Note: The complete HyperChem Lite manual is available in electronic form on your software CD. When you install the software, the Adobe Acrobat reader will be installed on your computer; you can use it to read the manual.

What is HyperChem Lite?

HyperChem Lite™ is a molecular modeling and simulation program that lets you perform complex chemical calculations.

Use the Glossary at the back of this book to look up terms and concepts you might be unfamiliar with. Use the master index to find subjects in this Reference Manual.

HyperChem Lite includes these functions:

- Drawing molecules from atoms and converting them to three-dimensional (3D) models
- Using molecules from other sources; for example, HyperChem molecular dynamics snapshot (*.SNP) files
- Rearranging molecules by, for example, rotating and translating them
- Changing display conditions, including stereo viewing, rendering models, and structural labels
- Setting up and directing chemical calculations, by molecular mechanical or semi-empirical quantum mechanical methods
What is HyperChem Lite?

HyperChem Lite: Summary of Major Functions

Creating and Editing
- draw molecules in 2D

Model Building
- Model Builder
- approximate 3D structures

Calculations
- single point
  - MM QM
  - total energy of one configuration
- geometry optimization
  - MM
  - a stable configuration

MM = Molecular mechanics
QM = Semi-empirical quantum mechanics
Sending Messages to the List

To send a message to all subscribers of the list, address your email message to:
hyperchem@hyper.com

These are Internet addresses. You can also send E-mail to Internet through gateways from other networks, including BITNET, CompuServe, and JANET. Contact your network administrator for details.

Messages sent to hyperchem@hyper.com are forwarded to all subscribers. Please do NOT send administrative messages such as requests for subscription and unsubscription to this address!

A Guide to Using HyperChem Lite

Note: The complete HyperChem Lite Manual is provided on the CD. It contains detailed tutorials and reference material, and describes features not covered in this document. From the Windows Program Manager or Explorer, open the Manual folder and double-click on a file to read it.

Introduction

This guide contains information on the following:

- opening a file
- moving and resizing molecules
- changing molecular display (rendering)
- drawing and modifying structures
- converting a 2-D sketch to a 3-D structure
- measuring angles and distances
- computing and viewing electronic properties
- playback of molecular dynamics simulations
- on-line help.
A Guide to Using HyperChem Lite

Opening a File

A collection of pre-built structures is supplied with HyperChem. From the File menu, choose Open. “.HIN” files are displayed automatically. Choose one and click on Open to begin. Additional files are found in the “Samples” folder (D: Samples).

Moving and Resizing Molecules

L-click on a toolbar icon to activate the desired tool. To use the tool in the workspace, hold the left mouse button down while moving the mouse.

Use the:

- X, Y-Rotation Tool to rotate about x- and y-axes.
- Z-Rotation Tool to rotate about the z-axis.
- X, Y-Translate Tool to move in x,y-plane
- Zoom Tool (L-drag up/down in the workspace) to enlarge or shrink the image.

Note: The x- and y- axes lie in the plane of the workspace, with x horizontal and y vertical. The z- axis is perpendicular to the plane of the workspace.

Changing Molecular Display

Under the Display menu, choose Rendering and then select the desired rendering style. Use the F2 key to toggle between the current and last-used renderings.

Drawing and Modifying Structures

L-click on the Draw Tool to activate it. Under the Build Menu, un-check Explicit Hydrogens.
Adding an Atom: First choose the element to be added: double L-click on the Draw tool to bring up the Element Table; L-click on desired element. L-click in the workspace to place one atom.

Drawing a Chain or Ring: Choose the desired element, then L-drag and release to place two connected atoms. Repeat to draw a chain or ring.

Suggestion: It is often easier to draw a structure with one element (for example, carbon) and then go back and change the heteroatoms after building.

Changing an Atom: Click on top of an existing atom to change its type to the current default element.

Deleting an Atom: R-click on the atom to be deleted with the Draw Tool active.

Connecting Atoms: L-click and drag from first to second atom.

Increasing or Decreasing the Bond Order: L-click on the center of a bond to toggle between single, double, triple, and aromatic.

Modifying Bond and Torsion Angles: Use the Select Tool to select the angle of interest. Under the Edit Menu, choose Set Bond Angle or Set Bond Torsion, and enter the desired value in the dialog box. Alternate Rotation of Torsion Angle (slightly tricky but worth it): with the select tool, double-L-click on one side of the rotation bond. Note that this selects all the atoms in the molecule on that end of the bond. Now activate the Z-Rotate tool ⌘ and R-drag to rotate the selected fragment about the rotation bond.

Converting a 2-D Sketch to a 3-D Structure

Quick Cleanup and Conversion of 2D Sketch: Under the Build Menu, choose Add H and Model Build; or double-L-click on the Select tool icon.

Molecular Mechanics Geometry Optimization. Under the Setup Menu, choose Molecular Mechanics. Under the Compute Menu, choose Geometry Optimization. Set Convergence Criterion and Maximum # cycles as desired; typical values are 0.1 and 100.

The MM+ energy is reported in the status line and the optimized structure is displayed.
Measuring Angles and Distances

Verify that both Atoms and Multiple Selections are checked (under the Select Menu. L-click on the Select Tool to activate it.

Measuring the Distance Between Atoms: With the Select tool active, L-click on each atom. The distance is reported in the status line at the bottom of the screen. R-click in the workspace to deselect the atoms.

Measuring a Bond Angle: L-click on the three atoms that define the angle; its value is reported the status line at the bottom of the screen. R-click in the workspace to deselect the angle.

Measuring a Torsion Angle: L-click on the atoms that define the angle; alternatively, L-drag from atom 1 to atom 4 of an angle 1-2-3-4. The angle is reported in the status line at the bottom of the screen. R-click in the workspace to deselect the angle.

Computing and Viewing Electronic Properties

Extended Hückel Calculation. Under the Setup Menu, choose Extended Hückel; then choose Options to set charge, etc. Under the Compute Menu, choose Single Point. The total energy is reported in the status bar.

View Orbitals and Charge Density. Under the Compute Menu, choose Orbitals. L-drag from top-left to bottom-right to zoom in on part of the energy level diagram. Choose Labels to see occupancy. To see charge or spin density, under Compute choose Contour Plot.

Molecular Dynamics Playback

These instructions are very condensed and meant to provide only a brief guide to use of this feature. Consult the HyperChem Lite Manual on your HyperChem Lite CD for detailed instructions.

To view dynamics simulations of chemical reaction and other snapshot files, with Display/Rendering set to Shaded Spheres, open a file from D:\Samples\Dynamics; for example, open elim_1.hin to view a simulation of an elimination reaction. Then under the Compute menu, choose Molecular Dynamics. Settings used to generate the file are visible. Click on Proceed to initiate playback.