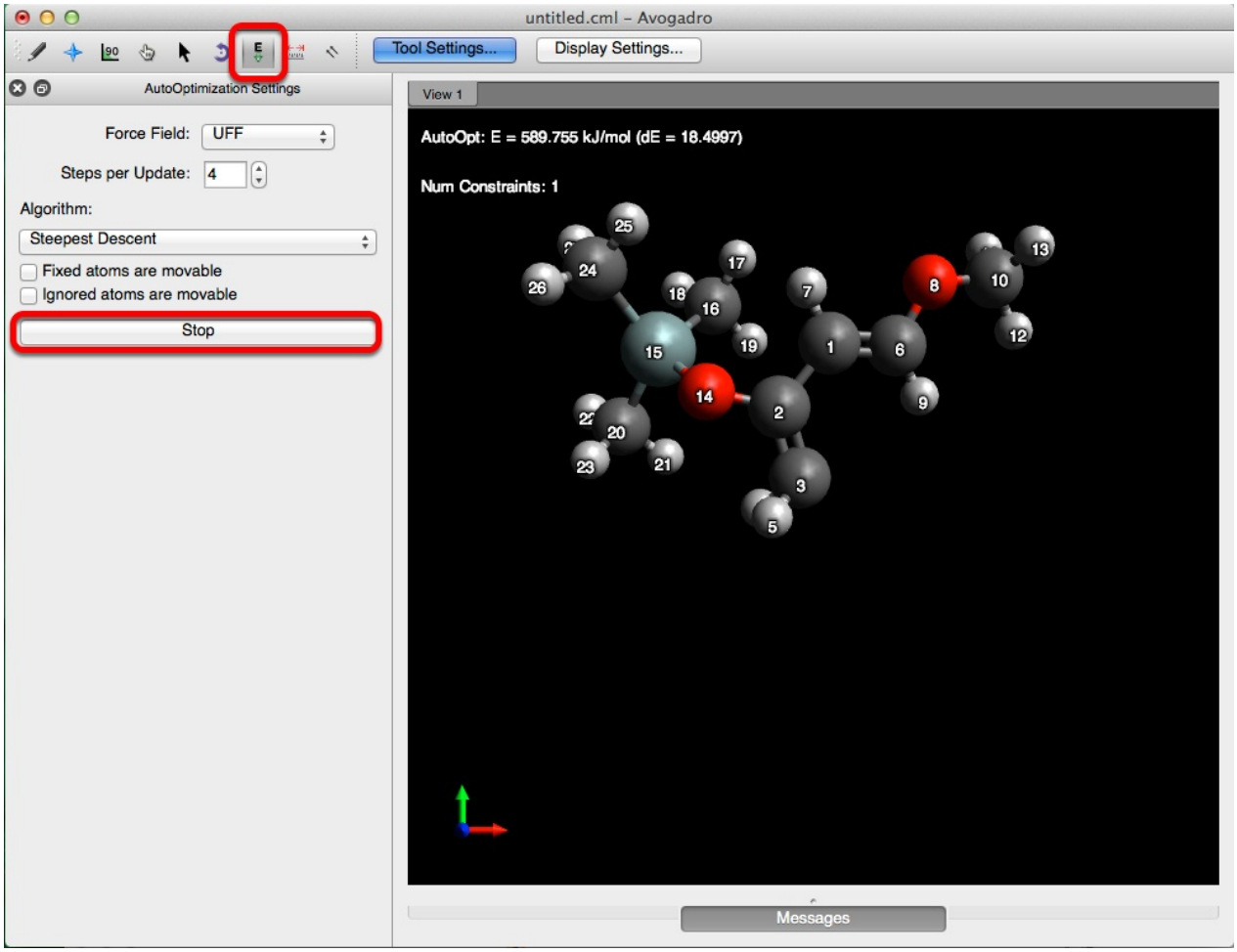


Optimizations

Optimizations can then be applied to work around the constraint. For more information about force fields refer to the "Molecular Mechanics and Force Fields" section of this manual.

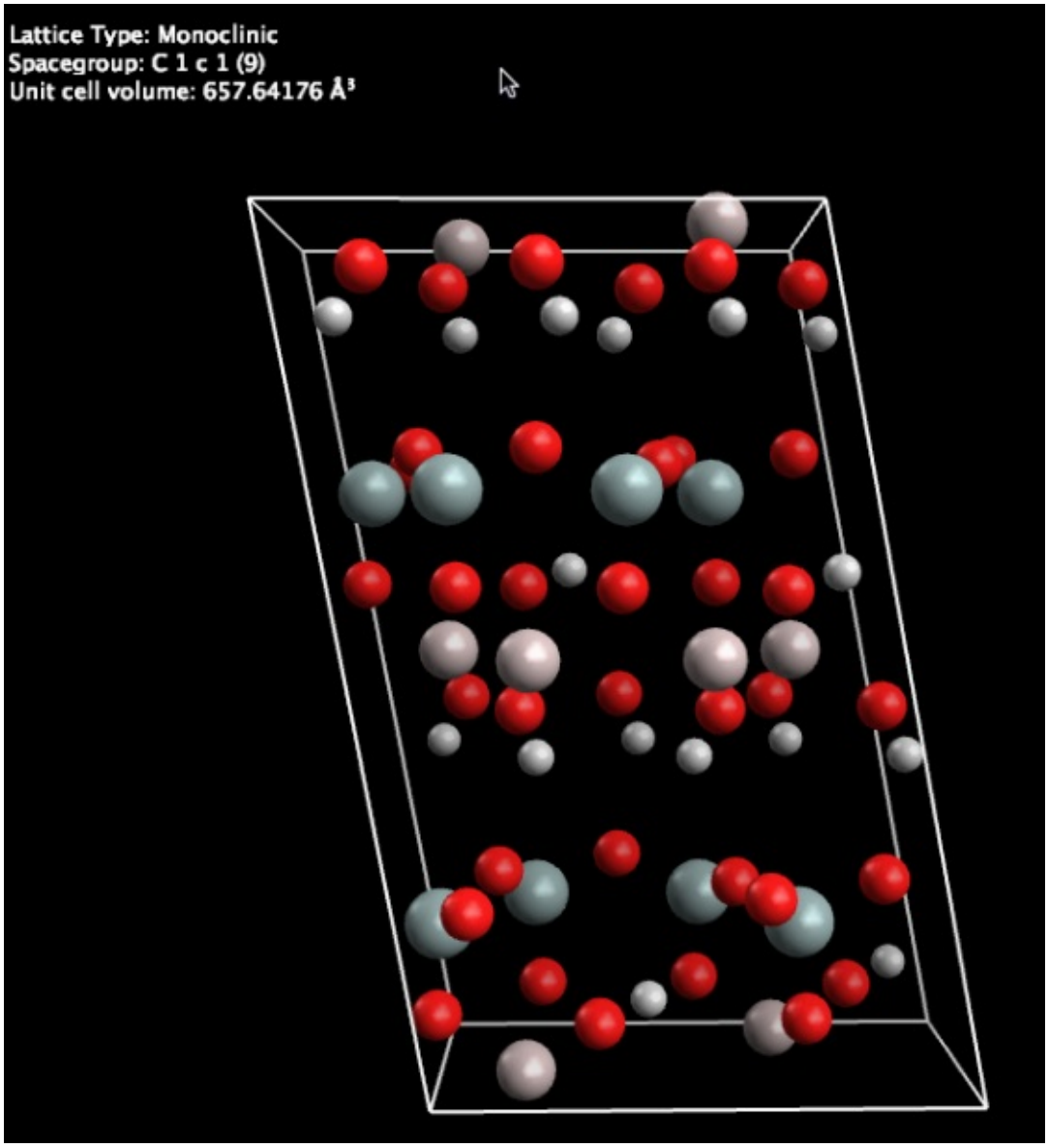
Example cont.

Now (post addition of constraint), Avogadro will selectively keep the cisoid conformation while concurrently adjusting the parameters of the other atoms in the molecule.

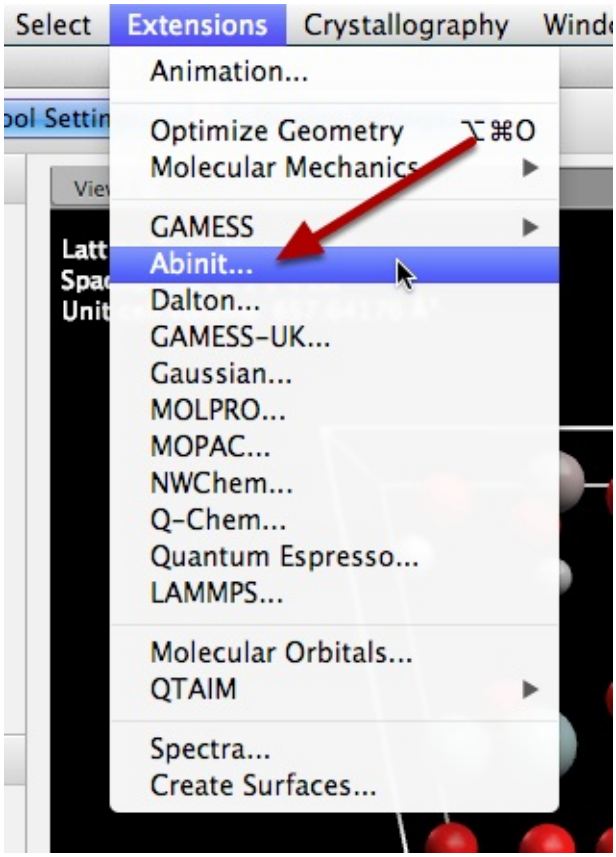

untitled.cml – Avogadro
Tool Settings...
Display Settings...
AutoOptimization Settings
Force Field:
UFF
Steps per Update:
4
Algorithm:
Steepest Descent
Fixed atoms are movable
Ignored atoms are movable
Stop
View 1
AutoOpt: E = 589.755 kJ/mol (dE = 18.4997)
Num Constraints: 1
Messages

ABINIT Generator

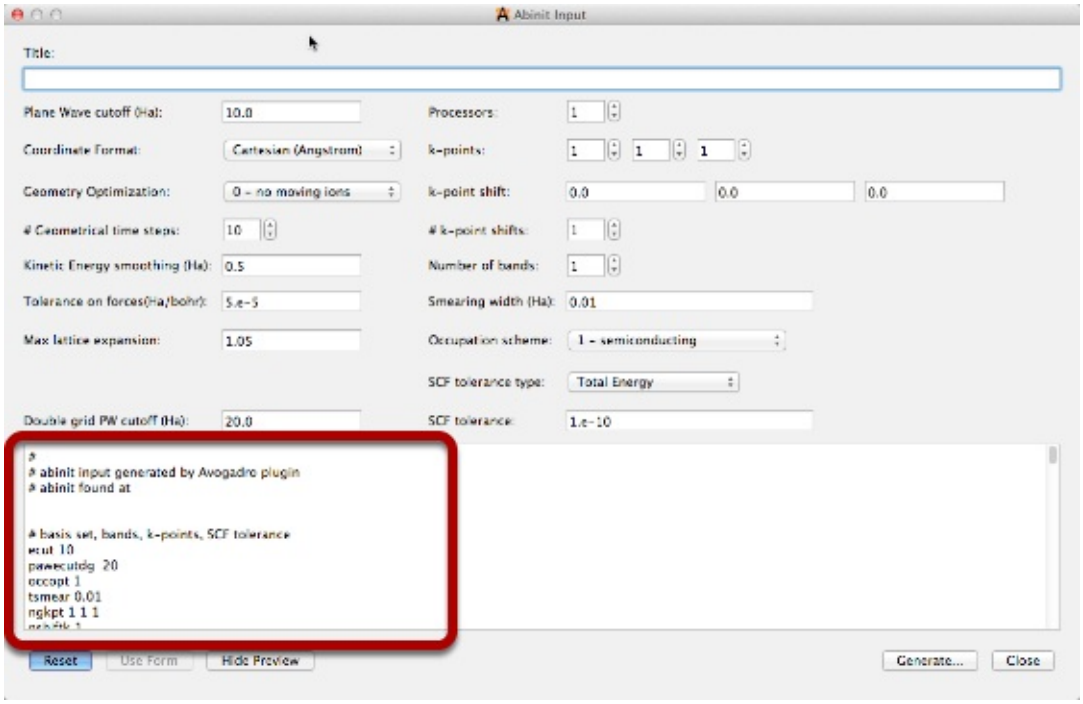
Avogadro has a new interface to the open source solid-state code ABINIT, provided by one of the ABINIT developers, Prof. Matthieu Verstraete



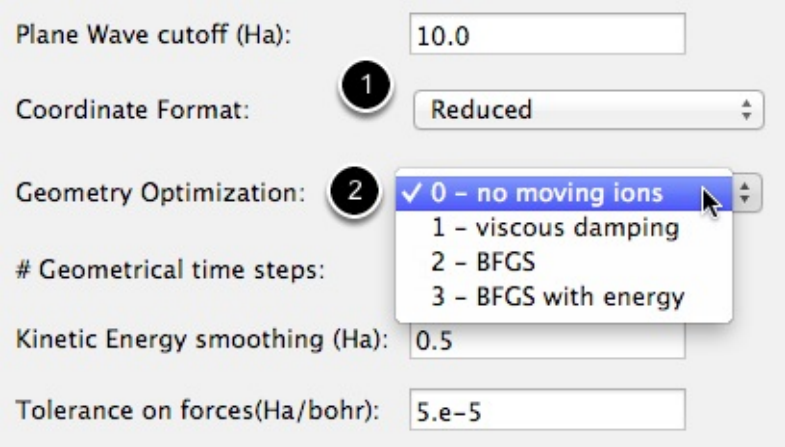
Start with a crystal structure — here a clay mineral from the new Avogadro crystal library.



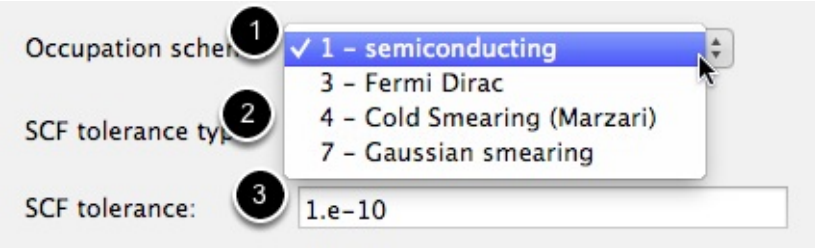
Open up the Abinit input generator under the Extensions menu



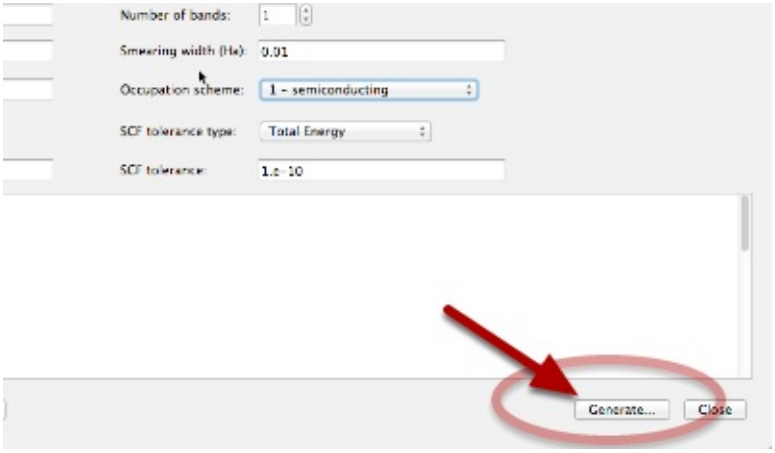
Most common options for Abinit are available here, with a text preview (highlighted in red) generated as you change options above.



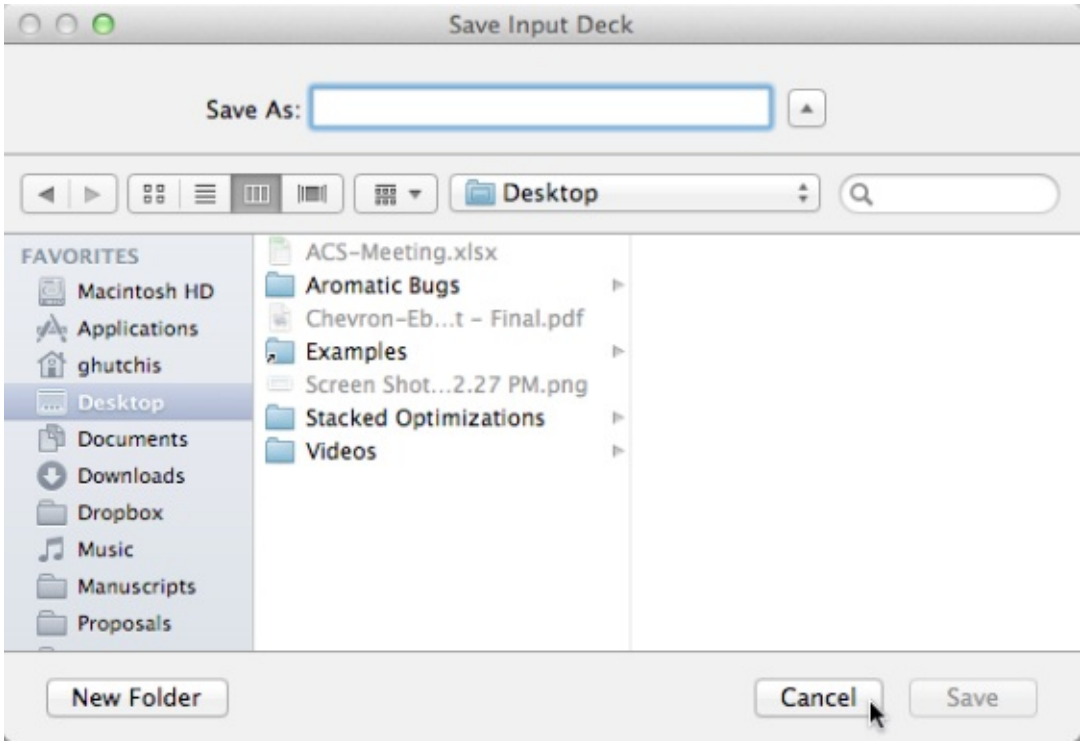
The input generator allows you to (1) pick the type of coordinates: real-space Cartesians or reduced coordinates and (2) pick the type of geometry optimization (if any).



Another important option is setting the occupation scheme (1) and SCF options (2) and (3).



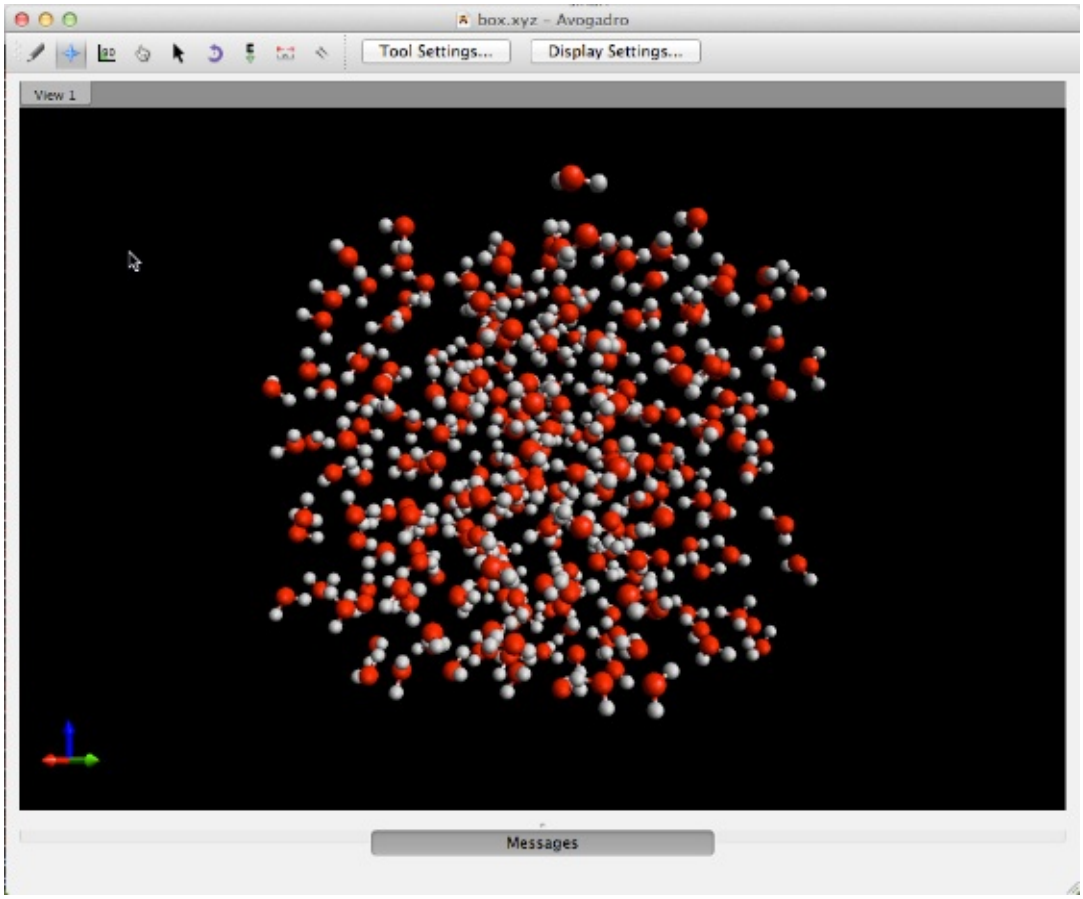
Finally, when finished, you can click the “Compute” button (not pictured) if Abinit is available locally on your computer, or “Generate” to save the input file for submission to a remote queue.



Save the input file and you‘re finished!

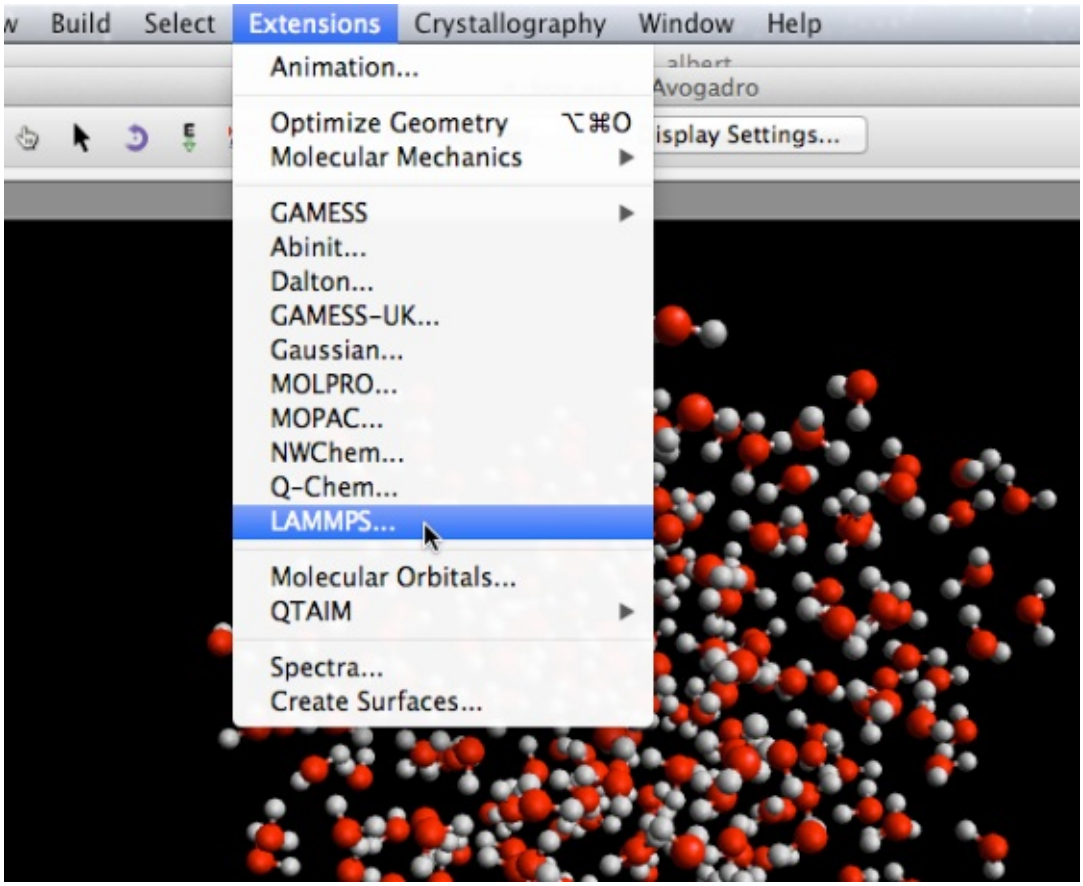
LAMMPS input for water

Prepare initial geometry

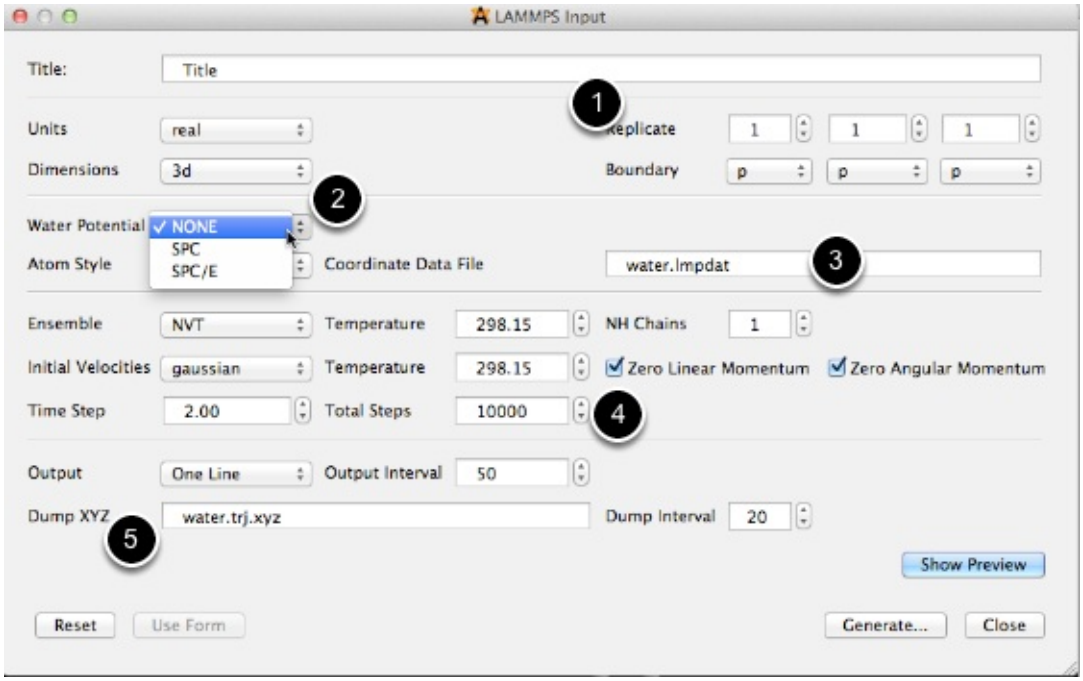


The independently developed Packmol extension can be used to generate a box of water molecules.

Open the LAMMPS input dialog

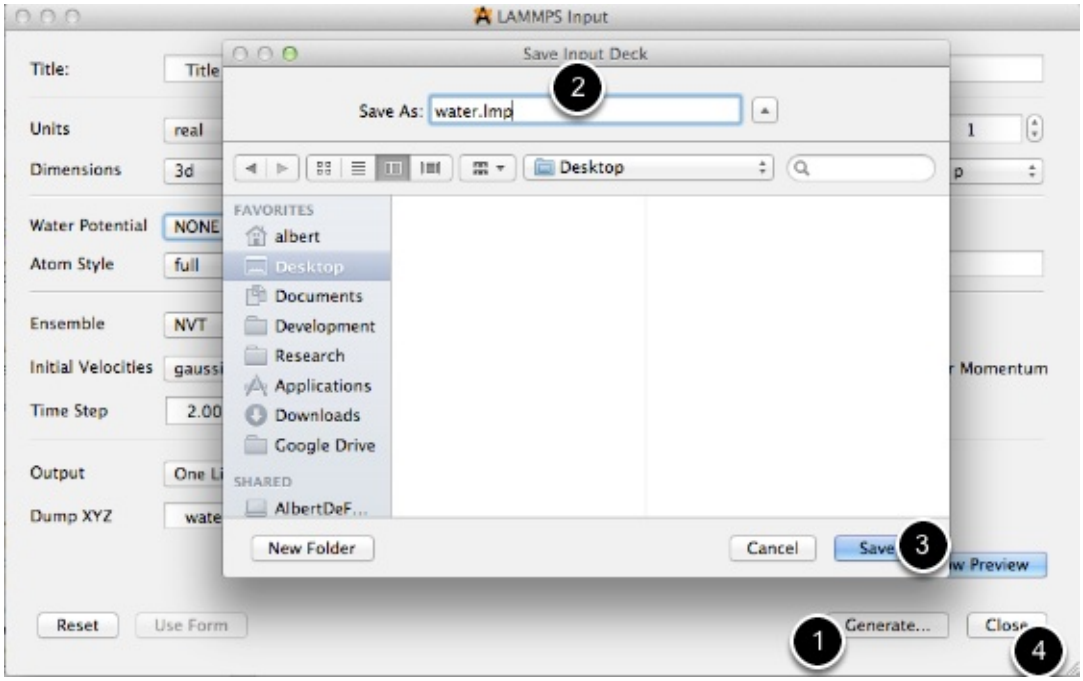


Prepare simulation parameters



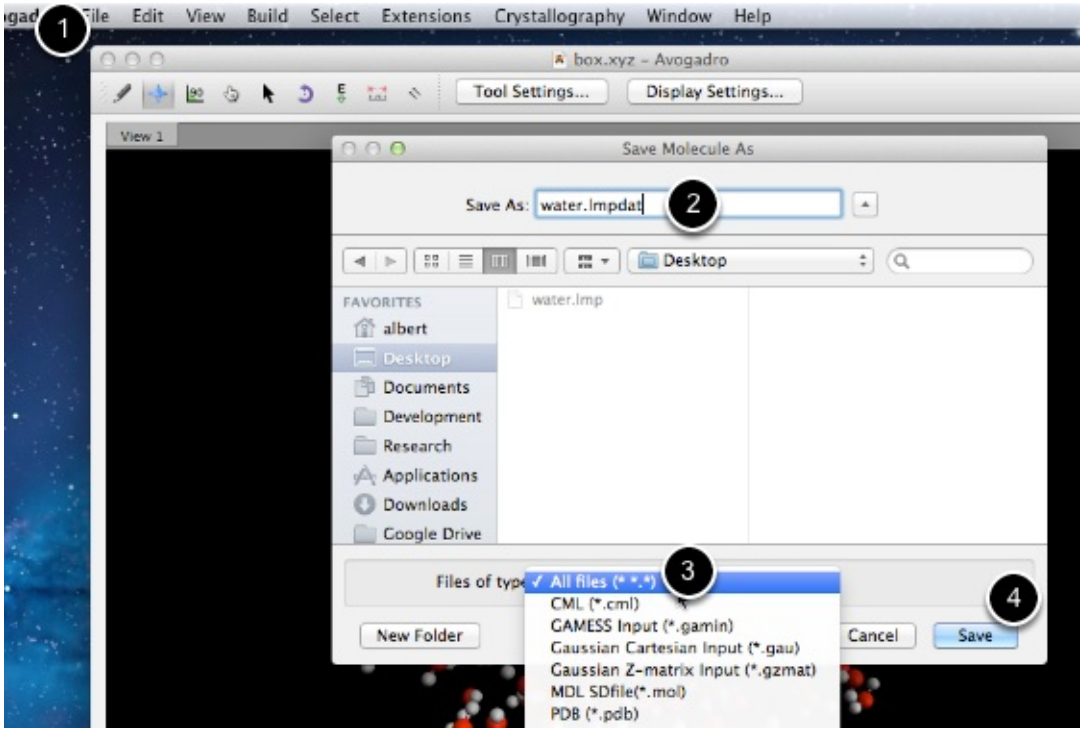
1. Choose the number of repeating units of the input coordintes in x, y and z directions
2. Choose the water potential. The current version supports SPC and SPC/E model potentials
3. Choose the name of LAMMPS formatted coordinates. The name will be used in a later step when the lmpdat file is created.
4. Choose the total number of MD steps.
5. Choose the file name of the XYZ formatted trajectory file.

Generate the LAMMPS parameters file



1. Click the Generate button
2. Choose a file name
3. Click save
4. Close the input generator dialog

Generate the LAMMPS Coordintes file



1. Select "Save As" from the file menu
2. Input the "water.lmpdat" file name from above
3. Select "All files"

4. Save the LAMMPS formatted coordinates file

Run LAMMPS

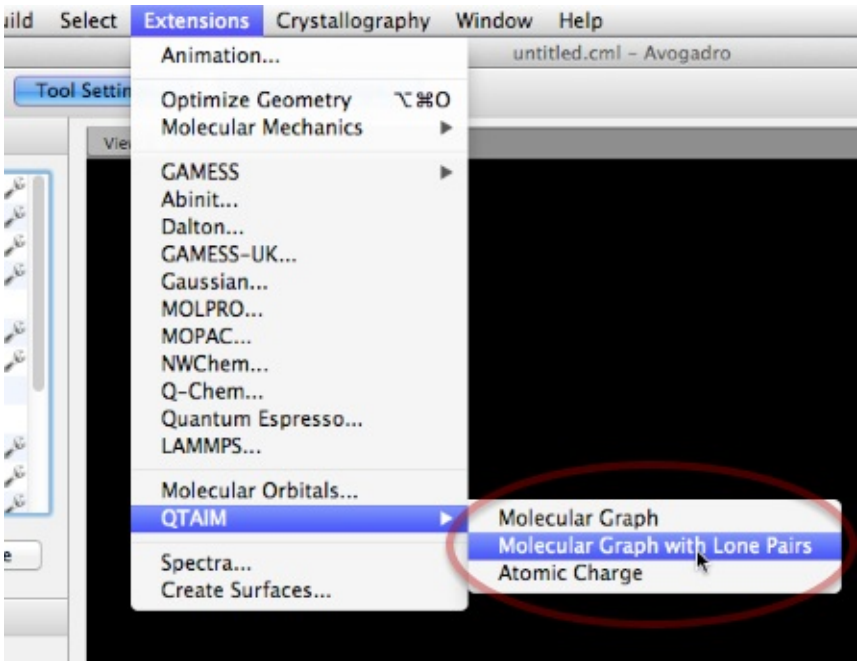
```
defusco@n4:Desktop>prun lmp_frank -c off < water.lmp
LAMMPS (25 Aug 2011)
Scanning data file ...
  2 = max bonds/atom
  1 = max angles/atom
Reading data file ...
  orthogonal box = (-10.501 -10.501 -10.501) to (10.5 10.5 10.5)

/
Truncated output
/

Step Temp E_pair E_mol TotEng Press
       0       298.15    25987.138            0    29782.897    158468.54
      50    270.80586   -18093.836            0   -14646.196   -1479.8204
     100    64.114374   -19915.375            0   -19099.132    -5390.092
     150    34.332422   -20991.539            0   -20554.451   -5729.3733
     200    35.213471   -20829.561            0   -20381.257   -5465.2238
     250    66.305262   -21542.975            0    -20698.84   -5071.9898
     300     195.9811   -22687.472            0   -20192.428    -3658.543
     350    597.99741   -23002.204            0   -15389.075    2351.6753
     400    598.67277    -16633.12            0   -9011.3935    3834.1146

/
Truncated output
/

    2700    296.25023   -16768.726            0   -12997.152   -2454.0595
    2750    303.27482   -21843.699            0   -17982.695    -3540.924
    2800    308.02588   -19563.062            0   -15641.572   -3368.5525
    2850    300.04115    -20470.31            0   -16650.474   -3832.0168
    2900    298.40475   -24216.521            0   -20417.518   -5042.3837
    2950    289.84633   -26874.461            0   -23184.416   -5638.2768
    3000    293.04234   -24533.617            0   -20802.883   -5090.3882
    3050    293.32283   -19844.799            0   -16110.494   -3470.8129

/
Truncated output
/
```

After 2700 time steps, the temperature is begining to stabilize.

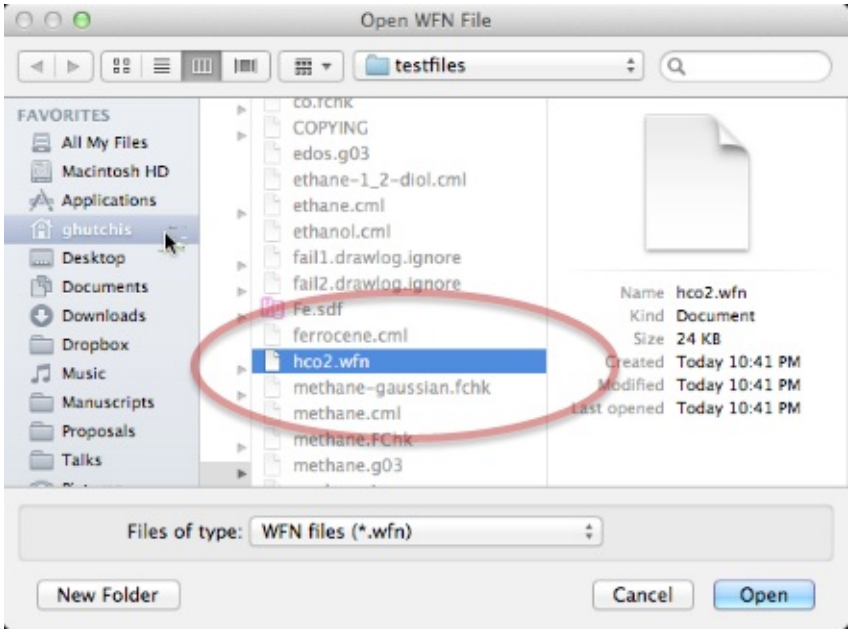
Using Atoms-In-Molecules (Bader) Analysis: QTAIM and WFN

Avogadro now includes support for the QTAIM analysis developed by Prof. Richard Bader and his group. This technique allows Avogadro to determine bond connections and bond orders directly from the quantum mechanical electron density.

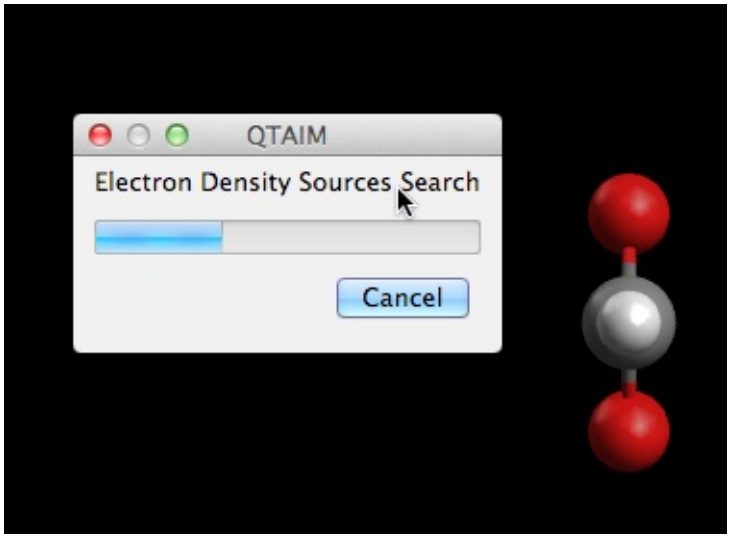
Start with a WFN File



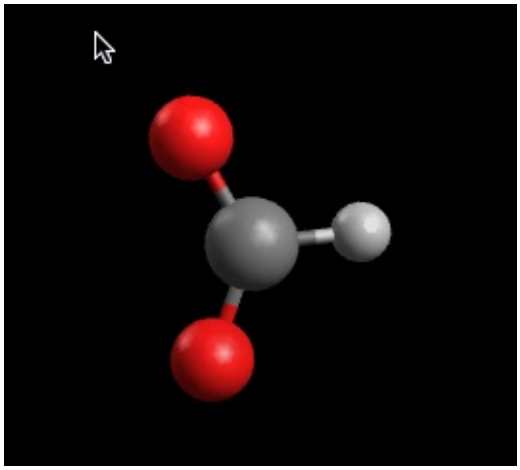
Most quantum chemistry software allows creating a WFN format file from the output of a calculation. We can read this file in through the QTAIM Extension for visualization and analysis. In the future, other formats will also be supported, including deriving the data directly from checkpoint files.



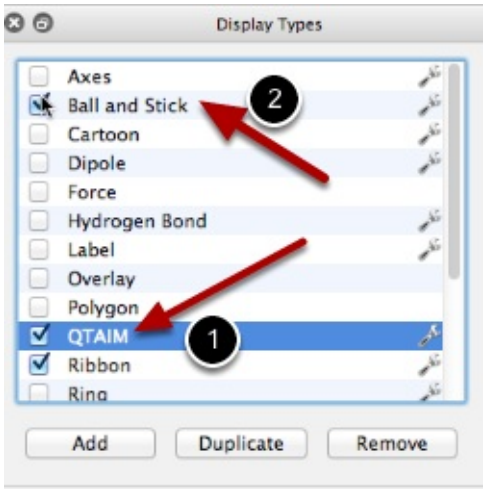
Here we've picked a WFN file of interest (HCO2) using the Molecular Graph + Lone Pairs command.



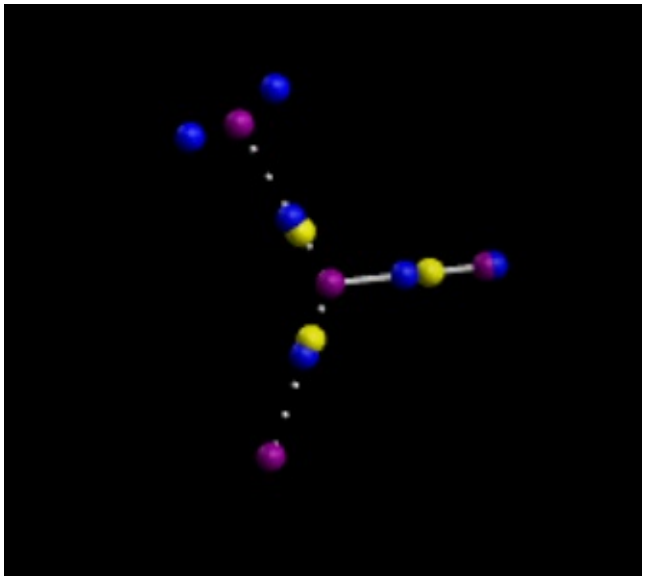
Avogadro's QTAIM support will read in the atoms, determine bonds and bond orders using AIM analysis and then continue with further analysis.



Initially, you may not see anything different. QTAIM includes a separate Display Type for viewing the results of the AIM analysis.



Here, we've enabled the QTAIM display, which will show lone pairs, bond critical points, etc. You may also want to turn off the Ball and Stick model to see all AIM annotations.

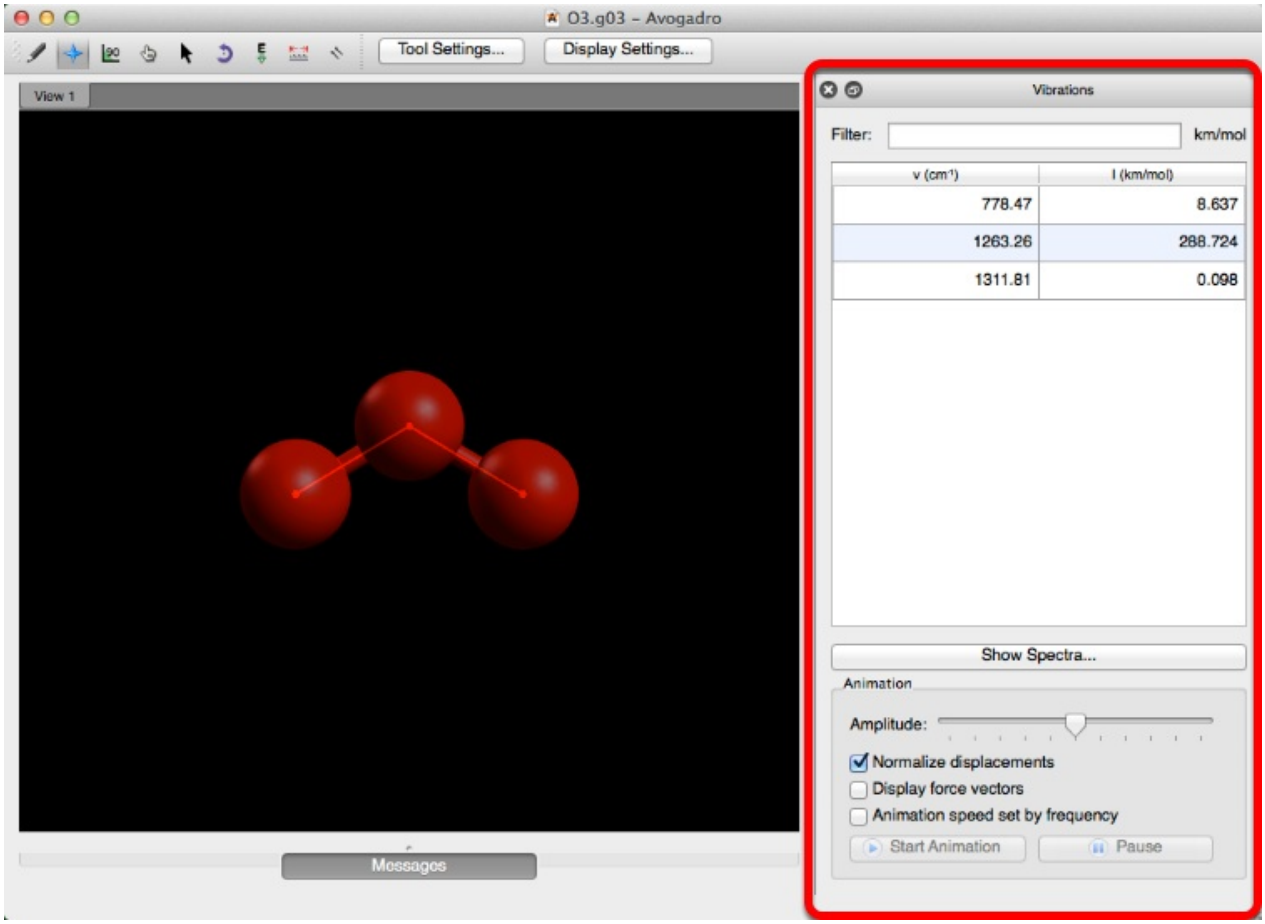


Here, we've also turned off the classical ball and stick display type to leave only the QTAIM view of HCO2.

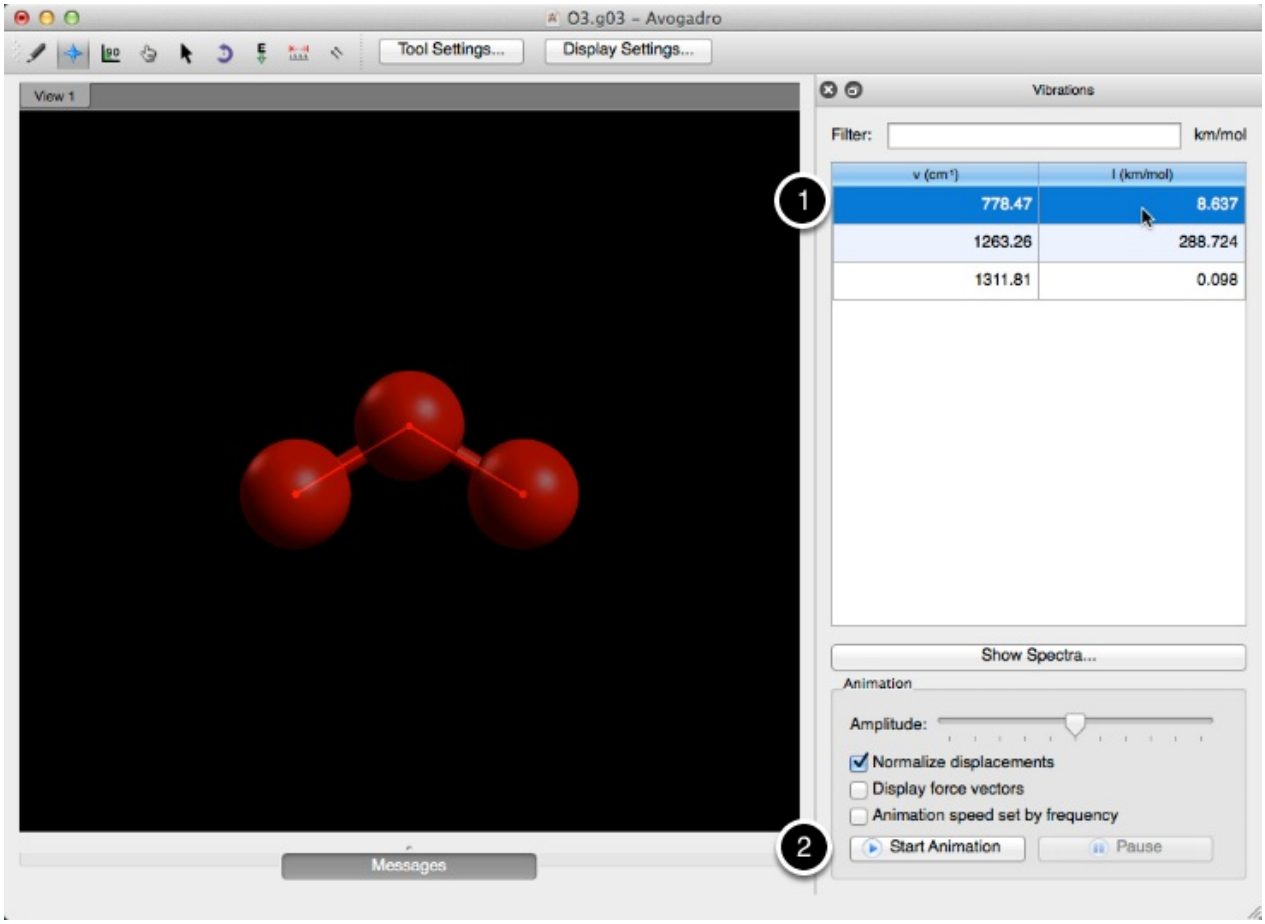
Viewing Vibrations

This feature allows visualizing vibrations from a "frequency" calculation with quantum chemistry codes (e.g., Gaussian, Q-Chem, etc.)

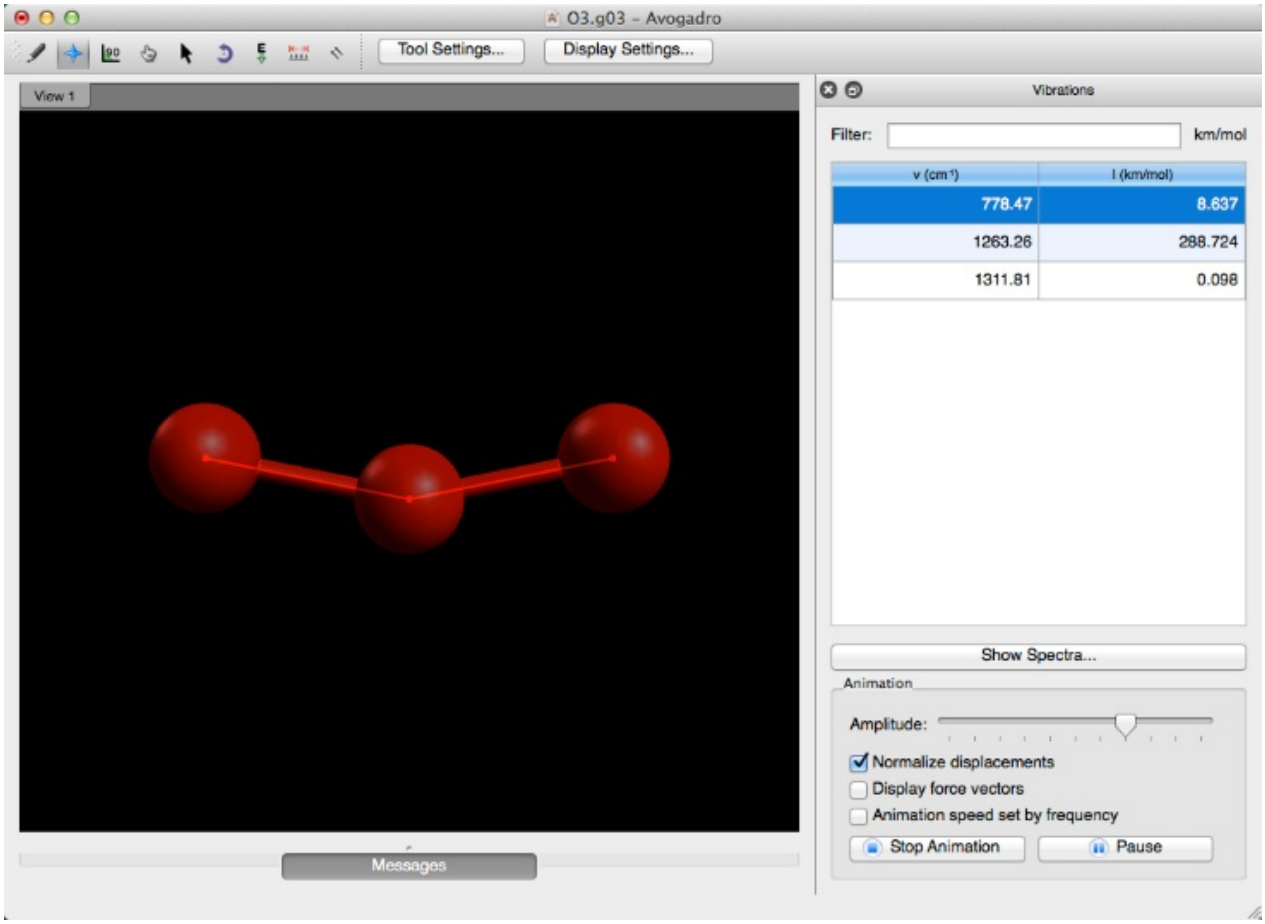
After opening an output file that has been run with the keyword "freq", the "Vibrations" toolbar will automatically open.



This toolbar allows you to view the various vibrations of a molecule. Selecting a frequency, and clicking "Start Animation" will begin a vibration.



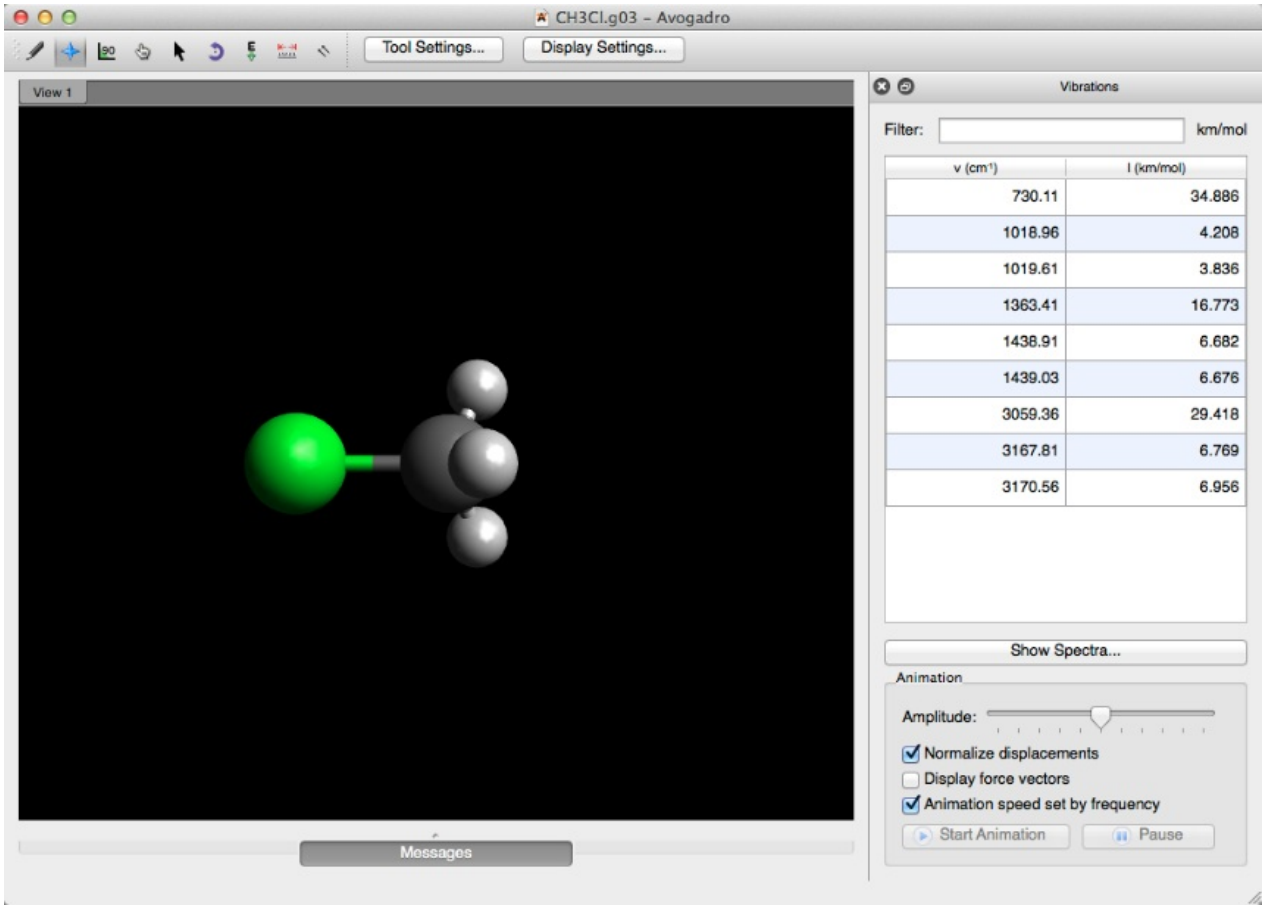
Avogadro then provides you with the ability to edit the vibration amplitude, it allows you to display the force vectors on the atoms present, and it allows you to adjust the animation speed by the frequency.


O3.g03 – Avogadro
Tool Settings...
Display Settings...
View 1
Messages
Vibrations
Filter:
km/mol
ν (cm⁻¹)
I (km/mol)
778.47
8.637
1263.26
288.724
1311.81
0.098
Show Spectra...
Animation
Amplitude:
Normalize displacements
Display force vectors
Animation speed set by frequency
Stop Animation
Pause

Viewing Spectral Properties

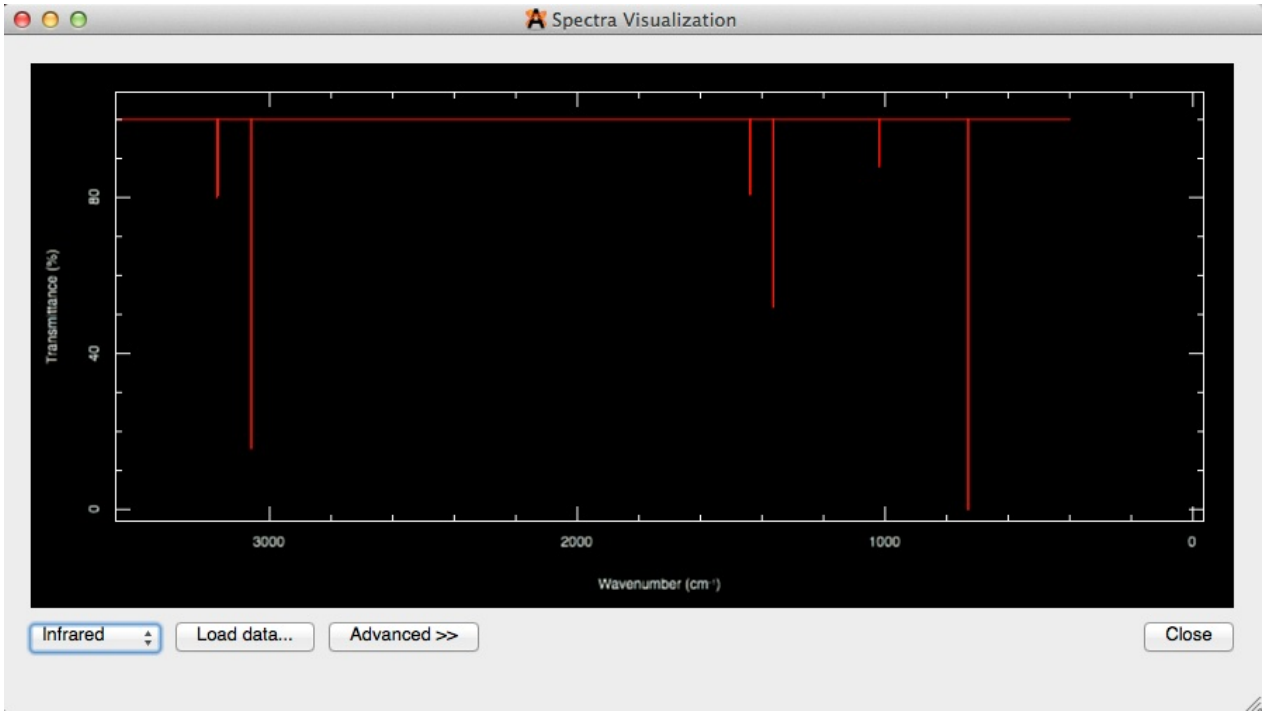
This tutorial covers plotting vibrational spectra, but other types of spectra are possible with the output files from quantum chemical programs

After opening an output file that has been run with the keyword "freq", the "Vibrations" toolbar will automatically open.

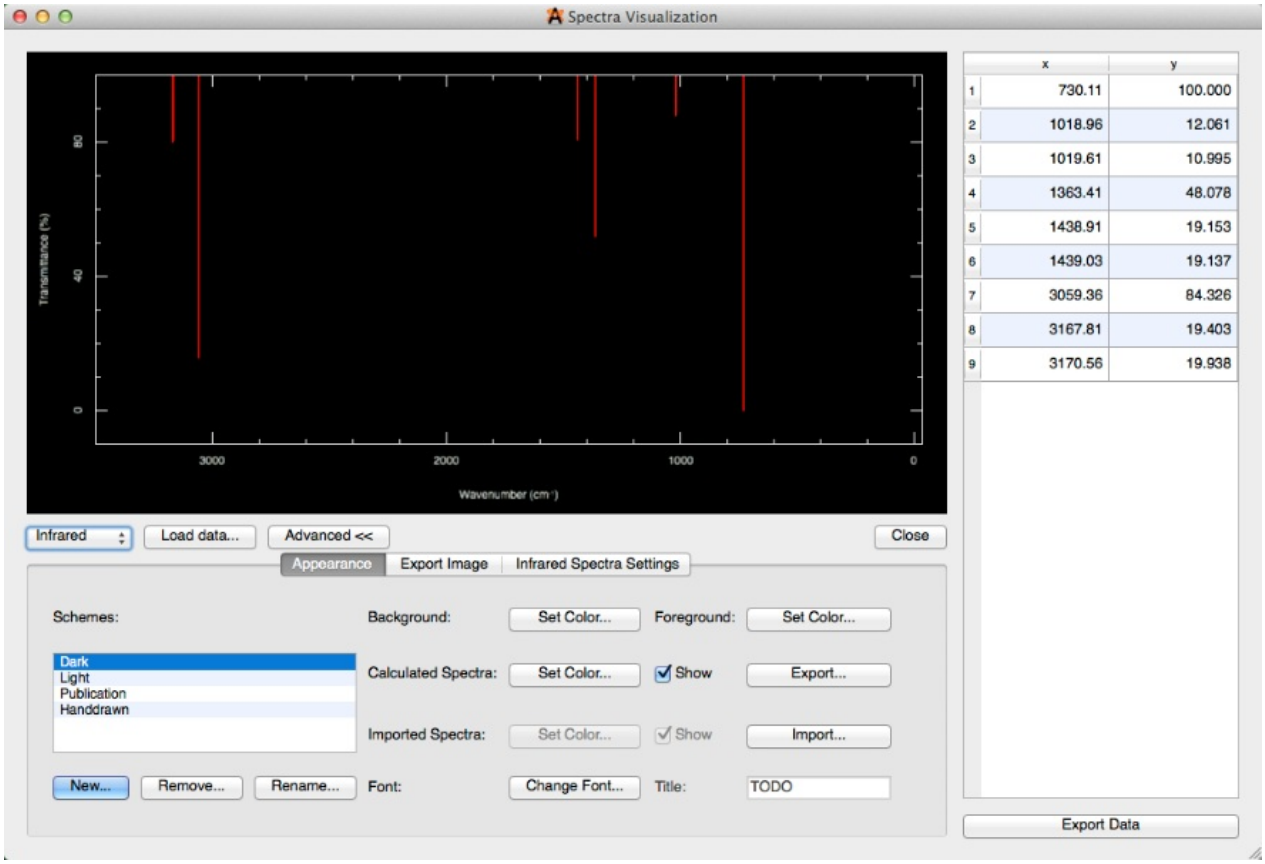


Show Spectra...

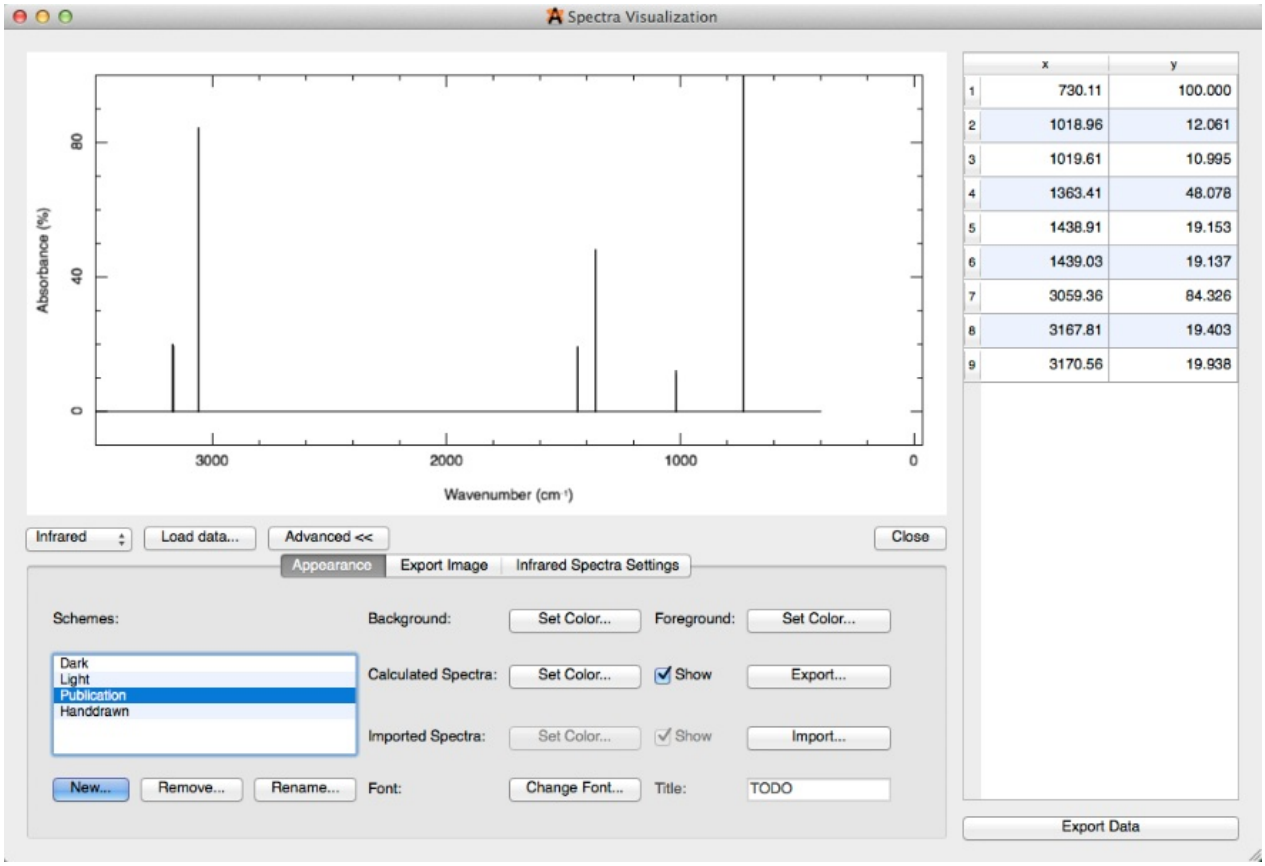
Clicking on "Show Spectra..." in the Vibrations toolbar, or selecting "Spectra..." under the "Extensions" menu will open a spectra visualization of the molecule (displayed below).



Selecting "Advanced>>" in the spectra visualization will allow you to change the visual settings, as well as the spectral settings, and export the image.



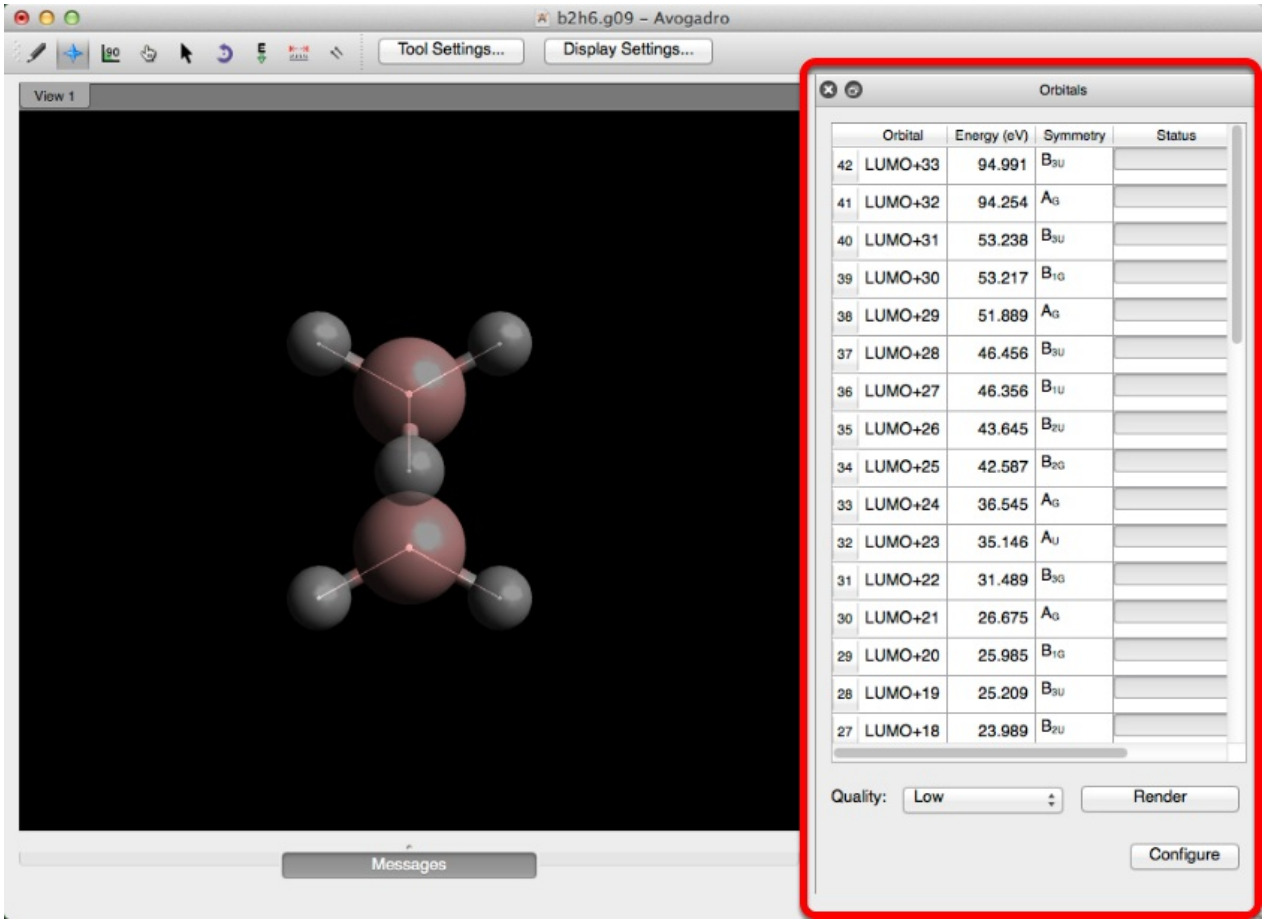
The "Advanced>>" selection provides a multitude of general edits to use at your convenience. For example, you can change % transmittance, to % absorbance (under Infrared Spectra Settings), and change the scheme from dark to publication (Appearance Settings).


Spectra Visualization
Absorbance (%)
80
40
0
3000
2000
1000
0
Wavenumber (cm⁻¹)
Infrared
Load data...
Advanced <<
Close
Appearance
Export Image
Infrared Spectra Settings
Schemes:
Dark
Light
Publication
Handdrawn
New...
Remove...
Rename...
Background:
Set Color...
Foreground:
Set Color...
Calculated Spectra:
Set Color...
Show
Export...
Imported Spectra:
Set Color...
Show
Import...
Font:
Change Font...
Title:
TODO
x
y
1 730.11 100.000
2 1018.96 12.061
3 1019.61 10.995
4 1363.41 48.078
5 1438.91 19.153
6 1439.03 19.137
7 3059.36 84.326
8 3167.81 19.403
9 3170.56 19.938
Export Data

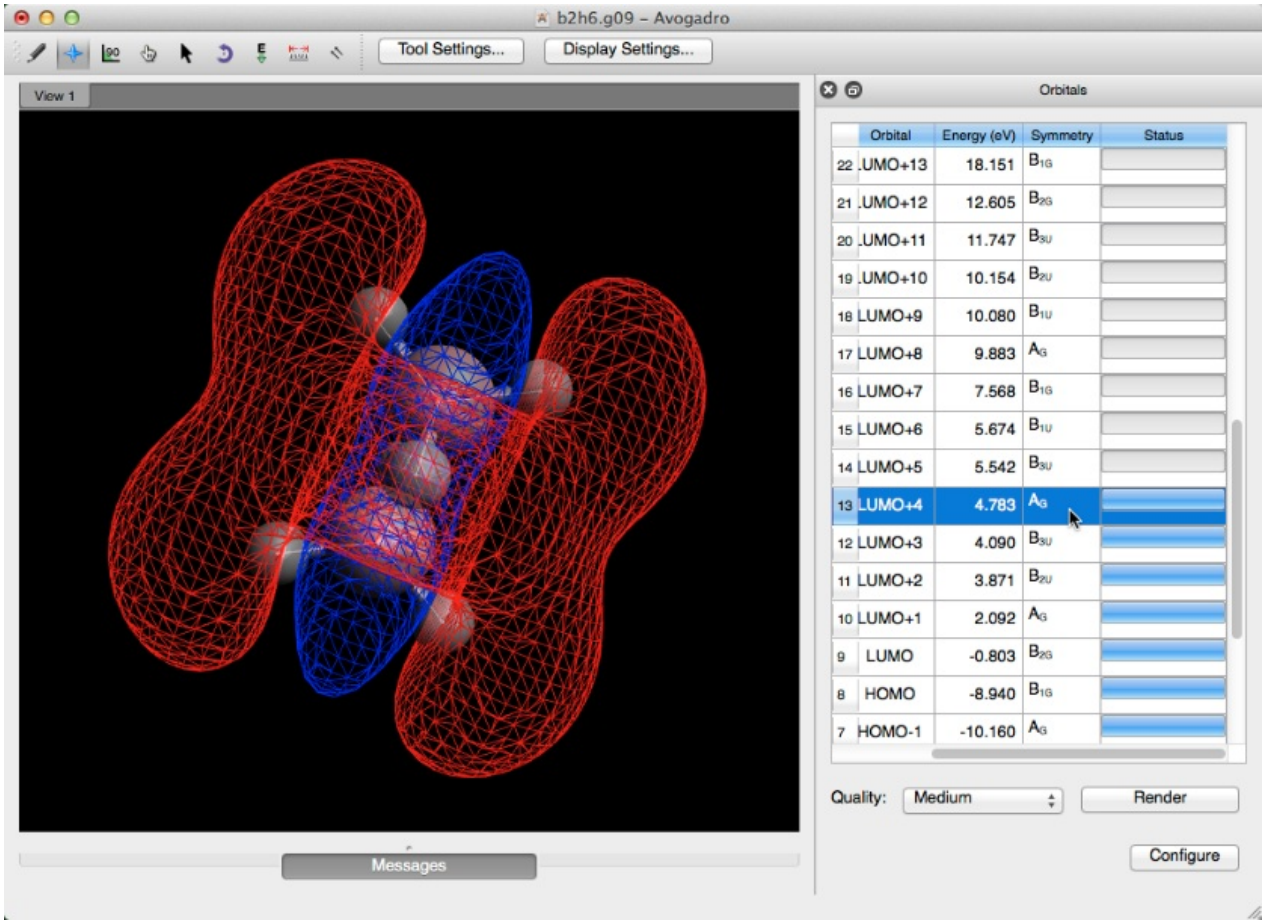
Viewing Molecular Orbitals

This feature requires a "checkpoint" or "formatted checkpoint" from quantum chemistry codes

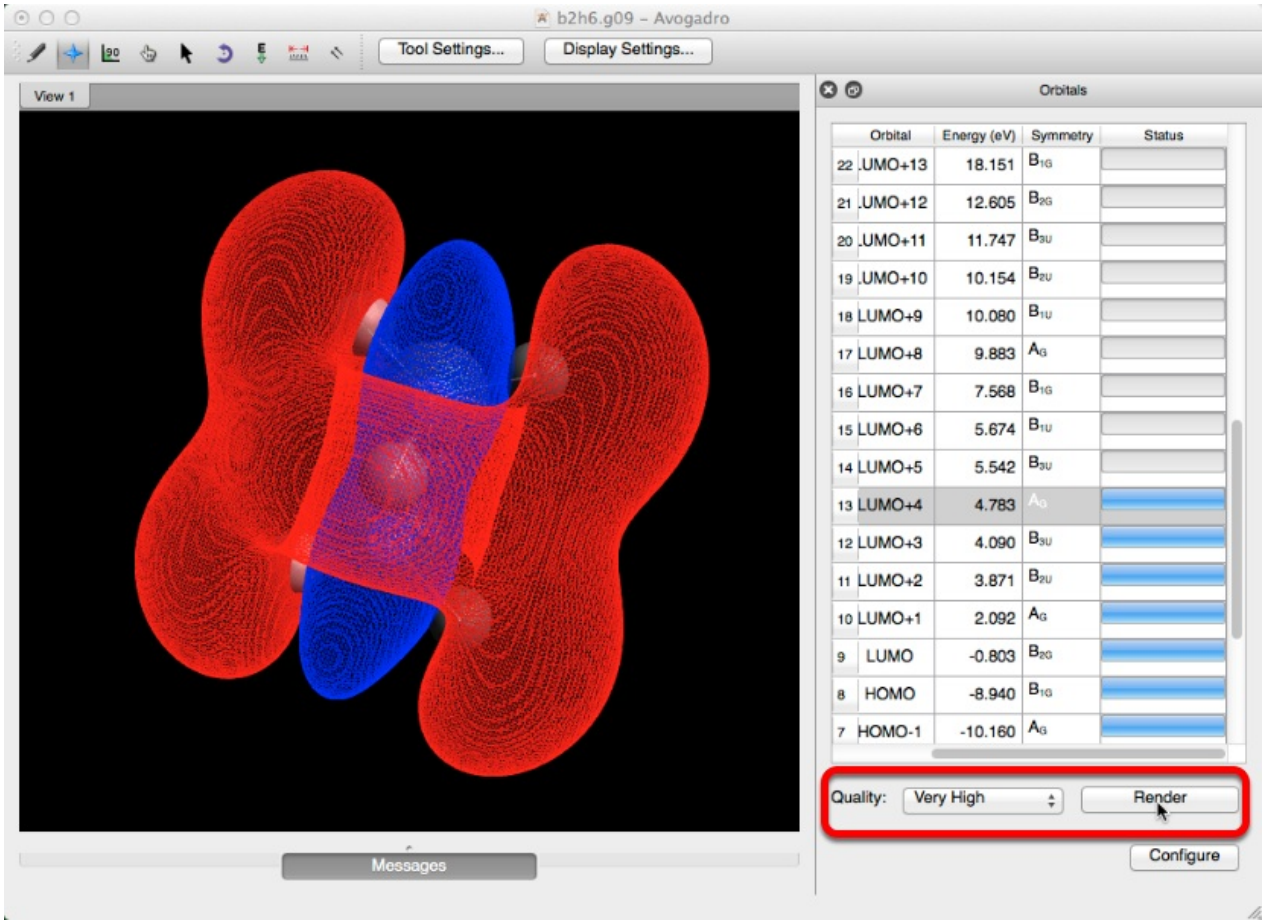
When the output file is opened, if a matching checkpoint file is found, it automatically opens the Orbitals toolbar.



All potential molecular orbitals will have full status bars (you may need to scroll down considerably to find the potential orbitals). Clicking in the row of an orbital, with a full status bar, will create a quick low quality rendition of the orbital.

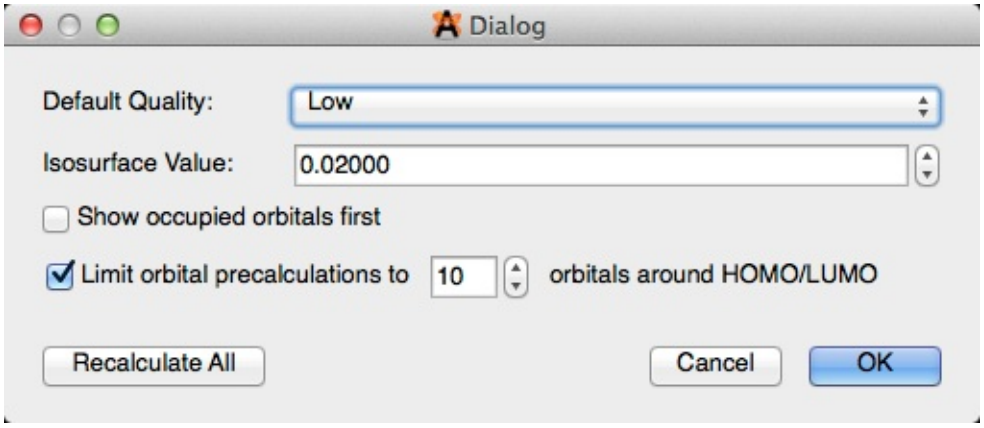


A higher orbital quality can be selected and applied if desired. This is done by selecting a new image quality from the drop down menu, and clicking "render". These renditions can take a moment to load.



Configure

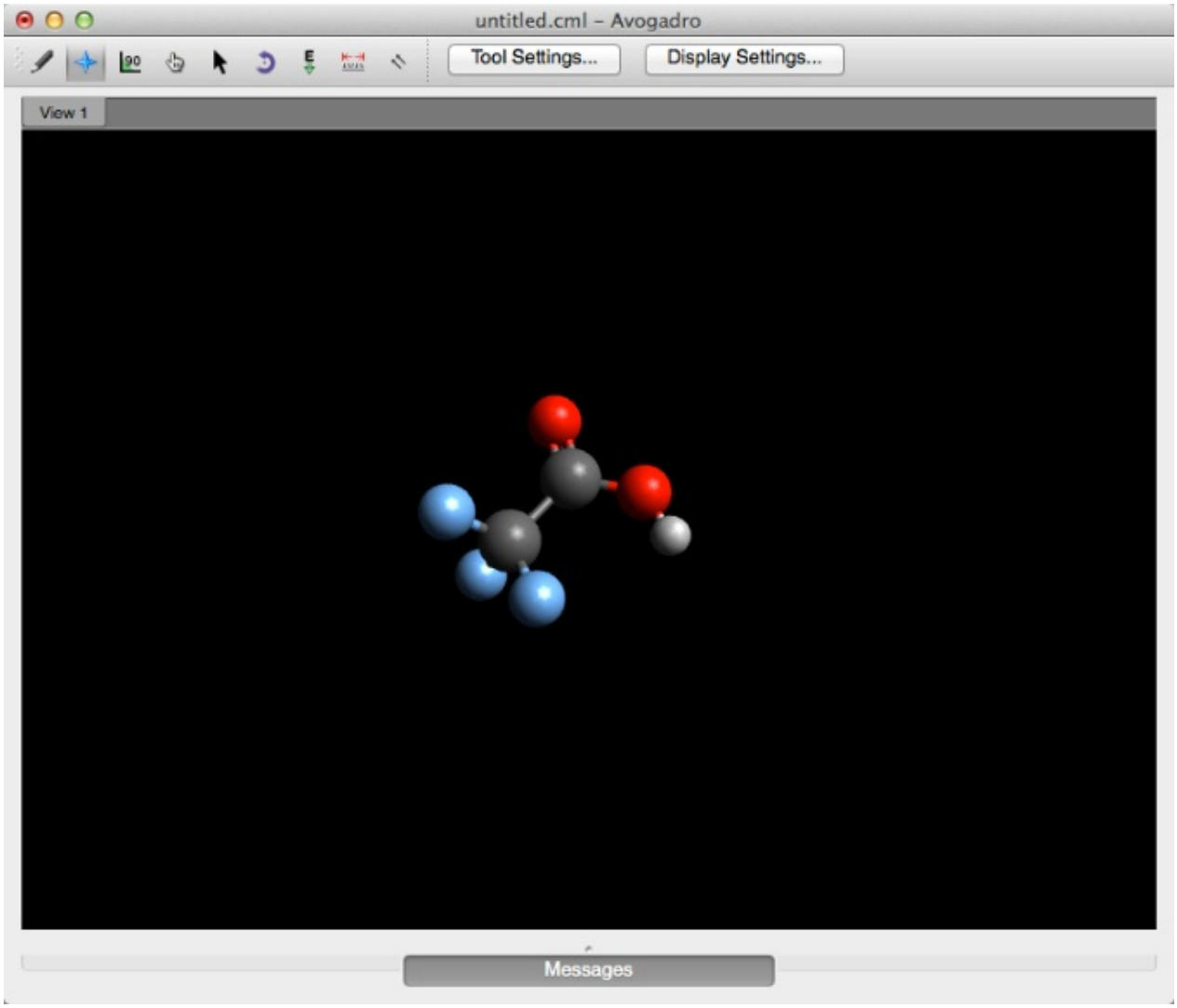
Selecting "Configure" allows you to adjust the default parameters for the orbital toolbar. Once the parameters have been adjusted, click "Recalculate All" before closing the dialog box. "Recalculate All" reevaluates, and updates all of the parameters.



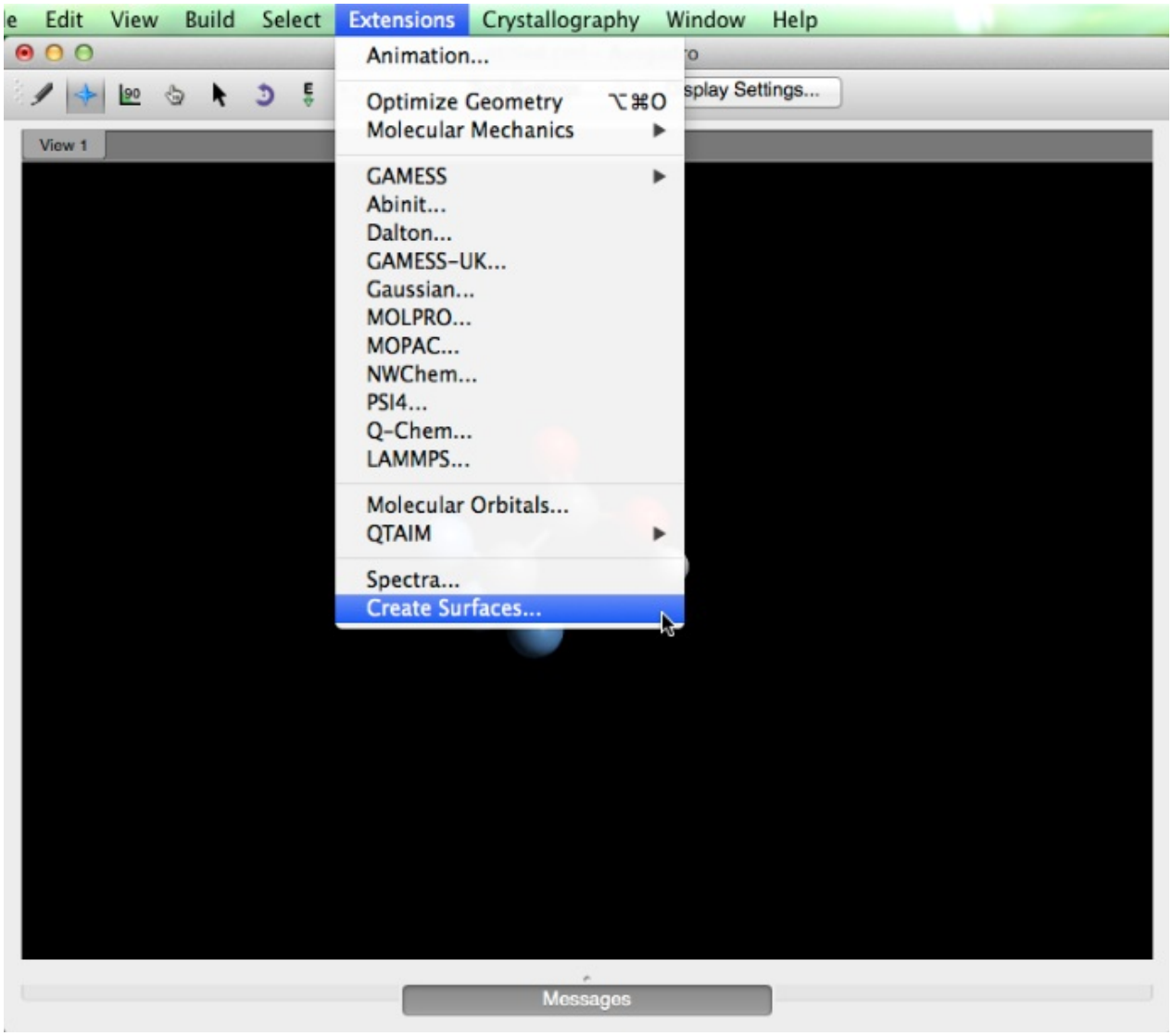
Viewing Electrostatic Potential Maps

The electrostatic potential maps help to visualize charge distribution, and other charge related properties of molecules.

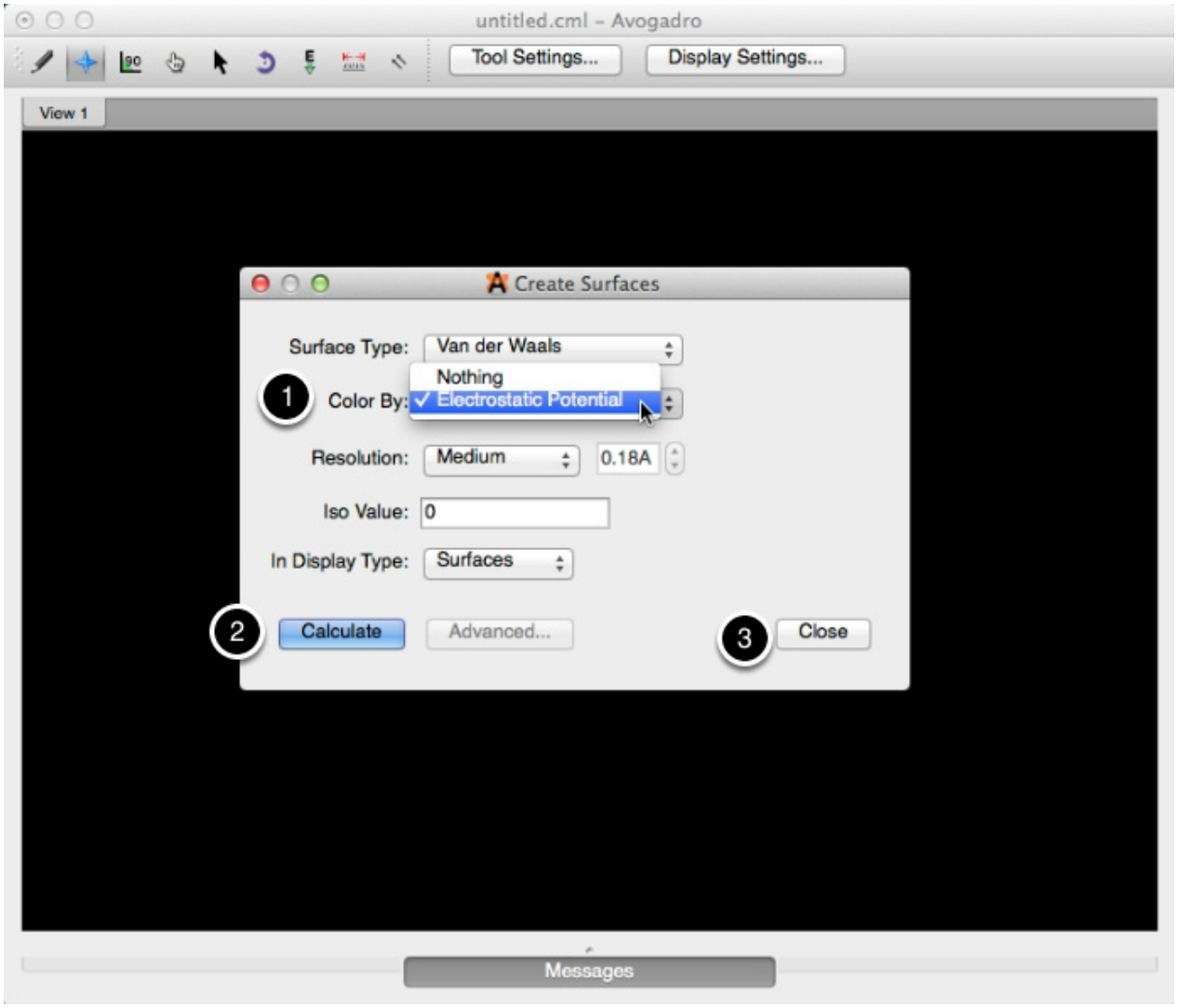
Overall, let's say you want to determine visually if a specific proton has more or less electron density. First, you'll want to begin with your molecule of choice (shown below is trifluoracetic acid).



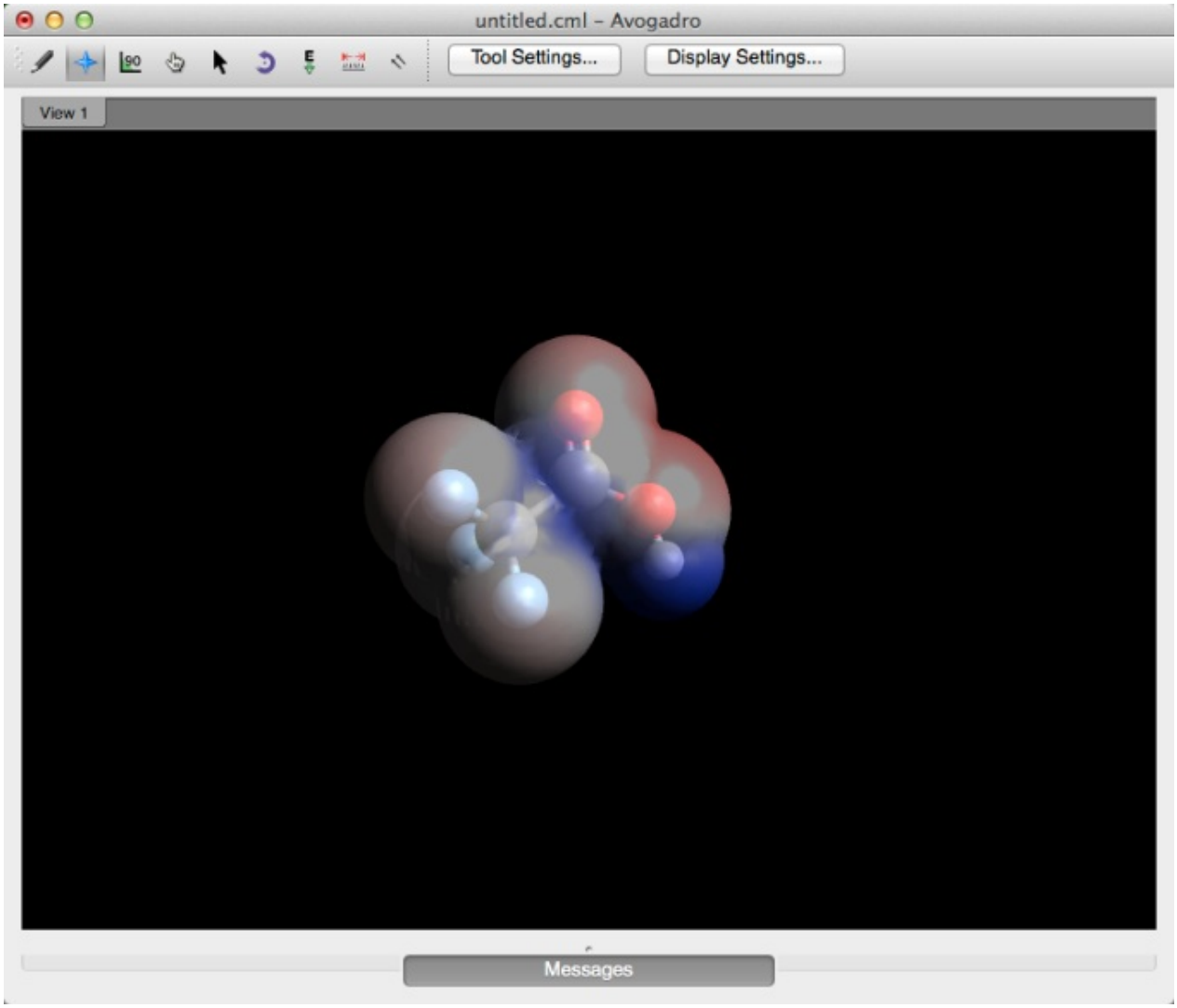
Then under the "Extensions" menu, select "Create Surfaces...".



A dialog box will pop up providing you with various surface options. Under "Color By:" select "Electrostatic Potential", and then click "Calculate". After Avogadro calculates the surface select "Close".



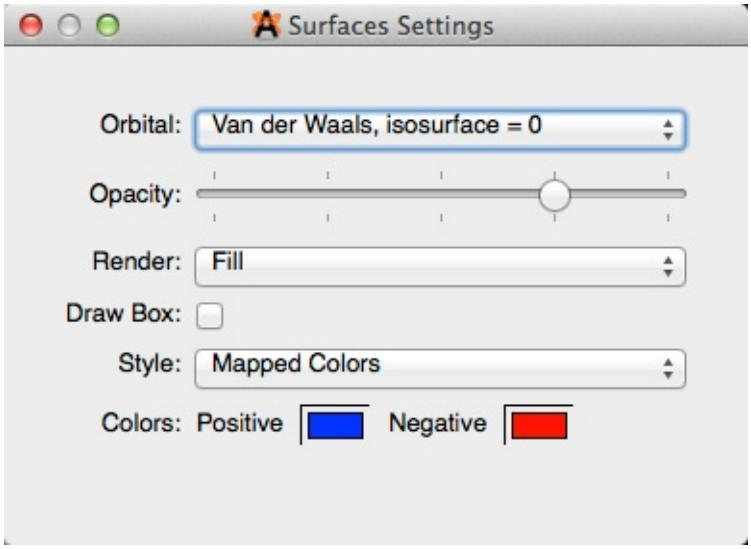
An electrostatic surface has now been created. From this surface, you can interpret where the most electron density resides (in the more red areas), and where the least electron density resides (deep blue areas). You can further determine, and compare the acidity of various protons, and how surrounding atoms impact the overall electron density.



This example was taken from "Exploring the Acidity of Organic Molecules with Avogadro" written by Tamika Madison.

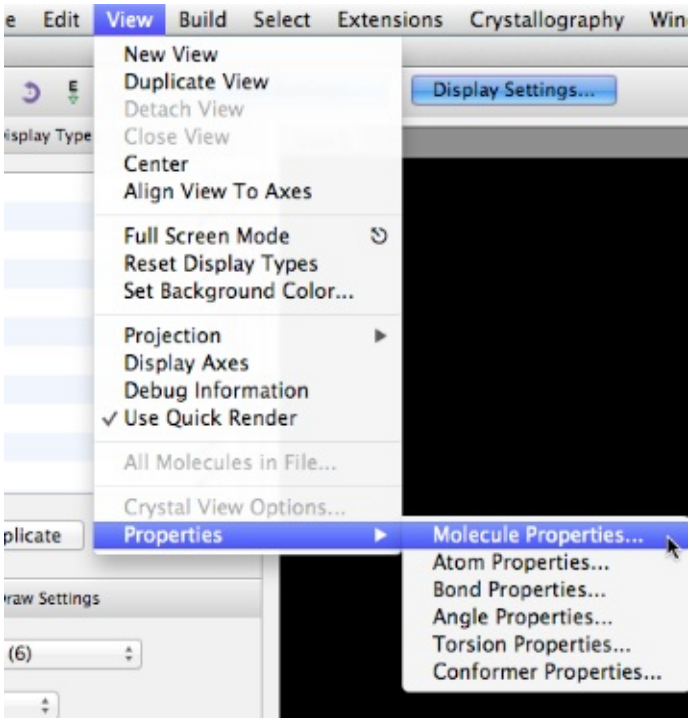
Changing Surface Settings

The opacity, rendition, and colors of the surface can the be changed by clicking the wrench next to the "Surfaces" display type.

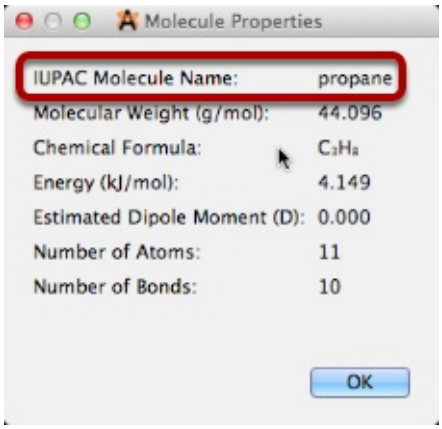


Naming a molecule with PubChem

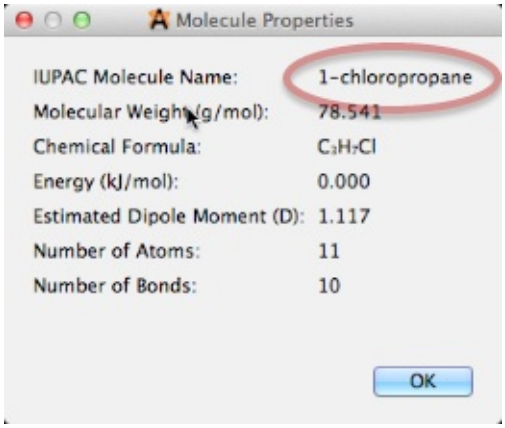
Avogadro 1.1 and later includes support for naming compounds using the NIH Chemical Resolver system and the PubChem database.



Open up the Molecule Properties window, under the View menu.



The IUPAC name will initially show as (pending) while the server returns the name, (unknown) if the molecule is not found in the resolver, or (unavailable) if your network connection is down or the resolver service is otherwise unreachable.



As you modify the molecule (e.g., adding a Cl atom), the name will update automatically with the other properties.