Instructions on how to use Cerius:

I. QUICK UNIX ORIENTATION !!!READ THIS FIRST!!!

(FYI UNIX is an operating system that runs on a computer much like Windows runs on most main stream computers.)

1. Right click and hold on an empty space in the desktop and select **programs** then select **console** in the menu that appears. This will open up a console window. Do this step twice so that you have two consoles available on the desktop.
2. The mouse pointer must be within the window you want to be working. So if you wish to work in the console that you just opened you must move the mouse pointer over the window and the window will change color indicating that it is selected. You may now type in that console window. Go ahead and separate the two consoles so that they are easily accessible. Also to select a console window you must left click on the border of the window.
3. These are some console commands that you may use if you return later to the cpu and need to amend files or directories. These commands are just for your information right now:
    - ls (this is a lower case L and S) <<enter>> gives a list of all files in the directory
    - cd (space) "some_directory_name" <<enter>> changes the directory to "some_directory_name"
    - Unix is case sensitive. Therefore (p) is not the same as (P).
    - rm (space) "some_file_name" <<enter>> deletes the file "some_file_name"
    - mkdir (space) "some_new_directory" <<enter>> makes the directory "some_new_directory"
    - rmdir (space) "some_old_directory" <<enter>> deletes the directory "some_old_directory"
    - cd (space) .. (these are periods without a space between them) <<enter>> moves up one directory step. If you are in the directory /home/some_user and you type cd .. <<enter>> you will then be in the directory /home

II. GETTING CERIUS2 TO RUN

1. After you have logged into a computer that is running a Unix operating system open two console windows.
2. Just as a warning Unix is case sensitive and does not like spaces in file names, so type everything just as you see it below.
3. In one of the console widows type:
   ssh (space) –l (dash lower case L) (space) "your_user_name" (space) cylon.engin.umich.edu <<hit enter>>
4. The console will prompt you for your password, go ahead and type in your password. <<hit enter>>
5. Now you are logged onto the cylon server. You must run Cerius2 from a directory where you have write privileges, so type the following:
   cd (space) /scratch <<hit enter>>
   mkdir (space) "your_user_name" <<hit enter>>
   cd (space) "your_user_name" <<hit enter>>
   pwd <<hit enter>> Wait until the prompt (cylon% appears before typing anymore)

pwd prints the directory you are currently in, the output should be:

/scratch/"your_user_name"

6. Now left click in the other unused console widow and type:

   uname (space) –n (dash lower case N) <<hit enter>>

   the output should be something like this:

   "computer_name".engin.umich.edu write this computer address down, you will need it shortly.
7. In the same console type:

   xhost (space) + <<hit enter>>

   this releases the computer and allows the cylon server to send information to your computers display.
8. Go back to the console where you logged onto the cylon server and type:

   setenv (space) DISPLAY (space) "computer_name.engin.umich.edu:0" (that is a colon and a zero at the end of the computer address). <<hit enter>>
9. Now type:

   /usr/local/cerius2-4.8/bin/cerius2 <<hit enter>>

   you should now see the Cerius2 window pop up.

III. QUICK MOUSE ORIENTATION

1. In Cerius the left mouse button selects and is the action button.
2. In the model window holding the middle mouse button and moving the mouse translates the molecule.
3. In the model window holding the right mouse button and moving the mouse rotates the molecule.
4. In the model window while holding the shift key + the middle mouse button and moving the mouse zooms in and out of the molecule.

IV. REACTANT CALCULATION SECTION

1. In the main Cerius2 window change form stick view to ball and stick view by left clicking on the light brown box labeled stick directly below the drop down menu bar.
2. In the drop down menu left click on **build** then left click on **3D-sketcher** and the sketcher window will open and. In the sketcher window left click on the **sketch.** Be sure that directly to the right of the sketcher button the carbon atom is selected, indicating that you will be drawing a carbon atom.
3. Before you draw anything minimize the model window by left clicking the first button in the upper right of the title bar of the modeling window. After it is minimized, maximize the window by double left clicking on the icon in the upper right of the desktop. There is a bug in the program that does not alow the out put to be refreshed in the modeling window unless we minimize and then maximize the modeling window. Draw a carbon atom by left clicking in the Cerius2 Models window once and then moving the pointer outside the model window. If you happen to make a mistake left click on the delete atom button and left click in the model window on the atom that you wish to delete.

4. Next to the sketch button in the sketch window left click on the drop down button next to the blue box where there should presently be a C and change to a N indicating that you will be drawing a nitrogen atom next.
5. Left click in the model window and then remove the pointer once again.
6. Draw a hydrogen atom in the model window also.
7. To bond these atoms left click the **edit bond** button in the sketch window and to the right select single bond and move to the model window and left click on the **H** then on the **C**. you should have drawn a single bond between them.
8. Now change to a triple bond and draw the bond between the carbon and the nitrogen.
9. Left click and hold on the **CLEAN** button in the lower left of the sketch window until the HCN molecule stops moving, indicating that the program has roughly minimized the molecules energy.
10. In the right portion of the visualizer window left click and hold on the light brown bar that is labeled **BUILDERS1** and select **QUANTUM1**
11. In the tiled windows below left click on the **MOPAC** tab, sending it to the front.
12. Now left click on **Run** in the blue menus, another window labeled MOPAC Run will pop up. This is where you will be able to tailor the calculations that you will be doing on these molecules.
13. First we will change the file name that this run will be saved under by left clicking in the blue box below the run button in the upper left hand corner.
14. Change the to a suitable file name for the reactant calculations
15. Left click and hold on the light brown rectangular bar labeled single point energy and change the calculation task to geometry optimization and frequency calculation.
16. Left click and hold on the light brown button below the calculation function chooser, here we can select different types of semi-empirical calculation methods such as PM3, AM1, MNDO, and MINDO3. Select the PM3 calculation method.
17. Further down in the MOPAC Run window you will find the electron spin, this specifies how many unpaired electrons we have residing in the system. There are zero unpaired electrons in the system so leave the spin at zero.
18. After all of the options you want are selected left click on the blue **RUN** button in the upper left had corner of the Run window. A small pop up window should appear as the computer calculates.
19. When the run window disappears the calculation is done. A graph window will pop up that contains the infrared spectra of the molecule, notice that there are three IR absorptions and then close the window. In the visualizer window in the right hand portion left click and hold on the **analyze** button. The properties that you may analyze are displayed here.
20. Left click on **files**, another pop-up window will appear with the heat of formation and dipole moment shown in the lower portion. Left click on the **Examine File button** to show a text form of the output of the calculation. Find the heat of formation, enthalpy, entropy, and heat capacity at 300 K and record these values, we will be using them later in this example.
21. Left click and hold on the **analyze button** and select the **vibrations** of the molecule.
22. With the model window visible select a frequency and left click the green **animate** button below the frequencies. These are the bends, stretches, and rotations that the molecule would be doing in its natural state. To stop the animation just click on another frequency.
23. Go ahead and close the vibrations window.

24. Left click and hold on **analyze** again and select **orbitals**. another pop up window should appear showing the different orbitals and their corresponding energies.
25. Left click on the **first orbital** and then left click on the **calculate** button in the upper left hand corner of the orbitals window. Another window will pop up and show that the orbital is being calculated. After the calculation is finished the HCN molecule in the models window should be surrounded by a somewhat spherical light blue orbital.
26. Left click on each orbital and calculate each to see what they all look like then go ahead and close the orbitals window.

V. TRANSITION STATE CALCULATION SECTION

1. In the visualizer window left click on the **file** drop down menu and select **new session**. This will reinitialize all of the Cerius2 programs options.
2. Again select ball and stick drawing, bring up the 3D sketch window and draw an HCN molecule.
3. Now in the sketcher window left click on the **angle button** so we can change the HCN angle. In the models window left click on the **hydrogen** then the **carbon** then the **nitrogen** to define the angle we will change. Be careful to left click exactly in the center of each atom because where you left click is the exact point the angle will be defined from.
4. Now left click and hold in the **black portion of the model window** and move the mouse up and down to change the HCN angle. Make the angle around 90 degree, it does not have to be exact as this is just a guess for the transition state.
5. Now open up the MOPAC calculation window.
6. Change the function to transition state optimization (geometry optimization to the
7. transition state)
8. Rename the file appropriately and change the calculation method from AM1 to PM3 left click on **RUN**
9. Analyze the output file and record the heat of formation, enthalpy, entropy, and the heat capacity at 300 K for the transition state.
10. Now there are some very interesting molecular orbitals that we can view for the transition state, but first for clarity we are going to change a viewing parameter so we can see the atoms a bit more clearly within the molecular orbitals.
11. Left click on **analyze** then on **surfaces**, there is a transparency % selection in the lower left corner or the surfaces window. Type 50 in the blue box and hit enter, then close the window.
12. Now open the orbitals window via the analyze menu and view the molecular orbitals of the transitions state HCN molecule.
13. Now that we have found the transition state geometry we can run a frequency calculation on it. Change the calculation function to frequency calculation and rename the file and run.
14. Go to the vibrations and look at the frequencies of the transition state. The top frequency is negative, which is the imaginary frequency along the direction of reaction that characterizes a transition state.
15. go ahead and close the freq window.

VI. PRODUCTS CALCULATION SECTION

1. Go ahead and start a new session (under file -> new session)
2. Now draw the products molecule with a triple bonded CN and the hydrogen bonded to the nitrogen.
3. Now run a geometry optimization and a frequency calculation on the molecule and take a look at the output file. Record the heat of formation, enthalpy, entropy, and heat capacity at 300 K.
4. Feel free to analyze the frequencies and molecular orbitals of the products.