

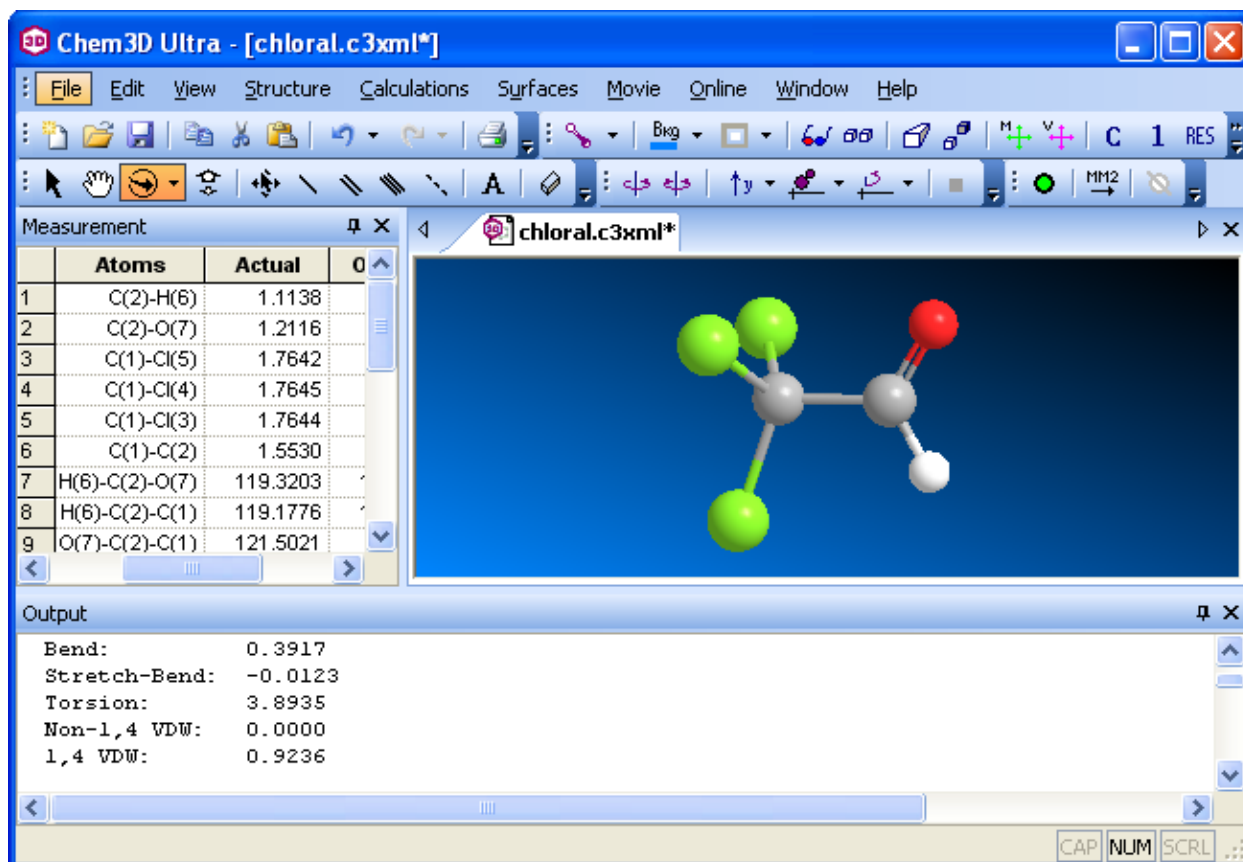
# MOLECULAR MODELING WITH CHEM 3D Pro v. 10

(GMU classroom)

Most of the instructions for using Chem 3D are taken from Chem3D **Help**. The **Help** and Tutorial features are quite good and you should expect to consult them if necessary. Choose **Help | Get Started** and choose Tutorials 2 and 3 for a quick start.

## Chem3D's Graphical Interface

When you first open Chem3D, you will see two main areas: the model window on the left and ChemDraw on the right. Close the ChemDraw window by clicking the **X** in the upper right of the window (or leave it open if you wish, but it takes up room). Because Chem3D is a Windows application, the GUI interface is already familiar to you and the **File**, **Edit**, **Window**, and **Help** menus are similar to those you've seen before.



Useful tools can be placed in the toolbar area. If you don't see the toolbar you need, choose **View | Toolbars**.

To open the three windows that you will commonly use, choose **View | Output Box** and **View | Measurement Table**. The windows can be detached and floated anywhere.

<b>Window Object</b>	<b>Description</b>
<i>Model area window</i>	Contains a molecular model you are viewing, building, or analyzing. The origin of the Cartesian axes (0,0,0) is always located at the center of this window. Regardless of how the model is moved or scaled, the Cartesian axes do not move relative to the window.
<i>Status bar</i>	Displays information about the active frame of your model and about hidden atoms in your model.
<i>Output window</i>	Contains all of the messages associated with a model.
<i>Measurement window</i>	Contains an area to display tables of measurements, for instance, the bond lengths, bond angles, dihedral angles and other such data. To generate measurements, choose <b>Structure   Measurements   Generate</b> and choose the measurement to display.
<i>Record Selector</i>	Used to select an entire record. Clicking a record selector highlights the corresponding atoms in the model window.

### **Tools palette**

In addition to menus and commands, there are tools that you can use for building and manipulating the model. These tools are available in the Tools palette described below:

<b>Tool Name</b>	<b>Use</b>
<i>Select</i>	Click or Shift+click or Drag or Shift+drag to select individual or multiple atoms or bonds.
<i>Translate tool</i>	Moves the model in the x,y plane of the model window.
<i>Trackball tool</i>	Use to rotate the molecule in the model window around all three axes. Hold down the left mouse button and drag.  When using the Trackball tool, move the cursor to the top edge of the model window. The Rotation bars will appear. Hold down the left mouse key and drag to rotate around the selected x, y, or z axis.
<i>Zoom tool</i>	Reduces or enlarges model in window.
<i>Single Bond</i>	Draw single bonds by dragging in the model window.

<i>Double Bond</i>	Draw double bonds by dragging in the model window.
<i>Triple Bond</i>	Draw triple bonds by dragging in the model window.
<i>Uncoordinated Bond</i>	Draw uncoordinated bonds by dragging in the model window.
<i>Text Building Tool</i>	Draw molecules or fragments by typing in text box or clicking on atoms. Case sensitive
<i>Eraser</i>	Erase bonds and atoms by clicking.

### ***Placing a structure in the model area window***

You can draw structures of molecules directly in the model area window. Chem3D, however, is not a great drawing program and there are many difficulties in drawing useful structures rapidly. Choose the Text tool. For simple molecules, you can type the molecular structure (not formula) in the model window. You must use appropriate upper and lower case letters. You can group like terms in parentheses [ (CH<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>CH<sub>3</sub> ] Use the Text tool to easily change one atom to another.

Most chemical drawing and visualization programs use interchangeable file formats and you can import some of these into the model area window. For example, Chem3D will open ChemDraw (*chm*), Protein DB (*pdb*) and MDL (*mol*) files. ChemDraw and Chem3D are part of the ChemOffice suite of programs. PDB and MDL files are used primarily in visualization programs such as DS Viewer and ChemSketch.

Recall that ChemSketch can Export drawings to many file formats, including *chm* and *mol* files. You can learn how to draw using Chem3D by trial-and-error and by consulting Chem3D Help Tutorials 2 and 3. But to get off to a fast start in this class, we'll assume you've drawn the relevant molecules in ChemSketch and saved them as *chm* files to open in Chem3D. Remember, when you want to save a ChemSketch drawing to another file format, you must choose **File | Export...** in the ChemSketch menu bar. In Chem3D, choose **File | Open...** to open the file.

### ***Cleaning a structure***

You may remember in ChemSketch that you could transform your 2D drawing in the drawing window. The program "cleaned" the bond lengths and angles to more "normal" values. You can do the same in the Chem3D window. Click on the background in the model window. Select the entire molecule (**Ctrl+A**). Notice that the atoms and bonds are now colored yellow (default). From the menu bar choose **Structure | Clean Up**.

### ***Rotating a molecule in the model area window***

Using the Trackball tool in Chem3D, you can perform a variety of rotations on the model:

- Choose the Trackball tool and drag in the window to freely rotate a molecule.
- or*
- Move the cursor to the top, bottom or right edge of the window to see the Rotate around X, Y and Z axes areas. Hold down the left mouse button and drag to rotate around the selected axis.
- or*
- Choose the Down arrow to the right of the Trackball tool button. Select an axis and the degrees of rotation.

### ***Selecting atoms and bonds***

Choose the Selection tool. Click on an atom. Click on a bond. To make multiple selections, hold down the [Shift] key while clicking on atoms and/or bonds. To choose a section of a molecule, or the whole molecule, hold down the left mouse button and draw a rectangle around the desired section. The selected atoms will be colored yellow (default).

### ***Moving atom(s) or molecules***

Use the Translation tool to move the entire molecule. Use the Move Objects tool to select and then move atoms in a molecule.

### ***Pop-up Information***

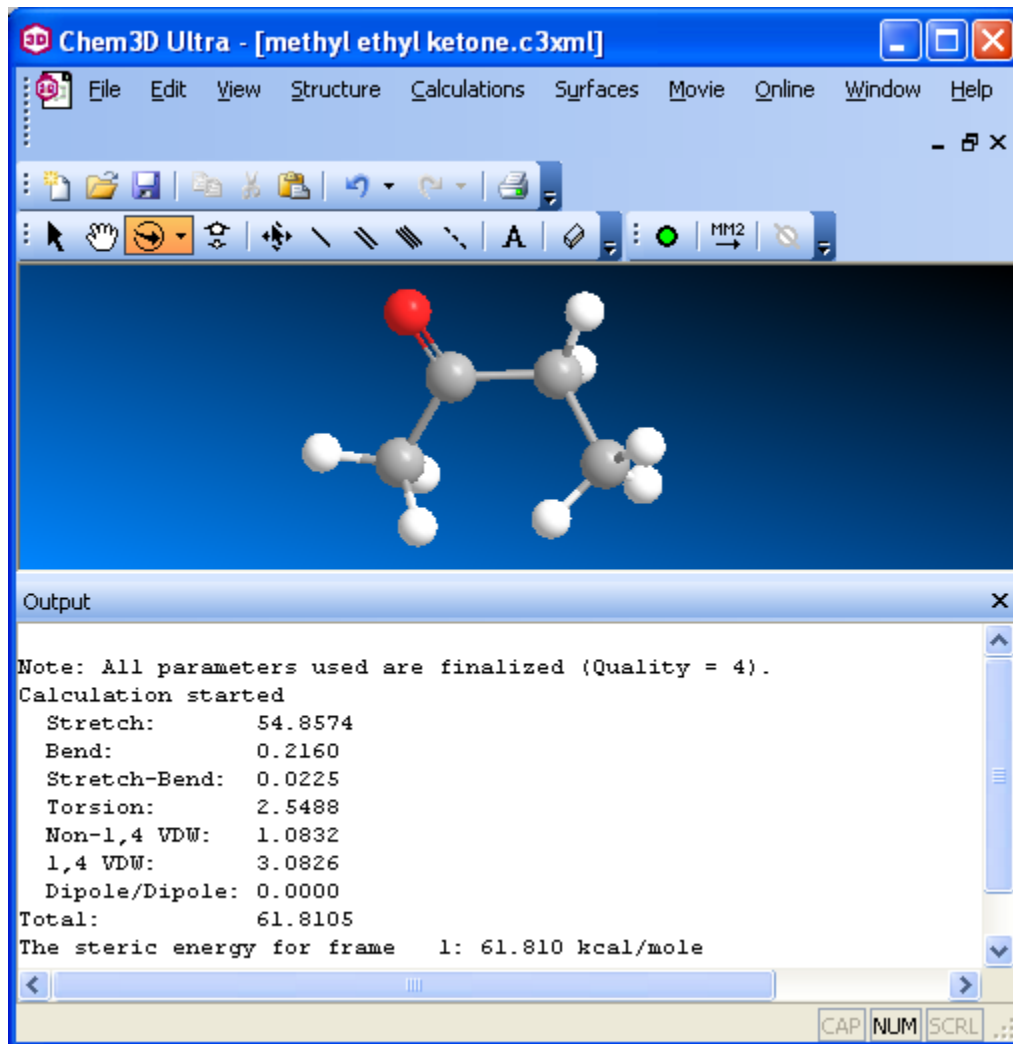
By default, Chem3D displays information about the atoms in the model when the cursor passes over them. Choose **File | Preferences | Popup Info** . The Pop-up Information control panel contains check boxes that you can select to determine what information appears as you point at atoms and bonds.

*Note:* Chem3D assigns "serial numbers" to uniquely identify each atom in the molecule. These numbers have no relationship to the numbering in nomenclature systems. In all directions for using Chem3D, the atom numbering refers to the nomenclature system, not the atom serial numbers.

## Single Point Energy Calculation

From the Chem3D menu, choose **Calculations | MM2 | Compute Properties...** Under the **Properties tab**, choose **Steric Energy Summary**. Make sure Compute Properties is chosen under the Job Type tab. Click the **Run** button.

Here is the output for one conformation of methyl ethyl ketone:



The units are kcal/mole for all terms. At the beginning of the computation the first message indicates that the parameters are of **Quality = 4** meaning that they are experimentally determined/verified parameters that are used in the force field.

The first steric energy term in the Messages table is the **Stretch** term. This term represents the energy associated with any bonds that are distorted from their optimal length.

The second steric energy term is the **Bend** term. This term represents the energy associated with any bond angles that are deformed from their optimal values.

The third steric energy term is the **Stretch-Bend** term. This term represents the energy required to stretch the two bonds involved in a bond angle when that bond angle is severely compressed.

The fourth steric energy term is the **Torsion** term. This term represents the energy associated with deforming torsional angles (dihedral angles) in the molecule from their ideal values.

The fifth steric energy term, **Non-1,4 van der Waals**, represents the energy for the through-space interaction between pairs of atoms that are separated by more than three atoms.

The sixth steric energy term, **1,4 van der Waals**, represents the energy for the through-space (non-bonded) interaction of atoms separated by two atoms.

The seventh and final term, the **dipole/dipole** steric energy, represents the energy associated with the interaction of bond dipoles.

Be sure you can identify the atoms and bonds referred to above. For example the Bend term involves the change in bond angle between 3 adjacent atoms.

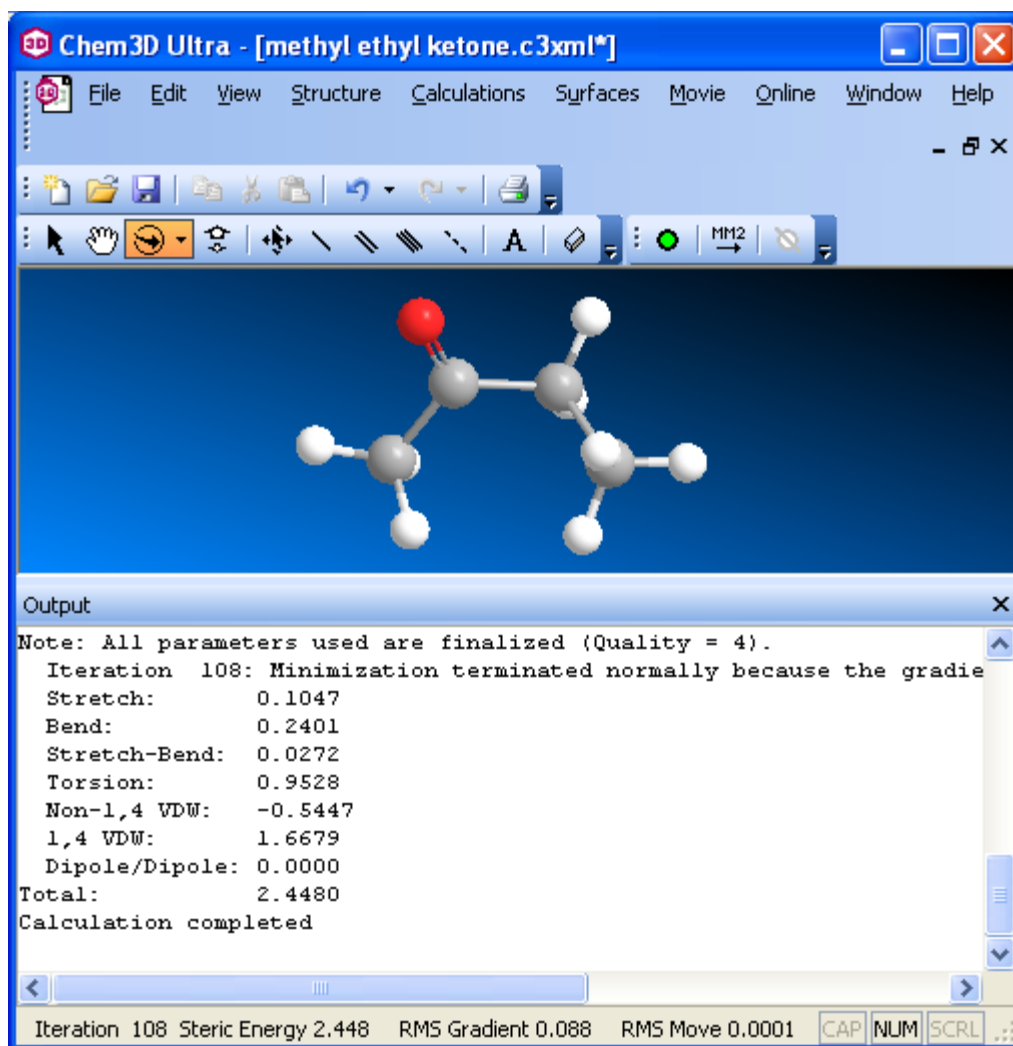
## ***Geometry Optimization/Energy Minimization***

From the Chem3D menu, choose **Calculations | MM2 | Minimize Energy....** Under the **Job Type tab**, choose **Minimize Energy** as the Job Type. Click on **Display Every Iteration**. Leave the Minimum RMS Gradient at 0.100. Click the **Run** button.

The output is shown below. The message that is cut off in the figure says: " Iteration 108: Minimization terminated normally because the gradient norm is less than the minimum gradient norm".

The total steric energy of the molecule is much less after geometry optimization. You can see the effect in the picture of the model. In which energy term did the largest relief of strain occur?

Note that this conformation might be a *local minimum* and not the most stable of all possible conformations, known as the *global minimum*.



Continue learning about CHEM3D by trying the **Exercises** in a separate document.