Conformational Analysis of Butane Derivatives

The method and procedure in this assignment are related to the Conformational Analysis of *n*-Butane that you should complete first and which is referred to in this document. Everyone in the class will be assigned a different substituted butane in order to generate a unique problem and solution for each student. The student molecule assignments appear at the end of this document.

PART I

Generating the Data in Chem3D

In this exercise you will calculate the single point energy of the molecule in various conformations with respect to internal rotation around the central C_2-C_3 bond and generate Excel charts of steric energy vs. dihedral angle. In Part II, you will analyze the conformations and the contributions to their steric energies.

1. Either open a structure drawing of the molecule or build one in Chem3D. Save the model. If you have used any method other than the Text Building tool in Chem3D, **Clean** the structure before proceeding. Orient the model in the window as you did for the conformational analysis of butane.

2. Open the Output box and Measurements table windows. Generate the dihedral angle measurements. Choose the C_1-C_2-C_3-C_4- dihedral angle and make it 180° in the Actual column. (If it changes to -180°, that's OK.)

3. Perform an MM2 Energy Minimization (**geometry optimization**). There will most likely be some slight changes in the model after optimization. This conformation should be either the global or a local minimum. Save the file.

> *Note*: If the dihedral angle is not 180 degrees, in the **Actual** column, change the angle to 180. You should see the model respond. Calculate a new **single point energy** for this slightly changed angle (*DO NOT optimize, just calculate*).

This is now the starting point for the conformational analysis. It might be helpful to delete any other messages in the Output box except for the one you just generated above as the starting point.

> *Note*: Any time you want to delete measurements or messages, select the text and press Delete or Ctrl X.

4. You are now going to change the designated dihedral angle by 30-degree increments and calculate the single-point steric energy after each rotation until it has been rotated through 360 degrees.

> Change the dihedral angle in the Actual column in the Measurements window to 150. Press Enter. If it says -150, it doesn't matter.

Calculate a **single point energy**. *DO NOT minimize the energy.* See "Single Point Energy Calculation" in the "Molecular Modeling with Chem3D" document.

Now change the angle to 120 (or -120 if the Actual column showed -150 previously). Calculate a single point energy.

Repeat the above steps, changing the rotation angle each time by 30 degrees until you reach -150° (or 150°, depending on the direction of the rotation). At each rotation, calculate a single point energy. The next step would be -180°, which will be equal to 180° and you've now rotated through the entire 360°. Confirm the internal rotations by looking at the dihedral angle in the Measurements window.

- If you scroll in the Output Box, you'll see the repetitive energy calculations after each rotation.

- Keep track of the actual dihedral angle in the Measurements window. Sometimes the sign of the rotation changes – it doesn't matter as long as you don't change the direction of the rotation. You can "undo" the last operation by pressing Ctrl-Z.

- *Periodically save the file* in case you make an error. Otherwise, you will have to start over.

Manipulating the Data in Excel

5. In this step, you are going to copy the energy data from Chem3D and paste it in an Excel workbook.

   Press **^A** while in the Chem3D Output box (selects all), then press **^C** (copy). Select a cell in Excel and press **^V** (paste). Sometimes (!?) the descriptors and numerical data appear in two adjacent columns. Other times, all the message window output will be in one column. If so, convert the text to columns in Excel (try the colon as a delimiter). Delete the **content** of the rows concerning parameter quality and "The steric energy for….". (Don't delete the rows themselves – they act as visual spacers.) Name the worksheet "Raw Data".

6. Activate a *new worksheet* in the Excel workbook. Name the worksheet "Data". Beginning in a cell in column A, type in the column headings **Dihedral angle**, **stretch**, **bend**, etc. for each of the energy terms corresponding to the message output. Adjust the column widths to accommodate the headings.

In column A, beginning with 180°, fill in the dihedral angles by 30-degree increments (use the auto-fill feature) for the full rotation.

7. Select the column range of energy data corresponding to the 180° dihedral angle in the "Raw Data" worksheet (the first single point energy measurement). Copy it. In the "Data" worksheet, click in the cell in column B corresponding to the dihedral angle. From the menu choose **Home** tab | **Paste** | **Transpose**.

Continue transposing each range of single point energy data from the first worksheet into a row corresponding to the dihedral angle in the second worksheet.

8. You now have all the data you need to plot the energy changes (*y*) as a function of dihedral angle (*x*).

> Make two charts **as separate sheets** (not embedded in a worksheet): one chart for only the total steric energy vs. dihedral angle and the other chart for all the individual component energy terms vs. dihedral angle. For the latter, plot each energy term vs. dihedral angle as a separate series on the same chart. Be sure to include a legend.

Choose a Chart Type that draws a smooth curve between visible data points. Your dihedral angle axis should have 30 degrees as the major unit (no minor unit). The y-axis major unit should be 1 kcal/mol and the minor unit 0.5 kcal/mol. The y-axis should cross the x-axis on the far left side of the plot. The x-axis should cross the y-axis a couple of units less than the y-axis minimum value. (The minimum might be different for the two charts.) Name the chart sheets.

Remember to include all the elements of good graphing in your chart as explained in class and in the Manual. The legend, if one is necessary, should appear within the plot area. Include the chart title, axis labels and units; no gridlines.

Checking your graph

You can verify your results for the total steric energy graph by generating a Dihedral Angle chart in Chem3D Ultra. Select the central C-C bond. Choose **Calculations** | **Dihedral Driver** | **Single Angle Plot**. You can click on the various maxima and minima to see the corresponding conformations. The energies and conformations should match yours. However, the plot might not *appear* exactly the same as your graph because the driver may assign the torsional angle to a different set of atoms than you did. Imagine the plot is wrapped around a cylinder and choose a starting point the same as for your graph.

9. Copy the model from Chem3D and embed it in the Data worksheet. Be sure the molecule is clearly presented in a staggered conformation. Use this method, which will allow interactivity for the embedded model: choose **Edit** | **Select All**, then **Edit** | **Copy As** | **Embedded Object**. In the destination, choose **Paste Special** | **HTML**.

Make sure that every page, every title, everywhere that it is relevant, includes the name of your compound.

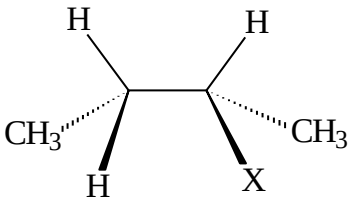
When you save the Excel workbook as *conf-XXX.xls*, save it with the Total Energy chart visible. The worksheet pages should appear in the workbook left-to-right in the order they were generated. Also, save the workbook so that the custom header and footer will be present on all pages when you print. (The embedded Chem3D model will not show.) There should be no extra worksheets in the workbook.

Save the Chem3D file as *chem3D-XXX.c3xml*.

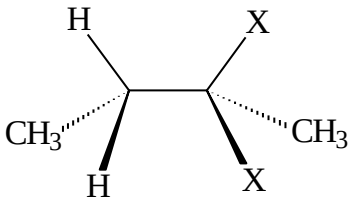
Print the two charts and "Data" worksheet from Excel in landscape mode. Include your name in a Custom header. Include the Sheet Names as Custom footers. Assemble and staple the printouts in order.

Publish the Excel workbook as an HTML file (non-interactive) on your web site in a new directory named "*conformation*". Link the page to your Chem 350 projects page with a descriptive title.

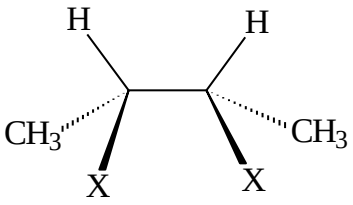
Submit the *.htm, xls* and *.c3xml* files to WebCT. The *htm* file and associated directory of subsidiary files must be zipped before submitting to WebCT.



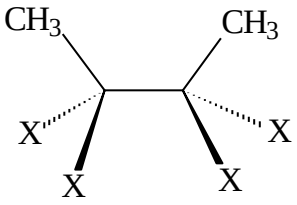
Computer	X
1	F
2	Cl
3	Br
4	I



Computer	X
12	F
13	Cl
14	Br
15	I

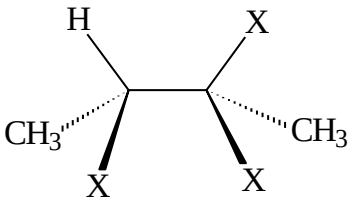


Note: stereochemistry ("threo") –build so that it appears in this conformation



Computer	X
20	F
21	Cl
22	Br
23	I

Computer	X
24	F
25	Cl
26	Br
27	I



Computer	X
9	F
	Cl
	Br
10	I