Exercises Using CHEM3D Pro

The exercises that follow are not merely exercises that depend on the earlier information presented but rather they are additional sections for learning to use any version of CHEM3D.

EXERCISE I

Open a *.sk2* file from ChemSketch , then save the structure drawing as a *.chm* file. Open the newly saved file in Chem3D. Practice rotating and selecting and moving the whole molecule as described earlier in the introductory instructions for using Chem3D.

Internal Rotations

Choose the rotation tool and as you slide the cursor around the Model window notice the gray rotation bars around the periphery of the window.

> Now choose the down arrow on the rotation tool button to see the pop-up rotation dial window. It can be detached for easier use. At the bottom of the window are buttons to rotate around the x, y, or z axis, or to use a free rotation trackball.

> Select two bonded atoms or the bond between them. At the bottom of the rotation dial window choose one of the two right-most tools (the Dihedral tool). Drag the pointer on the rotation dial to change the dihedral angle or type an angle in the angle box.

Measurements

The Measurements table contains internal measurements between various atoms in your model.

To open the model measurements window, choose **View** | **Measurement Table**. Then choose **Structure** | **Measurements** and then choose one of the commands in the menu (bond lengths, bond angles, dihedral angles, close contacts). You can only choose one at a time, but all of them will appear sequentially in the same table. You might have to resize the columns in the Measurements window so you can see all the text.

The "Actual" column measurements are the values associated with the model in the model display window – what you see. The "Optimal" column specifies optimal values for some measurements. These standard values are part of theChem3D program. Standard measurements are the optimal (or equilibrium) bond lengths and angles between atoms based on their atom type. The values for each particular atom type combination are actually an average for many compounds, each of which have that atom type (for instance, a family of alkanes). Standard measurements allow you to build models whose 3D representation is a fair approximation of the

actual geometry when other forces and interactions between atoms are not considered. If you change the value in the "Optimal" column, the new value is used instead of the standard measurement whenever that measurement is required (e.g. Clean Up Structure or energy minimization).

Using the same molecule, compute all the Measurements available. Notice that bond lengths are denoted by two atoms, bond angles by three atoms, dihedral angles and close contacts by four atoms.

Click on an open marker at the far left of a row in the measurements table. Selecting a measurement simultaneously selects the relevant atoms in the model area window. Select any two atoms bonded to each other in the Model area window (or the bond between them) and then find the corresponding selection in the Measurements table.

To select multiple bonds or atoms, **Shift**+**click** the open markers in the table, or hold the left mouse button and drag a rectangle around the measurements. To select all the measurements, press **Ctrl-A**.

Select any bond in the molecule. In the measurements table, change the Actual value to 3 Å. What happens in the model area window?

Select the atom in the Model window and move it a distance away from its initial position. What happens to the bond length Actual and Optimal values in the Measurements window?

Linking and Embedding Chem3D models

Draw or open a structure model in the Chem3D Model window. Select the entire molecule and **Copy** it.

In Word or Excel, **Paste** the selection (no need to use Paste Special although you can). In Word, if the pasted object is too small, you can resize it without too much distortion. Double-click on the object to edit it using the Chem3D window. When you are finished editing, in Chem3D, choose **File** | **Close & Return** or close the object window.

Go back to the Chem3D window. This time choose to **Copy As** an **Embedded Object**. Then Paste into the destination document. What is the difference between the two methods? What can you do with the embedded object now?

You can link the Chem3D object so that when the source Chem3D file is changed, the linked model is changed in the destination document. See the OLE instructions in the Manual.

EXERCISE II

Comparing the Steric Energy of *cis*- and *trans*-2-butene

1. Build or open a model of **trans-2-butene** in Chem3D.
  · Perform a *geometry optimization* by following the instructions in "Molecular Modeling with Chem3D". The four carbons in the molecule should all be in the same plane in the optimized structure.
  · Save the file.
  · Copy the output data in the Message/Output window to an Excel worksheet.*

2. Build or open a model of ***cis*-2-butene** in Chem3D.
  · Perform a geometry optimization. The four carbons in the molecule should all be in the same plane in the optimized structure.
  · Save the file.
  · Copy the output data in the Message/Output window to an Excel worksheet.*

> *Information in the Chem3D messages table can be copied to the Clipboard and pasted into another application as delimited or fixed-width text. Click in the messages table to activate it, then choose **Edit** | **Select All**, then **Copy**, to copy all text to the Clipboard, or **Shift+click** each record that you want to copy to the Clipboard.
>
> If you want to delete messages, select the messages to delete, then hit the Delete key or Ctrl-X.

3. In Excel, convert the text to columns of data. Align the data for *cis-* and *trans*-2-butene in adjacent columns, keeping only one column for the energy term labels so that the table looks like the one below.

A comparison of the steric energy components for cis-2-butene and trans-2-butene.

> NOTE: The values of the energy terms shown here are approximate and can vary slightly based on the type of computer processor used to calculate them.

Energy Term	*trans*-2-butene	*cis*-2-butene
Stretch:	0.0627	0.0839
Bend:	0.2638	1.3235
Stretch-Bend:	0.0163	0.0435
Torsion:	-1.4369	-1.5366
Non-1,4 van der Waals:	-0.0193	0.3794
1,4 van der Waals:	1.1742	1.1621

Dipole/Dipole:	0.0767	0.1032
Total:	0.137	1.5512

The significant differences between the steric energy terms for *cis-* and *trans*-2-butene are in the Bend (angle strain) and Non-1,4 van der Waals steric energy terms. The Bend term is much higher in *cis*-2-butene because the C(1)-C(2)-C(3) and the C(2)-C(3)-C(4) bond angles had to be deformed from their optimal value of 122.0° to 127.4° to relieve some of the steric crowding from the interaction of hydrogens on C(1) and C(4). The interaction of hydrogens on C(1) and C(4) of *trans*-2-butene is much less intense, thus the C(1)-C(2)-C(3) and the C(2)-C(3)-C(4) bond angles have values of 123.9°, much closer to the optimal value of 122.0°. The Bend and Non-1,4 van der Waals terms for *trans*-2-butene are smaller, therefore *trans*-2-butene has a lower steric energy than *cis*-2-butene.

Draw (or use previously drawn) *cis-* and *trans*-2-butene in ChemSketch. Be sure the Properties panel is set to show all carbons. Use the Numbering tool to number the carbon atoms 1-4 in each of the drawings. Use the Name tool to generate a name for each structure. Embed the drawings in the Excel worksheet and save.

4. Open your optimized *trans*-2-butene model in the Chem3D model window. Compute all the Measurements available for the model. Click the header row "Atoms" in the Measurements window. Copy it, and then paste it into a new worksheet in the Excel file you created earlier for the 2-butenes. Repeat the copying and pasting for the "Actual" and "Optimal" columns. Label the columns of data. You can delete the rows that do not have corresponding "Optimal" data.

Label a new column "Difference". Write an equation to calculate the difference between "Optimal" and "Actual" for the first row of data, and then copy the equation for the remaining rows.

Use a logical "IF" statement in the next column to find the Difference for which the absolute difference is greater than 1.8 (use ABS(cell) in the formula). Use the text "x" to denote true statements and "" (null) to denote false statements.) Copy the statement to all rows.

Repeat the exercise for *cis*-2-butene. Align the data measurements parallel to those for *trans*-2-butene.

As you compare the results, notice that the largest Differences are for bending, not stretching, terms. Notice also that the *cis*-butene has more and larger differences than *trans*-2-butene. Be sure you can identify the atoms that are involved in each of these energy terms.

Related Exercise

Choose one, or more, of the *cis-* and *trans*-cycloalkenes (C_7-C_{10})and compare their component steric energies. (Remember, you can only compare the stereoisomers -- you can't compare structural isomers or compounds with different molecular formulas.) What differences do you observe compared to the open-chain butenes?

When you draw the *trans*-cycloalkenes, start with your *trans*-butene, keep rotating it so you can add –CH_2- groups until finally you can join up the last –CH_2- with a –CH_3. Then select all the atoms and **Clean** the structure before starting other calculations.