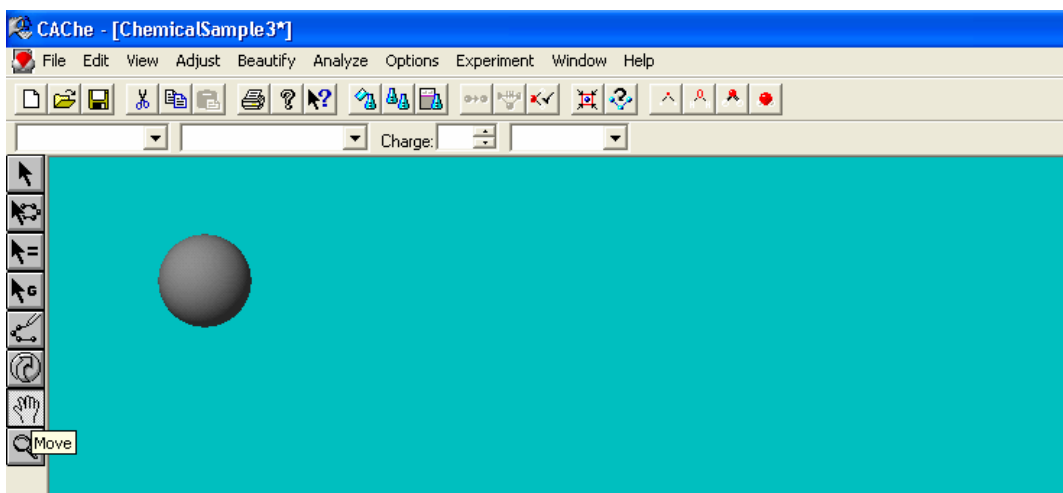


CAChe – A Practical Session

This exercise is designed to give you hands on experience with many of the basic functions that the CAChe program can do. Follow the instructions carefully, as these commands will be very helpful as you do the assigned problem set on your own.

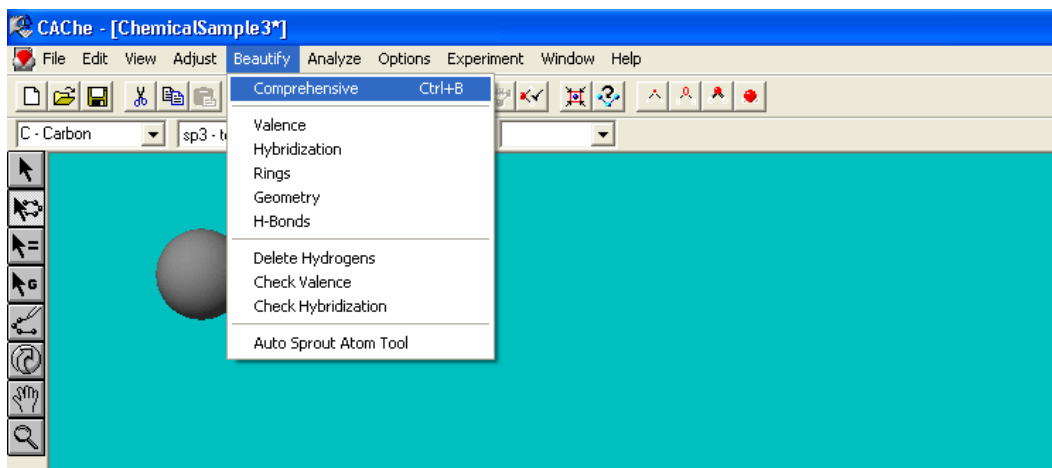
1) Draw Methane:

Click on *Drawing Pencil* on the left toolbar.
Make sure *Carbon* and *sp³* are selected on the top.
Click once in the drawing area to place a carbon.
Use the *Rotate* and *Move* tools to rotate and reposition the molecule.



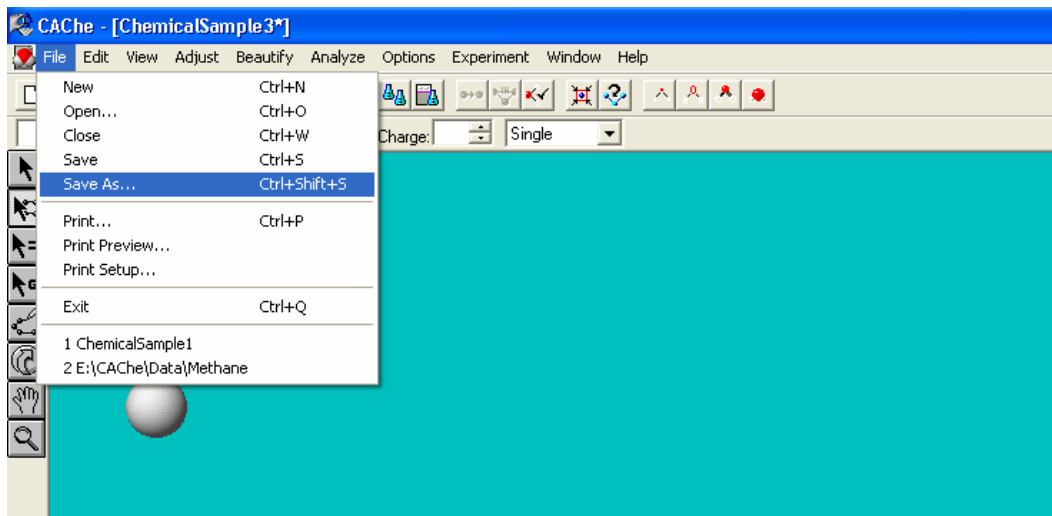
2) Beautify Methane:

Click on *Select Molecule* on the left toolbar.
Click on any atom in methane.
Under the *Beautify* drop down menu select *Comprehensive*.



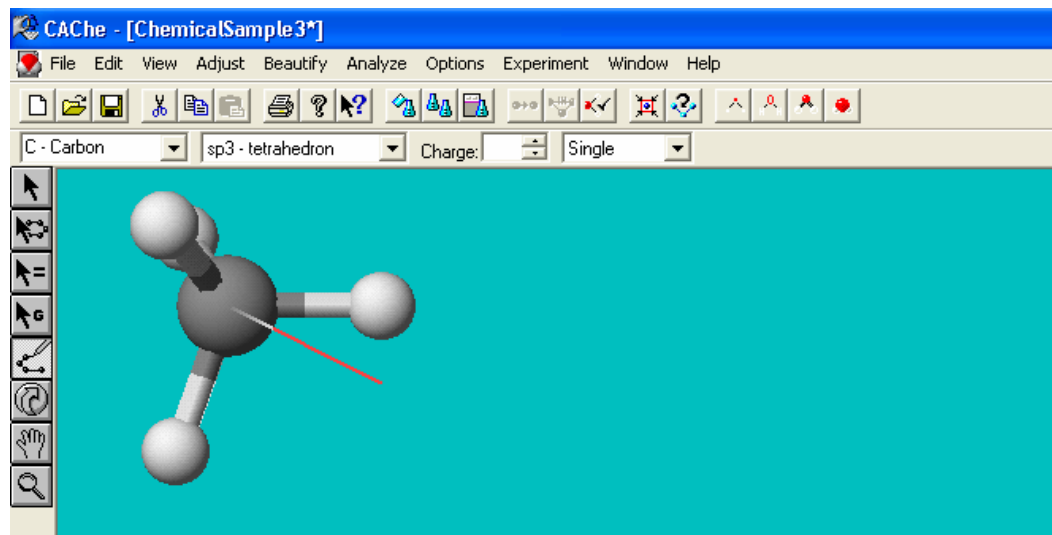
3) Save Methane:

Under the *File* drop down menu select *Save As*.
Navigate to the *My Documents* folder.
Save as *Methane*.
If asked to replace a file, select *Yes*.



4) Draw Ethane:

Click on *Drawing Pencil* on the left toolbar.
Click on the existing methane carbon.
Drag the pointer and release to form a new bond.
Click on select molecule and select ethane.
Beautify ethane.



5) Save Ethane:

Under the *File* drop down menu select *Save As*.
Navigate to the *My Documents* folder.
Save as *Ethane*.
If asked to replace a file, select *Yes*.

6) Draw Propane:

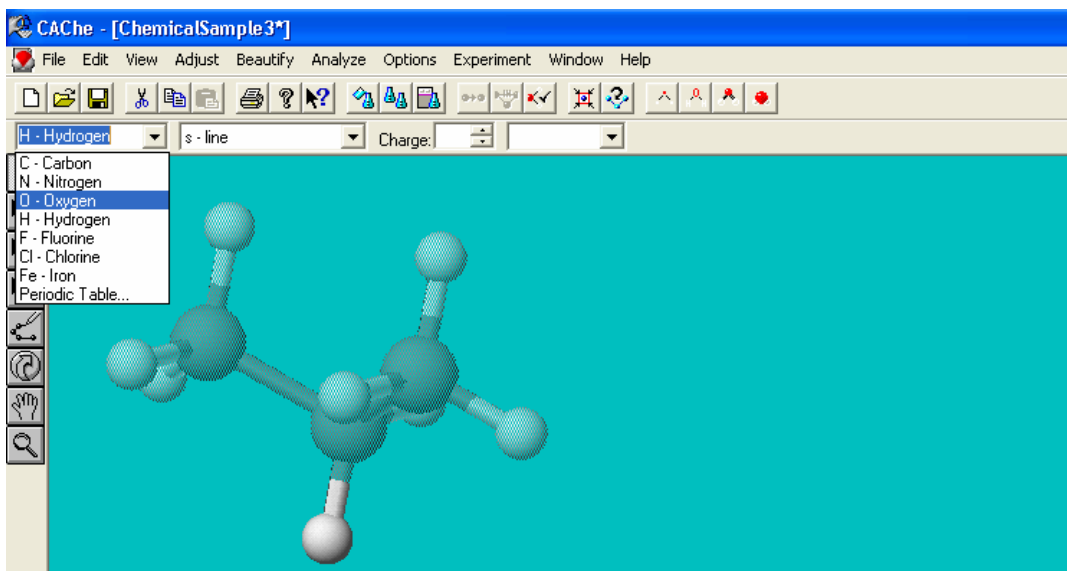
Draw propane by adding a carbon to ethane.
Beautify propane.

7) Save Propane:

Under the *File* drop down menu select *Save As*.
Navigate to the *My Documents* folder.
Save as *Propane*.
If asked to replace a file, select *Yes*.

8) Draw 2-Propanol:

Click on *Select* on the left toolbar.
Select a hydrogen atom on the 2-carbon of propane.
Click on the atom select toolbar above the drawing area.
Select oxygen in the drop down menu.
Beautify 2-propanol.

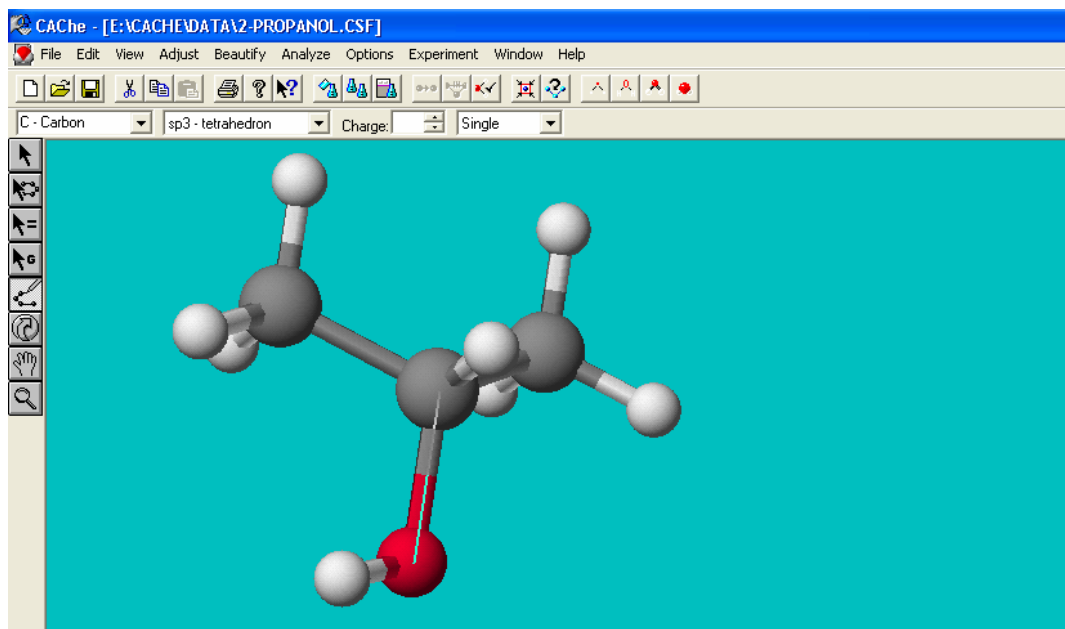


9) Save 2-Propanol:

Under the *File* drop down menu select *Save As*.
Navigate to the *My Documents* folder.
Save as *2-Propanol*.
If asked to replace a file, select *Yes*.

10) Draw Propanone:

Click on *Drawing Pencil* on the left toolbar.
Click on the 2-carbon of 2-propanol.
Drag the cursor to the oxygen.
Release the button to form a new bond.
Beautify propanone.



11) Save Propanone:

Under the *File* drop down menu select *Save As*.
Navigate to the *My Documents* folder.
Save as *Propanone*.
If asked to replace a file, select *Yes*.

12) Open ProjectLeader:

Open the ProjectLeader program located in the *CAChe* folder in the start menu.
This program automatically optimizes geometry of the molecule(s) in question and provides a workstation to run several experiments simultaneously.

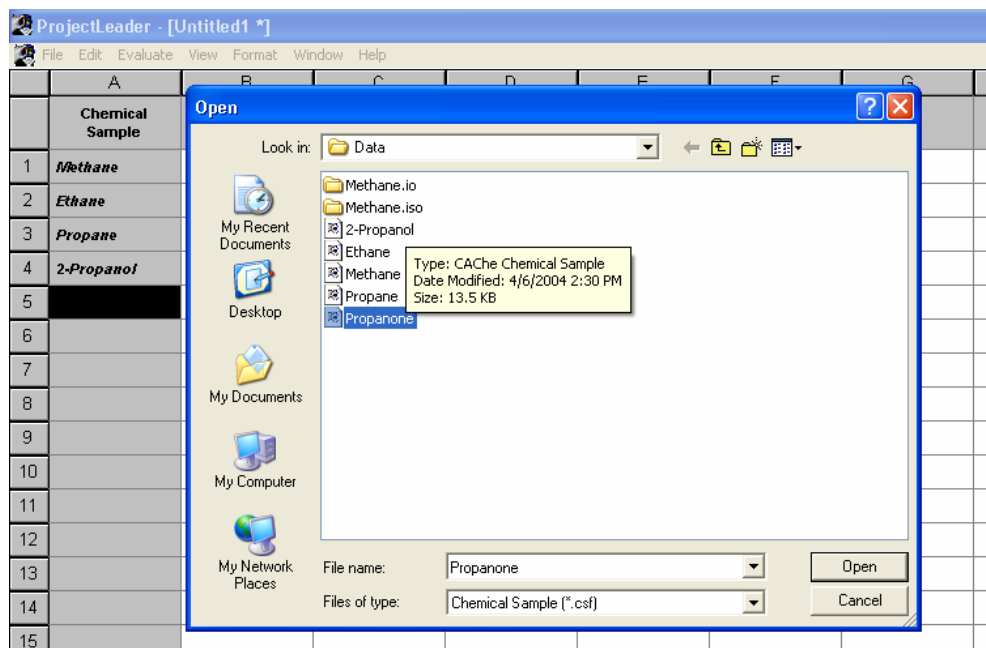
13) Import Molecules:

Double click on the grey cell labeled *A1* (under *Chemical Sample*).

Navigate to the *My Documents* folder.

Double click on *Methane*.

Fill cells *A2-A5* with *Ethane*, *Propane*, *2-Propanol*, and *Propanone*.



- 14) Add the Energy Property:** Double click on the grey cell to the right of *Chemical Sample*. Make sure *Chemical Sample* is selected in the *Property Of* menu and click *Next*. Select *Conformation Minimum Energy* and click *Next*. Select *Standard Procedure* and click *OK*. The grey cell will now contain the words *Conformation Minimum Energy (kcal/mol)*. No data will be displayed yet. This is ok.

The image displays two screenshots of the ProjectLeader software interface, showing the 'Enter Property' dialog box in a spreadsheet environment.

Top Screenshot: The spreadsheet shows a table with columns A-F and rows 1-14. Row 1 is labeled 'Chemical Sample'. The 'Enter Property' dialog box is open, showing the 'Kind' selection options:

- Chemical Sample
- Property of: chemical sample
- Sample Component
- Analysis
- Comment

 The 'Description' field contains the text: "The column will hold a chosen property of the chemical sample."

Bottom Screenshot: The spreadsheet is the same. The 'Enter Property' dialog box is open, showing the 'Kind of property' selection options:

- conformation minimum energy
- connectivity index 0
- connectivity index 1
- connectivity index 2
- dipole moment
- dipole vector X
- dipole vector Y
- dipole vector Z

 The 'Description' field contains the text: "Energy calculated for an optimized conformation of the chemical sample. Depending on which procedure is used, the calculated energy may be steric energy (from Mechanics), heat of formation (from MOPAC) or total energy (from ZINDO). The optimization procedures usually locate a minimum energy conformation near the starting geometry. Consequently, the resulting"

15) Add the Dipole Property:

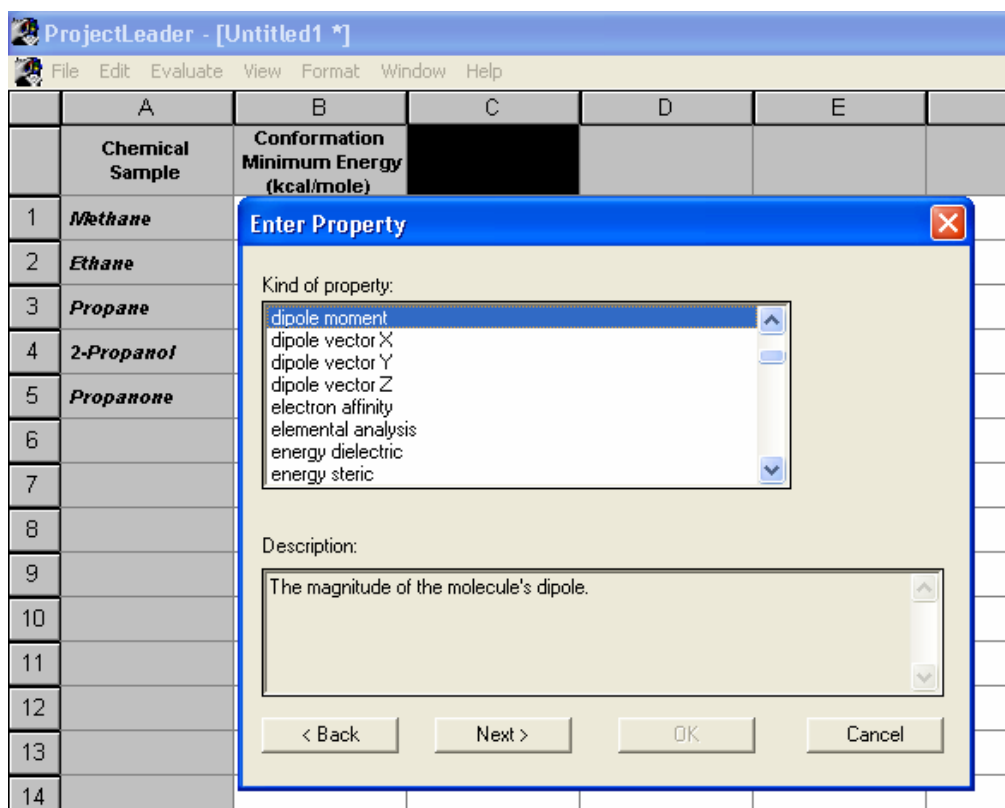
Double click on the grey cell to the right of the newly created property.

Make sure *Chemical Sample* is selected in the *Property Of* menu and click *Next*.

Select *Dipole Moment* and click *Next*.

Select *Standard Procedure* and click *OK*.

The grey cell will now contain the words *Dipole Moment (debye)*.



16) Choose Another Property:

Other properties can be analyzed as well.

View the list of accessible properties.

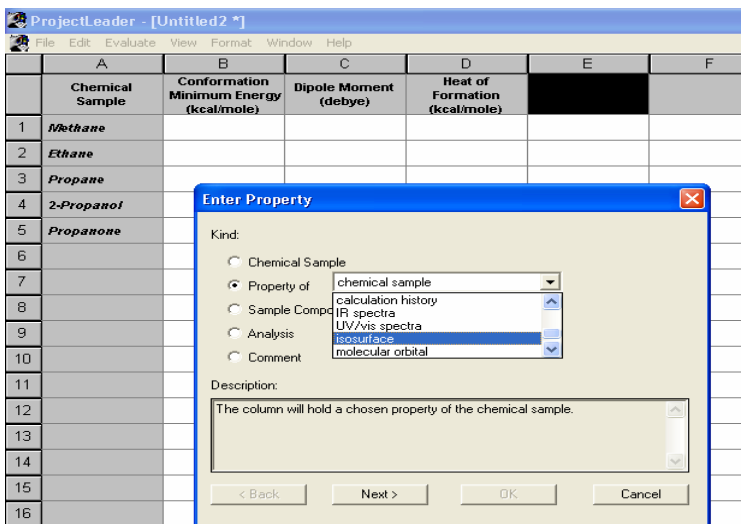
Choose an additional property to analyze.

If asked, select *Extract From Sample*.

If *Manual Entry* is the only option, choose a new property.

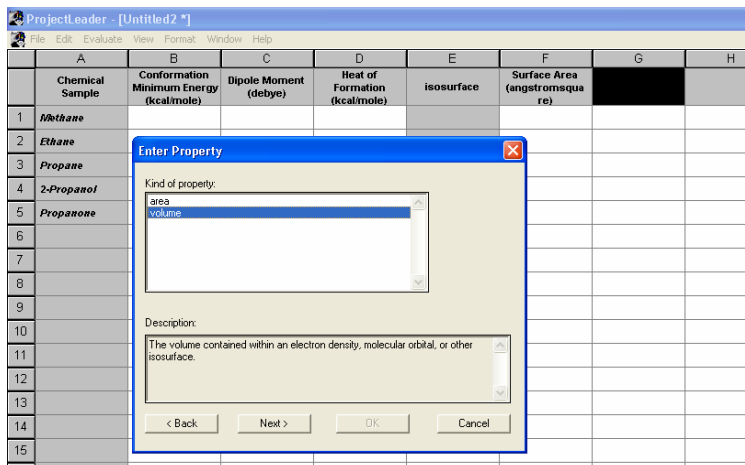
17) Add the Surface Area:

Double click on the grey cell to the right of the newly created property.
Select *Isosurface* in the *Property Of* menu and click *Next*.
Select *Area* and click *Next*.
Select *Standard Procedure* and click *OK*.
Two columns will be occupied, one containing the word *Isosurface* and the other *Surface Area (angstromsquare)*.



18) Add the Volume:

Double click on the grey cell to the right of the newly created property.
Select *Isosurface* in the *Property Of* menu and click *Next*.
Select *Volume* and click *Next*.
Select *Standard Procedure* and click *OK*.
The grey cell will now contain the words *Surface Volume (angstromcubic)*.



19) Analyze the Data:

Using the mouse, highlight the cells contained in the area of the molecules and properties. Under the *Evaluate* drop down menu select *Cell*. Some calculations will occur and the cells will be filled with data.

The isosurface value for each molecule will be shown twice. (Two 1's will be shown, etc.)

Two different isosurface values may be shown.

Select the data for the value at 1.

The second column is an error in the program.

Two different property values may be shown [e.g. Surface Area(1) and Surface Area (2)].

Select the data for the first property.

The second value is for negative surfaces on a dipole map.

The screenshot shows the ProjectLeader software interface with a menu open over the 'Evaluate' tab. The menu options are 'Cell' (Ctrl+E), 'Select Server...', 'Show Server...', and 'Stop Cell Evaluation'. The data table below has the following structure:

		C	D	E	F	G	H
	Chemical Name	Dipole Moment (debye)	Heat of Formation (kcal/mole)	isosurface	Surface Area (angstroms square)	Surface Volume (angstrom cubic)	
1	Methane						
2	Ethane						
3	Propane						
4	2-Propanol						
5	Propanone						
6							
7							
8							

20) Compare the Data:

Compare the data received for each molecule. Rationalize the differences found.