CS Chem3D for Apple Macintosh

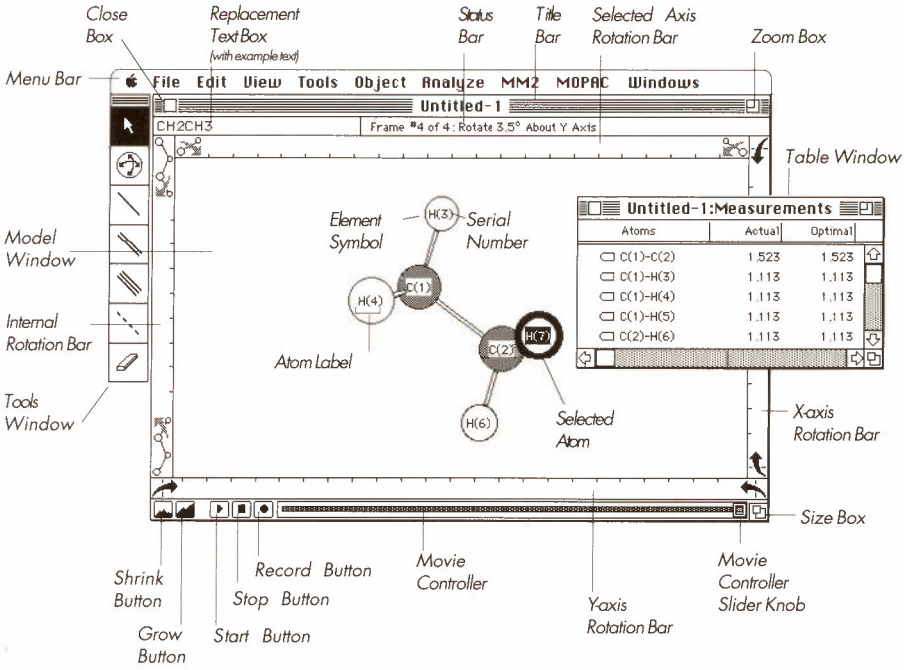
CambridgeSoft Corporation

Desktop Chemistry Software Leader

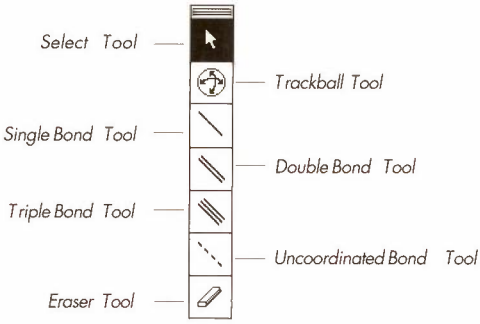
Chem3D for Macintosh

Quick Reference

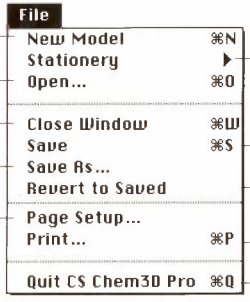
Window Elements



Tools



Menus



Create a new model window.

Open or import a model.

Close the active window.

Save a copy of the active model with a different name, location or file type.

Set paper size and other options affecting the printed output of your model.

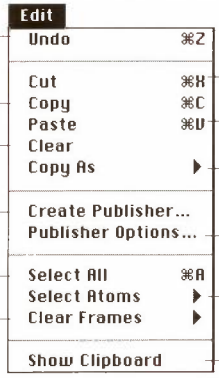
Display a submenu containing stationery in creating new models.

Save the active model to a file.

Discard changes to the active model since it was last saved.

Set print options and print your model.

Close the *Chem3D* application.



Undo your last action.

Copy selection to the Clipboard.

Delete selection from the active window.

Publish the current model in an edition file.

Select all atoms and bonds in a model, all text in the text box or all records in a table window.

Display a submenu where you can choose to delete all frames after the current frame before the current frame, or all but the current frame.

Remove selection and copy it to the Clipboard.

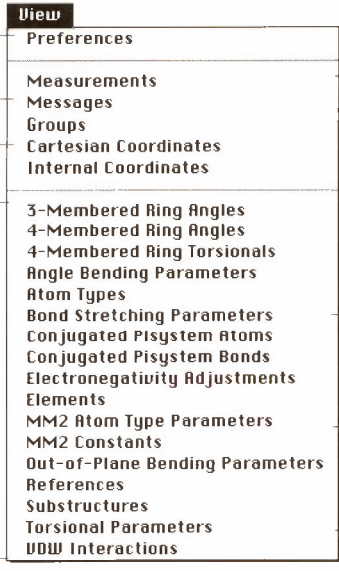
Place contents of the Clipboard into active window.

Display a submenu with a command for copying the active model to the Clipboard as a QuickTime™ movie or a two-Dimensional *ChemDraw* structure.

Set options for the published model regarding updating of the edition file.

Display a submenu with commands for selecting specific atoms within your model.

Display contents of the Clipboard.



Set options in control panels that affect building, analyzing and displaying your model.

Display any messages generated for the model.

Display the Cartesian coordinates for all atoms in the model.

Display tables containing parameters for building models and performing analyses.

Information in tables can be edited using the *Table Editor* application.

Display all measurements previously generated for the model.

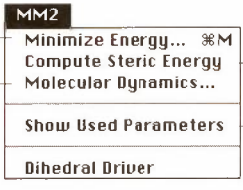
Display all groups defined for the model.

Display all distances and angles used to position atoms in the model.

Display a table of atom types you can use for building models.

Display a table of all elements you can use for building models.

Display a table of substructures you can use for building models.

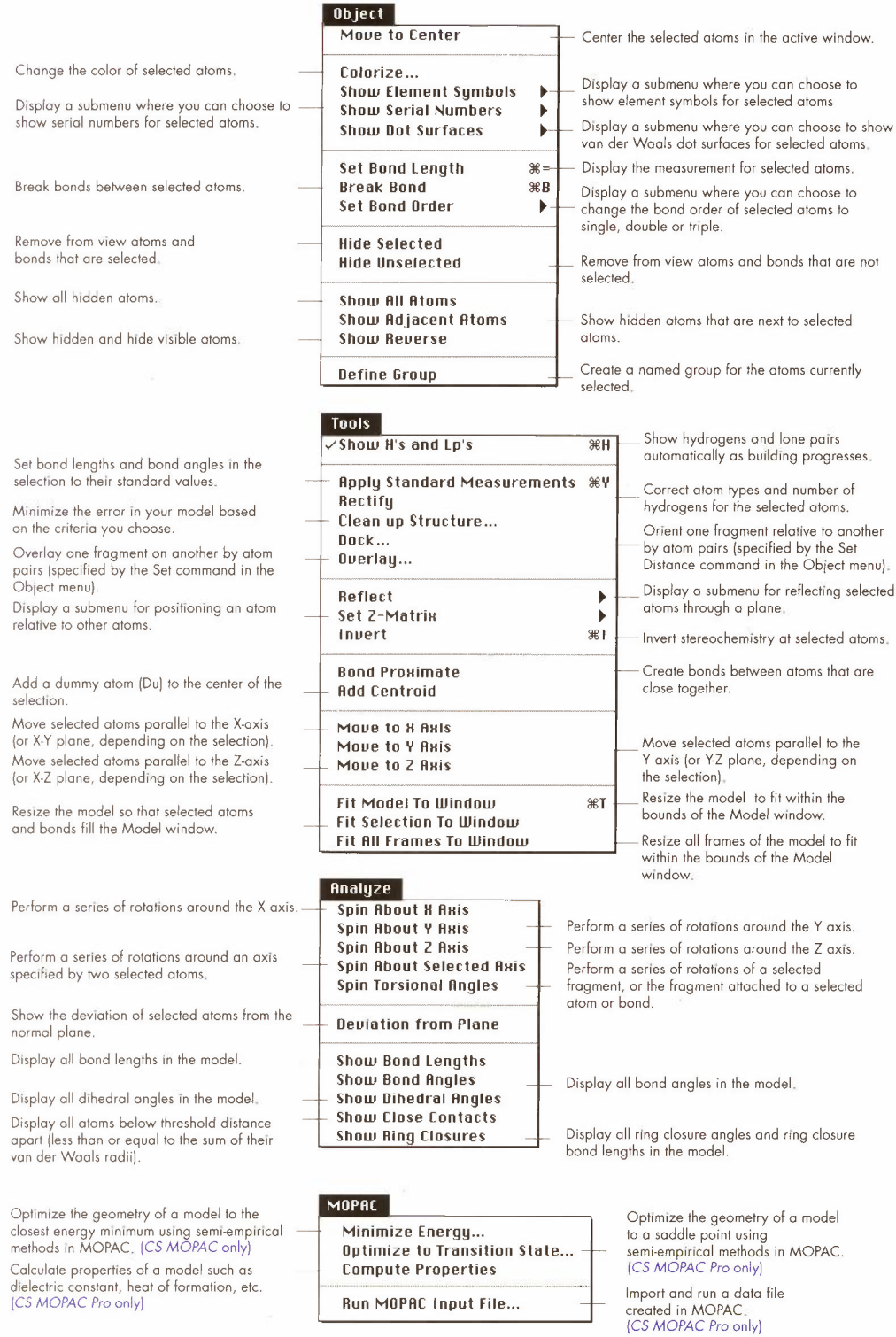


Optimize the geometry of a model to the closest energy minimum using molecular mechanics methods.

Perform a molecular dynamics computation using settings in the Molecular Dynamics control panel.

Calculate the steric energy of the model at the current conformation.

Display a list of parameters used in an MM2 analysis of the current model.


Object
Move to Center
Center the selected atoms in the active window.
Change the color of selected atoms.
Colorize...
Display a submenu where you can choose to show element symbols for selected atoms
Show Element Symbols
Display a submenu where you can choose to show serial numbers for selected atoms.
Show Serial Numbers
Display a submenu where you can choose to show van der Waals dot surfaces for selected atoms.
Show Dot Surfaces
Set Bond Length ⌘=
Display the measurement for selected atoms.
Break bonds between selected atoms.
Break Bond ⌘B
Display a submenu where you can choose to change the bond order of selected atoms to single, double or triple.
Set Bond Order
Remove from view atoms and bonds that are selected.
Hide Selected
Hide Unselected
Remove from view atoms and bonds that are not selected.
Show all hidden atoms.
Show All Atoms
Show Adjacent Atoms
Show hidden atoms that are next to selected atoms.
Show hidden and hide visible atoms.
Show Reverse
Define Group
Create a named group for the atoms currently selected.
Tools
✓Show H's and Lp's ⌘H
Show hydrogens and lone pairs automatically as building progresses.
Set bond lengths and bond angles in the selection to their standard values.
Apply Standard Measurements ⌘Y
Rectify
Correct atom types and number of hydrogens for the selected atoms.
Minimize the error in your model based on the criteria you choose.
Clean up Structure...
Dock...
Overlay...
Orient one fragment relative to another by atom pairs (specified by the Set Distance command in the Object menu).
Overlay one fragment on another by atom pairs (specified by the Set command in the Object menu).
Display a submenu for positioning an atom relative to other atoms.
Reflect
Set Z-Matrix
Invert ⌘I
Display a submenu for reflecting selected atoms through a plane.
Invert stereochemistry at selected atoms.
Add a dummy atom (Du) to the center of the selection.
Bond Proximate
Add Centroid
Create bonds between atoms that are close together.
Move selected atoms parallel to the X-axis (or X-Y plane, depending on the selection).
Move to X Axis
Move to Y Axis
Move to Z Axis
Move selected atoms parallel to the Y axis (or Y-Z plane, depending on the selection).
Move selected atoms parallel to the Z-axis (or X-Z plane, depending on the selection).
Resize the model so that selected atoms and bonds fill the Model window.
Fit Model To Window ⌘T
Fit Selection To Window
Fit All Frames To Window
Resize the model to fit within the bounds of the Model window.
Resize all frames of the model to fit within the bounds of the Model window.
Analyze
Perform a series of rotations around the X axis.
Spin About X Axis
Spin About Y Axis
Spin About Z Axis
Spin About Selected Axis
Spin Torsional Angles
Perform a series of rotations around the Y axis.
Perform a series of rotations around the Z axis.
Perform a series of rotations around an axis specified by two selected atoms.
Perform a series of rotations of a selected fragment, or the fragment attached to a selected atom or bond.
Show the deviation of selected atoms from the normal plane.
Deviation from Plane
Display all bond lengths in the model.
Show Bond Lengths
Show Bond Angles
Display all bond angles in the model.
Display all dihedral angles in the model.
Show Dihedral Angles
Display all atoms below threshold distance apart (less than or equal to the sum of their van der Waals radii).
Show Close Contacts
Show Ring Closures
Display all ring closure angles and ring closure bond lengths in the model.
MOPAC
Optimize the geometry of a model to the closest energy minimum using semi-empirical methods in MOPAC. (CS MOPAC only)
Minimize Energy...
Optimize to Transition State...
Compute Properties
Optimize the geometry of a model to a saddle point using semi-empirical methods in MOPAC. (CS MOPAC Pro only)
Calculate properties of a model such as dielectric constant, heat of formation, etc. (CS MOPAC Pro only)
Run MOPAC Input File...
Import and run a data file created in MOPAC. (CS MOPAC Pro only)

Preferences Control Panels

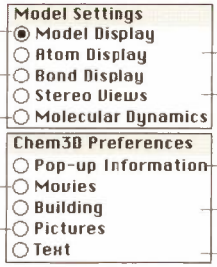
Change the rendering type for a model, atom coloring and fill and background color.

Specify the bond width and fill patterns.

Specify settings for performing molecular dynamics computations.

Specify how views of your model are captured for creating movies.

Specify whether PostScript information is included with pictures copied to the Clipboard.



Specify the font and size of atom labels, and display of dot surfaces, serial numbers and element symbols.

Specify whether stereo views of your model appear.

Change which information appears when you point at or hold down the mouse button over a bond or atom.

Specify what commands are automatically applied to your model as you build.

Specify the font and font size of text used in table windows.

Selecting

Select an atom or bond.	Click an atom or bond.
Add atoms or bonds to the selection.	Shift+click atoms or bonds not currently selected.
Remove atoms or bonds from the selection.	Shift+click atoms or bonds currently selected.
Select several atoms and bonds.	Drag diagonally across model using Select tool.
Deselect all atoms and bonds.	Click in empty space in the Model window.

Building

Change a bond type.	Drag over the bond using a different bond tool.
Change an atom type using the Replacement Text box.	Select an atom(s), type atom type (e.g. H Enol), press Enter.
Change an element using the Replacement Text box.	Select an atom(s), type an element (e.g. N or NH2), press Enter.
Reserialize atoms using the Replacement Text box.	Select an atom(s), type a starting number, press Enter.
Add a substructure using the Replacement Text box.	Select an atom(s), type a substructure (e.g. OEt), press Enter.
Create a dummy atom using a bond tool.	Click and drag using the Uncoordinated bond tool.
Move an atom.	Select and drag an atom.
Pull atoms towards you.	Option+drag the atoms down.
Push atoms away from you.	Option+drag the atoms up.
Convert a *ChemDraw* structure into a model.	Copy structure to Clipboard and Paste into *Chem3D*.
Place picture of a model in a *ChemDraw*.	Copy model to Clipboard and Paste into *ChemDraw*.
Convert a model into a *ChemDraw* structure.	Choose Copy *ChemDraw* Structure from Edit menu.

Rotating

Open the Rotate dialog box.	Double-click Rotation bar.
Rotate using the last entered rotation amount.	Triple-click a Rotation bar.
Rotate selected fragments.	Drag a rotation bar.
Rotate all fragments regardless of selection.	Shift+drag a rotation bar.
Save rotation frames as a movie.	Click the Record button before performing a rotation.
Stop recording frames.	Click the Stop button.
Replay recorded frames.	Click the Start button or drag the Movie Controller Slider knob.

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