**Opening the structures in Olex2**

1. Download and install Olex2 if it is not already on the computer you are using.
2. Download the cif from the *Organometallics* website.
3. Open Olex2 and then open the cif. Alternately, you may be able to just click on the cif and it will open in Olex2. During the installation of Olex2 it was probably set to be the default program to view a cif.
4. This should open the cif and have a picture of the structure.
5. One the right side of the Olex2 window there should be a secondary window named Multiple Dataset. Your window may look slightly different than the one shown below. The first two structures in the list are the ones of interest and you can switch between them by clicking on them.



1. The structure will first appear with the hydrogen atoms shown. This tends to make the structure very difficult to see. To turn off the hydrogen atoms type **Ctrl-H**.
2. If you hold a left click on the structure and drag the mouse, you should be able to rotate the structure in three dimensions. You can also manipulate the size of the structure by holding a right click and dragging the mouse.
3. Click on any two atoms of interest type **esd**. This will display the bond length with the esd in the text in the lower left of the window. You will need to click off any atoms you have previously selected in order to make the next measurement.
4. Measuring bond angles is performed similarly except three atoms are selected. The order that you choose the atoms for this is important; the second atom you choose will be defined as the vertex of the angle. Type **esd** to display the bond angle and esd in the text that is shown in the lower left side of the window.
5. Again, don’t forget to unselect atoms before making the next measurement.
6. The next step is to calculate the centroids (geometric center) and planes of the C5 rings. To do this select the five carbon atoms of one of the C5 rings. Type **mpln** and this will show a new ball in the center of the C5 ring and the ring should be filled in with a different color. The centroids can be selected as part of a bond angle. Typing **esd** will give the desired angle with esd in the text that is shown in the lower left side of the window.
7. By selecting just the centroids, you can measure the angle between the planes. Typing **esd** will cause a significant amount of text to be generated in the lower left portion of the window. Towards the top should be a line that reads Plane (list of 5 carbon atoms) to plane angle: followed by the angle and esd.
8. There are many other options available in Olex2. One other one you may wish to will display the structure in a slightly different way. First, you will want to turn the hydrogen atoms back on using **Ctrl-H**. Go to Select>All. The go to View>Quick Drawing Styles>Sphere Packing (the default is Ellipsoids (with Hydrogens)). This allows you to get a feeling for the steric crowding in your structure.

