

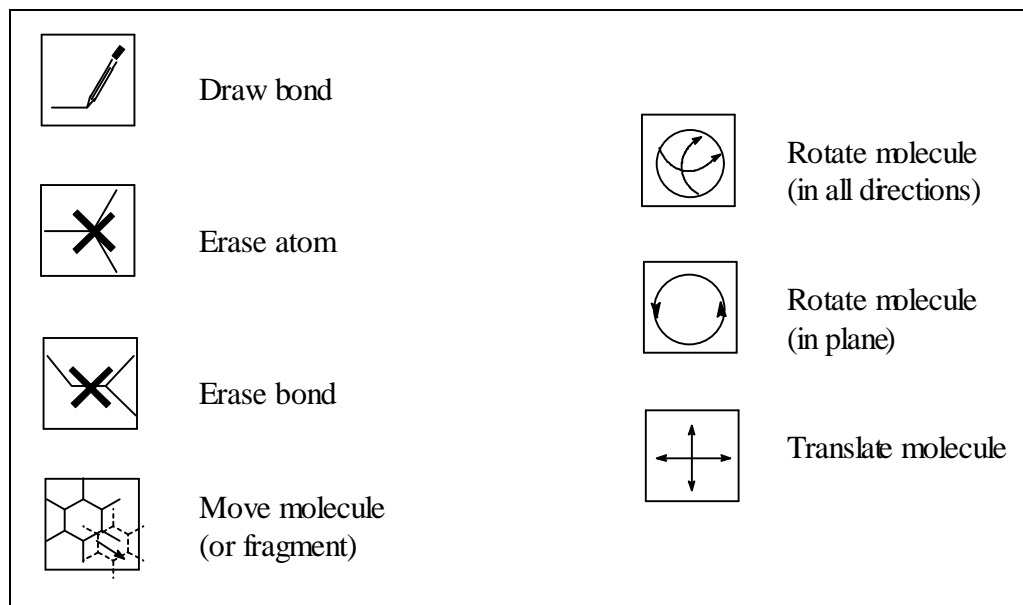
Introduction to Molecular Modeling Using *Alchemy2000* Dr. Ned Martin

(Mouse commands are given as L-click, R-click, or L-hold and drag)

Alchemy2000 tools used in this lesson:

From 2D Sketcher:

From Main menu:



Open Alchemy2000 by L-double clicking on its icon in the Applications Group or by using the Windows Start, Programs option and selecting Alchemy2000. Alchemy2000 opens with a black window in the upper left and a few colored element blocks to the right.

Building a model:

- R-click in the black window to obtain a menu window; select '2D Sketcher'.
- L-hold and drag to the open window on the left the appropriate ring or chain in upper right window after placing the cursor over a 'handle' at any atom (indicated by red square).
- If the available chains are longer or shorter than desired, they can be modified easily:

Adding bonds:

- L-click the 'Draw bond' (pencil) icon in upper left of screen, L-click-L-drag-L-click to draw bond (by default, this is a bond to carbon unless specified otherwise; see next entry).

Placing an atom or group other than C at the end of a bond:

- L-hold and drag into position the desired atom or group from either window at the right side of screen; release when red square appears. If other atoms or groups are needed, see Adding elements not in the 2D Sketcher, below.

Erasing groups or bonds:

- L-click on the 'Erase atom' or 'Erase bond' tool, L-click on an atom or bond to be erased. Do not be concerned about unfilled valences; the program will complete any unfilled valences for you automatically when the structure is converted to a 3D representation (see below).

Testing connectivity:

- L-click the 'Move molecule (or fragment)' tool from the menu at the left, L-hold on any handle (atom) in structure and drag. All connected atoms will move together. Groups/atoms not connected may be connected by L-holding and dragging them to position (at which point a red square will appear), then releasing the mouse.

Adding elements not in the 2D Sketcher

- Elements other than those listed can be added from the Main menu. If an element or group is not available in the 2D Sketcher, select (from the menu bar) 'File', 'Return to 3D' (at bottom of list).
- To obtain elements not listed in the colored boxes to the right, L-click on 'Elements', which opens a window containing a Periodic Table. L-click on the desired element and geometry (hybridization) choices available for that element will appear to the lower right of the screen. L-click on the appropriate one and click on the end of the bond in the active window to which the newly selected element should be attached (or on an atom to be replaced).

Converting to a 3D structure:

- When structure is complete or when it is desirable to render a partial structure in 3D representation, select (from the menu bar) 'File', 'Return to 3D' (at bottom of list).
- This places a structure color coded by atom type in the original black window. Right click within the black window to bring up a window and select '2D to 3D Builder'. This operation uses a very crude algorithm to establish a 3D structure, therefore this structure should be considered only the starting point for further 3D structure calculations.

Rotating the structure in any direction:

- L-click on the 'Rotate molecule (in all directions)' tool, L-hold anywhere in the active window (Alchemy2000 allows several windows with different structures to be displayed simultaneously) and move the mouse to rotate the structure as desired.

Rotating the structure around an axis perpendicular to the plane of the screen:

- L-click on the 'Rotate molecule (in plane)' tool, L-hold anywhere in the active window and move the mouse.

Translating (moving in plane of screen) the structure:

- L-click the 'Translate molecule' tool, L-hold and move mouse in direction you want to move the structure.

Finding the minimum energy (optimum) geometry of a 3D structure:

- On the menu bar L-click 'Compute', 'MM3', and 'Start Calculation'. Be sure that the box labeled 'single point calculation' is not checked. The default method employed under "Compute", 'Molecular mechanics' uses a forcefield (algorithm) called Sybyl, and results from Sybyl are generally not reliable.
- On the menu bar L-click 'Display', 'Molecular Properties'.
- The 'Total Steric Energy' (the sum of the computed energy contributions due to the various interactions in the structure, including the bond length compression/stretch, bond angle bending, van der Waals interactions, torsional interactions, dipole-dipole interactions, H-bonding and others) is at the top of the output, with the computed contributions to the steric energy listed below, along with the computed enthalpy of formation of the structure.
- This input can be moved into an Excel spreadsheet file by selecting 'Export to' and 'Excel'. This opens Excel and copies the data into a spreadsheet file; you may name the file and save it as an .xls file. Close the Molecular Properties window.

Displaying structural measurements (bond lengths, bond angles, and dihedral angles):

- On the menu bar L-click 'Display', 'Measurements', 'Bond Lengths' (or 'Bond Angles' or 'Dihedral Angles') to bring up a table of data for the molecule in the active window. This data may also be exported to an Excel spreadsheet. Each set of data is placed in a separate file (Book 1, Book 2, etc.) but you may combine the data into a single spreadsheet file by cutting (or copying) and pasting.

Determining elemental symbols or atom numbering

- On the menu bar L-click 'Display', 'Labels', and select Symbol (or Number, or Symbol and Number)
- Note that this menu can also be accessed by R-clicking within the active window

Rendering a structure differently:

- On the menu bar L-click 'Display', 'Rendering', select the rendering type desired, 'OK'.
- Note that this menu can also be accessed by R-clicking within the active window

Saving a structure file:

- On the menu bar L-click 'File', 'Save As', and assign the file a name. (Be sure to save files to your own floppy disk in drive A:) Alchemy2000 saves all information about a structure and allows recall of molecular properties and measurements upon re-opening the file without further calculation. Files of small organic molecules typically take 1 to 4 KB of disk space, but files of polypeptides may take 500KB or more.

It is important to realize that the calculated components of the steric energy are based on rather simplistic algorithms, and little physical significance should be placed on energy values of the individual components. Most forcefield methods have been parametrized for certain types of structures so that, for similar types of structures, the overall results (steric energy and enthalpy of formation) are usually quite close to experimental values.