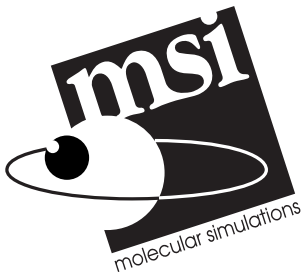
Cerius^2

Modeling Environment

April 1999

(Last Full Revision July 1998)



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Contents

1 How To Use This Guide

Important

If this is the first time you've used Cerius^2, please skip this chapter for now and go directly to *Introducing Cerius2*.

This documentation set, *Cerius^2 Modeling Environment*, is a complete guide to the Cerius^2™ modeling environment. It describes the integrated set of tools for session management and atomistic modeling that form the core of the Cerius^2 modeling environment. Topics described include molecular modeling tasks and their associated Cerius^2 procedures, combining conceptual, procedural, and reference material in one comprehensive information source.

Using this guide

You need not read this entire documentation set before you start using Cerius^2:

- First-time users should read *Introducing Cerius2* first.
- Everyone should read *How To Use This Guide*, which introduces the Cerius^2 modeling environment, and at least skim these sections, which describe how to perform basic modeling tasks:

  The Cerius2 Interface

  Building Models

  Managing Models and Sessions

  Geometry Analysis

  Viewing and Displaying Models
- You can glance through the headings in these sections, which describe modeling and other tasks that typically are performed less often or by fewer users:

  Enhancing Model Display

  Working with Graphs

  Working with Tables

Scripts and Licensing

Customizing the Interface

You can then read those sections that describe the tasks you want to perform and / or tools you want to use.

- Reference material is contained in these sections:

  References

  Definitions

  Mouse and Keyboard Actions

  File Formats

Who should use this guide

This documentation set is intended mainly for day-to-day users of Cerius^2 and should be of interest to all users, regardless of the type of work you are doing or the application modules you are using. *Enhancing Model Display* might also be used by a technical graphic artist in collaboration with a scientist-user of Cerius^2.

Prerequisites

You should already be familiar with:

- The windowing software on your workstation.
- Use of the mouse on your workstation.
- Basic UNIX commands.

Your workstation should have:

- A licensed copy of Cerius^2 installed.
- A home directory in which you have write permission.

Additional information sources

On-screen help

On-screen help is available within the Cerius^2 environment. It is accessed by clicking the right mouse button while the cursor is over the item in the interface about which you want information.

A brief identification of some items appears when you simply allow the cursor to linger over them. Additional help and some demos are accessed from the **Help** menu.

Other Cerius^2 documentation

You can find additional information about Cerius^2 in several other documentation sets:

- *Cerius^2 Builders*—Discusses the specialized builder modules that can be added to supplement the basic model sketching capabilities provided by the Cerius^2 modeling environment (that is, the Analog Builder, Crystal Builder, Surface Builder, Interface Builder, Polymer Builder, and Amorphous Builder modules).
- *Cerius^2 Tutorials*—Several guides illustrating the use of Cerius^2.
- *Forcefield-Based Simulations*, *CDiscover*, and *Cerius^2 Simulation Tools*—Discuss forcefields and orcefield-based calculations; CDiscover in the Cerius^2 and standalone modes; and the Open Force Field, Force Field Editor, Charges, Minimizer, Dynamics Simulation, and Analysis modules.
- *Command Script Guide*—Shows how to capture and replay a script of Cerius^2 commands and how to enhance your command scripts with the features of the Tool Command Language (Tcl).
- *Cerius^2 Installation and Administration Guide*—Provides step-by-step instructions for installing and administering Cerius^2 in your operating environment.

Typographical conventions

Unless otherwise noted in the text, *Cerius^2 Modeling Environment* uses these typographical conventions:

- Terms introduced for the first time are presented in *italic* type. For example:

Instructions are given to the software via *control panels*.

- Keywords in the interface are presented in **bold** type. In addition, slashes (/) are used to separate a menu item from a submenu item. For example:

  Select the **View/Colors...** menu item means to click the **View** menu item, drag the cursor down the pulldown menu that appears, and release the mouse button over the **Colors...** item.

- Words you type or enter are presented in **bold** type. For example:

  Enter **0.001** in the **Tolerance** entry box.

- UNIX command dialog and file samples are represented in a `typewriter` font. For example, the following illustrates a line in a .grf file:

```
CERIUS Grapher File
```

- Words in *italics* represent variables. For example:

```
> cerius2 -b outputfile scriptfile
```

  In this example, the actual name of the file to which text output should be directed replaces the value *outputfile*, and *scriptfile* is replaced with the name of a file containing the desired command script.

2 Introducing Cerius^2

Why read this section

If you've never used Cerius^2 before, please go through this section first! The idea is just to get you familiar with using basic controls in the interface, then you can find details on how to use these and other controls for your own scientific problems in other sections.

If it's been a while since you've used Cerius^2 or you just want a quick summary of some basic activities, you may start with *Starting Cerius2* and then skip to parts you find interesting.

This section includes instructions for:

Starting Cerius2

Building a model—caffeine

Saving a model

What you can do with a model display

Building another model—ferrocene

Reading in additional models

Managing multiple models

Printing a model

Controlling the 3D display

Exploring Cerius2 on your own

Prerequisites

- You need to have Cerius^2 already installed on your system (your own machine or an accessible machine on your in-house network).

  Either you or you system administrator should have done this, with the help of the *Cerius^2 Installation and Administration Guide*.

- You need to know how to log in to your machine, how to get around in your directory structure, and the basics of managing

your file system and working with your machine's user environment (see, for example, Todino & Strang 1990).

- You need a home directory in which you have write permission and can create subdirectories.
- You need to know how to start up Cerius^2 on your machine.

  Whoever installed Cerius^2 at your site can tell you how to start it. If their instructions differ from those given under *Starting Cerius2*, please follow the instructions for starting Cerius^2 *at your site.*

Layout of this section

> In general, activities that you must perform if you want this tutorial to work as designed are contained in boxes like this.

Optional activities are in plain text (not in boxes).

Explanations of what you are doing are in italics.

Note

If you want to perform only some of the optional activities or are interrupted and need to redo some of the initial activities, you need read only the boxed information.

Additional information

Detailed information on how to carry out the activities introduced in this section (as well as other activities) is contained in the other sections of this documentation set.

Starting Cerius^2

1. Preparing a work area

Starting in your home directory, you should first go to or make a subdirectory in which to run this tutorial. Do this by entering, for example, the following at your system prompt:

```
>cd
>mkdir CeriusIntro
>cd CeriusIntro
```

2. Starting Cerius^2

Enter at your system prompt:

```
>cerius2
```

Cerius^2 is a large program, and it takes a few moments for it to load and appear on your screen. Additional information on starting Cerius^2 can be found under Starting Cerius2.

If an outline of a window attaches to your cursor instead of being placed on the screen, use the mouse to move the outline to the upper left corner of your screen and click there to place a large black window labelled Cerius2 Models.

If nothing happens

It's possible that Cerius^2 was installed so that you need to use some other command to start it at your site. Please ask an experienced user at your site, or your system administrator, for this information. If *you* installed Cerius^2 and can't start it, please see the *Cerius^2 Installation and Administration Guide* and the Cerius^2 release notes for troubleshooting information. If after this you're still having trouble, please contact MSI's Customer Support, for example by sending email to support@msi.com.

3. Getting acquainted with the interface (optional)

Please feel free to take some time to explore the Cerius^2 interface on your own. You can't break anything!

Try using the left and right mouse buttons to click various buttons and other controls. If a list of items appears, continue to hold the left mouse button down and release it over an item to choose that item.

Try building or loading a model, if you want.

Important

If you do anything in this optional step, you should clean up the interface so that you can make a fresh start when you begin building your first model, as follows:

Use the mouse to move the cursor over the **File** menu at the top left corner of the main control panel. Click with the left mouse button and drag the cursor down to **New Session**. Release the mouse button. When a small window labelled Re-initialize All... appears, click its **Confirm** button with the left mouse button.

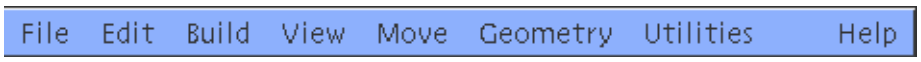
Everything now goes back to its condition when Cerius^2 first loaded. If you moved any main windows, you should put them back to where they were when you started.

You can close any open control panel by left-mouse clicking in the box  in its upper right corner.

Building a model—caffeine

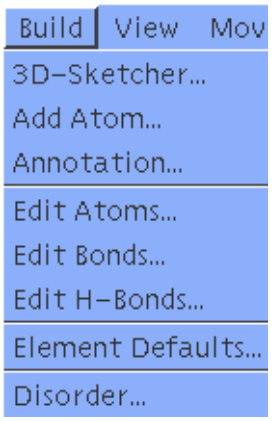
4. Locating the basic building tool

The top of the Visualizer main panel contains a menu bar (a row of menus) that looks like this:



Use the mouse to move the cursor over **Build** in the menu bar. Press and hold down the left mouse button.

A list of menu items, or pulldown menu, *appears:*



Continue to hold the left mouse button down, use the mouse to drag the cursor downwards, and release the mouse button over the **3D–Sketcher…** item in the list.

In other words

Select the **Build/3D–Sketcher…** menu item.

A window labeled Sketcher appears. This control panel *contains basic model-building tools.*

5. Sketching the ring system of caffeine

You will not necessarily build caffeine in the quickest possible way, since we want to show how several different sketcher tools work.

Locate the template tool in the Sketcher control panel. It is labeled **phenyl**, since a phenyl ring is the default template.

The template tool looks like:

Use the mouse to move the cursor over the template tool and click once with the left mouse button.

In other words

Click the template tool. (Always use the left mouse button to click items, unless otherwise indicated.)

The phenyl template tool changes color, indicating that it is active, and if you move the cursor into the large window, you will see that the cursor has changed to a T shape.

Move the cursor into the large window labelled Cerius2 Models.

Definition

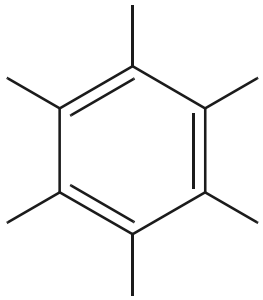
This is called the model window.

Click once near the center of the model window.

A benzene fragment appears, but it is not oriented conveniently.

Move the cursor so it's near any edge of the model window. Then hold down the *right* mouse button and move the cursor parallel to the closest edge of the window until one of the double bonds is vertical and on the right side of the fragment.

The model should now look something like this:



Note

Atoms are color-coded in the model window: the grey bonds connect two carbon atoms; and the half grey / half white bonds connect hydrogens (white) with carbons (grey). Atoms are not emphasized in the current display style, but one is located at the end of each bond.

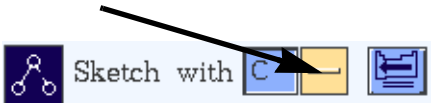
Click the **Sketch with** tool.

*The **Sketch with** tool looks like:*

The control panel indicates that you will sketch with C, whereas the ring you want to add contains 2 N's and only one C. So it might be more efficient to sketch with N instead of C:

Locate the popup control to the right of the **Sketch with C** entry box.

In other words, this control:

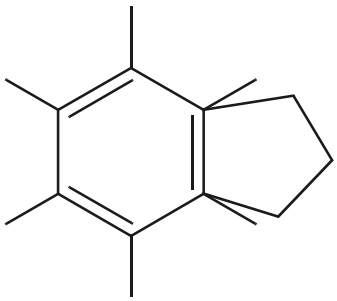


Click the popup control, then, while continuing to hold the left mouse button down, drag the cursor down and then release it over the **N**.

In other words

Choose **N** from the **Sketch with** popup.

In the rest of this step, you will try to make your model look something like this:



In the model window, click the carbon at the top end of the double bond on the right side of the model.

You will hear a beep to confirm that you succeeded in hitting the atom.

Move the cursor up and towards the right.

A dashed line follows the cursor, connecting it with the atom you

clicked and indicating where the bond to your next atom will lie.

Click in three places to the right of that double bond, then click the carbon atom at the bottom end of that double bond, forming a 5-membered ring that's fused with the 6-membered ring.

The new lines are blue-ish, indicating that all three atoms that you just added are nitrogens. The two carbons on the right side of the 6-membered rings now have too many bonds emanating from them. And the 5-membered ring might be oddly shaped. But don't worry—you'll correct these problems later.

If you make a mistake

The Sketcher control panel contains an **UNDO** button. It is active only when the previous Sketcher activity *can* be reversed.

If you really make a mess of your model, you can select the **Edit/Select All** menu item and then the **Edit/Delete** menu item to erase the entire model. Then start again at the beginning of Step 5.

6. Adding R groups to the basic ring structure

Cerius^2 often offers several ways of accomplishing the same activity, allowing you to use whatever method you find convenient. We'll demonstrate two different ways of adding groups of atoms to a model. But first we'll show a different way of changing the atom that you'll be sketching with .

Click in the **Sketch with** text entry box.

The N becomes highlighted. Anything you type in the box will now replace the N.

Type a **C** in the **Sketch with** text entry box and either press <Enter> on your keyboard or click anywhere else on the control panel.

In other words

Enter **C** in the **Sketch with** text entry box.

Click the bottom carbon in the 6-membered ring, then click below that carbon.

This adds a carbon, which will become a methyl group when you correct the hydrogens later.

(You may want to look at the picture of a complete caffeine model under Cleaning up the conformation for help in sketching your model.)

Here's another way of adding a methyl group:

Click the **Templates...** button in the Sketcher control panel.

*The **Templates...** button looks like:*

*Clicking the **Templates...** button causes the Sketcher Template control panel to appear. This control panel contains a file browser that*

allows you to navigate among directories and load selected files.

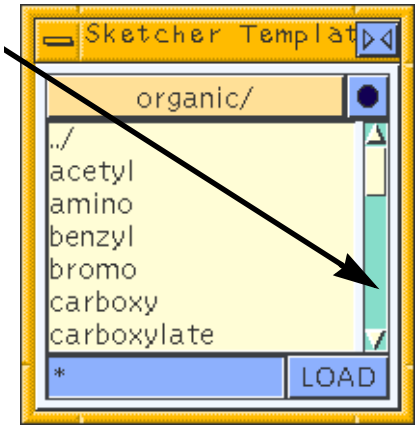
In the Sketcher Template control panel, double-click **organic/**.

This opens the directory named organic and displays a list of the filenames that are inside that directory.

Now scroll down the items in the list of filenames by clicking below the slider on the scroll bar to the right of the list box.

Stop when you see the filename methyl.

That is, click here:



You can also move the slider by clicking it, then dragging it down till you see the methyl filename.

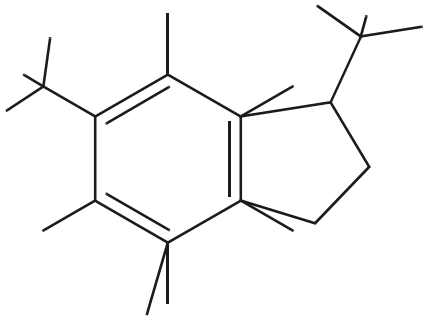
Click **methyl** and then click the **LOAD** pushbutton.

*The text next to the template tool in the Sketcher control panel becomes **methyl**, and the template tool is now active (highlighted).*

In the model window, click the hydrogen atom that's attached to the carbon atom in the upper *left* part of the 6-membered ring.

Next, click the uppermost N in the 5-membered ring.

Your model should now look approximately like this:



7. Correcting the atom types

In the Sketcher control panel, find and click the **Edit Element** tool.

*The **Edit Element** tool looks like:*

*The text entry box for this tool is already set to **C**.*

Click the middle N in the chain of N's in the 5-membered ring.

The two half-bonds connected to this atom become grey, indicating that the atom has been changed to carbon.

Change the **Edit Element** type to **O**, by choosing **O** from the associated popup or by entering **O** in the **Edit Element** text entry box.

Click the top H on the 6-membered ring.

Red indicates an oxygen atom.

Now click the bottom-left hydrogen that's directly attached to the 6-membered ring.

Change the **Edit Element** type to **N**.

Click each of the (two) carbons in the 6-membered ring to which the methyl groups are attached.

(Remember, the methyl group at the bottom of the 6-membered ring does not yet look *like a methyl group.)*

8. Correcting the bond order

In the Sketcher control panel, find and click the **Edit Bond** tool.

*The **Edit Bond** tool looks like:*

*The **Edit Bond** popup is already set to **SINGLE**.*

Click one of the nitrogens in the 6-membered ring.

Next click the carbon at the other end of the double bond that emanates from that nitrogen.

The double bond becomes a single bond.

Click the other nitrogen in the 6-membered ring, and then the carbon at the other end of its double bond.

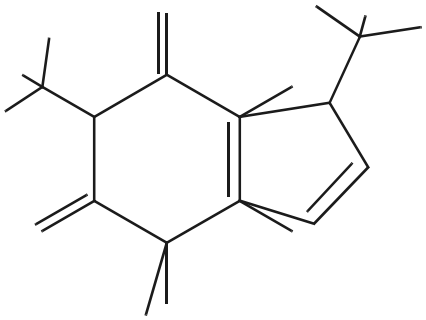
Now change the **Edit Bond** popup from **SINGLE** to **DOUBLE**.

Click the bottom N in the 5-membered ring and the right-most carbon in the same ring.

Click one oxygen and the carbon to which it is attached.

Do the same for the other oxygen.

Your model should now look approximately like this:



(Still bad, but you're getting there!)

9. Correcting the hydrogens

In the Sketcher control panel, click the **H ADJUST** button.

Now, except perhaps for some strange bond lengths or angles, your caffeine model is nearly finished.

10. Cleaning up the conformation

Still in the Sketcher control panel, click and hold the **CLEAN** button until the model stops moving.

Now your model should be finished and look like:

Note

In fact, your model may not really be "finished". The algorithm that the **CLEAN** button uses to improve the structure was written more for robustness and speed than for high accuracy. Therefore, if you want a model that is chemically even more realistic, and depending on the structural accuracy needed for your computational experiments, you would generally want to further optimize the structure. For this, you would use one of the forcefield- or quantum-based products (such as CDiscover or ADF), all of which have their own documentation.

Click the selection tool (the arrow icon in the upper left of the Sketcher control panel) to return the cursor to its selection function.

Alternatively, you can simply close the Sketcher control panel, since you don't need it for a while. The cursor should now be a plain arrow when it's in the model window.

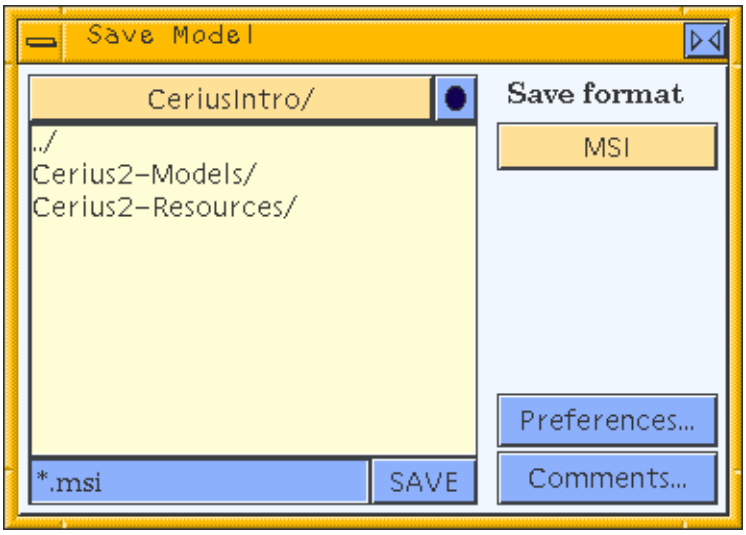
Saving a model

11. Saving your caffeine model

Now that you've built a model, you can save it:

Select the **File/Save Model...** menu item.

The Save Model control panel appears. If you named your working directory CeriusIntro as suggested in Step 1 and did not save any other files in this directory, the Save Model control panel should look like this:



Click in the text entry box next to the **SAVE** button. Change ***.msi** to **caffeine.msi** and click the **SAVE** button.

If you neglect to type the ".msi", Cerius^2 adds it automatically. The ".msi" helps you remember that the file is in Cerius^2's standard format.

12. Cleaning up your screen

By now, you have several control panels scattered about your screen. You can close one control panel:

Closing control panels

Click the close button  in the top right corner of any control panel.

Or you can close all open control panels at once:

Click the clear panels tool  on the toolbar of the Visualizer main panel.

The toolbar is just below the menu bar and looks like:

(By now, you might want to relax and have a cup of real caffeine!)

13. Interrupting this tutorial (optional)

If you need to quit your Cerius^2 session for any reason, you may do so now without losing any of your work.

To quit, simply select the **File/Exit** menu item and then click **Exit** in the Exit option… window that appears.

To resume this introduction to Cerius^2, **cd** to the directory that you made in Step 1 and start Cerius^2 as in Step 2.

To reload your caffeine model, select the **File/Load Model…** menu item. In the Load Model control panel's file browser, double-click (left mouse button) the name of the file that you saved in Step 11 (which should be caffeine.msi).

Close the Load Model control panel if you don't want it cluttering up your screen.

What you can do with a model display

If you've interrupted your tutorial, please see Step 13 before starting this section.

Now that you have a model, what kinds of things can you do with it in the Visualizer module of Cerius^2? (The Visualizer module is the one you've been using. It includes the controls that are accessed from the Visualizer main panel's menu bar and toolbar, as well as those on the left side of the Visualizer main panel. The stack of cards on the right side of the Visualizer main panel gives access to other modules.)

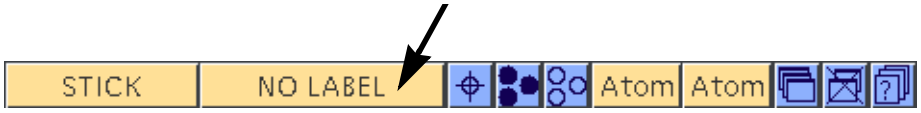
Note

This section shows you various ways of modifying the display of a model. None of its activities are required if you're mainly interested in features introduced in later sections of this tutorial.

14. Labeling a model

Find the label popup on the toolbar.

The label popup is this one:



Set the label popup to **ELEMENTS**.

That is, click the label popup, drag down the list that appears, and

*choose **ELEMENTS**.*

You can try using the label popup to replace the elements labels with labels that reflect other atomic properties. However, you have not defined some values (such as **FFTYPE** and **CHARGES**) and these labels display as question marks or zeros.

You can turn off labeling by setting the label popup to **NO LABEL**.

15. Moving a model

You can rotate and translate your model in 3D space. You can do this by controlling the cursor with your mouse:

With the cursor near the middle of the model window, hold down the right mouse button and move the cursor vertically and then horizontally.

The model is rotated around the x- and y-axes, respectively.

Keyboard shortcut

If you have an extended keyboard, you can rotate about the x- and y-axes in large increments by using the left, right, up, and down arrow keys while the cursor is in the model window.

Now place the cursor close to an edge of the model window and move it parallel to that edge.

The model is rotated around the z-axis.

Hold down the middle mouse button and move the cursor around in the model window.

The model is translated in the x,y-plane.

16. Zooming in or out on a model

You can control the magnification of the view of your model:

With the cursor in the model window, hold down the middle and right mouse buttons.

Moving the cursor up and / or to the right increases the magnification.

Moving the cursor down and / or to the left decreases the magnification.

Keyboard shortcut

If you have an extended keyboard, pressing the + and – keys on the keypad increases and decreases the magnification.

17. Returning the model to the center of the model window

Click the reset tool on the toolbar to reset your model to its initial position.

The reset tool looks like:

Keyboard shortcut

<Home> on an extended keyboard also resets the view.

18. Selecting atoms

Definition

Sometimes you will need to perform activities on only certain atoms, not on the entire model. For this purpose, you select *atoms. You can select them one at a time:*

Click any atom to select it.

A beep confirms that you've succeeded, and the atom is highlighted to indicate that it is selected.

Click another atom to select *only* it.

Hold down <Shift> and click one or more atoms to select *additional* atoms.

<Shift>-click an already selected atom to *deselect* it.

Click any one atom to select it and deselect all others.

Or you can select several atoms at once:

Hold down the left mouse button and drag out a rectangle in the model window, so as to enclose several atoms.

Drag out another rectangle to select a different group of atoms (or one atom).

<Shift>-drag to select an additional group of atoms.

<Shift>-drag some already selected atoms to deselect them.

You can select or deselect all atoms at once:

Click the selection tool  to select all atoms.

Click the deselection tool  to deselect all atoms.

Click empty space to deselect all atoms.

19. Measuring components of the model's geometry

Select the **Geometry/Measurements...** menu item.

The Measurements control panel appears.

Click the **Distance** tool in the Measurements control panel.

*The **Distance** tool looks like:*

Click any two atoms.

A dashed line and a distance (in angstroms) are displayed on the model.

Most tools on Measurements control panel work similarly: click the tool, then click the required number of atoms. If you need more information, look ahead to Step 20.

Clear the measurements:

Click the **DELETE Measurements** action button.

Definition

Even though this button is small, it is *an action button, as indicated by its blue color.*

20. Accessing on-screen help

To obtain help about any control in the Cerius^2 interface:

Move the cursor to a control about which you want information and click the right mouse button.

A help panel appears in the center of your screen.

Right-click any other control to replace the help with help about *that* control.

Right-click a blank area of a control panel to obtain general information about the entire control panel.

Click (left or right mouse button) the help window to make the help window disappear or click (left mouse button) any control panel to make the help window disappear.

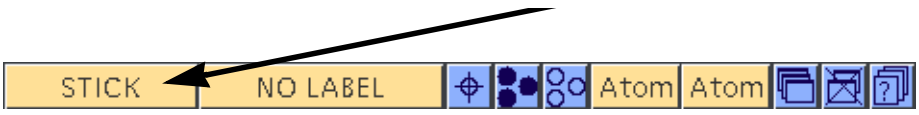
Caution

If you click a control while the help window is open, that control does perform its usual function.

21. Changing the display style

Find the display style popup on the toolbar.

The display style popup is this one:



Set the display style popup to **BALL**.

Try setting the display style to **BALL & STICK** and **CYLINDER**. (**ELLIPSOID**, **POLYHEDRA**, and **TRACE** are irrelevant to your current caffeine model.)

You can display different parts of the model in different styles by selecting atom(s) before applying a style.

22. Changing atom colors

Select the **Build/Element Defaults** menu item.

The Edit Elements control panel appears.

Enter **C** in the **Current Element** text entry box.

Change the **Display Color** popup to some color other than dark grey.

You can change the default colors for other elements in a similar way,

23. Coloring atoms according to a property

The functionality covered in this (optional) step is actually rather advanced, but it is new with release 3.0 of Cerius^2, so users interested in new features may find it useful.

Select the **View/Colors...** menu item.

The Color Selected Objects control panel appears. If we had defined a property such as charge or moveability, we could select all the atoms

in the model and then simply click one of the items in the ***Color by a Property*** *list to color the atoms. However, we haven't. So we will define our own property color map:*

Click the **Edit Mappings...** pushbutton in the Color Selected Objects control panel to access the Edit Color Mappings control panel.

The Edit Color Mappings control panel appears.

Enter the name **Mass** in the **New Map** entry box, choose **Mass** from the **Attribute** popup, and set the **Type** popup to **CONTINUOUS**.

Set the **Min**imum and **Max**imum **Attribute Values** between-which the color range is to extend to 0.5 and 15.5, respectively. Check the **Use Range** check box and choose **PEN_COLORS** from the **Use Range** popup.

You can label atoms with their mass if you want. The atomic masses range from 1.01 (H) to 16.00 (O).

We use 0.5 and 15.5 rather than 1 and 15 so that divisions between colors occur between *the atomic weights of atoms in our model. In addition, we use 15.5 rather than 16.5 because the PEN_COLORS color range contains 15 useable color entries, as we can see by displaying the color range:*

Check the **Show Range** check box.

A color range appears on the right side of the model window. The first entry (zero) is invisible, since it is black and so is the window back-

ground.

Set the the **Min**imum and **Max**imum range-color entry numbers (in the **Color Scheme** section of the control panel) to 1 and 15, respectively.

Select all atoms. Then, go to the Color Selected Objects control panel and choose Mass from the **Color by a Property** list.

All atoms except the oxygens are colored according to their atomic mass. We can color the oxygens by treating masses above 15.5 as outliers:

In the Edit Color Mappings control panel, click the **Outliers...** pushbutton next to the **Max** entry box to access the Maximum Outlier Handling control panel.

Check the **Pin to Maximum** check box.

Oxygen is colored according to the maximum color entry number, 15.

Check the **Use Pen** check box and choose a color from the **Use Pen** popup.

Oxygen is colored with your chosen color.

You can experiment with some of the other controls in this control panel.

24. Cleaning up the display or interrupting this tutorial (optional)

Close the open control panels if you have too many cluttering up your screen.

Use the **File/New Session** menu item to set all controls to their defaults and remove the model from the model window.

Reload your caffeine model. Or, if you want to stop for a while, please see Step 13 for exiting Cerius^2 and restarting this tutorial.

Building another model—ferrocene

If you've interrupted your tutorial, please see Step 13 before starting this section.

25. Adding a new model space

You already have a caffeine model, but we want to make an additional, separate model, ferrocene. To do this, we first make a "space" to contain the new model:

To open an additional model space, click the + tool  just above the model table (which is the bottom-left part of the Visualizer main panel).

A new, empty model space becomes current, and the caffeine model is hidden.

26. Sketching an iron atom

Ferrocene can be built much faster than caffeine:

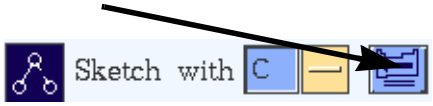
Use the **Build/3D–Sketcher...** menu item to open the Sketcher control panel.

*Iron isn't listed in the **Sketch with** popup; you can get it by using the*

periodic table.

Click the periodic table tool that's to the right of the **Sketch with** tool.

In other words, this control:



Click **Fe** in the Periodic Table window.

*The **Sketch with** entry box is filled in with **Fe**. (Actually, you could have just entered Fe in the **Sketch with** entry box by typing, but we wanted to show you the periodic table.)*

Click once somewhere near the center of the model window.

The single Fe atom is represented as a cross.

If you prefer the Fe to be represented as a ball, select the **View/Display Attributes...** menu item. Then, in the Display Attributes control panel, click the **Preferences...** button. In the Style Preferences control panel, set **Lone Atom Style** to **BALL**.

27. Adding the ligands

Click the **Templates...** button in the Sketcher control panel.

In the Sketcher Template control panel, double-click **ligands/** and then double-click **pentadienyl**.

(You may have to move up out of the organic directory, if you haven't restarted Cerius^2 since the beginning of this tutorial.)

The template tool is now selected and allows you to add pentadienyl ligands to the iron.

Click the Fe atom.

This adds one ligand.

Click the Fe atom again.

Select the selection tool in the Sketcher control panel, and move the model so that the rings appear to be nearly superimposed.

*You'll notice that the ferrocene model is not symmetrical and that pressing the **CLEAN** button does not make it exactly symmetrical.*

If you have purchased one of the QUANTUM 1 applications (ADF, DMol^3, GAUSSIAN, MOPAC, or Zindo), you may use their symmetry function to fully symmetrize the model:

Click the popup above the deck of cards (it should be labeled **BUILDERS 1**) on the right side of the Visualizer main panel and choose **QUANTUM 1**. The menu card for any of these quantum chemistry applications contains a **Geometry/Symmetry** menu item. Select it to access a Symmetry control panel. Change the **Tol-**

erance popup to **COARSE**. Click the **Find symmetry** action button.

Reading in additional models

28. Reading in more models

Click the **File/Load Model...** menu item to access the Load Model control panel.

In the control panel, double-click Cerius2-Models and then double-click one of the subdirectory names. If you obtain another list of subdirectories, double-click the desired one.

Double-click the name of any model you think might be interesting.

A third model space is created, displaying the chosen model. Both the caffeine and ferrocene (named Model2) model spaces are hidden.

Locate the model table in the lower left of the Visualizer main panel. In the list of model names, click Model2 and type **ferrocene**, then press <Enter>.

You may save the ferrocene model if you want.

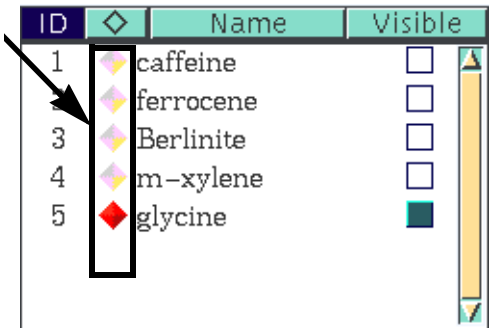
Use the Load Model control panel to load a few (2–4) more models. If you want a model from a different subdirectory, you can double-click **../** to go up one directory level or use the popup above the files list box to go directly to any parent directory.

Managing multiple models

29. Finding the name of the model shown in the model window

Notice the column of diamonds in the model table.

That is, these items:



The diamond that is highlighted in red and looks 3-dimensional indicates the name of the current model.

Definition

In the above example, glycine is the active model. It is both current (activities done in control panels or with the mouse affect it) and the only model visible in the model window.

30. Viewing a hidden model

Say you'd rather look at ferrocene than the currently active model:

Click the empty diamond next to the ferrocene model name.

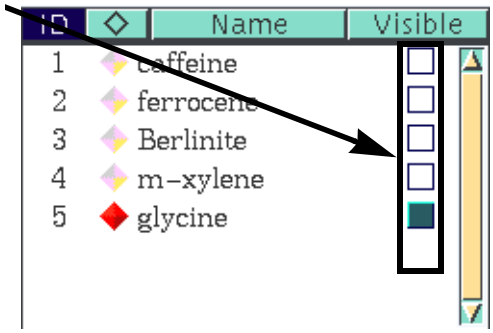
That diamond becomes highlighted and ferrocene replaces the other model in the model window.

You may make other individual models current by clicking their diamonds.

31. Viewing several different models simultaneously

Notice the column of squares in the model table.

That is, these items:



The square that is highlighted in cyan and looks somewhat 3-dimensional indicates the visible model.

Click one of the empty squares.

The model window becomes divided into one large square display area

and a border of smaller square display areas. The current model (ferrocene, if you performed only the boxed instruction in Step 30) is in the largest square display area. The model you just specified is displayed in one of the smaller square display areas.

Click one or more additional empty squares in the model table.

Each model is displayed in one of the smaller square display areas.

Click a square that's already highlighted in blue.

That model now becomes hidden.

Notice the display mode tools.

That is, these tools:

The border mode tool is currently active.

Select the grid mode tool (directly above the currently selected border mode tool).

The display is divided into 4 or 9 (or 16, etc., depending on how many visible models you have) equal-sized display areas. The current model

is displayed in the lower-left corner of the model window.

Select the overlay mode tool (the topmost one of these three tools).

All visible models appear in the same display area.

Click the border mode tool again, so that the current model appears in a large square display area, with the others in smaller square display areas.

32. Adding and deleting model spaces

You've already learned (in Step 25) how to add a new, empty model space by clicking the + tool. You can also clear an existing model space (i.e., remove the model, leaving its model space empty) or delete a model space (i.e., remove both the model and its space from the current Cerius^2 session):

To delete a model space, click a diamond to make the desired model current, then click the – tool  . Click **OK** in the confirmation window that appears.

The number of models listed in the table decreases by one (the remaining models are not renumbered).

To clear a model space, click a diamond to make the desired model current, then click the clear tool  . Click **OK** in the confirmation window that appears.

The model space and the current display area are cleared, but the

model name and number remain in the model table. You may sketch a new model in this display area (and model space). You may also copy one of the other models into the cleared space (if you, say, wanted to make an analog of caffeine):

33. Copying models from one model space to another

Leave the cleared model space defined as current (the largest display area is empty).

Click in an empty part of one of the other display areas, continue holding down the mouse button, and drag the cursor into the current (empty) display area.

In other words.

Click and drag from a noncurrent to a current model space.

The copied model now exists as two separate models in two separate model spaces.

To avoid confusion, you should rename the current model space so that the name reflects the model that's currently occupying that space (or the name of the analog or complex that you intend to construct from the newly copied model).

For example, click the name of the current model in the model table and change it to **caffeine analog**.

You can also copy a model into a currently occupied model space, if, say, you want to join them together into a complex or new model:

Click in an empty part of one of the other display areas and drag the cursor into the current (occupied) display area.

The models will be on top of one another, but you can move them apart as follows:

Go to the right atom selection popup on the toolbar of the Visualizer main panel. Click and drag to change it from **Atom** to **Frag**.

Click an atom in one of the fragments in the current model space. Holding down <Ctrl> and the middle-mouse button, drag that fragment away from the other. Make sure both atom selection pop-ups are set to **Atom** when you are finished.

34. Cleaning up the display or interrupting this tutorial (optional)

Close the open control panels if you have too many control panels cluttering up your screen.

Use the **File/New Session** menu item to set all controls to their defaults and remove the models from the model window.

Reload your caffeine model. Or, if you want to stop for a while, please see Step 13 for exiting Cerius^2 and restarting this tutorial.

Printing a model

If you've interrupted your tutorial, please see Step 13 before starting this section.

If you've deleted caffeine from your Cerius^2 session, please reload it (see Step 13 if you need instructions). You may have to use the file browser in the Load Model control panel to navigate back up to the directory in which you stored caffeine.msi.

If several models are visible, make caffeine the only visible (and active) model by assuring that the visibility controls (square blue icons in the model table) are toggled off for all other models and on (highlighted) for caffeine.

Change the display style from **STICK** to something else if you prefer (see Step 21).

Select the **File/Print...** menu item.

In the Print control panel, change the **Command** to the statement that you usually use to specify printing to a postscript printer.

An experienced user at your site, or your systems administrator, should know this command if you don't.

Either select the **PRINT** button or change the settings of some of the other controls and then select the **PRINT** button.

If nothing happens

Please ask an experienced user at your site, or your system administrator, how to access your printer(s).

Controlling the 3D display

35. Depth cueing

Depth cueing gives an impression of 3-dimensionality by causing the atoms that appear to be closest to the viewer (you) to appear brighter, and those farther away, to fade into the background. You may want to adjust or turn off this feature.

Select the **View/Graphics** menu item.

*When you drag the cursor down to the **Graphics** item, a* pullright menu *appears.*

Continue dragging the cursor (to the right and then down) and release the mouse button over the **View/Graphics/Depth Cueing...** menu item.

In the Depth Cueing control panel, click the control on the **Depth Cue Factor** slider and drag it to the right.

*The **Depth Cue Factor** slider and entry box now look like:*

You can also change the depth cue factor by entering a number in the ***Depth Cue Factor*** *entry box.*

A depth cue factor of 1 turns depth cueing off. Setting it to zero results in extreme depth cueing (the atoms farthest away from you will probably appear black).

Now set the **Depth Cue Factor** to some value less than 1.0.

When the depth cue factor set to some value less than 1, you can use the **Far Distance** and **Near Distance** sliders to adjust the points at which depth cueing takes effect. The adjustments take effect immediately and are more easily seen at lower values of the depth cue factor. Since caffeine is a nearly planar model, you can see the effects of depth cueing more readily by turning it so that it is no longer parallel to the computer screen.

36. Lighting your model

Lighting effects are more dramatic if you have a model with some solidity, so:

Change the display style to **BALL**.

Select the **View/Graphics/Lighting...** menu item.

The Lighting control panel appears. You can experiment with the controls on and accessible from this panel. Remember, you can click with the right mouse button to obtain help on any control.

You can, for example:

- Change the color of the global ambient light by adjusting the **Color** sliders in the Lighting control panel. Make it a rather dim, neutral color, so that you can more easily see the effects as

you add light sources (*More lights*). You can even turn it off by setting **Gray** to 0.0.

- Click the **Color...** button to access the Lightsource Colors control panel, where you can change the colors and brightness of the various components of LIGHT 1.

If nothing happens

If some of these controls appear to have no effect, you are probably not running Cerius^2 in OpenGL mode (see *Important*).

Click the **Position...** button in the Lighting control panel to access the Lightsource Position control panel, where you can change the light from directional to positional and then change its position. For example, set the **X**, **Y**, and **Z** values to 1, -1, and 10, respectively, to place a light in front of the model, somewhat to its lower right.

Click the **Spotlight...** button in the lighting control panel to access the Spotlight Settings control panel, where you have additional control over the positions of spotlights (positional light sources).

For example, set the **Latitude** and **Longitude** controls on this control panel to 5.68 and 174.29, respectively, to shine the light back towards the model. Narrow the **Cutoff** to, say, 20° to make a narrow beam of light. Try increasing the **Falloff** value to smooth the transition from the light to the dark area.

Iteratively change the **Position** controls in the Lightsource Position control panel and the **Direction** controls in the Spotlight Settings control panel so as to, for example, illuminate a particular atom or center the light on the 6-membered ring.

Click the **Attenuation...** button in the Lighting control panel to access the Lightsource Attenuation control panel. Try increasing the **Linear** or **Quadratic** factor to make atoms farther from the lightsource appear dimmer. The effect is more apparent if the illuminated part of the model is nearly parallel to the direction of the light beam.

More lights

- Add a second light source by changing the **Light** popup in the Lighting control panel to LIGHT 2 and checking (i.e., clicking, so that a checkmark appears in the check box) the **Enabled** check box.

Use the Lightsource Colors control panel to change the color of LIGHT 2. Make it different from LIGHT 1 so you can more easily see what's happening as you adjust the lights.

37. Changing the model window's background color

Select the **Utilities/Customize/Pen Colors…** menu item.

In the Pen Colors control panel, set the **Background** popup to **OTHER** or set the **Pen** popup to **BACKGROUND**.

Use the color sliders to customize your background's color.

Or just set the **Background** popup to one of the predefined color choices.

Exploring Cerius^2 on your own

38. Using the Help menu

Select the **Help/Getting Started…** menu item.

You can use the buttons in the Getting Started control panel to find out more about:

- The names of the parts of Cerius^2's graphical environment and how to manage all the windows.
- Loading models.
- Manipulating models in the model window, including:

  Access to on-screen summaries of mouse- and keyboard-actions for selecting and moving models.

  Information on changing the display style and atom colors, as well as on labeling atoms.

- Building models (icons in some of these help panels function just as they do in the Sketcher control panel).
- Performing simple and complex selections and simple editing of your selections.

You can also access many of these subtopics directly, by selecting the **Help/Topics** menu items.

Select the **Help/Examples…** menu item.

The Example files control panel allows you to load and automatically play back some pre-recoreded examples of many things that can be done with Cerius^2. Most of these examples use other modules, in addition to the basic Visualizer controls. Try some of them! (You must, of course, have licensed copies of any programs used in these tutorials.)

Select the **Help/About Cerius2…** menu item.

The About Cerius2 control panel contains information on contacting Molecular Simulations, Inc. It includes our website's URL and the email and other addresses for obtaining customer support.

39. Experimenting with other features of the interface

Now that you've gained some familiarity with Cerius^2, you can explore more of its features on your own. You cannot cause any permanent damage:

- Unless you specifically save, for example, changes you make via the **Utilities/Customize** menu items, Cerius^2 will revert to all its default settings the next time you start it.
- You can use the **File/New Session** menu item to, in effect, restart Cerius^2 without actually quitting and reloading it.
- Many module cards have a **Reset** function, which returns control settings to their defaults.

40. Finding additional information

Detailed information on all the functions of the Visualizer are found in the other sections of this documentation set.

Tables of the mouse and keyboard functions can be found under *Mouse and Keyboard Actions.*

Detailed information about modules other than the Visualizer are found in the documentation for the applications to which those modules belong.

41. Quitting your Cerius^2 session

Select the **File/Exit** menu option. Click **Exit** in the confirmation window that appears.

Summary—Some of what you've learned

Sections of this book where you can find additional information are listed in ***bold type*** in this list.

- Using and managing menus, windows, and other controls in the Cerius^2 interface (e.g., *Locating the basic building tool*, *Cleaning up your screen*, see also ***The Cerius2 Interface***).
- Building models (see *Building a model—caffeine*, *Building another model—ferrocene,* see also ***Building Models***).
- Sketching with templates and ligands (see *Sketching the ring system of caffeine*, *Here's another way of adding a methyl group:*, *Adding the ligands,* see also ***Adding templates (groups of atoms)***).
- Changing atom elements and bond types (see *The Edit Element tool looks like:*, *Correcting the bond order*, see also ***Changing atoms and their bonding types***).
- Using the periodic table (see *Sketching an iron atom*).
- Adding the correct number of hydrogens (see *Correcting the hydrogens*, see also ***Adding hydrogens***).

- ❏ Cleaning up the conformation (see *Cleaning up the conformation*, see also ***Refining the conformation***).
- ❏ Using file browsers to find models and templates (see *Stop when you see the filename methyl.*, *Reading in more models*, see also ***Managing Models and Sessions***).
- ❏ Saving and loading models (see *Saving your caffeine model*, *Reading in more models*, see also ***Managing Models and Sessions***).
- ❏ Labeling a model (see *Labeling a model*, see also ***Labeling and annotating models***).
- ❏ Moving a model (see *Moving a model*, *Zooming in or out on a model*, *Returning the model to the center of the model window*, see also ***Moving models on the screen***).
- ❏ Changing a model's display style (see *Changing the display style*, see also ***Model display style***).
- ❏ Selecting atoms and groups of atoms (see *Selecting atoms*, see also ***Selecting atoms and groups of atoms***).
- ❏ Measuring parts of a model (see *Measuring components of the model's geometry*, see also ***Geometry Analysis***).
- ❏ Managing multiple models (see *Adding a new model space*, *Reading in more models*, *Managing multiple models*, see also ***Handling multiple models***).
- ❏ Coloring a model according to atomic properties and creating property maps (see *Coloring atoms according to a property*, see alse ***Coloring atoms by properties***, ***Property–color mapping***).
- ❏ Manipulating lighting and colors (see *Changing atom colors*, *Controlling the 3D display*, see also ***Enhancing Model Display***).
- ❏ Printing a model (see *Printing a model*, see also ***Printing models and graphs***).
- ❏ Accessing on-screen help (see *Accessing on-screen help*, *Using the Help menu*, see also ***On-screen help***).

3 Tutorials

This chapter contains several tutorials covering the basics of working within the Cerius^2 modeling environment. The tutorials in this chapter are:

Basic GUI Functions

Using the 3D Sketcher

Managing Models and More

Managing and Modifying Graphs

Basic Molecular Simulation: Minimization & Dynamics

Basic GUI Functions

This section contains an introductory Cerius^2 Visualizer tutorial. It shows you the basics of the GUI including loading, viewing, and display of simple models; manipulating control panels; and exiting the program. You learn about functions on the menu bar and the tool bar.

This chapter is divided into three parts:

- **Before you begin**— provides some introductory and background information.
- **Step-by-step tutorial** — gives you specific instructions to follow.
- **Review** — summarizes the exercise by giving a checklist of the skills you've learned and points you to MSI documentation that provides more detailed information about the functions introduced in the tutorial exercise.

Before you begin

To complete this tutorial, you need a licensed copy of Cerius^2 and a directory into which you can save the files you create during the tutorial.

In this tutorial, you familiarize yourself with the look and feel of the Cerius^2 GUI and Visualizer. You use the Cerius^2 menu bar (**File**, **Edit**, **Build**, etc.) and the tool bar immediately below it. You learn how to load a model and then practice viewing, displaying, and selecting it. The tutorial concludes with a brief exercise about control panels.

Summary of tutorial

The tutorial is divided into four short exercises:

A. Loading and displaying a molecular model

B. Viewing and labeling a model

C. Selecting atoms

D. Manipulating control panels

Step-by-step tutorial

This section takes you through a series of short progressive exercises designed to familiarize you with some basics of the Cerius^2 Visualizer.

A. Loading and displaying a molecular model

In the following steps, you load an msi format structure file of trimethylbenzene and display it in both Stick and Ball styles.

1. Start Cerius^2 and load the model.

If Cerius^2 isn't already open, type

```
> cerius2
```

in a UNIX shell to run the program.

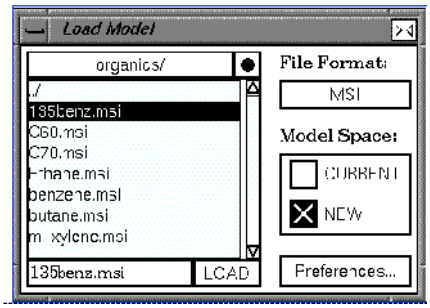
The program takes a few seconds to initialize; a welcome screen appears briefly and then the Cerius^2 GUI appears.

Troubleshooting

If typing cerius2 does not start the program, consult the *Cerius^2 Installation and Administration Guide* for help on setting up the correct environment for running Cerius^2.

Select **File/Load Model...** to open the Load Model control panel.

Remember to use the left mouse button for choosing menu items.

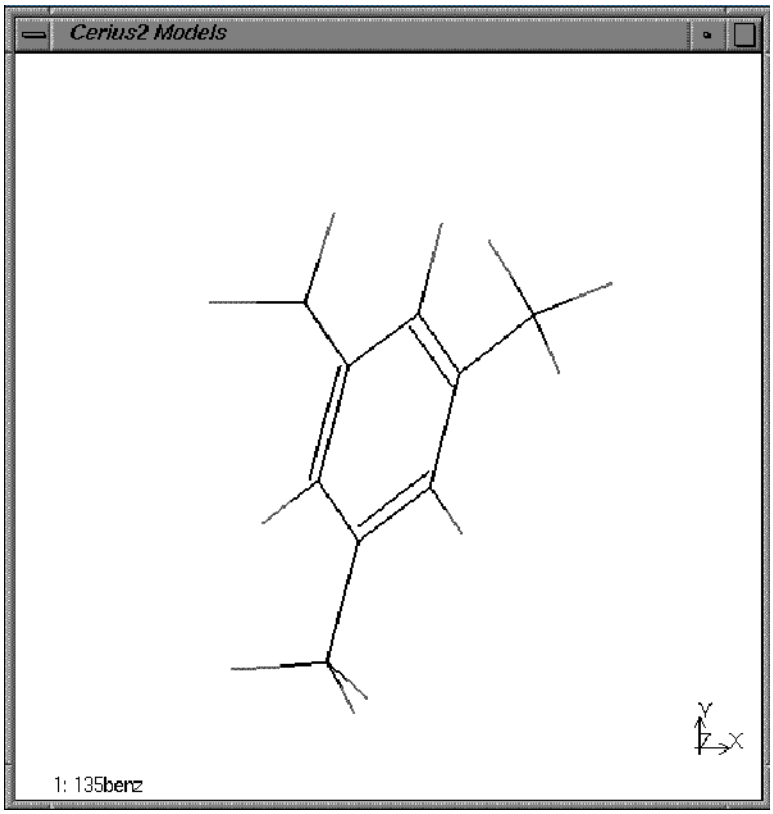


Load the model 135benz.msi from the directory Cerius2-Models / organics: double-click the **Cerius2-Models/** directory name in the browser box to open that directory; double-click the **organics/** directory to open the organics directory; then double-click the **135benz.msi** filename to load the file.

Note

You may need to use the scroll bar at the side of the file list to locate the **organics/** directory.

Your model window should look similar to this:



Troubleshooting

If you need to return to the Cerius2-Models/ directory, choose the Run directory selector  at the top right of the browser box.

If you can't find the file in the organics/ directory, make sure that the **File Format** popup reads **MSI** and that the text box at the foot of the panel reads ***.msi**.

2. **Change the display style of the model.**

Use the **Display Style** popup menu on the left end of the tool bar to change the display style to **Ball**.

The atoms are displayed as spheres. By default they are filled to 0.7 of their van der Waals radii.

Troubleshooting

If some of the atoms stayed in stick display? If not all the atoms appear in Ball display?

You may have inadvertently selected some of the atoms in the model window. If any atoms were in a selected state, then only those selected atoms will appear as balls. To correct this, click in some empty space in the model window: this deselects any previously selected atoms. Then reselect **Ball** from the **Display Style** popup.

Select **Stick** from the **Display Style** popup menu.

The model returns to stick display where all bonds drawn as lines.

B. Viewing and labeling a model

The following steps show you how to rotate and translate the trimethylbenzene model. You also learn how to label atoms in the model by element name.

1. **Manipulate the model's presentation using the mouse.**

Rotate the model by placing the cursor over the model window and then dragging while holding down the right mouse button. Familiarize yourself with the action of the mouse.

If the cursor is near the center of the screen, it rotates the model about an axis in the plane of the screen and perpendicular to the direction in which you drag. If the cursor is towards the edge of the screen, it rotates the model around an axis perpendicular to the screen.

Translate the model by dragging over the model window with the middle mouse button depressed.

Scale the model by dragging over the model window with the middle mouse button and the <Shift> key depressed, or with both the middle and right mouse buttons depressed.

Try rotating the model in some other display styles. Then return the display style to **Stick**.

Note that rotation is quickest in the stick display.

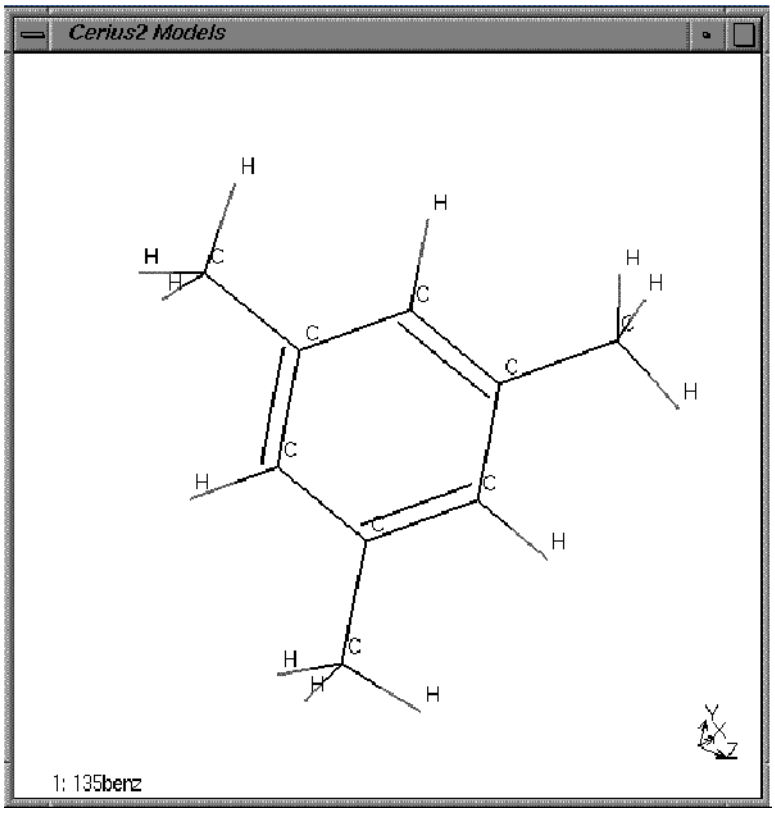
[Aside: The Ellipsoid style is for models for which temperature factors have been defined. The Polyhedra style is used to display coordinated cations, for example, in zeolites.]

2. Label the atoms in the model with their element type.

Change the **Atom Labeling** popup on the tool bar from **No Label** to **Elements**.

All the atoms in the model window should now be labeled as hydrogens or carbons, either C or H.

If the display style isn't stick, the labels may be difficult or impossible to see.



Troubleshooting

If some of the atoms are not labeled, you may have inadvertently selected some of the atoms in the model window. If any atoms are selected, then only those selected will be labeled. To correct this, click the **Deselect All** icon in the tool bar, and then reselect **Elements** from the **Display Style** popup.

C. Selecting atoms

In the following steps, you learn several techniques for selecting and deselecting atoms.

1. **Select an atom.**

   Use the left mouse button to pick one of the atoms in the model.

   In stick display, when the atom is selected it is highlighted. Cerius^2 beeps to let you know that you've selected the atom. The atom is also identified in the text window.

   Select several more atoms by holding down the <Shift> key as you select them.

   You should now have three or four atoms highlighted in the model window.

2. **Change the display style.**

   Use the **Display Style** popup to change to **Ball & Stick**.

   Note that the new display style only applies to the selected atoms. In the ball and the cylinder display styles, selected atoms are indicated with thin stripes.

3. **Select and deselect all atoms.**

   Deselect all atoms by clicking on empty space in the model window.

Find the **Select All** and **Deselect All**  icons on the tool bar. They look like the icons in the margin.

Next, you use these buttons to select and deselect atoms in the model window.

Choose the **Select All** button then changethe **Display Style** popup to **Ball**.

All the atoms in the window are highlighted and then appear as balls wrapped in thin blue lines.

Choose the **Deselect All** button.

All the atoms are deselected — the thin blue lines disappear.

D. Manipulating control panels

In the following steps, you learn about control panels: how to open, close, scale, and stack them. You use on-line help to get information about the controls on the panels. And finally you learn how to re-initialize and / or exit from Cerius^2.

1. Close and open control panels.

Close the Load Model control panel by clicking on the close box  in the right corner.

All control panels can be closed this way.

Open the Save Model control panel by choosing **File/Save Model...** .

Notice that those pulldown menu items that open control panels all have names that end in ellipses (…).

2. **Open more control panels.**

Choose **Build/Element Defaults** to open the **Edit Elements** control panel.

You would use the Edit Elements control panel if you wanted to alter any element properties such as the display color used in Cerius^2.

Choose **View/Display Attributes...** to open the Display Attributes control panel.

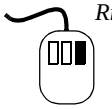
*The Display Attributes control panel has the same functionality as the **Display Style** and **Atom Labeling** tool bar popups, which you have already used.*

*You can select the **Preferences** button to change the defaults for the different displays. For example, you can change the size of the spheres in the Ball display from 0.7 to 1.0 in van der Waals radii of the atoms.*

3. **Access help for a command in a control panel.**

Click the **Preferences...** button on the Display Attributes control panel to open the Style Preferences control panel.

Again, control panel buttons with names ending in ellipses (…) open other control panels.



Right mouse button for help

Click with the right mouse button on a command in one of the control panels.

This brings up a help text panel that describes the function.

Click in the help text panel to close it.

Try clicking with the right mouse button in other items in the GUI: check boxes, buttons, popups, sliders, menu items, and so on.

4. **Access the Stereo control panel from a pullright menu.**

Select **View/Graphics>** and then move the mouse to the right to select the **Stereo…** item on the pullright menu.

The Stereo control panel opens. You would use the Stereo view control panel if you wanted to view the model as a stereo pair or with the Crystaleyes stereo hardware.

Right arrows at the end of pulldown items indicate that there are pullright menus for these items.

5. **Move and resize control panels.**

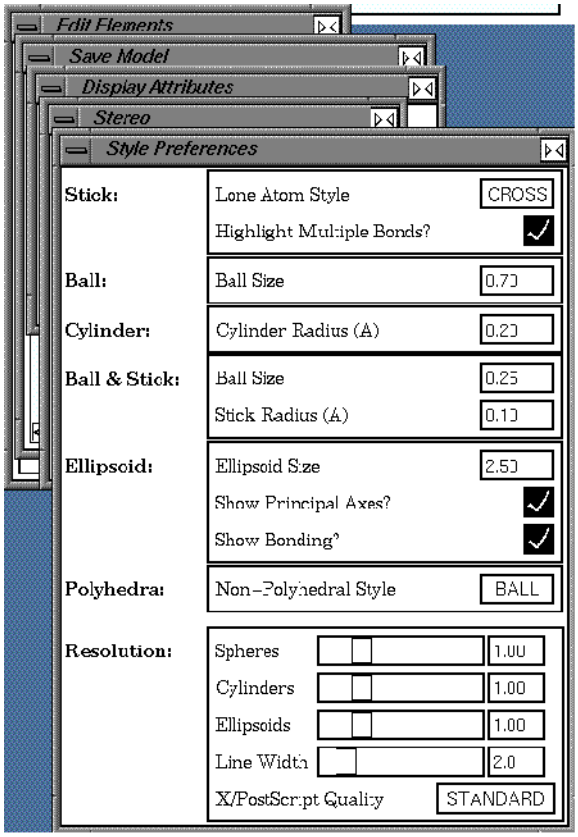
Click and drag some control panel title bars to different screen locations.

Cascade Panels

Resize some control panels by clicking and dragging their edges or corners.

Click the **Cascade Panels** button on the tool bar.

This stacks all the open control panels with their title bars visible.



Bring the last panel to the front by clicking on its title bar, and close it by selecting its close box (in the top right corner).

6. **Close the control panels.**

Clear Panels

Select the **Clear Panels** button on the tool bar.

The remaining control panels close.

7. **If you are going to continue immediately with another tutorial:**

Re-initialize the program by selecting **File/New Session** and selecting the **Confirm** button on the **Re-initialize** dialog box.

Re-initialization *resets all the Cerius^2 control panels to their original defaults.*

Alternatively, if you want to stop now:

Choose **File/Exit** to quit from Cerius^2, and select the **Exit** button on the **Exit Option...** dialog box.

Review

In this tutorial you learned how to:

- Load an msi structure file
- Change the display style of all or some atoms
- Rotate, translate, and scale the model view in the model window
- Label atoms by element type
- Open, close, and move control panels
- Display help text panels for control panels and menu items
- Re-initialize and exit from Cerius^2

You may now want to proceed to the next tutorial, "Using the 3D Sketcher", where you learn how to build your own models.

Alternatively, you may want to learn more about the Visualizer by reading the user manual sections listed below.

Related material

The Visualizer is discussed in detail in the *Cerius^2 Modeling Environment*. The sections listed here will provide you with more detailed information about atom display and selection than are included in this tutorial book.

1. Sections in the *Introducing Cerius^2* and *Viewing and Displaying Models* chapters of the *Cerius^2 Modeling Environment*.
2. The section, *Selecting atoms and groups of atom*s in the *Building Models* chapter of the *Cerius^2 Modeling Environment*
3. The *Managing Models and Sessions* chapter of the *Cerius^2 Modeling Environment*.

Using the 3D Sketcher

This chapter contains a tutorial on molecular sketching. It introduces the Cerius^2 3D Sketcher. You learn how to draw and edit models in 3D and how to use the Clean function to do simple optimization of model geometry. You also learn how to save the models, which you build, into structure files.

This chapter is divided into three parts:

- ***Before you begin*** — provides some introductory and background information.
- ***Step-by-step tutorial*** — gives you specific instructions to follow.
- ***Review*** — summarizes the exercise by giving a checklist of the skills you've learned.

Before you begin

To complete this tutorial, you will need a licensed copy of Cerius^2 and a directory into which you can save the files that you create during the tutorial.

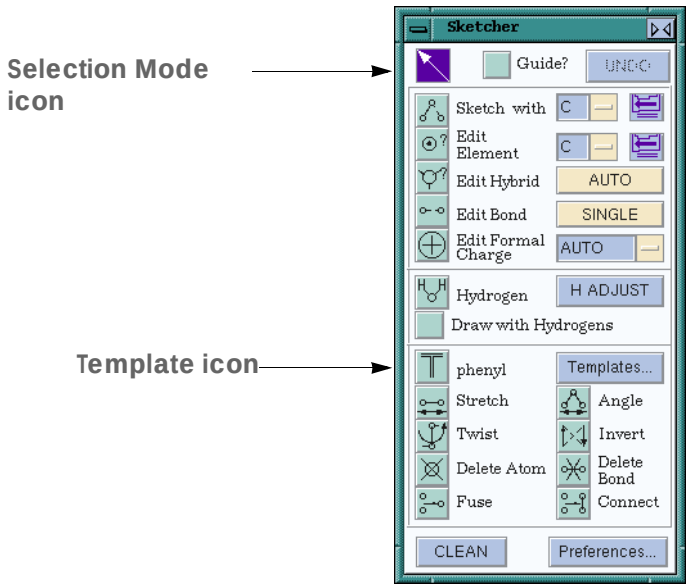
Before you begin the tutorial on page 50, you should be familiar with the contents of the section *Basic GUI Functions*. If you have not read this section, you should ensure that you know how to do the review items listed in the *Review* on page 61 before beginning this tutorial.

In *Basic GUI Functions*, you loaded a model from file into the model window. The purpose of this tutorial chapter is to show you how you can build your own models using the 3D molecular Sketcher. The Sketcher is the principal building tool of the Cerius^2 Visualizer.

Note

There are other ways to build models in Cerius^2: using the Analog, Crystal, Surface, Interface, Polymer, and Amorphous builders. You may have licensed some or all of these modules with your configuration of Cerius^2. The tutorials in the *Cerius^2 Tutorials: Materials Science* and *Life Science* demonstrate the use of some of these sketchers.

Below is an illustration of the Sketcher control panel. The Sketcher provides tools for mouse-driven sketching, editing, and cleaning of models. The operation of the Sketcher is *modal*, that is, the function of the left mouse button in the model window is determined by which icon is currently selected in the Sketcher control panel. The default setting is to have the **Selection mode** icon highlighted. This allows normal Cerius^2 operation, with the mouse button selecting atoms (just as in the previous tutorial). It is a good habit to always highlight the **Selection mode** icon before closing the Sketcher control panel.



Summary of tutorial

The tutorial is divided into five short exercises:

A. Building cyclohexane and saving the structure to file

B. Converting cyclohexane into the boat conformation

C. Editing cyclohexane to make benzene

D. Editing benzene to make phenol

E. Building xylene from template fragments

Step-by-step tutorial

This section takes you through a series of short progressive exercises designed to familiarize you with some basics of the Sketcher.

A. Building cyclohexane and saving the structure to file

In the following steps, you open the Sketcher panel and use its **Sketch**, **H Adjust**, and **Clean** tools to build a model of cyclohexane. After you build cyclohexane, you save it into a structure file.

1. **Start Cerius^2 and open the Sketcher.**

   If Cerius^2 isn't already open, type

   ```
   >    cerius2
   ```

   in a UNIX shell to run the program.

   The program takes a few seconds to initialize; a welcome screen appears briefly at first, and then the Cerius^2 GUI appears.

   Open the Sketcher control panel by selecting the **Build/ 3D-Sketcher...** item.

   The Sketcher control panel appears.

2. **Sketch the cyclohexane model.**

   Choose the **Sketch** icon:  x

   *Note the Sketch With element is set to **C** for carbon. Notice also that in the model window the mouse cursor appears as an inverted V; this indicates that the mouse is now in sketching mode.*

   Click once in the model window.

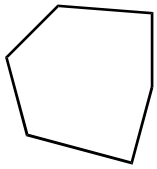
   A single carbon atom appears, represented as a cross, and a dotted "guideline" follows the mouse cursor. Keep the cursor within the model window — if the cursor moves out of the model window, you lose the guideline.

Troubleshooting

If you lose the guideline, click once on the first carbon atom (with the mouse still acting in Sketch mode), and the guide line will reappear. (If you click directly on the existing carbon, you won't generate a second atom.)

Click somewhere else to put down a second atom and continue to build a ring of six carbon atoms —terminate the ring by clicking on the original atom.

You should now have a hexagonal form somewhat similar to this in the model window:



*You can correct any mistakes with the **Undo** button.*

3. **Set the sketching mode back to Selection.**

Highlight the **Selection mode** icon once more so that all future clicks in the Model window do not result in new atoms!

4. **Adjust the hydrogens and minimize the structure.**

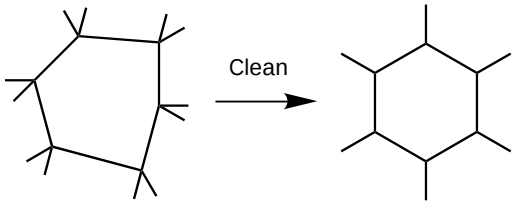
Click the **H Adjust** button.

The H Adjust command adds (or deletes) hydrogens to all atoms in order to satisfy their valences. In this case, H Adjust adds two hydrogen

atoms to each of the carbon atoms.

Hold down the **Clean** button. Release the button when the atoms stop moving.

***Clean** attempts to adjust bond lengths and angles to reasonable values. Note that recleaning after manipulating or deforming the structure may find a different structure.*



You have built a cyclohexane ring. The cyclohexane ring that you see on the screen is probably in the "chair" conformation.

5. **Experiment with the display and view of the model.**

Try altering display styles and rotating and rescaling the model to view it. (If you need hints on how to do this, refer to the *Basic GUI Functions* tutorial lesson.)

Reset the view — use the  icon beside the label popup on the tool bar.

6. Save the cyclohexane model into a structure file.

Select **File/Save Model...** to open the Save Model control panel.

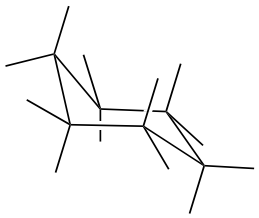
Type **cyclohexane.msi** into the filename text box, which is next to the **Save** button, then select the **Save** button to save the structure to a file. Use the directory selector popup and the file browser on the panel to find the correct directory before you save the file.

B. Converting cyclohexane into the boat conformation

In the following steps, you learn how to move atoms to convert the chair conformer of cyclohexane into the boat conformer.

1. Adjust your view of the model.

Use the mouse to rotate the model to view the “chair” from the side.

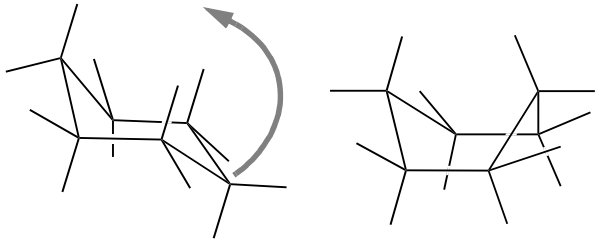


Select the carbon on one end of the ring as you look at it, and select the two hydrogens attached to that carbon.

(Remember you need to hold down the <Shift> key to select multiple

atoms.)

Hold down the <Control> key and drag with the middle mouse button to move the selected atoms. Drag these atoms well to the other side of the plane defined by the four carbons in the seat of the chair.



Clean the model.

You should now have either the boat form or the twist-boat form of cyclohexane. The boat form is shown above.

Note

If cleaning returns the model back to the chair form, drag the CH_2 group even farther above the seat of the chair than it was in step 3 and even closer to the back of the chair. Then repeat the **Clean** step.

Rotate and view the model.

C. Editing cyclohexane to make benzene

In the following steps, you learn how to edit bonds and to edit and delete atoms, and so build benzene from cyclohexane.

1. **Delete the hydrogens from cyclohexane.**

Find the two popups on the tool bar that currently read **Atom**. Change the second of these to **El** for element.

*Both of these popups control the selection rules for atom picking. Setting the second popup to **El** means that all atoms of the same element type are selected when one atom of that type is picked.*

Select one hydrogen atom.

All hydrogens appear selected in the model window.

Double-click the **Delete Atom** icon in the Sketcher control panel.

All the hydrogens in the model are deleted.

This delete procedure has illustrated the alternative way of applying the Sketcher icons — double clicking on an icon carries out its action on all selected atoms.

2. **Make the double bonds.**

Change the second selection rule popup back to its default **Atom** setting. Also, highlight the **Selection mode** icon once more.

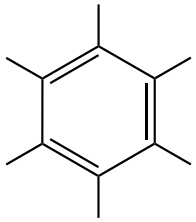
Change the **Edit Bond** popup from **Single** to **Double** and click any carbon atom. Pick an adjoining carbon atom.

A dotted guideline appears and then becomes the double bond between the carbon atoms.

Repeat to make alternate bonds in the ring double.

3. Adjust the hydrogens and minimize the model.

Use the **H Adjust** and **Clean** buttons, then rotate and view this planar benzene.



D. Editing benzene to make phenol

In the following steps, you add an OH group to benzene to make phenol. Also, you learn how to use the Sketcher tools to alter torsion angles, bond angles, and bond lengths.

1. Add an oxygen.

Use the popup adjacent to the **Edit Element** text box to select **O** for oxygen.

The popup is a fast way to choose commonly used element symbols.

Select the periodic table icon after this popup.

A periodic table appears.

Select any element in the table.

The element is written to the text box.

*You can also change the element by typing a new element symbol into the **Periodic Table** text box.*

Close the periodic table. If necessary, restore the **Edit Element** symbol to **O**.

Pick any one of the hydrogens to change it to an oxygen.

In Edit Element mode, the mouse cursor is a circle.

Use the **H Adjust** and **Clean** buttons. Highlight the **Selection mode** icon once more.

Rotate and view the model; try some other display styles, then return to the Stick display.

Choose the **Twist** icon.

In the model window, the mouse cursor for twist mode is shaped like a bow tie.

You must select four atoms to define a twist torsion.

Pick the hydrogen attached to the oxygen, the oxygen itself, the carbon attached to the oxygen, and one of the adjoining ring carbons.

In this case, don't hold the <Shift> key down; the atoms don't become highlighted when they are selected in Twist mode.

Drag the mouse over the model window with the left mouse button depressed to increase / decrease the torsion.

The change in the torsion angle is interactively updated. Note that the atom picked last is the one that moves.

2. **Try the other geometry manipulation tools.**

Use the **Stretch** and **Angle** tools, which work similarly to **Twist**.

3. **Save the new structure.**

Save the phenol structure into a file called **phenol.msi**. If necessary, see Step 6 on page 68 for a reminder of how to save.

Clear the model window.

E. Building xylene from template fragments

In the following steps, you use the template tool to create a model of p-xylene. The template tools let you sketch with predefined molecular fragments (called templates) — for common structures, this is often more convenient than sketching atom-by-atom.

1. Create a model from the phenyl template.

Template Icon

Click the **Template** icon on the Sketcher — this looks like a "T" and is located about halfway down the box.

The current template is phenyl.

Click in the model window.

A phenyl ring appears.

2. Add a methyl fragment from a template to make toluene.

Click the **Templates...** button in the Sketcher.

Double-click the **organic/** directory and find the template file **methyl**.

Double-click **methyl**.

*A file browser opens on a directory called templates/ and the template name in the Sketcher changes from **phenol** to **methyl**, indicating that the methyl template has been successfully loaded.*

Pick one of the phenyl hydrogens.

The hydrogen atom is replaced by a methyl group to make toluene.

3. **Add another methyl group.**

> Select another of the phenyl hydrogens — choose the one farthest away from the methyl group to make *p*-xylene.

4. **Save the model.**

> Save the p-xylene structure into a file called **xylene.msi**. If necessary, see Step 6 on page 68 for a reminder of how to save.

5. ***If you are going to continue immediately with another tutorial:***

> Re-initialize the program by selecting **File/New Session** and selecting the **Confirm** button on the **Re-initialize** dialog box.

Re-initialization resets all the Cerius^2 control panels to their original defaults.

Alternatively, if you want to stop now:

> Choose **File/Exit** to quit from Cerius^2 and select the **Exit** button on the **Exit Option…** dialog box.

Review

In this tutorial you learned how to …

- ❑ Sketch atoms
- ❑ Move and delete atoms

- ❑ Edit atom and bond types
- ❑ Edit bond angles and lengths
- ❑ Adjust hydrogens in a model
- ❑ Use the template tool
- ❑ Clean a model
- ❑ Save a model to file

You may now want to learn more about the Sketcher by:

- ♦ practicing what you have learned by sketching some models of your choosing
- ♦ reading the *Basic building* section in the *Building Models* chapter of the *Cerius^2 Modeling Environment*

Or you may proceed immediately to the next tutorial, *Managing Models and More*.

Managing Models and More

This chapter contains a progressive tutorial designed to show you some more functions of the Visualizer including managing multiple models, copying between model spaces, measuring models, and printing. You also get additional practice at loading, saving, and sketching models.

This chapter is divided into three parts:

- ♦ ***Before you begin*** — provides some introductory and overview information.
- ♦ ***Step-by-step tutorial*** — gives you specific instructions to follow.
- ♦ ***Review*** — summarizes the exercise in a checklist of the skills you've learned and suggests what to do next and points you to MSI documentation that provides more detailed information about the functions introduced in the tutorial exercise.

Before you begin

To complete this tutorial, you need a licensed copy of Cerius^2 and a directory into which you can save the files that you create during the tutorial.

Before you start this tutorial lesson (page 50), you should have read (or be familiar with the contents of) *Basic GUI Functions*, and have done the tutorial exercises in *Using the 3D Sketcher*.

In this tutorial, you load in and use the models that you created in *Using the 3D Sketcher*.

Summary of tutorial

The tutorial is divided into five short exercises:

A. Using the model manager

B. Making picric acid from phenol (transferring data between model spaces)

C. Building a model of indigo

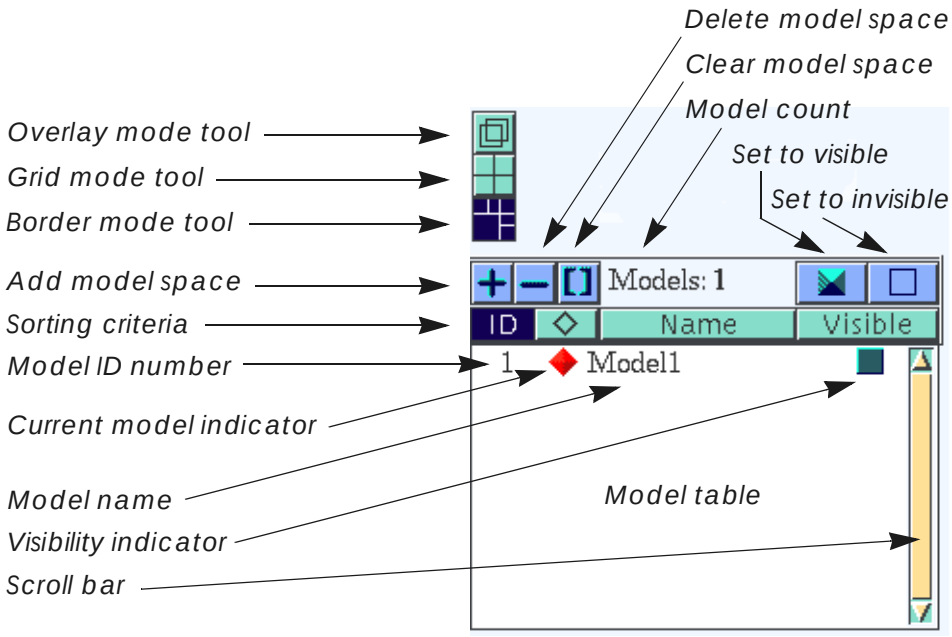
D. Measuring the indigo model

E. Generating hard copy

Step-by-step tutorial

This section includes a series of short progressive exercises describing various aspects of the Cerius^2 Visualizer: model management, measuring models, and creating Postscript images for printing. You will use the controls in the model manager to complete the steps of

this tutorial. The components of the model manager are named in the illustration below.



A. Using the model manager

The model manager is used to view collections of models, sort models by name and by identity number, and discard models from the Visualizer.

1. Load the models.

> If Cerius^2 isn't already running, type **cerius2** in a UNIX shell to start the program.

Choose **Load Model...** from the **File** pulldown menu.

Use the Load Model control panel to load models from the previous tutorials: phenol.msi, cyclohexane.msi, and xylene.msi.

The file names, without the ".msi" extensions, appear in the model manager list in the same order that the files are loaded in.

Load butane.msi and napthalene.msi from the Cerius2-Models / organics directory.

There are now five models in the system. Each is named and numbered on the model manager list. The diamond after the model number is the current model indicator (i.e., the displayed model on which calculations will be performed). The current model is marked with red.

Click the diamond for the different models in the list. After trying the other models, select **phenol** to be displayed.

The model displayed in the window changes with each selection. Phenol should be the last one displayed.

*It is possible to display multiple models on the screen at any one time in a variety of display styles. The **Model Display Selector** boxes to the right of the model names (under the heading **Visible**) show which models are displayed. Displayed models are indicated by a filled blue box, the visibility indicator.*

The current model is always marked visible.

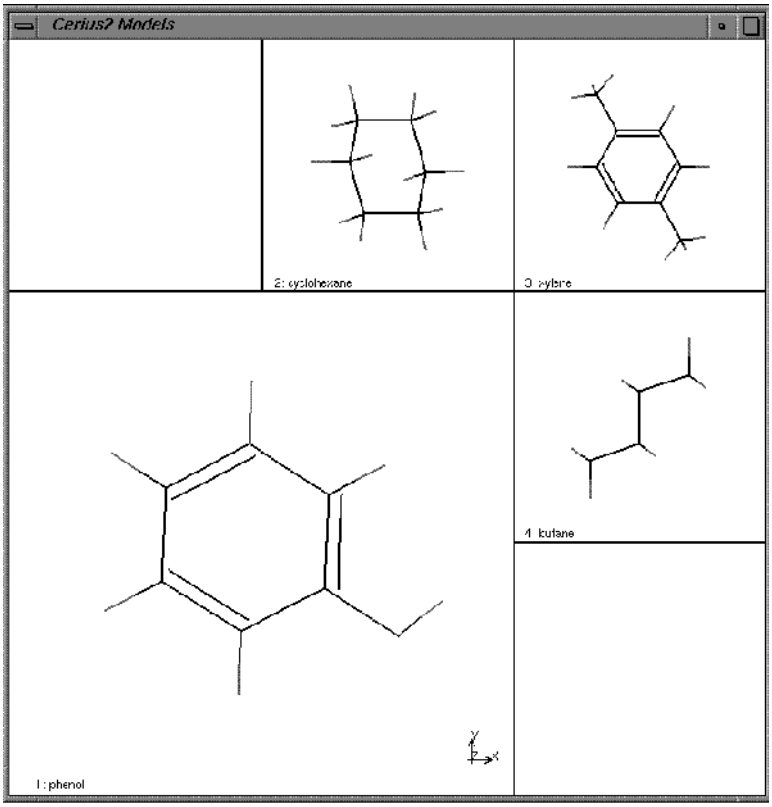
Check the **Model Display Selector** box for **xylene**.

The model window divides into border mode, and the xylene model

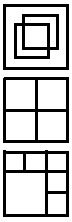
appears in the top right corner of the window.

Select two more models.

The four models are displayed in border mode, with the current model (phenol) as a large model surrounded by smaller images of the other models.



2. Try rotating and translating the models.



Use the mouse to rotate and translate the models in various ways.

Notice how all are rotated together.

To the left of the Cerius^2 logo are three icons that control display style.

Click on the middle **Display Mode** icon to get a grid display.

Click the top icon.

It overlays all currently visible models

Return to border display mode by clicking the bottom icon.

Click the filled blue box on the bar above the Model Manager list.

All models should now be displayed.

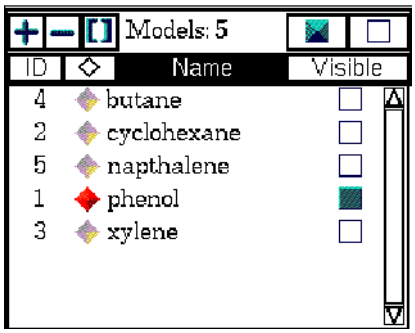
Click the adjacent empty box icon.

Only the current model is displayed.

Click the **Name** button immediately above the list.

This orders the models according to the first letter of the model names. (This is case sensitive: names beginning with uppercase letters are listed before those beginning with lowercase letters.)

Try clicking on the **ID**, A, and **Visible** buttons to sort models in other ways.



Make **napthalene** the current model.

Click the "**–**" icon above the Model Manager list and choose the **OK** button when prompted by the dialog box.

This deletes the model.

Make **cyclohexane** the current model.

Click the "**[ ]**" icon and choose the **OK** button when prompted by the dialog box.

This clears the model — leaving it in the list but removing all data from it.

B. Making picric acid from phenol (transferring data between model spaces)

In the following steps, you learn how to create a new model space and to copy atoms from one model space and paste them into another. You copy the phenol model into the new model space and then use the Sketcher to modify the phenol model to form picric acid (2,4,6-trinitrophenol).

1. Copy the phenol model.

Set the current model to be **phenol**.

Select all the atoms in the phenol model.

*(You can do this with the **Select All** item from the ccpulldown or use the*  *icon.) All the atoms in the current model will be highlighted.*

Choose the **Copy** option from the **Edit** pulldown.

This copies the phenol model into the buffer.

Choose the "+" icon on the Model Manager.

A new model space, called Model6, is created.

Choose **Paste** from the **Edit** menu.

The phenol model is copied into the new model space.

2. Edit the model to create 2,4,6-trinitrophenol.

Open the Sketcher, and click the **Fragments** button.

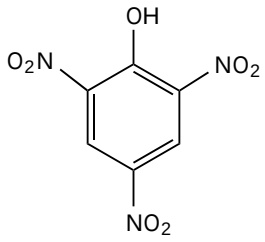
Load the nitro template — the templates / organic / nitro file.

Use the nitro template to create 2,4,6-trinitrophenol.

This molecule, 2,4,6-trinitrophenol, is also called picric acid..

Return the highlight to the selection mode icon  once more.

Clean the model and give it the name **ferrocene** in the Model Manager list.



C. Building a model of indigo

In the following steps, you use the Sketcher to build a model of indigo. In doing this, you review sketching while also learning some important new things:

- How to duplicate a model
- How to select by fragment
- How to move one fragment relative to another

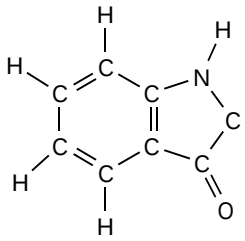
1. **Sketch the indigo model.**

> Create a new model space by choosing the "**+**" button on the Model Manager.

> Rename this new model space "**indigo**".

You're going to sketch the indigo model in this space.

Because indigo is centro-symmetric, save time by sketching only half of the molecule and then doubling it.



Half an indigo molecule

2. **Sketch this fragment.**

Hint: you may want to begin by using the template tool with the phenyl fragment.

> Choose the **Select All** item from the **Edit** pulldown menu or the  icon.

All atoms are highlighted.

> Choose the **Duplicate** item from the **Edit** pulldown menu.

A second copy of the molecule is pasted into the model window.

Pick in the Model window and hold down the left mouse button while you drag the mouse to create a box enclosing the whole of one molecule.

Hold down the <Ctrl> key, and use the rotate and translate mouse controls.

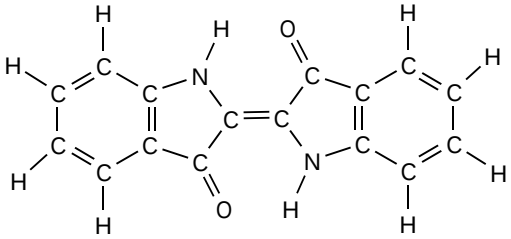
Only the selected molecule moves.

Move one fragment relative to the other until the two carbon atoms at the ends of the five-membered rings are about a bond length apart.

Link the two fragments by a double bond using the **Edit Bond**  option in the Sketcher. **Clean** to complete the indigo molecule.

Return the Sketcher to selection mode, and then close the Sketcher control panel.

D. Measuring the indigo model



In the following steps, the Measurements control panel is used to measure the geometry of the indigo model from *C. Building a model of indigo.*

1. **Measure the distance between two atoms.**

   Open the Measurements control panel from the **Geometry** pulldown menu.

   Click on the **Distance** icon.

   As in the Sketcher, these icons determine the function of the mouse in the model window.

   Pick any two atoms.

   The distance between them will be marked on the model. You may need to rotate the model or zoom in on it to see the measurement clearly.

2. **Try some of the other measurement tools.**

   Pick three atoms to measure angles, four to measure torsions or inversions, and six to measure the angle between two planes.

   Choose the **List Measurements** button.

   Pick three atoms to measure angles, four to measure torsions or inversions, and six to measure the angle between two planes.

   All measurements you have made will be written out to the text window. (You may want to label the model by Numbers to match up the atom serial numbers in the text window with the atoms in the model window.)

3. **Optional step**:

Load the model Cerius2-Models / molecular-crystals / pigments / indigo_1.msi.

This is a crystal structure of indigo.

Perform the same measurements on this model as you made on the indigo that you sketched. Compare the results.

*Because the model that you made was only crudely minimized by the **Clean** tool and not affected by crystal packing constraints, you'll notice significant differences between the two models.*

Finish by choosing the **Delete Measurements** button.

This removes all the measure lines and values from the models.

E. Generating hard copy

In the following steps, you output the contents of the model window to a PostScript file, and then print a view of the trinitrophenol model in ball display.

Note

This exercise assumes that you are able to print grayscale PostScript files from your workstation.

Make trinitrophenol the current model and the only model visible.

Set the display style to **Ball**.

If necessary, rotate, scale, or translate the model in order to get a pleasing view of it in the model window.

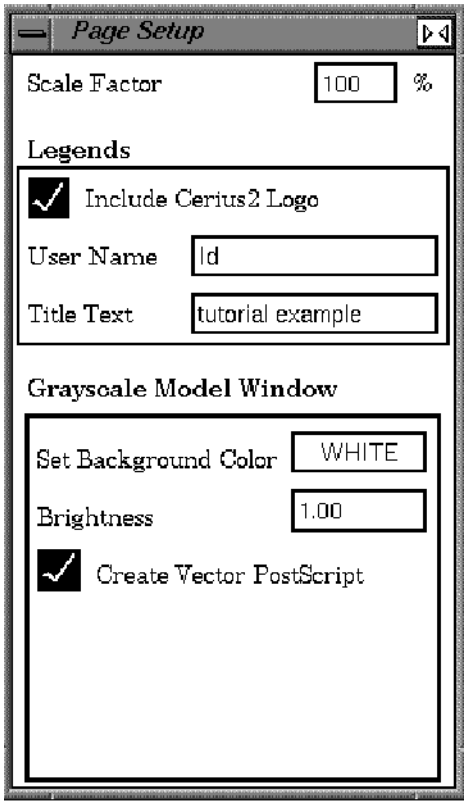
Open the Print control panel by selecting **Print...** from the **File** pulldown menu.

Choose the **Page Setup...** button to open the Page Setup control panel.

On the Page Setup control panel set the background **Color** popup to **White**.

The model window background turns to white. (A white background will save toner when the image is printed.)

If you want your name or any other text to appear on the image, type into the **User Name** and **Title Text** boxes.



Make sure that no windows or control panels are overlapping the Model Window.

Choose **File** to be the **PostScript Destination** and enter **trinitrophenol.ps** in the text box that currently reads **CERIUS.ps**.

Choose the **Print** button.

A message is written to the text window:

```
Starting to output image ...
..................Image Captured
```

The PostScript image will be written to a file called rinitrophenol.ps.

If you are running Cerius^2 on an SGI, choose the **Preview** button. (If you are running on another platform skip to step 4, below.)

This calls the xpsview program to give a preview of how the PostScript image will look on the page. The preview gives you a chance to alter the model view or the page setup controls before printing.

Close the xpsview window by choosing **Exit** from the xpsview **File** menu in the top left corner.

4. **Select one of two methods to print the file.**

There are two ways that you can print the file:

The first is to change the **PostScript Destination** back to **Printer**, and choose the **Print** button. If the laser printer that you want is not the system default, you will also need to edit the print command **lp -c.**

Or

The second is to print the trinitrophenol.ps file from a UNIX shell in the way you would normally print any PostScript file. In the simplest configuration, the print command would be **lp trinitrophenol.ps**.

On the Page Setup control panel, set the background **Color** popup back to **Black**.

The model window background returns to black. (You may have found that the white background is hard on your eyes.)

Note

It is also possible to use the SGI snapshot utility or the xv program to capture rgb images from Cerius^2.

5. Exit or continue to another tutorial.

Either:

Re-initialize the program by selecting **New Session** from the **File** pulldown menu and choosing the **Confirm** button on the Re-initialize dialog box.

Re-initialization resets all the Cerius^2 control panels to their original defaults.

Alternatively, if you want to stop now:

Choose **Exit** from the **File** pulldown menu to quit from Cerius^2, and choose the **Exit** button on the **Exit Option...** dialog box.

Review

In this tutorial you learned how to:

- ❑ Display multiple models using the Model Manager
- ❑ Remove and clear models from the Model Manager list
- ❑ Create a new model space

- ❑ Copy atoms between model spaces
- ❑ Duplicate selected atoms
- ❑ Move one model fragment relative to another
- ❑ Measure model geometry
- ❑ Generate a PostScript image from the model window

Now, you may want to proceed to the next tutorial, *Managing and Modifying Graphs.*

Related material

The model manager is discussed in detail in the *Cerius^2 Modeling Environment*. If you haven't already done so, you may want to read the introductory tutorial in Chapter 2 of that book. Other sections of that book that relate to the activities in this lesson include:

Using the main control panel in Chapter 2

Controls and control panels in Chapter 2

Basic building in Chapter 4

Printing models and graphs in Chapter 7

Managing and Modifying Graphs

This chapter contains a tutorial exercise about graphs in Cerius^2. It introduces the basics of viewing, modifying, saving, and loading graphs that are created by Cerius^2.

This chapter is divided into four parts:

- ♦ ***Before you begin*** — provides some introductory and background information.
- ♦ ***Step-by-step tutorial*** — gives you specific instructions to follow.
- ♦ ***Review*** — summarizes the exercise by giving a checklist of the skills you've learned.
- ♦ ***Related material*** — points you to MSI documentation that provides more detailed information about the functions introduced in the tutorial exercise.

Before you begin

To complete this tutorial, you need a licensed copy of Cerius^2 and a directory into which you can save the files you create during the tutorial.

In this tutorial, you learn about the Cerius^2 **Graphs** card. Nearly all the Cerius^2 materials science modules produce some output to the graph window. It's important that you understand how the **Graphs** card works so that you can get the most from your graphical results.

You can use the functions on the **Graphs** card:

- To load and save graph files
- To edit text on graphs
- To set new colors and plotting styles
- To make graphs and data-sets visible or invisible
- To combine data-sets from different graphs
- To control version over-writes

You have opportunity to do all these things in this tutorial exercise.

Cerius^2 Graphs terminology

The Cerius^2 graph system is based on a hierarchy of three structures:

- Gallery
- Graph
- Data-set

These are defined below and shown symbolically in the figure.

Data-set

At the bottom of the hierarchy is the *data-set*. The data-set must be one of three types:

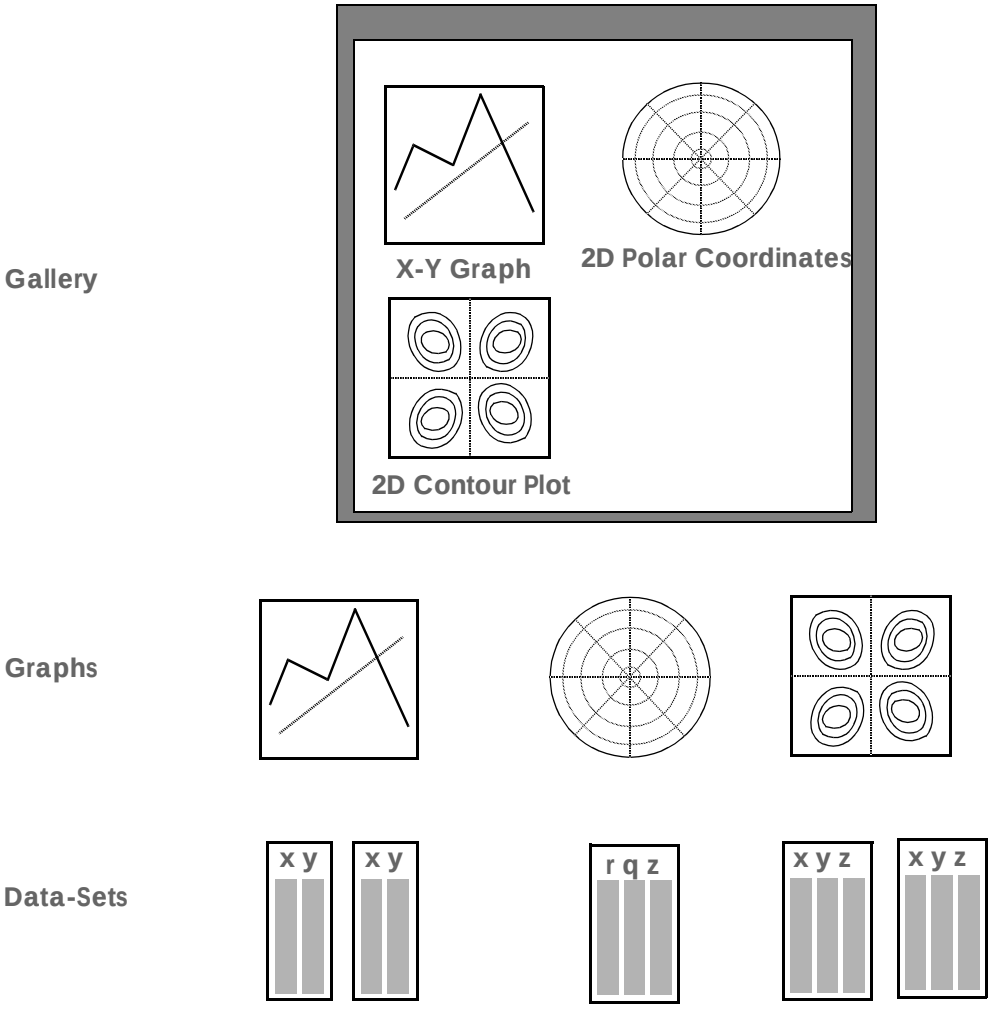
- An array of xy coordinates (for a normal 1D plot)
- A set of grid points with an intensity or a contour height (for a 2D cartesian plot)
- A set of radii, angles, and value coordinates (for a 2D polar plot)

Graph

At the middle level of the hierarchy is the *graph*. A graph is made up of one or more data-sets displayed on axes.

Gallery

At the top of the hierarchy is the *gallery*. The gallery is the name given to the group of graphs on display in the graph window at a given time.



Summary of tutorial

The tutorial is divided into six exercises:

A. Loading graphs and using the Gallery Manager

B. Using the Graph Manager and setting plotting attributes

C. Scaling graphs

D. Annotating graphs

E. Saving graph files

F. Creating new graphs and using expert functions

Step-by-step tutorial

This section takes you through a series of short progressive exercises designed to familiarize you with the Cerius^2 **Graphs** card.

A. Loading graphs and using the Gallery Manager

Graphs are saved in files with .grf extensions; this format is described in the "File Formats" appendix of the *Cerius^2 Modeling Environment*.

Files generated using Insight II can also be loaded; these have the extension .tbl and are described at the MSI website, www.msi.com.

The sample graphs that you load for this tutorial were created by the Blends module and the Sorption module. The contents in themselves are irrelevant for this tutorial, and you needn't have licensed the Blends or the Sorption modules to load or manipulate these graphs.

1. Load the graph files.

Find the **Graphs** card (on the **Tables & Graphs** card deck).

If the card is not already at the front of the deck, click on the card title to bring it to the front.

Open the Load Graphs control panel by choosing the **File -> Load Graphs** item on the **Graphs** card. Find the directory Cerius2-Resources /EXAMPLES/data.

*Be sure that the filename text box at the bottom of the browser box reads *.grf.*

Load the file **EM_MM_DG.grf**: pick its name on the browser box and then click the **Load** button.

A confirmation message like the one shown below appears in the text window. The graph appears in the graph window.

```
Loading Grapher file: ./Cerius2-Resources/EXAMPLES/data/EM_MM_DG.grf
Loading Done.
```

Place the graph window in the top left corner of the screen over the Model window. Enlarge the graph window (click and drag a corner of the window) until the window is almost as large as the Model window.

You do not need the Model window for this tutorial.

Now load two more graph files from the EXAMPLES/data directory: **EM_MM_Emix.grf** and **Loading.grf**.

Close the Load Graphs control panel.

2. Arrange the graphs in the Gallery.

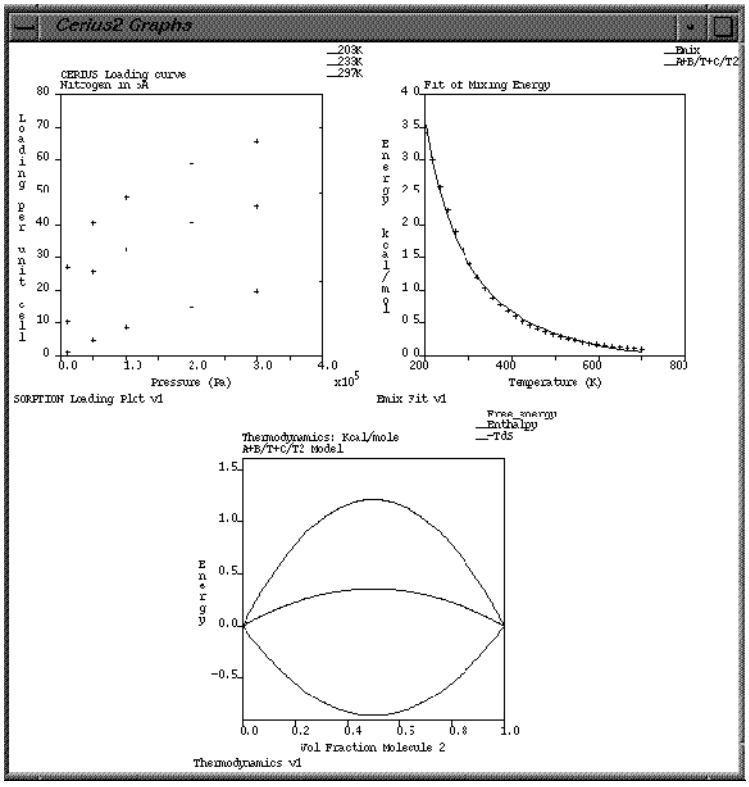
Open the Gallery Manager control panel by choosing **Gallery -> Manager** from the **Graphs** card.

In the Graph Chooser list box, you will see the names of the *three* graphs that you've loaded into the system.

They are: Sorption Loading Plot v1, Emix Fit v1, and Thermodynamics v1. Only the Sorption Loading Plot is on display.

Click on the **Display** check boxes next to **Emix Fit v1** and **Thermodynamics v1**.

Three graphs should now be on display in the graph window.



*Notice that the **Gallery Width** and the **Gallery Height** popups on the Gallery Manager control panel are both set to **Auto**. This automatically arranges the graphs to best effect in the graph window.*

Change the **Gallery Width** to **3** and the **Gallery Height** to **1**, and note the result. Try some other width / height combinations before returning both settings to **Auto**.

Note

If you specify a gallery size that is too small for the number of graphs, graphs will disappear from the Gallery window. To redisplay a lost graph, set the gallery size large enough for all the graphs and then select again the missing graphs on the **Graph Chooser** list box of the Gallery Manager control panel.

Set the **Label Graphs** check box to **on**. Note the appearance of the graph labels in the graph window.

Uncheck the **Emix Fit v1** and the **Thermodynamics v1** graphs on the **Graph Chooser** list box to leave only the Sorption Loading Plot on display in the graph window. Be sure that the **Edit** box for the Sorption Loading Plot graph is toggled **on**.

B. Using the Graph Manager and setting plotting attributes

Now that you've looked at the Gallery Manager and used it to edit the layout of graphs in the graph window, you learn how to edit the graphs themselves using the Graph Manager.

1. Open the Graph Manager

Open the Graph Manager control panel by clicking the **Graph Manager...** button at the bottom of the Gallery Manager control panel. (Alternatively open the control panel by choosing **Graph -> Manager** from the **Graphs** card.)

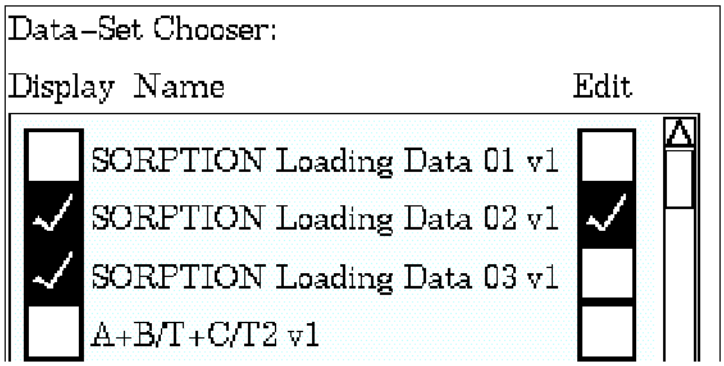
*The Graph Manager control panel has a **Data-Set Chooser** list box that parallels the G**raph Chooser** browser box in the Gallery Manager. In the D**ata-Set Chooser** are listed the data-sets of all three of the loaded graphs, but only the data-sets currently displayed on the Sorp-*

tion Loading Plot are checked.

Uncheck the **Display** button for the **Sorption Loading Data 01** data-set in the **Data-set Chooser** list box to leave the **Sorption Loading Data 02** and the **Sorption Loading Data 03** data-sets on display in the graph window.

Set the check boxes in the Edit column so that the **Sorption Loading Data 02** data-set can be edited but the **Sorption Loading Data 03** data-set cannot be.

*The top portion of your **Data-Set Chooser** should look like this:*



Click the **Plotting Attributes...** button at the base of the Graph Manager control panel to open the Plotting Attributes control panel.

Change the **Style** popup (currently reading **Point**) to **Line**.

Observe that the data plot style changes from points to a line.

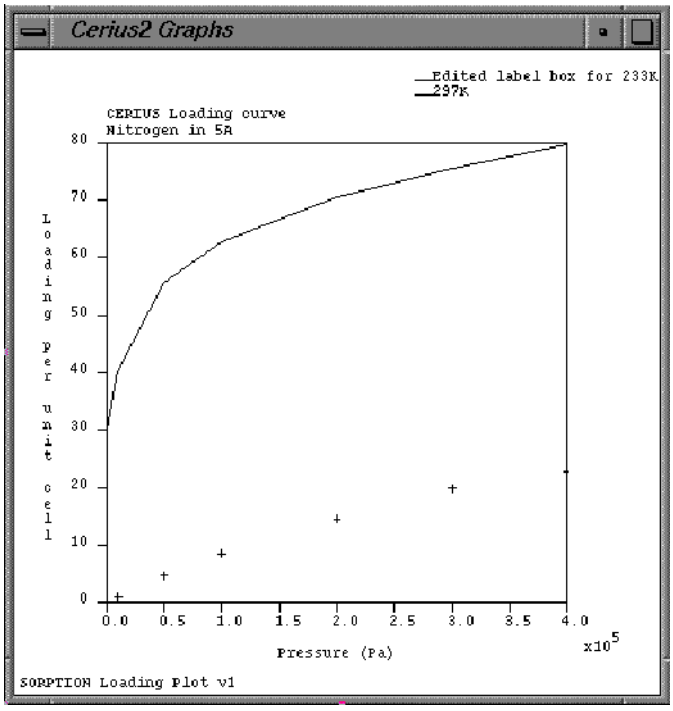
Use the **Color** popup (currently reading **YEL**) to change the line color to light green (**LGR**).

Edit the **Label** text box.

Observe that the text for the green line is modified.

Edit the **Y Offset** text box: for example, change it to **30**.

Observe the Y shift in the data plotted.



2. Editing more than one dataset at a time.

On the Graph Manager control panel, select all the Sorption data-sets for both **Display** and **Edit**.

Return to the Plotting Attributes control panel.

*Notice how the **Style** and **Color** popups show the –> symbol and the **Y Offset** and **Label** text boxes are blank. This is because the attributes are not the same for all of the data-sets. The 01 and 03 data-sets are in point style, and the 02 is in line. Furthermore, the colors of all three are different, and the key labels and Y offsets also differ.*

Set the **Y Offset** to **0** (zero).

Experiment with the **Style** popup: set it to **Histogram**, to **Delta**, to **Point**, and finally to **Line**.

*You could also use the **Color** popup to set all the lines to the same color or the **Label** text box to make the labels the same for all of the datasets — but these would not be very useful.*

Close the Plotting Attributes control panel.

C. Scaling graphs

In the following steps, you learn four ways to alter the scale of a graph:

- Using the scaling text boxes

- Using the scroll and zoom buttons
- Using the mouse
- Using the **Axis Scaling** popup

1. Use the text boxes to scale a graph.

Open the Graph Scaling control panel by choosing the Graph -> Scaling item on the Graphs card or by choosing the Graph Scaling… button at the foot of the Graph Manager.

Enter a value of **-1e5** in the **Min X** text box and a value of **-20** in the **Min Y** text box.

Notice the effect on the graph axes.

2. Try the zoom and scroll buttons and observe their effect.

[+] *increases the zoom level*

[-] *decreases the zoom level*

[●] *resets the graph to its original scale*

You can use the % text box associated with the zoom buttons to specify the magnitude of the zoom buttons' effect.

Alter its value from **5** to **20%** and notice the effect on the zoom rate.

Use the zoom buttons to adjust the graph scale so that the origin of the graph is not visible.

Now use the scroll buttons until you can see the origin back on the graph.

The scroll buttons work very similarly to the zoom ones. The arrows indicate the scroll directions, and the central button resets the scale. The scroll % text box is used to set the percentage of the axis scrolled in one button click.

Next, you try the mouse/keyboard shortcuts for scrolling and zooming.

3. Manipulate the graphs with the mouse.

Try mouse scrolling: put the cursor within the axes of the graph, and move the mouse while holding down the middle mouse button.

By moving the mouse diagonally, you can scroll in both the x and y directions at once.

Try mouse zooming: put the cursor within the axes of the graph, and move the mouse while holding down both the <Shift> key and the middle mouse button.

Click the **Zoom Reset** button to return the graph to its original scale.

Click the **Axis Scaling** popup to view the choice of scale settings. Then click again using the right mouse button to display the help text that describes the five sorts of scaling.

When you have finished reading the help text, click it to make it disappear.

Try the **Auto-XY** setting, and then the **Nice-XY** setting.

*Notice the change in the **Max Y** value when you do this.*

Exit from the Graph Scaling control panel.

D. Annotating graphs

In the following steps, you learn how to use the **Annotation Option** popups to display (or not display) graph axes and various text items. You also edit the text for the graph title and axes.

(Remember, you've already learned how to edit the text for the graph key, or legend, in the *Edit the Label text box.* step on page 102.)

1. Experiment with the Graph Annotations.

Open the Graph Annotation control panel by choosing **Graph -> Annotation** from the **Graphs** card or by clicking the **Graph Annotation…** button at the foot of the Graph Manager.

Change the popup options from **Yes** to **No** and back again so you can identify the various components of the graph: Axes, Label, Title, and Key.

*The **Cell** option only applies to 3D graphs.*

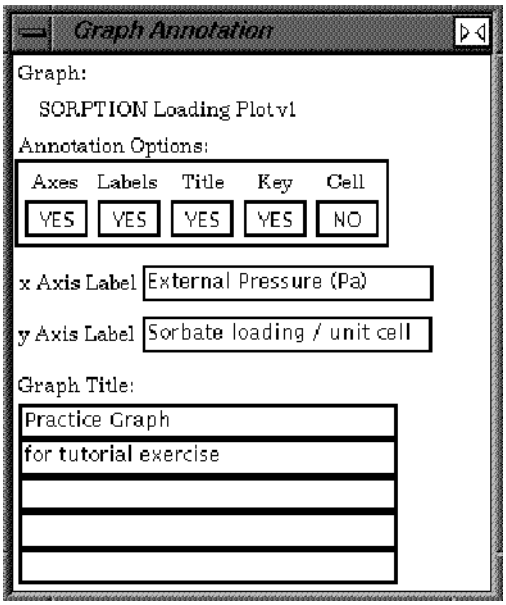
Note

You will never want to select **-->** because it has no effect. However, Cerius^2 may set a popup to **-->** to indicate that this option is not unique for the graphs in the edit list.

Edit the **X Axis Label**, the **Y Axis Label**, and **Graph Title** text boxes.

Notice that the text on the graph is updated with the new labels and

title.



Close the Graph Annotation control panel.

E. Saving graph files

A graph (.grf) file can contain a single graph or multiple graphs. Each of the graph files that you loaded in section A (page 96) contained only one graph. In the following steps, you save a gallery of two graphs into one .grf file. Then, you reset the Graphs card and load back in the two-graph file that you saved.

1. Save multiple graphs into one file.

On the Gallery Manager control panel select the **Emix Fit** and the **Thermodynamics** graphs to be displayed (and do not display the **Sorption Loading Plot** graph).

Open the Save Graphs control panel by choosing **File -> Save Graphs** from the **Graphs** card.

Type **two_graphs.grf** into the filename text box and click the **Save** button.

A confirmation message like the one shown below is written to the text window.

```
Saving Gallery File: ./two_graphs.grf
Saved GRAPHS file.
```

2. **Delete graphs from the Gallery.**

Choose **Reset** from the **Graphs** card, and choose **Re-initialize Graphs** from the dialog box to confirm the reset.

Reset *deletes all graphs from the Gallery Manager and returns all* ***Graphs*** *controls to their default settings.*

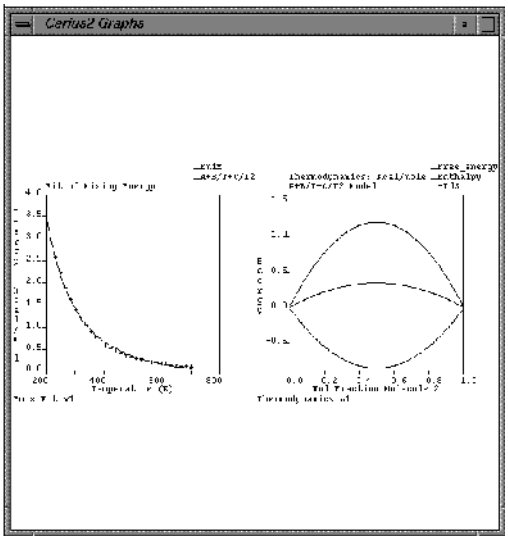
The Gallery and graph window should now be empty.

3. **Load the saved file of multiple graphs.**

Open the Load Graphs control panel by choosing **File -> Load Graphs** from the **Graphs** card.

You may have to move up several directories to return to your working directory where the two_graphs.grf file is located.

Load back the two_graphs.grf file.



F. Creating new graphs and using expert functions

In this final section of the Graphs tutorial, you create a new User Graph and copy datasets from other graphs onto it. You also learn how to use the Expert Functions: Clean, Data Placement, and Keep Same.

Clear

In part E (page 108), you deleted all the graphs from the Gallery Manager by resetting the **Graphs** card. In the following steps, you learn how to selectively remove graphs from the gallery.

Data Placement & Keep Same

There is another version of the Emix Fit graph saved in the file Cerius2-Resources / EXAMPLES / data / EM_PM_Emix.grf. Here, you load this graph to illustrate the usefulness of the **Keep Same** and **Data Placement** options of the Graphs Expert Functions control panel. In this exercise, *you* load the second version from file, but, in practice, it will usually be a Cerius^2 module that creates a new version of a graph and pipes it into Graphs. However, the principle is the same regardless of whether the graph is loaded or piped. The **Data Placement** control lets you decide how to treat new versions of the same graph. The **Keep Same** controls let you apply the graph formatting that you've specified for one graph to subsequent versions of the graph.

1. **Create a User graph.**

Open the Gallery Manager control panel by choosing **Gallery -> Manager** from the **Graphs** card.

Create a new User Graph by checking the third (empty) **Display** box in the **Graph Chooser** list box.

This causes the list box to update with the name User Graph v1, and an empty set of axes appears in the graph window.

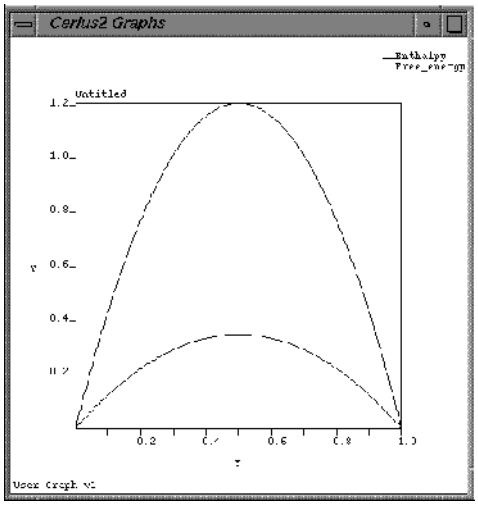
Next, you copy a dataset from the Thermodynamics graph to the new user graph.

Be sure that the **Edit** box of the User Graph is toggled **on** and that the **Display** boxes for the Emix Fit and the Thermodynamics graph are toggled **off**.

Open the Graph Manager control panel by clicking the **Graph Manager...** button on the Gallery Manager control panel.

Toggle **on** the **Display** boxes for the Enthalpy and the Free Energy data-sets.

These two datasets are plotted on the User Graph.



Optional: You may want to review what you learned in the previous exercises (pages 100–106) by customizing this graph: altering plot style, changing colors, scaling axes, and editing text.

2. Delete extra graphs from the Gallery.

Open the Graphs Expert Functions control panel by choosing **Gallery -> Expert Functions** from the **Graphs** card.

In the **Graph Chooser** list box of the Gallery Manager control panel, choose to display only the Emix Fit graph.

Click the **CLEAR** button on the Gallery Manager / Graphs Expert Functions control panel.

*Clicking the **CLEAR** button deletes from the Gallery Manager all graphs that are not currently on display in the graph window. The **Graph Chooser** list box should now look like the figure below (the Thermodynamics and the User Graphs graphs are gone).*

3. **Add a second graph.**

   Set the **Data Placement** popup of the Graphs Expert Functions control panel to **Additional Graph**.

   Open the Load Graphs control panel (**File -> Load** from the **Graphs** card), and load the file Cerius2-Resources / EXAMPLES / data / EM_PM_Emix.grf.

   *There are now two Emix Fit graphs listed in the **Graph Chooser** list box, and two Emix Fit graphs on display in the graph window.*

4. **Delete the second graph.**

   On the Gallery Manager control panel, set the second version of the Emix Fit graph to **off**. Then choose the **CLEAR** button of the Graphs Expert Functions control panel.

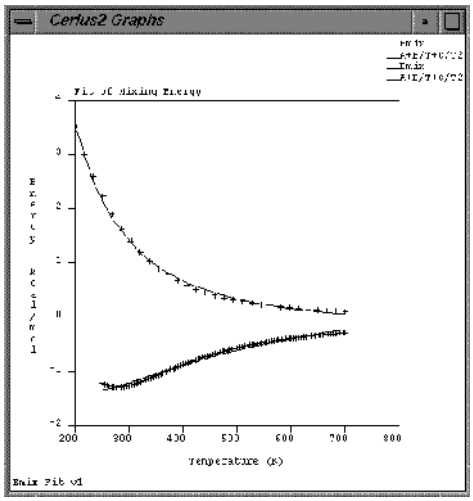
   This deletes the second version of the Emix Fit graph.

5. **Combine the data-sets from the two graphs.**

   Set the **Data Placement** option to **Combine With Existing**. Re-load the Cerius2-Resources / EXAMPLES / data / EM_PM_Emix.grf graph file.

   This time, when you load the second version of the Emix Fit graph, the data-sets from the two versions are combined and displayed on the same

axes.



Now set the **Data Placement** popup to **Replace Existing** and reload the Cerius2-Resources/ EXAMPLES/data/EM_ PM_Emix.grf.

Now, the older version of the graph is overwritten by the new one. ***Replace Existing*** *is the default for* ***Data Placement****; when a computational module creates versions of the same graph, the* ***Replace Existing*** *option prevents these many obsolete versions from accumulating in the gallery.*

6. Make two graphs with identical axes.

Open the Graph Scaling control panel (**Graph -> Scaling** from **Graphs** card), and set the scale of the X axis to **300 – 600** and the scale of the Y axis to **-1.3 – 2.0**.

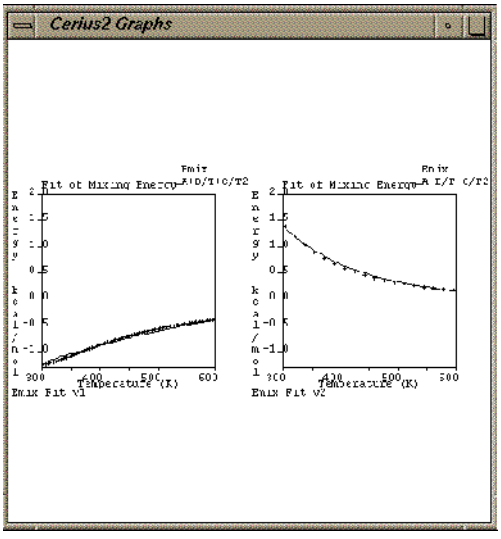
Open the Plotting Attributes control panel (**Data -> Plotting Attributes** from **Graphs** card), and set the **Color** popup to your favorite color.

Set the following option values in the Graphs Expert Functions control panel:

Data Placement	**Additional Graph**
Keep Same: Graph Axes	**On**
Keep Same: Plot Attributes	**On**

Reload the file Cerius2-Resources/EXAMPLES/ data/EM_MM_Emix.grf.

*Because the **Keep Same** options are toggled on, the scale and plot attributes for the new graph are not the ones stored in the file, but instead, they are the same as the previous version of the graph.*



7. Exit or continue to new tutorial.

If you are going to continue immediately with another tutorial:

> *Re-initialize* the program by selecting **New Session** from the **File** pulldown menu and choosing the **Confirm** button on the **Re-initialize** dialog box.

Re-initialization resets all the Cerius^2 control panels to their original defaults.

Alternatively, if you want to stop now:

> Choose **Exit** from the **File** pulldown menu to quit from Cerius^2 and then choose the **Exit** button on the **Exit Option...** dialog box.

Checklist review

In this tutorial you learned how to...

- ❑ Load and save graph files
- ❑ Display graphs using the Gallery Manager
- ❑ Display data-sets using the Graph Manager
- ❑ Alter the data plot style and color
- ❑ Specify a Y-offset value for data-sets
- ❑ Edit text for graph titles, axes, and keys
- ❑ Use the Expert Functions to selectively remove graphs and to control version overwrites

What next?

In this tutorial exercise, you have encountered only the xy linear graph. Many Cerius^2 modules also create 2D cartesian and polar graphs. These graphs can be manipulated (loaded, saved, modified) in much the same way as the xy graphs. When a polar or cartesian

contour graph is selected for editing, the appearance of the Graph Scaling and Plotting Attributes control panels are automatically altered to show the special controls you need to modify 2D plots. You may now want to run one of the Cerius^2 example files that creates a 2D graph and practice scaling it and modifying its plot attributes. For more information about 2D plots, see the *Graphs* chapter of the *Cerius^2 Modeling Environment*.

These are some of logfiles that generate 2D plots:

ANL_exafs_SiAs.log	ANL_hrtem_particle.log
ANL_gsas_inorganic.log	QM_mopac_SN2.log
POL_diff_crys.log	POL_diff_am.log

Alternatively, you may want to learn more about the graphs in Cerius^2 by reading the user manual selection listed under the *Related material* heading below.

You may now want to proceed to the tutorials in *Cerius^2 Materials Sciences Tutorials* or *Cerius^2 Life Sciences Tutorials*, or you may prefer to explore other Cerius^2 modules on your own with the aid of the Cerius^2 user's reference books and the on-line help text.

Related material

1. The *Graphs* chapter of *Cerius^2 Modeling Environment*.
2. The *File Formats* appendix of *Cerius^2 Modeling Environment*.

Basic Molecular Simulation: Minimization & Dynamics

This chapter shows how to use molecular mechanics techniques to simulate the behavior of a system on an atomistic scale. The example used is a simulation of beta-D-glucose in water.

The tutorial has four parts:

A. Building an initial model of the glucose molecule using the 3D Sketcher

B. Refining the model using molecular mechanics minimization to optimize bond lengths, angles etc.

C. Adding water (for the purposes of this tutorial only a small amount of water is included)

D. Simulating the behavior of the glucose / water system over time using molecular dynamics.

The purpose of this lesson is to introduce the most basic tools for atomistic level simulation. More advanced simulation and analysis options are described in *Cerius^2 Tutorials—Materials Science* and *—Life Science.*

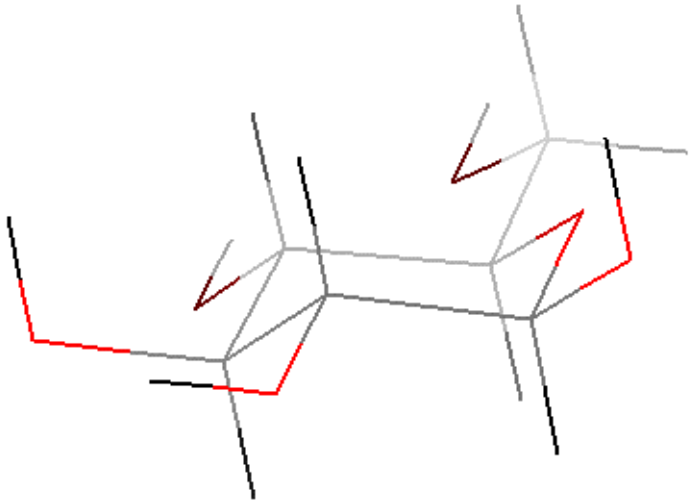
A. Build a model of the glucose molecule

1. Construct a glucose model

To start Cerius^2, enter **cerius2** in a UNIX window. After Cerius^2 starts, open the 3D Sketcher from the **Build** pull-down and construct a model of glucose.

See Using the 3D Sketcher, for guidance on using the 3D Sketcher.

Click and hold the **CLEAN** button in the Sketcher control panel to clean the structure.



B. Minimize the glucose energy

During a molecular mechanics simulation the movement of the atoms (the changing of bond lengths, angles, etc., and the interactions between non-bonded atoms and molecules) are controlled by a mathematical function usually referred to as the forcefield. The accuracy of a molecular mechanics simulation depends critically on the choice of forcefield. The PCFF forcefield has been shown to give accurate models of a wide range of organic molecules and polymers and is used in this tutorial. Information about other forcefields and theoretical background about atomistic-level simulation using molecular mechanics can be found in the *Forcefield-based Simulations* book.

1. Load the forcefield.

Open the **OFF SETUP** card deck and locate the **OPEN FORCEFIELD** card. Load the pcff_300_1.01 forcefield.

You may need to scroll down through a number of other forcefields to locate pcff. Note that references are written to the textport for your

information.

A molecular mechanics forcefield contains different sets of parameters (different bond lengths, etc.) for atoms in different bonding environments. For example, the oxygen in a carbonyl group will be modeled using different parameters than those used for oxygen in an ether group or in water; carbon in benzene will be given different parameters to carbon in ethanol or in ethene. Before running the simulation it is necessary to identify these different atom types.

2. **Identify the atom types.**

Open the **Atom Typing** menu by holding down the **Typing** option on the **OPEN FORCEFIELD** card and selecting **Atoms**.

Select the **Run** button next to **Calculate using typing rules** to ask Cerius^2 to identify the atoms types for all the atoms in the current model (the glucose molecule).

Change the **Atom Labeling** popup on the tool bar from **NO LABEL** to **FFTYPE**, and then to **CHARGES.**

Note that the oxygen atoms and carbon atoms in different bonding environments have been identified as different atom types. Once the atom types and bonding environment were identified, partial charges were automatically allocated to each atom.

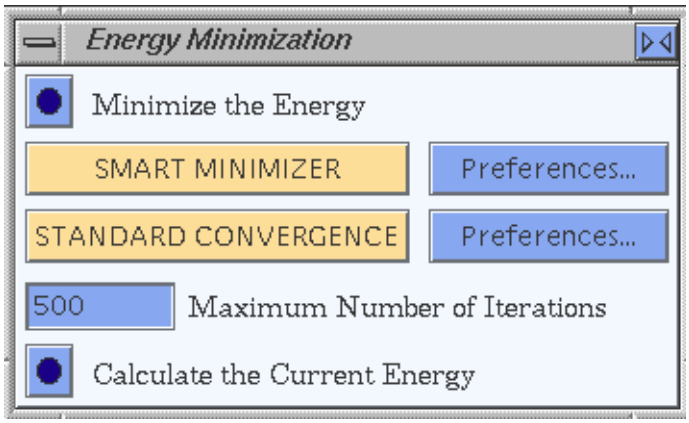
3. **Minimize the energy of the model.**

Select the **MINIMIZER** card from the **OFF METHODS** card deck (it is usually the first card in this deck).

During molecular mechanics minimization the positions of the atoms in

the model are altered to find lower energy conformations of the molecule.

Open the **Energy Minimization** menu by selecting **Run** from the **Minimizer** card.



The **Smart Minimizer** works through a series of minimization algorithms that have been found to give the most efficient minimization for molecular models. Pick the **Smart Minimizer** with the right-hand mouse button to read about the methods used. With the options set as shown, up to 500 iterations (changes in the molecular model which reduce its energy) will be carried out. The minimization will stop either at 500 interactions, or earlier if a minimum energy structure is located.

Select the **Preferences...** button to see the convergence criteria used.

Select the **Run** button to minimize the energy.

C. Add water to the system

1. Create water molecules with the Sketcher

If the **3D-Sketcher** menu is not still active, open by selecting it from the **Build** pulldown menu. Change the **Sketch with element** to oxygen, and double-click at five or six random locations around the glucose molecule.

This sketches five or six isolated oxygen atoms —shown by default as small red stars.

Select the **H ADJUST** button on the **Sketcher** menu to automatically add hydrogens to satisfy the oxygen valences.

This produces five or six water molecules.

D. Simulating the behavior of the glucose/water system

1. Identify the atom types

Return to the **OFF SETUP** card deck and open the **Forcefield Atom Typing** menu (select **Typing/Atoms** on the **OPEN FORCEFIELD** card). Calculate the atom types using typing rules.

This identifies the atom types in the water molecules and assigns appropriate partial charges.

You can select **CHARGES** from the **Atom labelling** popup menu to view these charges. Change back to **NO LABEL** before continuing.

Before carrying out a molecular dynamics simulation it is always wise to run a few steps of molecular mechanics minimization to relax any "hot spots".

Select the **MINIMIZER** card from the **OFF METHODS** card deck. Open the **Energy Minimization** card by selecting **Run** from this card. Reduce the **Maximum Number of Interactions** to **200** and **Minimize the Energy**.

*The most significant interactions between the glucose molecule and the surrounding water will be hydrogen bonds. The PCFF forcefield does not contain an explicit hydrogen bond term, but correctly models hydrogen bonding as a result of electrostatic and van der Waals interactions between non-bonded atoms. You can use the **Edit H-bonds** command under the **Build** pulldown menu to view the predicted hydrogen bonding.*

2. Calculate hydrogen bonds

Select the **Build/Edit H-bond** from the top menu bar. Click the **Preferences...** button to see the criteria that will be used to judge the presence of hydrogen bonds. Click the **CALCULATE** button to display the pairs of atoms that fall within the H-bond criteria.

Turn on the **Enable Automated Recalculation** so that the changing hydrogen bonding pattern will be displayed during the molecular dynamics simulation.

3. Simulate the system dynamics

Select the **Dynamics Simulation** card from the **OFF METHODS** card deck and open the **Dynamics Simulation** menu by selecting **Run**.

This model is fairly small so the number of dynamics steps can be increased to 2000 without making the simulation too time consuming. Each step simulates 0.001 ps, so the entire run will simulate the behavior of the glucose/water system for 2 ps.

A certain amount of analysis is carried out during the simulation and results will be displayed in the graphics and graph windows, but further analysis, after the simulation completes, requires data to be saved.

Select the **Trajectory...** button at the bottom of the **Dynamics Simulation** menu, or select **Trajectory ->** from the **Dynamics Simulation** card to open the **Dynamics Trajectory Output** menu.

Select to **Create a Dynamics Trajectory** file with an update every 100 steps (**Trajectory Update Frequency**). This means that during the 2000-step simulation, 20 trajectory frames will be saved for later analysis. Type in **glucose_water** as the **Filename Prefix**.

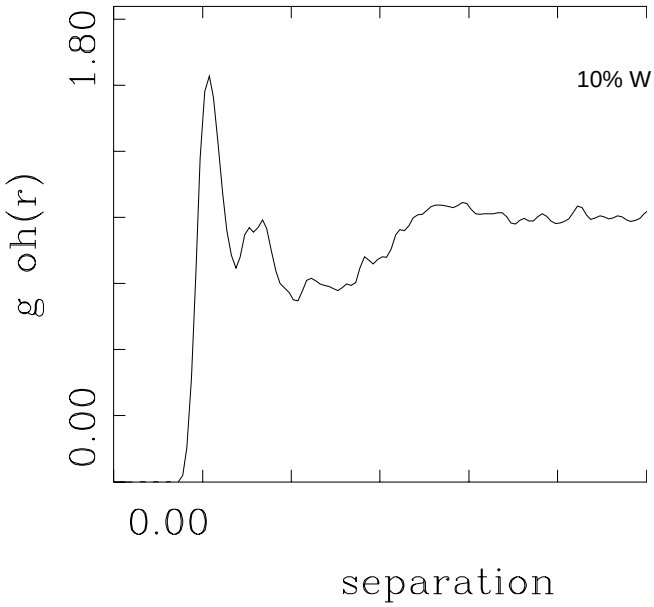
Return to the **Dynamics Simulation** menu and select the **Run Dynamics** button.

As the simulation continues, the structure on the graphics screen is updated every 25 steps.Notice the changing H-bond pattern. The graphs show that the temperature of the simulation fluctuates around

the requested 300K.

What to do next

This simple simulation might be useful to provide insight into hydrogen bonding patterns and dynamic behavior. To obtain a more quantitative measure of hydrogen bonding between water and beta-B-glucose the calculation could be repeated with a larger number of water molecules using periodic boundary conditions. The resulting trajectory file could be analyzed to predict the pair correlation function between the hydroxyl groups on the glucose and the water.



The area under the h-bond peaks is proportional to the number of hydrogen bonds in the system and can be compared to results for other systems (for example to other carbohydrates).

It is known that monosaccharides in water undergo structural isomerization. Processes that involve bond breaking and formation will not be observed using molecular mechanics, but could be stud-

ied using quantum mechanics models (for example, using Fast-Structure).

4 The Cerius^2 Interface

The Cerius^2 product line is a range of molecular modeling software, all based on the core control and presentation platform called the Cerius^2 *Visualizer*. The Visualizer is an integrated collection of tools whose functions include Cerius^2 session management, session logging, building and visualizing atomistic models, model management, saving and loading models, 3D graphical representation, data presentation, and environment customization.

The Visualizer supports numerous specialized Cerius^2 application modules. These plug into the Visualizer and are all controlled with a consistent mouse-driven graphical user interface (*GUI*). The GUI provides intuitive control of all functions, maintaining a consistent look and feel throughout the Cerius^2 environment.

This section explains

This section tells you how to run Cerius^2 and introduces basic features of the graphical interface. It includes:

Starting Cerius2

Initial layout of the Cerius2 screen

Using the mouse—the basics

Using the main control panel

Controls and control panels

Information sources

Other windows

Related information

The rest of this guide describes in detail how to use the Visualizer. Another guide, *Cerius^2 Builders*, describes the specialized builder modules you can add to the Visualizer to supplement its basic model-sketching capabilities. Each other optional application module or group of related modules includes its own documentation.

Starting Cerius^2

Cerius^2 is started by invoking the **cerius2** script, which is typically located in ~msi/cerius2/runtools. On your system, the script may have been copied or linked to a standard directory in your search path, such as /usr/local/bin. If not, you may want to set up and use an alias. If you are not sure how your system is configured, please ask your system administrator.

Once you are correctly set up, you should make a working directory in which to run Cerius^2. You should have write access to such directories. (Write access is necessary because symbolic links and log files are created in the startup (run) directory during a Cerius^2 session.) You may want to create subdirectories in which to store related Cerius^2 files for each of your projects and use one of these as your run directory.

Start a regular Cerius^2 session by changing (**cd**) to the desired run directory and entering at the UNIX prompt:

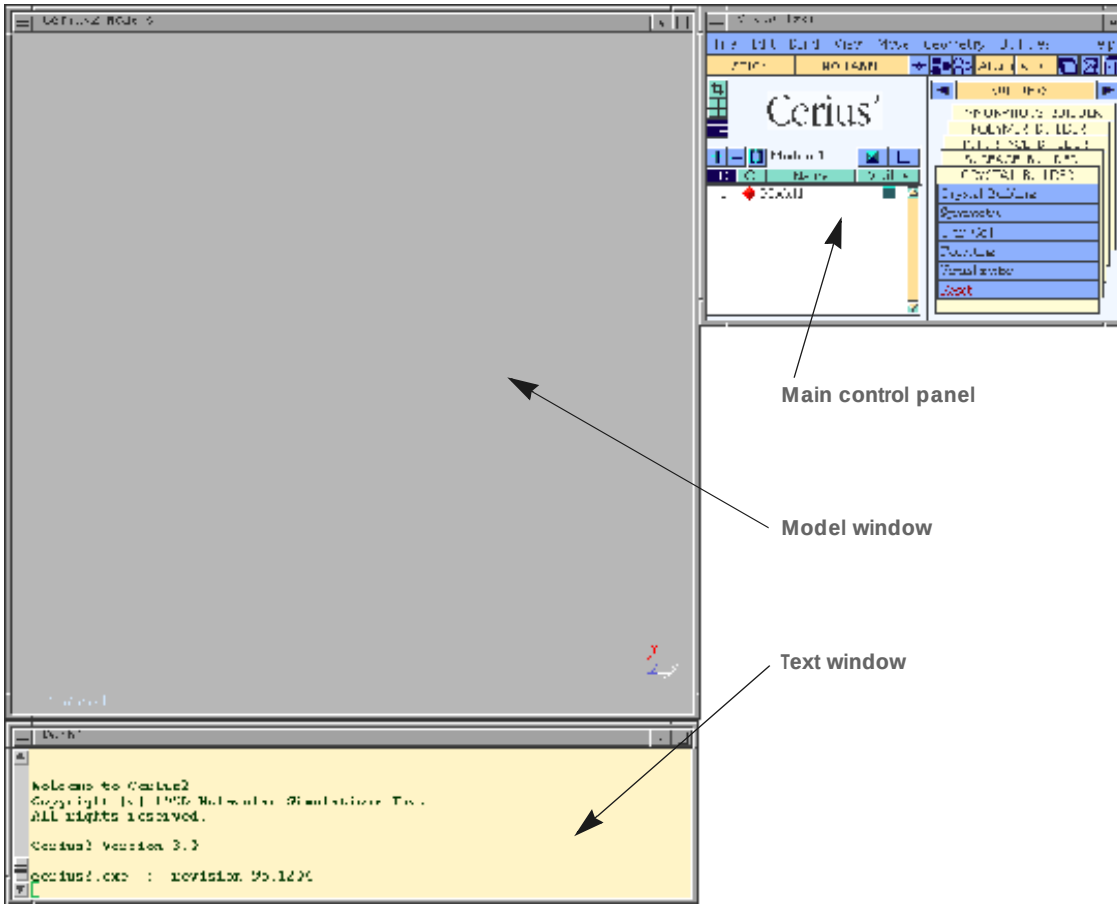
```
> cerius2
```

Example

A specific example of starting Cerius^2 is presented under *Starting Cerius2*.

Initial layout of the Cerius^2 screen

The key GUI elements are the *main control panel*, which contains the Visualizer controls, the *model window*, in which models are displayed, and the *text window*, which is used to display text messages. Their initial screen orientation is shown below (except that the large square window should be black on your screen)



Main control panel

The main control panel contains the Visualizer controls and is therefore your primary point of interaction with Cerius^2. All control panels are obtained directly or indirectly from the main control panel. Unlike ordinary control panels however, the main control panel should not be resized. You may stow (iconify) the main control panel by clicking the stow button on the window border. This stows all open Cerius^2 windows to a single icon on your desktop. If you try to close it, a warning message appears, asking you to confirm that you want to quit the Cerius^2 session.

For details on using the main control panel, please see *Using the main control panel*.

Model window

Cerius^2 provides real-time 3D graphic display of models in the model window. The models displayed, the style of display, model orientation, and so on are determined primarily by Visualizer controls accessible from the main control panel (see, for example, *Managing Models and Sessions* and *Viewing and Displaying Models*). The mouse, function keys, and cursor keys can also be used to effect rotations, translations, and scaling. The mouse is also used to select atoms for various operations.

Mouse and keyboard shortcuts

Summaries of mouse and keyboard shortcuts available in the model window are accessible from the **Help** pulldown menu on the main control panel menu bar (by selecting **Help/Topics/Mouse Operations...** or **Help/Topics/Keyboard Operations...**). Information on mouse and keyboard operations can also be found in *Mouse and Keyboard Actions*.

Text window

Cerius^2 uses the text window primarily to display text messages. However, you can use it to enter shell commands (prefixed by an exclamation point), Tcl scripting language commands, and comments. To learn more about Cerius^2 scripting, see *Using Cerius^2 Command Scripts*.

Caution

However, do not try to start programs that take over the window (such as vi or rn) in this window.

Using the mouse—the basics

Mouse buttons

Cerius^2 controls are operated with the mouse. The mouse has three buttons that perform different general functions:

- Left button = the action button. Used to click a control panel button, drag a slider, select an option from a pulldown menu or popup, and so on.
- Middle button. Used by your system's native window manager and also for certain model-manipulation activities.
- Right button = the help button. Used to obtain help text for GUI controls. For details, see *On-screen help*.

Note

The actions of the mouse buttons can differ, depending on whether the cursor is over control panels, in the model window, or over tables or graphs. A summary of all mouse button functions is contained in *Mouse and Keyboard Actions*.

Mouse activities

Certain words are generally used in indicating what to do with the mouse. Unless otherwise specified, they always mean to use the *left* mouse button. (The types of controls are described under *Types of controls*.)

Definitions

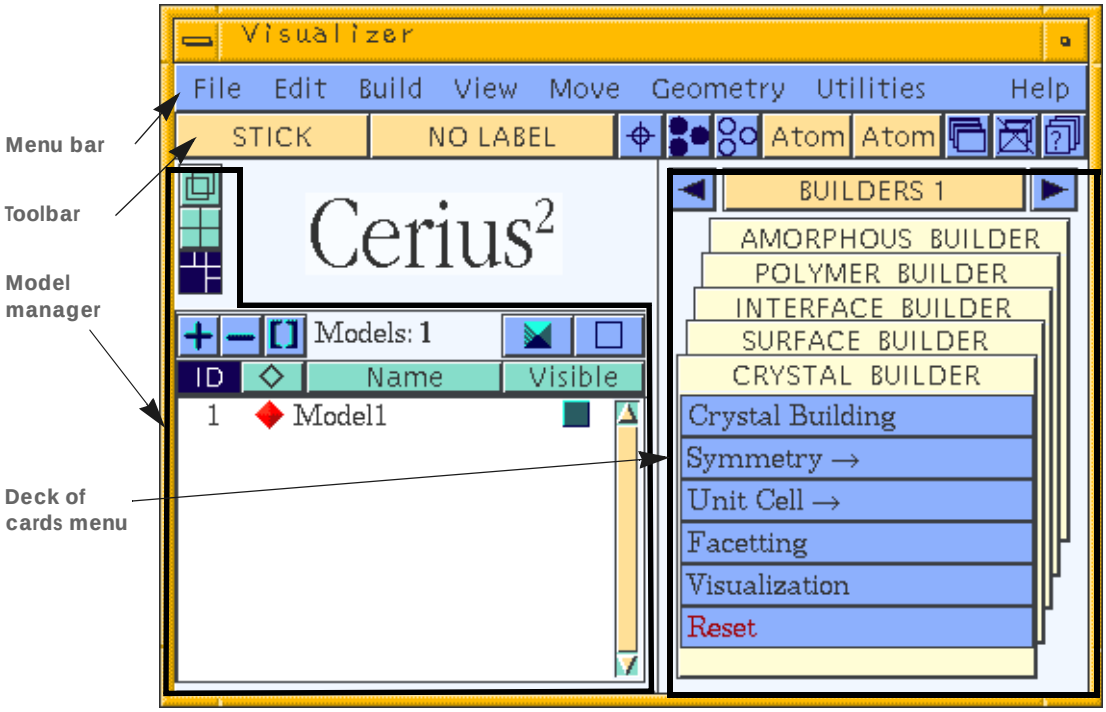
- *Click* = move the mouse so as to place the cursor over the control or other item mentioned and then press and immediately release the left mouse button.
- *Double click* = place the cursor over the control or other item mentioned and then click the left mouse button twice in succession (relatively quickly).
- *Click and drag* = place the cursor over the control or other item mentioned and then press the left mouse button and, while keeping the button depressed, move the cursor to the item mentioned and then release the button when the cursor is over

that item. For menus, popups, and similar controls, a list of items usually appears as soon as you click.

- *Select, choose, set the popup to a value,* etc., = click or click and drag. It will be clear from the context.
- *Pick* = click an item (usually an atom) in the model window.
- *Check* and *uncheck* = click a check box so that it contains or does not contain (respectively) a checkmark.
- *Toggle* = click an on / off control to change its state from on to off or vice versa.

Using the main control panel

The main control panel controls the Cerius^2 • Visualizer. Functionalities are collected into related groups of controls:



Parts of the main control panel

The *menu bar* contains pulldown menus that provide access to all Visualizer tools. For descriptions of the menu bar entries, see *The menu bar*.

The *toolbar* provides a set of frequently used Visualizer tools, some of which are duplicated in control panels relating to model viewing and selection. For full details, see *The toolbar*.

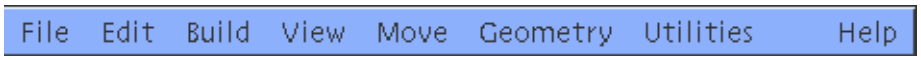
The *model manager* enables you to control the selection, editing, and saving of models in the Cerius^2 modeling environment. The model manager is described fully under *Handling multiple models*.

Application modules are represented by *menu cards* grouped into *card decks* in the *deck of cards* menu. For more information, see *Deck of cards menu*.

Window manager controls, located in the window border, allow you to stow all open Cerius^2 windows to a single icon on your desktop.

The menu bar

The menu bar is found at the top of the main control panel:



The items on the menu bar provide click-and-drag access to related sets of controls:

- **File**—Access to session control, output, and file operations. These include working with Cerius^2 sessions, loading and saving structure files, and printing. See *Managing Models and Sessions*, *Printing models and graphs*.
- **Edit**—Access to atom selection and editing tools. See *Selecting atoms and groups of atoms* and *Basic editing*.
- **Build**—Access to the Visualizer's general model building (including the 3D-Sketcher) and attribute editing tools. See *Building Models*. Builder modules that provide additional, specialized model building functionality are accessed from the deck of cards menu and are described in *Cerius^2 Builders*.
- **View**—Access to tools that enable you to manipulate the view of models in the model window, as well as to produce high-quality displays and renderings of those models. See *Viewing and Displaying Models* and *Enhancing Model Display*.
- **Move**—Access to tools that enable you to alter the 3D geometry of models by moving atoms. See *Translating and rotating atoms* and *Aligning and positioning atoms*.
- **Geometry**—Access to geometry analysis tools, which enable you to examine the 3D structure of models. See *Geometry Analysis*.
- **Utilities**—Access to Visualizer utilities, which enable you to control, record, and play back Cerius^2 sessions, customize various aspects of the Cerius^2 modeling environment, and access and control external applications. See *Customizing the Interface* and *Scripts and Licensing*.

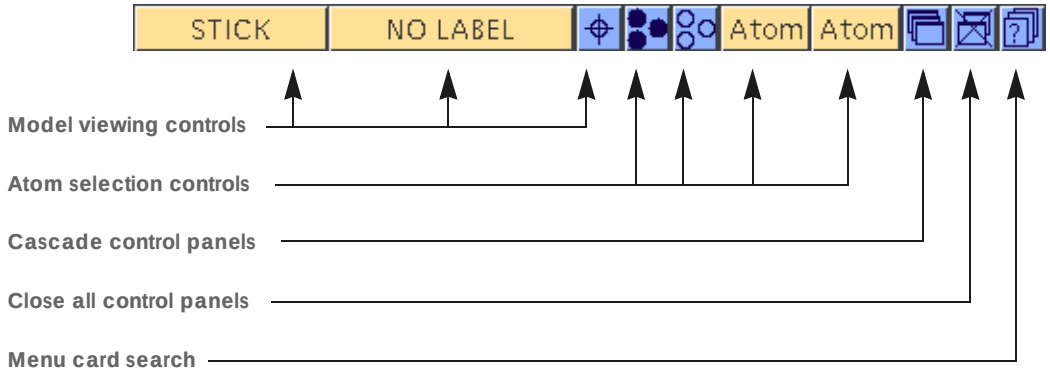
- **Help**—Access to on-screen help on the basics of the Cerius^2 modeling environment and to some prerecorded demonstrations. Simply select the topic that you are interested in. See also *On-screen help*.

Keyboard shortcuts

The functions of several pulldown menu items can also be carried out by using keyboard shortcuts (generally <Alt>–key combinations) when the cursor is in the model window. Relevant key combination are shown beside the item on the pulldown menu itself. See also *Keyboard shortcuts*.

The toolbar

The toolbar is located just below the menu bar in the main control panel:



Some controls on the toolbar duplicate functions of control panels relating to model viewing and selection; others provide unique functionality.

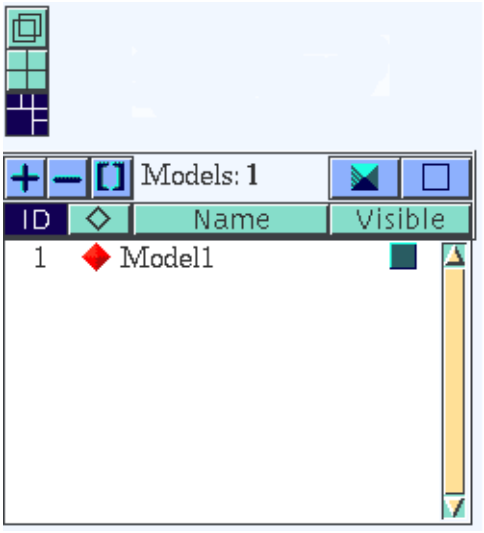
Types of controls in the toolbar

- Model viewing controls—Use these controls to change the model's display style; add, change, or remove labels; and reset the position of the model. See *Model display style*, *Labels*, and *Setting position and orientation*.
- Atom selection controls—Use these tools to control atom selection. See *Selecting atoms and groups of atoms*.

- Cascade control panels—Click to reorganize all open control panels into an ordered cascade, which helps prevent screen clutter.
- Close all control panels—Click to close all open control panels.
- Menu card search—Click to access the Menu Card Search control panel, which enables you to search for words in the deck of cards menu hierarchy and in the menu bar menus (*Menu card searching*).

The model manager

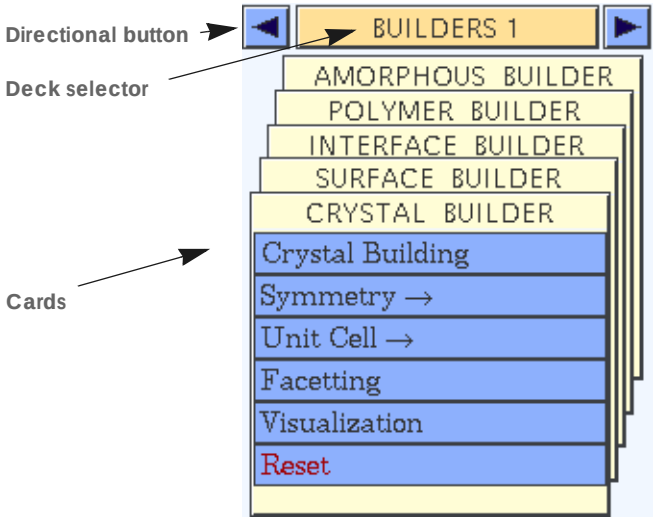
The model manager enables you to control the selection, editing, and saving of models in the Cerius^2 modeling environment.



The model manager is described fully under *Basic model management tasks*.

Deck of cards menu

The deck of cards menu on the main control panel provides easy access to application modules and their controls



Access to application modules

The exact appearance of the deck of cards menu depends on which application modules you have purchased. Each module that is added to the Cerius^2 interface is represented by a menu card. Some menu card entries provide direct access to control panels; others (whose labels end with an arrow) give access to pullright menus, which each give access to a control panel. A **Reset** control (shown in red letters) appears on most cards and can be used to reset the controls for that module.

You can select a specific deck of cards from the deck selector popup (by clicking and dragging). Alternatively, you can cycle backwards or forwards through available card decks by clicking the left or right directional buttons next to the deck selector popup.

Menu cards are grouped into decks of 1–5 cards, which usually represent modules having related functionality. To bring any card in the current deck to the front, simply click the card's title.

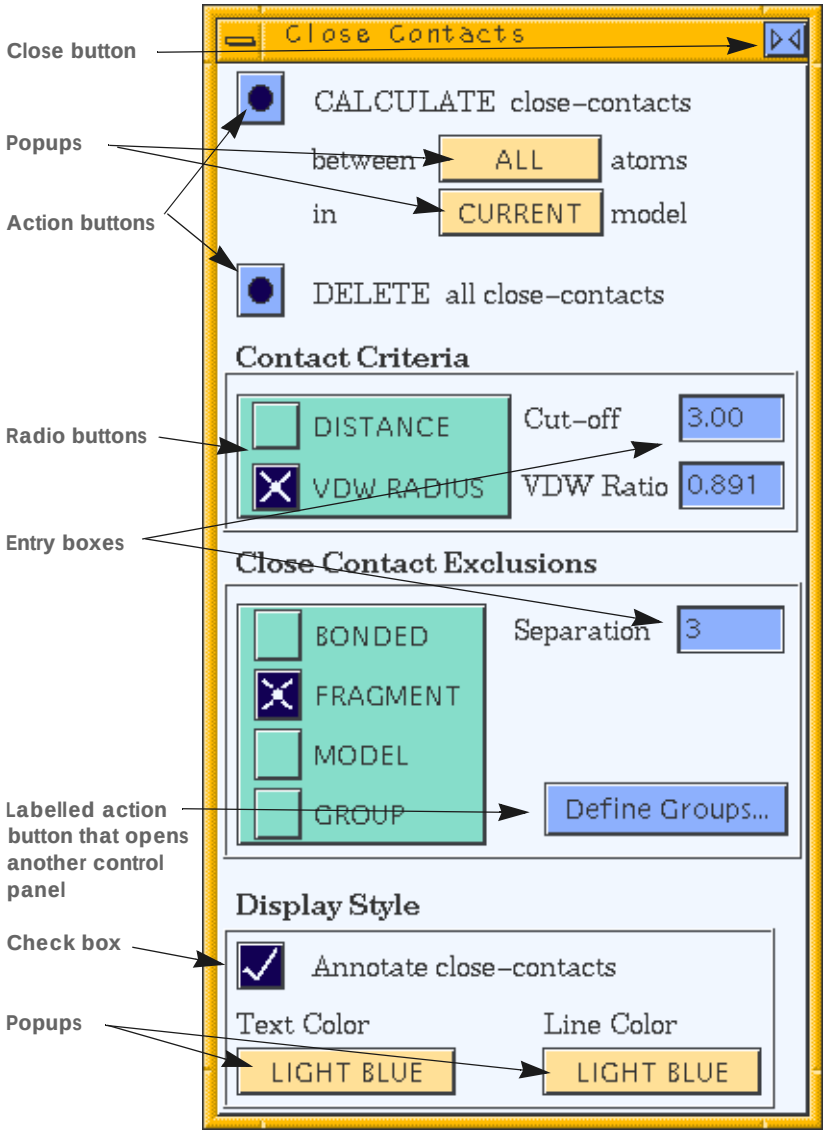
Customization

You can customize the deck of cards menu by using controls in the **Utilities** pulldown menu on the main control panel's menu bar. You can make new decks, name them, change the card order, and so on. For details, see *Customizing the Interface*.

Controls and control panels

Definition

Control panels are windows that contain functionally grouped Cerius^2 controls. Many different control types are available, each designed to provide an intuitive method of invoking an action, providing a value, setting an option, or selecting an item. The control panel below illustrates many types of controls.


Close button
Popups
Action buttons
Radio buttons
Entry boxes
Labelled action button that opens another control panel
Check box
Popups
Close Contacts
CALCULATE close-contacts
between
ALL
atoms
in
CURRENT
model
DELETE all close-contacts
Contact Criteria
DISTANCE
VDW RADIUS
Cut-off
3.00
VDW Ratio
0.891
Close Contact Exclusions
BONDED
FRAGMENT
MODEL
GROUP
Separation
3
Define Groups...
Display Style
Annotate close-contacts
Text Color
Line Color
LIGHT BLUE
LIGHT BLUE

Types of controls

Color-coding

Different types of controls are distinguished by their appearance. For instance, popups are yellow, two-state controls (which can be on or off, checked or unchecked, etc.) are purple or green (respectively), and buttons that perform an immediate action when clicked are blue.

Labels and shape

A control's function is generally indicated by labels (words) on or next to the control and / or by a graphical icon. A control's function may also be suggested by its shape (e.g., a slider or a dial, which you manipulate by clicking and dragging).

Except for the deck of cards itself, all buttons and menu items that provide access to a control panel are followed by an ellipsis (…). For example, selecting a menu item or clicking a button labeled **Preferences…** brings up a control panel that enables you to set related preferences.

Functions of typical controls

The label on a *labeled button* indicates what action occurs if you click the button.

- *Radio buttons* are used to select only one of a group of options.
- An *action button* (or *run button*) performs the associated action (usually indicated by the label and / or some nearby text) when you click it.
- *Popups* and similar controls display a list of options when clicked, from which you can select one by dragging the cursor.
- *Entry boxes* are used to display current values and enter new ones.

Tip

To enter the exponent portion of a double-precision number in an entry box that is used for entering numbers, use an E followed by a signed number, for example, enter 1.234e-4 for 0.0001234 and enter 1.234e4 for 12340.0.

Functions of specific controls

If you are unsure about the function of a particular control, click it with the right mouse button to obtain help (see *On-screen help*).

Buttons in the control panel window border

Clicking the *close button* in the upper right corner of the control panel border closes the control panel.

Clicking the button in the upper left corner gives access to some of your system's window-manager functions.

Managing control panels

Opening control panels

To access a control panel, you select a menu item from the main Visualizer control panel (*The menu bar*), select an item from a card (*Deck of cards menu*), or click a pushbutton in an open control panel. Instructions for accessing particular control panels are given throughout this guide.

Tip

Often, a control panel can be accessed in several different ways. Since Cerius^2 is *amodal*, it makes no difference how you access a particular control panel or whether you close and reopen it or just leave a frequently used panel open on the computer screen.

Closing control panels

To close a control panel, click the close button  in the upper right corner of the control panel's border.

To close all open control panels, click the clear panels tool  on the toolbar of the Visualizer main panel.

Cascading control panels

To group all open control panels into an orderly cascade, click the cascade panels tool  on the toolbar of the Visualizer main panel.

Stowing all Cerius^2 windows to an icon

To stow all open Cerius^2 windows to a single icon on your desktop, click the stow button on the upper window border of the main control panel. To open the windows again, simply click the icon on your desktop.

Additional information

More advanced management of control panels, including customization so that certain control panels are opened whenever you start Cerius^2, is discussed under *Control panel management*.

Information sources

On-screen help

While using Cerius^2, you can obtain information about every control and menu item by using the on-screen help facility. To obtain a help window, move the cursor over the control or menu item and click the right mouse button. A window containing the requested help text appears in the center of the screen. Click the help window to close it or click the right mouse button over another item to obtain more help.

If you allow the cursor to rest over many controls, a small balloon help message appears, identifying the tool's function.

General information about Cerius^2 and basic GUI operations is available from the **Help** pulldown menu on the main control panel's menu bar.

Example

An example of using the Cerius^2 help facility is presented in *Accessing on-screen help*.

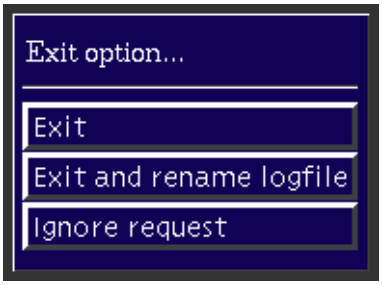
Menu card searching

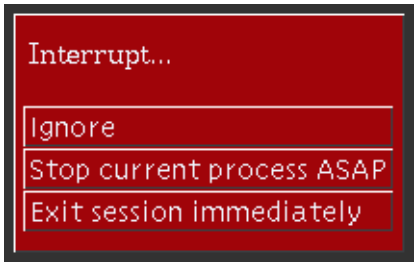
The menu card search tool on the main control panel's toolbar gives access the Menu Card Search control panel. You can use this control panel to search for a keyword used anywhere in the menu card deck hierarchy or in menu items accessed via the menu bar. The search is case-insensitive, and wildcards can be used. For details, see the on-screen help associated with the controls in this control panel.

Messages and status information

Warnings

When you request that Cerius^2 perform some procedure with potentially important consequences (e.g., loss of data), a warning message window appears. These windows typically give you a chance to confirm or cancel your request or to make an alternative request, by clicking a push-button control.





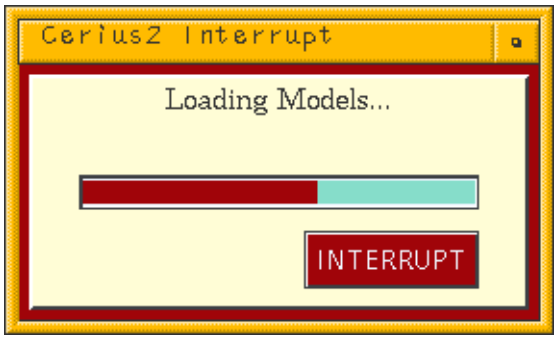
Typical controls include:

- **Ignore** or **Ignore request**—Command processing continues from the point at which it was interrupted.
- **Stop Current Process ASAP**—The tool or application stops processing as soon as possible, that is, when Cerius^2 determines that it can do so cleanly.
- **Exit Session Immediately**—The Cerius^2 session is ended immediately.

Time-consuming processes

When Cerius^2 is busy processing a command issued from the Visualizer or an application module, a Cerius^2 message window indicating the status of the job may be displayed. This window can take several forms, depending on the nature of the command in process. In some, a moving bar indicates progress. In others, where progress is less easily quantifiable, a diamond-shaped activity indicator appears.

During such periods of prolonged activity, you cannot perform any other Cerius^2 tasks except basic mouse-controlled model-viewing actions. If the command in process can be stopped cleanly before its scheduled conclusion, the message window contains an **INTERRUPT** button.



Click the **INTERRUPT** button (if present) to stop processing the command. A warning window (see *Warnings*) with several options appears, giving you the chance to confirm your choice or change your mind.

When Cerius^2 is iconified

If a process is running when you stow the main control panel to a desktop icon (see *Managing control panels*), the Cerius^2 icon displays a progress meter.

Other windows

Other windows, containing controls and/or static or dynamic information, appear as needed. Some examples (and where you can find more information on them) are:

- Graph window (*Working with Graphs*).
- Table window (*Working with Tables*).
- Rendering windows (*Rendering and ray-tracing*).
- Periodic table window (*Building Models*, e.g., *Dummy atoms*).

5 Building Models

The Cerius^2 • Visualizer provides a variety of tools for making new models and changing existing models. These include a mouse-driven 3D-Sketcher for constructing and editing models (this section), as well as features that enable you to position atoms precisely (*Precise positioning of atoms during building*), edit the properties of selected atoms or elements (*Editing element and bond attributes*), change bonding (*Changing the hybridization and adjusting the valence*), and introduce disorder (*Introducing substitutional disorder*). You can also annotate the model by adding items such as text, arrows, and boxes (*Viewing and Displaying Models*).

These general-purpose basic and advanced building and editing tools are directly available from the **Build**, **Edit**, and **Move** pull-down menus on the main control panel's menu bar.

Other builders designed for constructing more specialized models are available as separate modules and are accessed with the deck of cards menu. They have separate documentation.

This section explains

Basic building

Selecting atoms and groups of atoms

Basic editing

Advanced building and editing

Other builders

Table 1. Finding information about building models

If you want to know about:	Read:
Strategy for building models.	*Strategy*.
Example procedure.	*Building a model—caffeine*, *Building another model—ferrocene*.
Mouse buttons and keyboard use.	*Mouse and Keyboard Actions*.
Adding functional groups.	*Adding templates (groups of atoms)*.
Specifying bond lengths, angles, and torsions.	*Examining and changing bond lengths*.
Specifying, editing, drawing (etc.) hydrogen bonds.	*Hydrogen bonds*.
Inverting a chiral center.	*Inverting about an atomic center*.
Moving models and parts of models.	*Translating and rotating atoms*, *Aligning and positioning atoms*, *Managing Models and Sessions*.
Optimizing the conformation.	*Refining the conformation*.
Introducing disorder into a structure.	*Introducing substitutional disorder*, *Introducing positional disorder*.
Adding labels, arrows, etc.	*Labeling and annotating models*.
Changing color and display style.	*Model display style*, *Enhancing Model Display*.
Specifying temperature factors.	*Temperature factors*.
Changing default properties and functionality.	*Editing element and bond attributes*, *Control of the model-cleaning function*.
Saving a constructed model.	*Saving model structure files*.
Saving preferences.	*Using saved sessions as preferences settings*.

Basic building

Why read this section

This section tells you where to access the basic building tools and how to perform tasks that are typically associated with building the basic skeleton of a small model. It contains information on:

Starting to construct a new model

Adding atoms and bonds

Adding templates (groups of atoms)

Fusing and connecting fragments

Adding hydrogens

Related information

Basic editing tasks, including changing element types, bonding, and model conformation, are presented under *Basic editing*. The final task you would perform for building almost any model would be to optimize its configuration (*Refining the conformation*). Storing models in files is presented under *Saving model structure files*.

Selecting atoms is presented under *Selecting atoms and groups of atoms*.

Tasks that may be less often or less typically performed, such as editing atom attributes and changing defaults and preferences, are covered in *Advanced building and editing*.

You should already know...

If you have never used Cerius^2 before or are unfamiliar with the terminology used to indicate how to use its interface, please go through the model-building example in *Introducing Cerius2* before continuing with this section. How to start Cerius^2, the names of parts of its interface, as well as basic mouse usage and how to access on-screen help, are covered in *The Cerius2 Interface*,

Starting to construct a new model

Strategy

Why develop a strategy

You can probably construct a model of almost any small model you want, simply by straightforward trial-and-error use of the 3D-Sketcher. This procedure will probably be good enough if you have to build only a few models. However, Cerius^2 building tools typically offer several ways of accomplishing the same end.

Therefore, depending on the types and number of similar models you need to work with, a more considered approach (including the use of model-building or -generating tools other than those contained within the Visualizer and not documented here) may prove

more efficient. So, it should be helpful for you to obtain some familiarity with all the relevant tools as you develop your own model-building style, using whatever combination of tools and order of tasks that works best for your purposes.

Task-oriented information

This section presents information in a task-oriented way, generally presenting simpler or default methods first. The organization assumes you would build the complete skeleton of a structure first and then edit it as desired. However, the task orientation (rather than tool orientation), as well as ample use of headings and labels, should facilitate your finding information, no matter what approach you use.

Note

This guide does not necessarily replicate control-specific information that can be found by using the on-screen help.

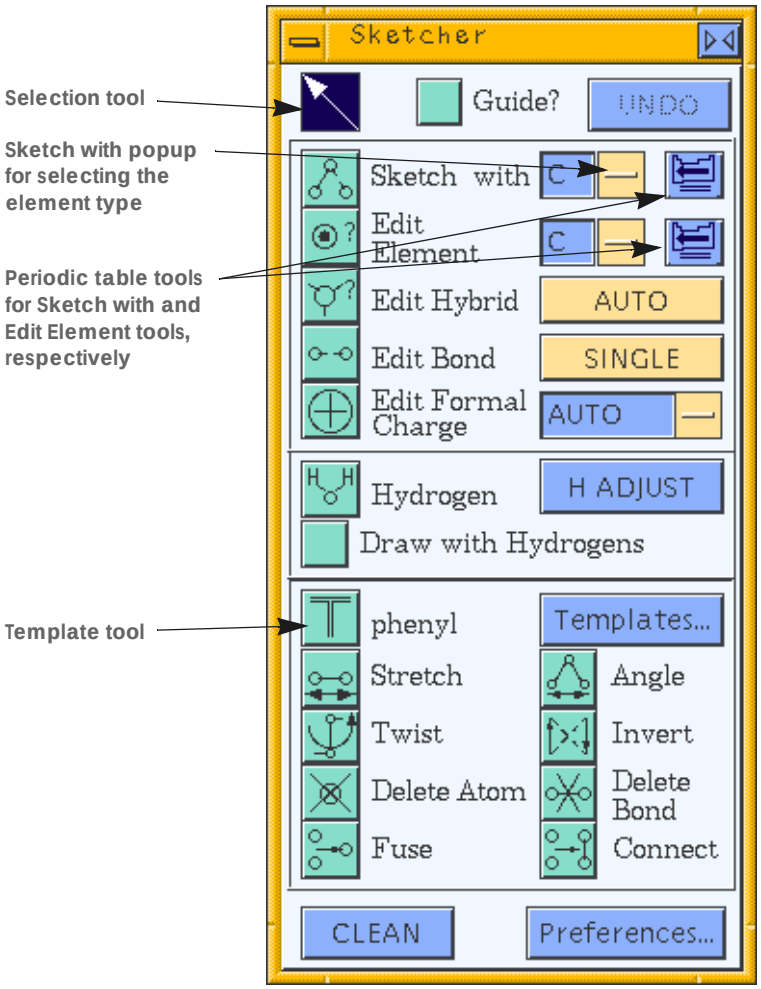
Some possible approaches

A few of many possible approaches include:

- Build a model using carbon atoms and available templates, then edit the element and bond types as desired.
- Add hydrogens as the heavy-atom skeleton is being built or after it is complete.
- Keep the conformation and topology as correct as possible while building a model or build a distorted model and then adjust its conformation and / or connectivity.
- Add several identical templates simultaneously at several points of a base model, then edit the individual functional groups as needed.
- Build a small model, copy it, edit both copies as desired, and then join the fragments into one larger fragment.
- Build small fragments, then use them as the basis for constructing larger models or as starting structures for use with the more specialized builders available as other Cerius^2 modules.
- Load templates from disk, then edit, fuse, and / or connect them to form a larger fragment.
- Load or generate a periodic system (*Other builders*), then edit it.

The 3D-Sketcher

You access the 3D-Sketcher by selecting the Build / 3D-Sketcher… menu item from the Visualizer's main control panel. This causes the Sketcher control panel to appear. This control panel provides a range of tools for mouse-controlled sketching, editing, and refinement of model structures:



How it works

Clicking any of the icon tools on the Sketcher control panel alters the function of the left mouse button. *Selection mode*, when the

selection tool (the arrow in the upper left of the Sketcher control panel) is highlighted, is the default for cursor behavior. Clicking other icon-type tools enables you to use the cursor, for example, to place atoms, manipulate angles, or change an atom's element type.

Many of the functions can be performed on several atoms simultaneously. This is done by first selecting (*Selecting atoms and groups of atoms*) the atoms, then double-clicking the appropriate tool. (If the tool is already active, only one click is needed to perform the action.)

In some Sketcher modes, a property of the structure can be changed by moving the mouse in the model window. Generally, dragging left-to-right or bottom-to-top while holding down the left mouse button increases a value (e.g., a bond length), and dragging in the opposite direction decreases the value.

Recovering from mistakes

An **UNDO** button, provided at the top of the control panel, can be used to cancel one or a series of previous commands for many types of operations. The **UNDO** button is greyed out when it is not usable.

Help

Checking the **Guide?** check box gives you on-screen help (in the upper left corner of the model window) on the 3D-Sketcher.

Examples

Detailed examples of using the Sketcher control panel to build caffeine (*Building a model—caffeine*) and ferrocene (*Building another model—ferrocene*) are included in this guide.

Other basic building tools

Other building tools are also accessed from the Visualizer's **Build** menu. Use of some of these is covered under *Advanced building and editing*, but others have functions that are similar to those in the 3D-Sketcher control panel. Among the latter are the **Add Atom…**, **Edit Atoms…**, **Edit Bonds…**, and **Edit H-Bonds…** menu items.

Most of these enable better control over exactly how the controls operate than does the 3D-Sketcher control panel and may therefore enable faster building under certain circumstances.

These alternatives to the sketcher often provide full support of periodic models in areas where the Sketcher does not (for example, to add atoms to a periodic system, you have to use the Add Atom control panel rather than the 3D-Sketcher control panel).

Some items in the **Edit** menu may provide quicker action than equivalent tools in the Sketcher control panel (especially if the Sketcher control panel is not open and you need to make only a few changes).

Adding atoms and bonds

The simplest procedure for building the basic structure of a model is to draw in the model window, manually placing atoms (connected by single bonds) at desired positions (see *Adding atoms and single bonds*). The model is then generally edited, and finally its conformation is optimized (*Refining the conformation*). Precise positioning of atoms as they are added is also possible (*Precise positioning of atoms during building*).

Note

This section refers to using the Sketcher control panel (*The 3D-Sketcher*), unless otherwise indicated.

Selecting the element type

The sketching element type is listed in a text entry box to the right of the **Sketch with** tool:

You can change the sketching element type, if needed, in any of several ways:

- Click this entry box and enter an element name in it.
- Choose an element from the popup immediately to the right of this text entry box. This popup lists several commonly used elements.
- Select the periodic table tool to the far right of this text entry box. When the Periodic Table window appears, select the desired element.

Changing the element type automatically activates the **Sketch with** tool.

Adding atoms and single bonds

To begin sketching, simply click the **Sketch with** tool to activate it (if it is not already active—when an icon-type tool is active, it is colored dark purple.) When you move the cursor into the model window, it is shaped like a triangle, indicating that you are in *sketch mode*, that is, that clicking the left mouse button places an atom and/or bond rather than selecting an atom (or some other activity). The element that is used in sketching is specified as described under *Selecting the element type*.

You can use the **Sketch with** tool to start building a new model and to add atoms to existing models.

Placing the first atom

Click anywhere in the model window to place the first atom. Move the cursor away—a dashed line follows the cursor, connecting it with the atom you clicked and indicating where the bond to your next atom will lie.

Tip

If you already have one or more models loaded into (or built during) your current Cerius^2 session, you need to create a new, empty model space in order to start building a new model (please see *Creating, clearing, and deleting model spaces*).

What next?

After placing the first atom or when adding to an existing model, you can use the sketch mode for several tasks:

- To place a second atom, click where you want it to appear. Continue clicking to place subsequent atoms in a chain.
- To end a chain, double-click when you place the last atom, click again on the last atom added, or move the cursor outside the model window. The dashed line no longer appears.

Tip

When you click an atom, Cerius^2 beeps to indicate that you succeeded.

- To close a ring or connect a chain to an existing ring or chain, click the appropriate existing atom.

- To place a bond between two atoms that are not bonded to each other, click each atom. (You can also use the **Connect** tool or the **Edit Bond** tool for this purpose—see *Connecting fragments* and *Changing the bond type*.)
- To start a new chain or ring, end the first one (see above) and then click in empty space.
- To add a branch to an existing chain or ring, click the atom that is to be the branch point, then click in empty space.
- To sketch with a different element type, select a different element type (*Selecting the element type*), then click the atom in the model window to which you want to add the new element.

Tip

You do not need to specifically add hydrogen atoms—this can be done automatically while sketching or (more quickly) after sketching is completed (*Adding hydrogens*).

Other sketch-mode functionality

While in sketch mode, you can also:

- Change the type of bond from single to double (or from double to triple) by clicking the atoms at each end of the bond.

Precise positioning of atoms during building

When you use the 3D-Sketcher, you manually place atoms in the model window, then refine the atom positions later (see *Refining the conformation*). Another builder tool, the Add Atom control panel, enables you to add atoms to the current model one at a time at specified coordinate positions. You can use it to build models and to add to existing models. Although less convenient to use than the Sketcher control panel, the Add Atom control panel allows precise control over the positions of atoms, which is particularly useful for duplicating published crystal structures or inorganic structures.

To access the Add Atom control panel, select the **Build/Add Atom…** menu item from the main control panel.

Set the element type by entering the desired element name in the **Element** entry box or by accessing the Periodic Table window from the Add Atom control panel.

Specify the coordinate system to be used for positioning atoms by choosing from a popup: Cartesian coordinates (**XYZ**), crystal fractional coordinates (**ABC**), or surface fractional coordinates (**UVd**)

for nonperiodic, 3D periodic, or 2D periodic systems. Then click the associated entry box and enter the exact coordinates at which to place the atom.

Other properties

Several other atom properties can optionally be specified before placing an atom in the model window: hybridization, charge, occupancy, the atom name, and temperature factors (*Specifying temperature factors*)—see the on-screen help for details. Hybridization is also discussed under *Changing the hybridization and adjusting the valence*—the hybridization popup in the Add Atom control panel functions the same as in the Sketcher control panel.

Placing the atom

After setting all desired parameters, click the **ADD ATOM** action button to place the atom in the model window. The most recently added atom can be deleted by clicking the **UNDO** button.

Adding templates (groups of atoms)

The efficiency of the building process can often be improved by adding groups of atoms ("templates") rather than single atoms. You may start sketching a new model by placing a template in the model window, or you can add templates to an existing model.

Note

This section refers to using the Sketcher control panel (*The 3D-Sketcher*), unless otherwise indicated.

Selecting templates

The current template (the one that is used if you click in the model window while the template tool is active) is printed on the Sketcher control panel, just to the right of the template tool, for example:

To use a different template, click the **Templates...** pushbutton to the right of the template tool. This causes the Sketcher Template control panel to appear. This control panel contains a file browser that allows you to navigate among directories and load selected files that contain templates.

Using the file browser to navigate the directory structure is fairly intuitive. The procedure is described under *Loading model structure files*.

Example

A specific example of using the file browser to find and load a template is demonstrated under *The Templates… button looks like:*.

Loading a template

Once you find the desired template file, load it by:

- Selecting its name and then clicking the **LOAD** button.

  or:

- Double-clicking its name.

The new name should appear next to the template tool, and the template tool becomes active (as indicted by highlighting).

Adding templates to a model

Once the desired template is chosen (see *Selecting templates*), click the template tool to activate it, if it is not already active. The cursor is now shaped like a T when it is over the model window. You can use the template to start building a model or to add a group to an existing model:

- To add the template as a separate (or new) fragment, click in empty space.
- To add the template at an existing atom, pick that atom. It is attached in a reasonable way (e.g., by replacing a hydrogen).
- To add identical templates simultaneously to several atoms, first select the atoms (*Selecting atoms and groups of atoms*), and then double-click the template tool (or single-click if it is already active). Hydrogen atoms are replaced as appropriate.

Custom templates

If you often need a particular template that doesn't exist, you can construct it as a model and save it as a custom template. How to do this is discussed more fully in the presentation of the Analog Builder in *Cerius^2 Builders*, since that builder can both check a template structure for some errors and save it.

To save a template if you don't have the Analog Builder, follow these steps:

1. Construct the template model, making sure you are satisfied with its final structure and conformation (this section).
2. Decide which hydrogen atom should be the point at which the template is to be added to other models.
3. Replace this hydrogen with a dummy element of type X (*Changing the element type*).
4. Save the model in .msi format (*Saving model structure files*).

You should now be able to use your template just as you do any other template, except that the Sketcher Template control panel does not find it automatically unless you were able to save it in the default Cerius2-Models / templates directory.

Fusing and connecting fragments

The Sketcher control panel includes tools for fusing or connecting two entities to form one model.

Fusing fragments

Fusing two fragments (in the model window) means to join them so as to delete a heavy (non-hydrogen) atom. For example, two benzenes could be fused to form naphthalene, or many cyclohexanes and cyclopentanes could be fused in building buckminsterfullerene.

The **Fuse** tool on the Sketcher control panel can be used in several ways:

- To fuse two fragments at one point, select the **Fuse** tool, then pick an atom in each fragment. Click the second atom again to perform the fusion. The first atom picked is deleted, and the rest of the fragment is bonded to the second atom.
- To fuse several atom pairs simultaneously:

  Select the **Fuse** tool and pick each pair in succession. Then click the last atom a second time.

  or:

While in selection mode, select all the atom pairs to be fused (*Selecting atoms and groups of atoms*), then double-click the **Fuse** tool.

Connecting fragments

Connecting two fragments means to join them by a bond (deleting only hydrogens as necessary). For example, two benzenes could be connected to form biphenyl or connected twice to form biphenylene.

The **Connect** tool on the Sketcher control panel can be used in several ways:

- To connect two fragments by a single bond, select the **Connect** tool, then pick each of the two atoms to be connected by a bond. The fragments become oriented so as to give a reasonable bond length and orientation, and extra hydrogens are deleted as appropriate.
- To place a bond between two atoms in the same model, select the **Connect** tool, then pick each of the two atoms.

You can also select the two atoms first (*Selecting atoms and groups of atoms*) and then double-click the **Connect** tool. Bonds can be formed only one at a time.

Tip

You can also connect fragments with the **Sketch with** tool (see *What next?*).

Adding hydrogens

Note

This section refers to using the Sketcher control panel (*The 3D-Sketcher*), unless otherwise indicated.

You may add hydrogens to your model at any time and in several ways.

- Wait until you have finished building and editing your structure, then click the **H ADJUST** button. Hydrogens are added to or deleted from *all* atoms (as needed) in the current model so that their valences are satisfied.

- Select the **Hydrogen** tool and then pick atoms whose valences you want to satisfy by adding or deleting hydrogens. Alternatively, select these atoms first (*Selecting atoms and groups of atoms*), then double-click the **Hydrogen** tool.
- Check the **Draw with Hydrogens** check box. Hydrogens are automatically added to or deleted from atoms as you sketch your model.
- Use the **Sketch with** tool with the **Sketch with** entry box set to **H** (*Adding atoms and bonds*).
- Use the Add Atom control panel (*Precise positioning of atoms during building*) if you need to control hydrogen positions exactly.
- Change selected atoms to H, using editing tools (*Changing the element type*).
- To delete all hydrogens, select hydrogens by element (*Selecting and deselecting individual atoms*), then use the **Delete Atom** tool in the Sketcher control panel or the **Edit/Delete** menu item in the main control panel (*Deleting atoms and bonds*).

Hybridization state

If any of the automatic tools give the wrong number of hydrogens at some atom(s), you can change their hybridization state (*Changing the hybridization and adjusting the valence*), formal charge (*Changing the formal charge*), and / or the bond type between that atom and another heavy atom (*Changing the bond type*) and then adjust the hydrogens again.

Selecting atoms and groups of atoms

Why read this section

You need to *select* one or more atoms when you want to perform some function (e.g., editing, labeling, changing the display style) on only certain atoms.

You can select atoms individually or according to some criterion, such as a common property or their membership in a group. Selection criteria may be quite complex.

This section contains information on:

Selecting and deselecting individual atoms

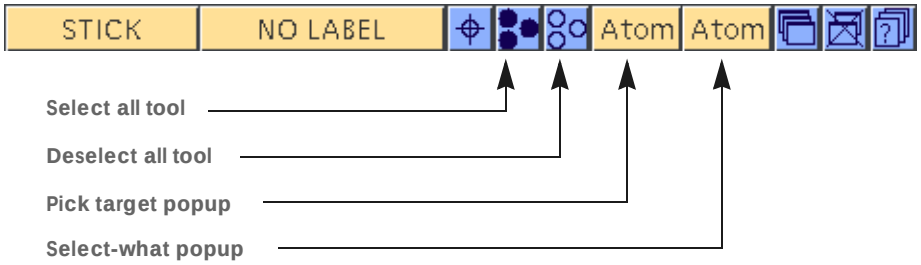
Selecting atoms in several models

Selecting and deselecting collections of atoms

Customized atom selection

The controls

The **Edit** pulldown menu and the toolbar in the Visualizer's main control panel offer several ways of selecting one or more atoms. There are also four atom selection tools in the toolbar:



Example

Several ways of selecting individual atoms are demonstrated under *Selecting atoms*.

Related information

You can also select atoms in several models simultaneously (*Selecting atoms in several models*).

Selecting and deselecting individual atoms

The mouse is in *selection mode* when the selection tool in the Sketcher control panel is highlighted. (In addition, the cursor is shaped like an arrow pointing to the upper left when it is in the model window.) This tool is also found in other control panels, and selection is always the default mode.

You always use the *left* mouse button to select atoms in the model window.

Single-atom picking

- To select only one atom, simply click it. A beep confirms that you've succeeded, and the atom becomes highlighted.
- To select only one different atom, click it.

- To select additional atoms, keep <Shift> depressed and click the appropriate atoms (in other words, <Shift>-click them).
- To deselect some (but not all) selected atoms, <Shift>-click them.

Using a selection rectangle

- To select only all atoms in some area of the model window, click nearby and drag out a selection rectangle that encloses the desired atoms. (The atoms must be visible to be selected; see *Visibility of polymer backbones*.)
- To add all atoms in another area of the model window to the selection, <Shift>-drag a selection rectangle around them.
- To deselect a group of already-selected atoms, <Shift>-drag a selection rectangle around them.

Operating on all atoms

- To select all atoms, drag out a rectangle enclosing the entire model, select the **Edit/Select All** menu item, press <Alt> **a** on the keyboard, or click the select all tool (see toolbar illustration at *The controls*).

Tip

For some functions, selecting all atoms has the same effect as selecting none (e.g., changing the display style, *Model display style*, or applying labels, *Labels*). Other functions (e.g., deleting all atoms, *Deleting atoms and bonds*) require that all atoms actually be selected.

- To deselect all atoms, click in empty space (in the model window) or click the deselect all tool in the toolbar.

Selecting atoms in several models

You are not restricted to selecting atoms only in the current model. Atoms in any number of displayed models can be selected. This capability is useful for activities like monitoring close contacts between models (*Calculating close contacts*) and comparing models by superimposing them (*Superimposing models*).

You should already know…

Managing and displaying multiple models is documented in *Managing Models and Sessions*.

How it works

Selecting atoms works differently, depending on how the models are displayed (see *Controlling model visibility and the display mode*):

- In overlay mode, all the single-atom picking and selection-rectangle methods listed above (*Single-atom picking*) can be used to select atoms in all displayed models.
- In border mode, all the single-atom picking methods listed above (*Single-atom picking*) can be used to select atoms in all displayed models. The selection-rectangle methods function only for the current model (see *Specifying the current model*).
- In grid mode, all the single-atom picking methods listed above (*Single-atom picking*) can be used to select atoms in all displayed models.

Selecting and deselecting collections of atoms

Selecting according to properties

Pick target

A single pick in the model window (by the same selection process as described under *Selecting and deselecting individual atoms*) can act on different *pick targets*. A single click can pick a single atom, all atoms in one residue, all atoms in one chain, or all atoms in one model. Similarly, using a selection rectangle can pick only the atoms within the rectangle, or all residues, chains, or models that have at least one atom within the rectangle.

To change the default behavior (i.e., picking individual atoms), change the pick target popup on the toolbar (see *The controls*) from **Atom** to **Res**idue, **Chain**, or **Model**. Residues and chains are not present in all models, but may be defined in other Cerius^2 modules, which are documented separately.

What is selected

When you pick a target, other items (in addition to the target) might also be selected, depending on your *selection criteria*.

Selection can apply to only the single atoms actually picked; or to all atoms with the same name, same element type, or same forcefield type; or to all of a bonded set of atoms (a *fragment*) or of the smallest set of bonded atoms leading away from the main model and starting after the selected atom (“short end”).

To change the default behavior (i.e., picking individual or contiguous atoms), change the select-what popup on the toolbar (see *The controls*) from **Atom** to **Name**, **El**ement, **FF** (forcefield type), **Frag**ment, or **End** (short end). Names atoms are not present in all mod-

els, but may be defined in other Cerius^2 modules, which are documented separately. You can also name atoms with the Edit Selected Atoms control panel (*Atom properties*).

Depending on the setting of the pick target popup, you can also select all residues of the same **Type** or **Id**entifier or all chains of the same **Name**. The default is to select all atoms in a residue, chain, or model.

Selection is within...

In addition to the selection criteria, you can restrict or expand the *selection scope*; for example, whether atoms are selected in the current model or all models, etc. To change the default selection scope (i.e., within the current model, use the Atom Selection control panel (see *Additional selection criteria*).

How it works

Not all combinations of pick target, selection criterion, and selection scope make sense or are allowed. The supported combinations are shown in Table 2.

Additional selection criteria

Select the **Edit/Selection...** menu item to access the Atom Selection control panel. This control panel enables you to specify the **Pick target**, **Select atom(s) which are**, and **Within** criteria when the mouse is used for selection (see *Selecting according to properties*).

In addition, more selection criteria are available. These functions are not linked to mouse activity in the model window, but occur when an icon or action button in the control panel is clicked.

For example, you can select all atoms within a specified radius of a selected atom, all atoms in a named group, or all backbone atoms in a polymer. See also *Defining and selecting groups* and *Customized atom selection*.

Additional information

Please see the on-screen help for details on the functioning of each control in the Atom Selection control panel.

Defining and selecting groups

Defining groups

You can define any collection of atoms as a “group” and then perform group-based selections.

To define and name such groups, access the Groups control panel by selecting the **Edit/Groups...** menu item. You can also rename, redefine, or delete the group definitions.

Table 2. Possible combinations of pick target, selection criterion, and selection scope

pick target	what is selected	selection can be within...
atom[1]	The atom(s) actually picked1[1]	In one model.[1] In all[2] models (see *Selecting atoms in several models*).
atom[1]	All atoms of the same name. All atoms of the same element type. All atoms of the same forcefield type.	All in the same residue. All in the same chain. All in the same model.[1] All in all[2] models.
atom[1]	All atoms in the same fragment. Smallest set of bonded atoms.	In one model.[1] In all[2] models.
residue	All atoms in the residue(s) actually picked.[1]	In one model.[1] In all[2] models.
residue	All atoms in all residues of the same type. All atoms in all residues of the same ID.	All in the same chain. All in the same model.[1] All in all[2] models.
chain	All atoms in the chain(s) actually picked.[1]	In one model.[1] In all[2] models.
chain	All atoms in all chains of the same name.	All of this chain name in the same model.[1] All of this chain name in all[2] models.
model	All atoms in the model picked.[1]	All atoms in all[2] models.

[1]Default value.
[2]Or in all visible models or in selected models.

Selecting groups

You can select groups by clicking the **Select objects** action button in the Groups control panel or the **Select Group** button in the Atom Selection control panel.

Customized atom selection

You can set up sophisticated and/or multiple selection criteria and/or obtain even more precise control over what is selected when you pick an atom.

Accessing the tools

Select the **Edit/Selection...** menu item to access the Atom Selection control panel. Click the **Custom Selection...** pushbutton to access the Customized Atom Selection control panel.

Setting multiple and customized criteria

To set up customized selection criteria, you can pick properties from the popups in the Customized Atom Selection control panel and enter additional subcriteria in the associated entry boxes.

Wildcards are allowed in the subcriteria. Also, multiple subcriteria may be entered into an entry box—separate the individual subcriteria with a colon (**:**).

For example, you can select all atoms whose name starts with c, which have a desired range of charge values, and are located within residues of a certain type.

For maximum flexibility, you can also use raw object reference language to select atoms. Please see the on-screen help for the syntax.

Finding atom information

To enter information into the subcriteria boxes, you of course need to know what an atom's properties are.

You can query atom properties by shift-clicking the atom with the right mouse button (*Tip*). This displays a temporary message box and also prints to the text window.

You can also choose to have brief information on atom properties sent to the text window whenever you click an atom. To do this, select the **Utilities/Customize/Environment...** menu item to access the Customize Environment control panel. Check the **Echo object reference** check box.

Additional information

Please see the on-screen help for the precise syntax for entering subcriteria and for details on the functioning of each control in the Customized Atom Selection control panel. The help that is accessed with the **?** buttons on this control panel is context-sensitive; that is, what help is displayed depends on what the associated popups are set to. The cumulative criteria are displayed in the **Object Reference** entry box as they are built up with the other controls in this control panel. The context of the **Object Reference** entry box may be edited.

Basic editing

Why read this section

Most models require some editing after the basic skeleton is built or while the model is being built. You may also want to edit models that were read in from a file. This section tells you where to

access the basic editing tools and how to perform tasks that are typically associated with editing a model. It contains information on:

Changing atoms and their bonding types

Editing the structure

Refining the conformation

Related information

Basic building tasks are presented under *Basic building*.

Tasks that may be less often or less typically performed, such as editing atom attributes and changing defaults and preferences, are covered in *Advanced building and editing*. Displaying labels and other information about atoms in a model is presented in *Labels*.

You should already know…

You need to know how to select atoms in your model (*Selecting atoms and groups of atoms*), so you can edit them. You also of course need to know how to build a model (*Basic building*) and / or load a model from a file (*Loading model structure files*).

You may want to review the basics of how the controls in the Sketcher control panel work (see *How it works*).

Note

This entire section refers to using the Sketcher control panel (*The 3D-Sketcher*), unless otherwise indicated. Most of its editing functions work with both nonperiodic and periodic (*Other builders*) systems.

Changing atoms and their bonding types

This section includes:

Changing the element type

Changing the formal charge

Changing the bond type

Changing the hybridization and adjusting the valence

Changing the element type

To change the element type of an existing atom in the model window, you use the **Edit Element** tool.

Specifying the element type

The edit element type (i.e., the element that you want the atom to become) is listed in an entry box to the right of the **Edit Element** tool:

You can change the edit element type in any of several ways:

- Click this entry box and enter an element name in it.
- Choose an element from the popup immediately to the right of this text entry box. This popup lists several commonly used elements.
- Select the periodic table tool to the far right of this text entry box. When the Periodic Table window appears, select the desired element.

  If the Periodic Table window is already open, click the periodic table tool to link it to the **Edit Element** function.

Tip

The Periodic Table window can function with any of several controls or control panels. The control or panel that it is currently *linked to* is listed near the top of the Periodic Table window. To change the link (and therefore also the entry box that the periodic table affects), click the appropriate periodic table tool in the desired control panel.

Changing the default element type automatically activates the **Edit Element** tool. If the edit element type is already correct, you can activate the **Edit Element** tool by clicking it.

Changing the element type

You can change atoms in the model window to the element type specified in the element type entry box in several ways:

- Select the **Edit Element** tool and then pick the desired atom(s).
- Select the desired atom(s) (*Selecting atoms and groups of atoms*) and then double-click the **Edit Element** tool.

Changing the element type together with other properties

If you want to edit both the element type and other properties simultaneously, select the **Build/Edit Atoms...** menu item. This gives access to the Edit Selected Atoms control panel.

Additional information

Please see the on-screen help for details on the functioning of each control in the Edit Selected Atoms control panel.

Changing the formal charge

To change the formal charge on an atom, use the **Edit Formal Charge** button in the Sketcher control panel.

Specifying the formal charge

Choose **AUTO** or the desired value of the formal charge from the popup to the right of the **Edit Formal Charge** tool.

Changing the default formal charge automatically activates the **Edit Formal Charge** tool. If the formal charge is already correct, you can activate the **Edit Formal Charge** tool by clicking it.

Changing the formal charge

You can change the formal charge on atoms in the model window to the value specified by the formal charge popup in several ways:

- Select the **Edit Formal Charge** tool and then pick the desired atom(s).
- Select the desired atom(s) (*Selecting atoms and groups of atoms*) and then double-click the **Edit Formal Charge** tool.

Tip

To see the effect of changing the formal charge, either click the **H ADJUST** button after changing the formal charge or check the **Draw with Hydrogens** check box before changing the formal charge. You can also label atoms (*Labels*) according to their formal charge.

Changing the formal charge together with other properties

If you want to edit both the formal charge and other properties simultaneously, select the **Build/Edit Atoms...** menu item. This gives access to the Edit Selected Atoms control panel.

Additional information

Please see the on-screen help for details on the functioning of each control in the Edit Selected Atoms control panel.

Changing the bond type

To change the bond type between any two atoms, use the **Edit Bond** button in the Sketcher control panel.

Specifying the bond type

Choose **SINGLE**, **DOUBLE**, **TRIPLE**, or **RESONANT** from the popup to the right of the **Edit Bond** tool.

Changing the default bond type automatically activates the **Edit Bond** tool. If the bond type is already correct, you can activate the **Edit Bond** tool by clicking it.

Changing the bond type

You can change bonds in the model window to the type specified by the bond type popup in several ways:

- Select the **Edit Bond** tool and then pick two atoms. If a bond exists between the atoms it is changed to the type specified. If no bond exists, one (of the desired type) is created.
- Select the desired atom pair(s) (*Selecting atoms and groups of atoms*) and then double-click the **Edit Bond** tool. Existing bonds are changed to the type specified. No new bonds are created if more than two atoms are selected.

Tip

You can also change the bond type while in sketch mode (see *While in sketch mode, you can also:*).

Additional controls over bonding

If you want to edit the bond type and also change how bonds are calculated (see *Editing element and bond attributes*), select the **Build/Edit Bonds...** menu item. This gives access to the Edit Connectivity and Bonding control panel.

Additional information

Please see the on-screen help for details on the functioning of each control in the Edit Connectivity and Bonding control panel. (Setting the bond calculation preferences is discussed under *Bond properties*.)

Changing the hybridization and adjusting the valence

Generally, Cerius^2 automatically determines what the hybridization should be. However, you can specify the hybridization manually.

To change the hybridization for any selected atom, use the **Edit Hybrid** tool.

Tip

You can label atoms (*Labels*) according to their hybridization.

Specifying the hybridization

Choose the desired type of hybridization from the popup to the right of the **Edit Hybrid** tool. **AUTO** means to allow Cerius^2 to automatically determine the hybridization; the specific types listed in the popup are self-explanatory; **OTHER** should be used for high-coordination centers not specifically included in the list of choices. (Setting the hybridization to **OTHER** where appropriate allows the cleaning function (*Refining the conformation*) to work optimally.)

Changing the default hybridization type automatically activates the **Edit Hybrid** tool. If the hybridization type option is already correct, you can activate the **Edit Hybrid** tool by clicking it.

Changing the hybridization

You can change atoms in the model window to the hybridization type specified in the hybridization type popup in several ways:

- Select the **Edit Hybrid** tool and then pick the desired atom(s).
- Select the desired atom(s) (*Selecting atoms and groups of atoms*) and then double-click the **Edit Hybrid** tool.

Other ways to change the hybridization

You can change the hybridization before adding an atom by using the Add Atom control panel (*Precise positioning of atoms during building*). You can also edit the hybridization of existing atoms (and other properties simultaneously) with the Edit Selected Atoms control panel (*Changing the element type together with other properties*).

Editing the structure

This section includes:

Deleting atoms and bonds

Duplicating parts of a model

Examining and changing bond lengths

Examining and changing angles

Examining and changing torsions

Inverting about an atomic center

Translating and rotating atoms

Aligning and positioning atoms

Deleting atoms and bonds

Deleting atoms and associated bonds

To delete an atom and all bonds leading to it, use the **Delete Atom** tool in the Sketcher control panel.

You can:

- Select the **Delete Atom** tool and then pick the atom(s) to delete.

  or:

- Select the desired atom(s) and then double-click the **Delete Atom** tool to delete all selected atoms simultaneously.

You can also:

- Select atom(s) and then select the **Edit/Delete** menu item or the **Edit/Cut** menu item.
- Select atom(s) and then press <Ctrl> <Delete> (simultaneously) while the cursor is in the model window.

Deleting only bonds

To delete a bond between two atoms without deleting any atoms, use the **Delete Bond** tool.

You can:

- Select the **Delete Bond** tool and then pick the atoms whose bond you want to delete.

  or:

- Select the desired bonded atom pairs(s) and then double-click the **Delete Bond** tool to delete all bonds between selected atoms simultaneously.

You can also:

- Delete bonds between all atoms or between selected atoms with the **Delete bonds** action button in the Edit Connectivity and Bonding control panel. Access this control panel by selecting the **Build/Edit Bonds...** menu item.
- Delete hydrogen bonds (*Hydrogen bonds*) between all or selected atoms with the **Delete H-bonds** button in the Edit Hydrogen Bonding control panel. Access this control panel by selecting the **Build/Edit H-Bonds...** menu item.

Duplicating parts of a model

To make copies of all or part of a model, select the desired atom and then select the **Edit/Duplicate** menu item or press <Alt> **l** on the keyboard. This performs a copy-and-paste operation, producing an offset copy of the selected atoms.

You can also copy or move parts of models, or entire models, from one model space to another (see *Moving models between model spaces*).

Examining and changing bond lengths

Important

Cleaning a structure (*Refining the conformation*) automatically optimizes all bond lengths. You can change bond lengths before cleaning if you want to bias the final structure. However, if you want a different specific bond length than that determined automatically, change it *after* using the clean function, do not use cleaning, clean only selected atoms (*Control of the model-cleaning function*), or change the default properties used for setting bond lengths (*Bond properties*).

Changing a bond length manually

To change the length of a bond manually, select the **Stretch** tool in the Sketcher control panel.

Then click two bonded atoms. The length of the bond (in angstroms) is displayed next to it in the model window when you click in empty space. To change the length, click and drag the cursor in empty space in the model window. Dragging up and / or to the right lengthens the bond; dragging down and / or to the left

shortens it. You cannot make bonds very unreasonably short or long.

You can also modify bond lengths by moving selected atoms manually (*Translating atoms manually*). You can also examine bond lengths and other distances with the Measurements control panel (*Distances*).

Precise change in bond length

To change the length of a bond precisely, select the **Move/Bond Geometry…** menu item to access the Bond Geometry control panel.

Additional information

Please see the on-screen help for details on using the controls in the Bond Geometry control panel to measure and change bond lengths, valence angles, and torsions and to specify which atoms are moved in the process.

You can also modify bond lengths by translating (*Translating atoms precisely*) or positioning (*Aligning and positioning atoms*) atoms to specified locations. You can also examine bond lengths and other distances with the Measurements control panel (*Distances*).

Default bond lengths

You can change the defaults that Cerius^2 uses in calculating bonds. To change the default radii of atoms, please see *Element properties*. For covalent bond calculation preferences, see *Bond properties*. For setting the hydrogen bond length criterion, see *Hydrogen bonds*.

Examining and changing angles

Important

Cleaning a structure (*Refining the conformation*) automatically optimizes all valence angles. You can change angles before cleaning if you want to bias the final structure. However, if you want a different specific angle than that determined automatically, change it *after* using the clean function, clean only selected atoms (*Control of the model-cleaning function*). or do not use cleaning.

Changing an angle manually

To change a valence angle manually, select the **Angle** tool in the Sketcher control panel.

Then click three contiguous bonded atoms. The angle between them (in degrees) is displayed next to the angle in the model window when you click in empty space. To change the angle, click and

drag the cursor in empty space in the model window. Dragging up and / or to the right increases the angle; dragging down and / or to the left decreases it. Angles in rings cannot be changed.

You can also modify angles by moving atoms manually (*Translating atoms manually*). You can examine angles between any three atoms with the Measurements control panel (*Angles*).

Precise change in angles

To change an angle precisely, select the **Move/Bond Geometry...** menu item to access the Bond Geometry control panel.

Additional information

Please see the on-screen help for details on using the controls in the Bond Geometry control panel to measure and change valence angles, bond lengths, and torsions and to specify which atoms are moved in the process.

You can also change angles in the course of translating (*Translating atoms precisely*), aligning, or positioning (*Aligning and positioning atoms*) atoms to specified locations. You can also examine angles between any three atoms with the Measurements control panel (*Angles*).

Default angles

You can implicitly control default valence angles through setting the hybridization state of the atoms involved (*Changing the hybridization and adjusting the valence*). For setting the hydrogen bond angle criterion, please see *Hydrogen bonds*.

Examining and changing torsions

Important

Cleaning a structure (*Refining the conformation*) automatically optimizes all torsion angles. You can change torsions before cleaning if you want to bias the final structure. However, if you want a different specific torsion angle than that determined automatically, change it *after* using the clean function, clean only selected atoms (*Control of the model-cleaning function*), or do not use cleaning.

Changing a torsion manually

To change a torsion angle manually, select the **Twist** tool in the Sketcher control panel.

Then click either two or four contiguous bonded atoms. Click two bonded atoms and then click the second atom again to define the

bond that you want to twist. Click four atoms to define the specific torsion angle to be changed.

The torsion angle (in degrees) is displayed next to the torsion in the model window when you click in empty space. To change the torsion angle, click and drag the cursor in empty space in the model window. Dragging up and / or to the right increases the angle; dragging down and / or to the left decreases it. Torsions in rings cannot be changed.

You can also modify torsions by rotating parts of models manually (*Rotating atoms manually*). You can also examine torsions or the angle between any two planes with the Measurements control panel (*Torsions*).

Precise change in torsions

To change a torsion angle precisely, select the **Move/Bond Geometry…** menu item to access the Bond Geometry control panel.

Additional information

Please see the on-screen help for details on using the controls in the Bond Geometry control panel to measure and change torsions, bond lengths, and valence angles and to specify which atoms are moved in the process.

You can also change torsions by rotating parts of models to specified orientations (*Rotating atoms precisely*). You can examine torsions or the angle between any two planes with the Measurements control panel (*Torsions*). For inverting a chiral center, please see the next section.

Default torsions

You can implicitly control default torsion angles through setting the hybridization state of the atoms involved (*Changing the hybridization and adjusting the valence*).

Inverting about an atomic center

The most straightforward way of inverting about a chiral center is to use the **Invert** tool in the Sketcher control panel. (Although inversion can be applied to any atomic center, it should be most useful when the center is chiral.)

You can:

- Select the **Invert** tool and then pick the atomic center whose chirality you want to invert. Two fragments attached to that

atom are rotated 180° about the axis that bisects the bond angle between the fragments. The fragments that are rotated are those that result in the fewest atoms being moved.

or:

- Select the desired atomic centers) and then double-click the **Invert** tool to invert the chirality at all selected centers simultaneously.

Note

Inversions cannot be done for centers that are part of complex ring structures, i.e., for those in which one fragment makes more than two attachments to the selected atomic center.

You can examine inversions with the Measurements control panel (*Inversions*).

Translating and rotating atoms

Translating atoms manually

You can translate selected atoms in all three dimensions by using the mouse to control the cursor in the model window. To translate selected atoms:

- *In the x, y plane*—Drag the cursor while holding down <Ctrl> and the middle mouse button.
- *Along the z axis*—Drag the cursor while holding down <Ctrl>, <Alt>, and the middle mouse button.

If symmetry constraints do not allow the requested translation, the closest permitted translation is made instead.

Tables of mouse button and keyboard combinations are included in *Mouse and Keyboard Actions*.

Translating atoms precisely

To translate selected atoms a precise distance in a specified direction, select the **Move/Atoms Translate...** menu item to access the Translate Atoms control panel.

You can specify the direction in Cartesian (**XYZ**), crystal (**ABC**), or surface (**UVW**) coordinates or specify that the direction be calculated as the best-fit vector through the currently selected atoms (not necessarily the same atoms that you select to move).

If symmetry constraints do not allow the requested translation, the closest permitted translation is made instead.

Additional information

Please see the on-screen help for details on the functioning of each control in the Translate Atoms control panel.

Rotating atoms manually

You can rotate selected atoms around all three axes by using the mouse to control the cursor in the model window. To rotate selected atoms:

- *Around the x axis*—Drag the cursor vertically while holding down <Ctrl> and the right mouse button.
- *Around the y axis*—Drag the cursor horizontally while holding down <Ctrl> and the right mouse button.
- *Around the z axis*—Place the cursor close to an edge of the model window and drag it parallel to that window edge while holding down <Ctrl> and the right mouse button.

More than one atom should be selected. Symmetry considerations in periodic systems may not allow certain rotations.

Tables of mouse button and keyboard combinations are included in *Mouse and Keyboard Actions*.

Rotating atoms precisely

To rotate selected atoms by a precise angle around a specified rotation axis and center, select the **Move/Atoms Rotate...** menu item to access the Rotate Atoms control panel.

More than one atom should be selected. You can specify the rotation axis and center in Cartesian (**XYZ**), crystal (**ABC**), or surface (**UVW**) coordinates. Alternatively, you can specify that the axis be calculated as the best-fit line through the currently selected atoms and / or the rotation center as their geometric center. (You can change which atoms are currently selected, for specifying each definition.)

If symmetry constraints do not allow the requested rotation, the closest permitted rotation is made instead.

Additional information

Please see the on-screen help for details on the functioning of each control in the Rotate Atoms control panel. You can rotate the selected atom(s) by clicking and dragging a slider or a dial or by entering the angle in the associated entry box.

Aligning and positioning atoms

Aligning atoms

To accurately align selected atoms with respect to a coordinate system, select the **Move/Atoms Align...** menu item to access the

Align Atoms control panel. You specify one intra-model vector that is to be aligned with one coordinate axis and another intra-model vector to be aligned with a coordinate plane that includes that axis. You also specify the point about which the selected atoms are rotated.

You specify the intra-model vectors to be aligned with the coordinate axis and plane and the rotation center, using Cartesian (**XYZ**), crystal (**ABC**), or surface (**UVW**) coordinates. Alternatively, you can specify that the first intra-model vector (the one to be aligned with a coordinate axis) be calculated as the best-fit vector through the currently selected atoms. Similarly, you can specify that the second intra-model vector (the one to be aligned with a coordinate plane) be calculated as the best-fit vector through the currently selected atoms. You can also specify that the rotation center be calculated as the geometric center of the currently selected atoms. (You can change which atoms are currently selected, for specifying each definition.)

If symmetry constraints do not allow the requested alignment, it is not performed.

Additional information

Please see the on-screen help for details on the functioning of each control in the Translate Atoms control panel.

Positioning atoms

To accurately position selected atoms in space, select the **Move/ Atoms Position...** menu item to access the Position Atoms control panel. You specify both a reference point and a destination point, then the selected atoms are moved in a way that maintains their spatial relationship with the reference point (i.e., the reference point is moved together with the atoms).

You can specify the reference and destination points in Cartesian (**XYZ**), crystal (**ABC**), or surface (**UVW**) coordinates and / or specify that these points be calculated as the geometric center of the currently selected atoms. (You can change which atoms are currently selected, for specifying each definition.)

If symmetry constraints do not allow the requested translation, it is not performed.

Additional information

Please see the on-screen help for details on the functioning of each control in the Position Atoms control panel. (You can position atoms while adding them to a model, with the Add Atom control panel, see *Precise positioning of atoms during building*.)

Refining the conformation

Cleaning the structure

The model structure as initially drawn is usually not chemically reasonable. Thus, it needs to be "cleaned" (i.e., its structure needs to be optimized). Initial optimization is often done with the **CLEAN** button in the Sketcher control panel. Simply click the **CLEAN** button and keep the left mouse button depressed until the structure in the model window stops changing. (You can adjust how the clean function works—please see *Control of the model-cleaning function*.)

You may adjust the structure as desired after you clean it (e.g., *Examining and changing bond lengths*). However, a better approach may be to apply constraints before additional optimization or to apply symmetry (next paragraph).

Additional optimization

If you want an even more chemically correct structure than the clean function is capable of, you may want to use a forcefield-based minimizer such as the OFF Minimizer or optimize the structure to an energy minimum or a transition state with one of the quantum applications. You can also use the quantum applications to enforce space-group symmetry. Documentation for these modules is supplied separately.

Advanced building and editing

Why read this section

This section tells you where to access some building and editing controls, such as editing atom attributes and changing defaults and preferences, that are not as commonly used as those discussed earlier in this section. It contains information on:

Editing element and bond attributes

Introducing substitutional disorder

Introducing positional disorder

Temperature factors

Control of the model-cleaning function

Related information

Basic building tasks are presented under *Basic building* and basic editing tasks under *Basic editing*.

Displaying labels and other information about atoms in a model is presented under *Labels*.

Saving nondefault settings for later use is described under *Working with Cerius2 sessions*.

You should already know...

You need to know how to select atoms in your model (*Selecting atoms and groups of atoms*), so you can edit them. You also of course need to know how to build (*Basic building*) and edit (*Basic editing*) a model and / or load a model from a file (*Loading model structure files*).

You may want to review the basics of how the controls in the Sketcher control panel work (see *How it works*) or how controls work in general (*The Cerius2 Interface*).

Editing element and bond attributes

Cerius^2 allows you to edit the default properties of elements (*Element properties*), change how bonds are determined (*Bond properties*), and adjust the criteria for determining hydrogen bonds (*Hydrogen bonds*).

Related information

Changing the properties of individual selected atoms (i.e., not necessarily of all atoms of a given element type) is covered under *Changing atoms and their bonding types*. Setting temperature factors is discussed under *Temperature factors*.

You should already know...

You should have already worked with the types of models and the various application modules that you typically use, before deciding whether and how much you should change the default behavior of Cerius^2. And of course there is no substitute for chemical knowledge and intuition. This section is for experienced Cerius^2 users.

Element properties

What element properties can be edited

Element properties are stored within Cerius^2 and used for calculations and display attributes. These properties include mass, van der Waals radius, atomic radius, covalent radius, metallic radius, ionicity, hydrogen bonding nature, and display color. Cerius^2 "ele-

ments" include chemically real elements, "mixture" elements, and "dummy" elements.

Editing element properties

Select the **Build/Element Defaults...** menu item to access the Edit Elements control panel. Changing element defaults changes the properties for atoms of that element type that already exist in the model, as well as for all atoms added to models later in the current Cerius^2 session.

Among other properties, you can, for example, change:

- The van der Waals radius that is used in producing BALL displays (*Atom and bond display styles*) of atoms.
- The atomic radius, which is used by the clean function (*Refining the conformation*).
- The color used to display an element.

Additional information

Please see the on-screen help for details on the functioning of each control in the Edit Elements control panel.

"Mixture" elements

Mixture elements are special Cerius^2 elements (with atomic symbols T, TT, M, and MM) whose properties you can specify as proportions of those of up to eight real elements. Such a mixture can be useful, for example, in studying disordered structures (*Introducing substitutional disorder*).

Mixture elements are defined using the Element Mixtures control panel, which you access by clicking the **Mixtures...** pushbutton on the Edit Elements control panel. You can also examine the compositions of predefined mixture elements with this control panel.

Dummy atoms

Cerius^2 also allows you to use predefined dummy atoms. These nonstandard "elements" (as well as the mixture elements, deuterium and other nonstandard "elements") are listed at the bottom of the Periodic Table window. (You can access the periodic table by clicking the periodic table icon in several control panels, including the Edit Elements control panel.)

Tip

To find the atomic number, atomic mass, symbol, and name of any real or dummy element, click the element in the Periodic Table window. This information is listed in a box near the top of the window, below the line stating what control panel the periodic table is linked to.

Atom properties

You can also edit properties of individual selected atoms (rather than of all existing and future atoms of a given element type): the element type, hybridization state (*Changing the hybridization and adjusting the valence*), charge, formal charge, mass, occupancy, the atom name, and temperature factors (*Specifying temperature factors*). To do so, select the **Build/Edit Atoms…** menu item to access to the Edit Selected Atoms control panel.

Additional information

Please see the on-screen help for details on the functioning of each control in the Edit Selected Atoms control panel.

Most of these atom properties can alternatively be specified before placing an atom in the model window with the Add Atom control panel (*Precise positioning of atoms during building*).

Bond properties

Bonds can be drawn and then optimized automatically (*Refining the conformation*). Alternatively, unbonded atoms can be placed in the model window (see *Precise positioning of atoms during building*) and then bonds can be calculated for all or selected atoms. In either event, the calculated bond lengths are based on distance and other criteria. For cleaning, Cerius^2 uses these criteria in deciding what is the optimum bond length. For placing bonds, Cerius^2 uses them to decide which atom pairs to join by bonds.

Editing bonds

Elementary bond editing with the Sketcher and the Edit Connectivity and Bonding control panels is presented under *Changing atoms and their bonding types* and *Editing the structure*. These tasks include deleting bonds, changing the bond type and order, and making bonds between selected atoms.

Accessing the tools

For more advanced bond editing tasks or for performing several elementary tasks simultaneously, select the **Build/Edit Bonds…** menu item to access the Edit Connectivity and Bonding control panel.

You can bond selected atoms or delete bonds, calculate bonding from a connectivity map, change the bond order, and change how resonant bonds are displayed.

Additional information

Please see the on-screen help for details on the functioning of each control in the Edit Connectivity and Bonding control panel.

Specifying how bonds are calculated

To define the criteria by which bonds are calculated, click the **Preferences...** pushbutton to the right of the **Calculate connectivity** check box in the Edit Connectivity and Bonding control panel to access the Bond Calculation Preferences control panel.

Covalent, general (Slater, i.e., atomic), and (where appropriate) metallic radii are stored for each atom. Depending on the selected **Bonding Method**, the appropriate radius is used in bond calculations. The stored radii can be edited by specifying an element and method and then entering the radius in the corresponding radius entry box. These radii can also be changed with the Edit Elements control panel (*Element properties*).

You can also define a **Bonding Tolerance** (effectively the proportion of the relevant atomic radius to be used in looking for contacts). For example, if the tolerance factor is 1.5 and the ideal bond length is 1.4 Å, a bond is created if the two atoms are within 2.1 Å (1.4 x 1.5) of one another.

You can inhibit the creation of bonds to certain categories of elements (that is, alkali metals, transition metals, and lanthanides / actinides) during bonding calculations using the appropriate check boxes. This inhibition works by effectively zeroing the bonding radius for a given atom. Inhibition of bonding to a specific element can be achieved by actually zeroing the bonding radius for that element.

Additional information

Please see the on-screen help for details on the functioning of each control in the Bond Calculation Preferences control panel.

Specifying automatic determination of bond types

To specify whether Cerius^2 should determine the bond types automatically by valence satisfaction, check the **Calculate bond types** check box. To specify how this algorithm works, click the **Preferences...** pushbutton next to the **Calculate bond types** check box in the Edit Connectivity and Bonding control panel to access the Bond Type Calculation Prefs control panel.

Additional information

Please see the on-screen help for details on the functioning of each control in the Bond Type Calculation Prefs control panel.

Calculating bonds

To request bond calculation between all atom pairs that meet the criteria, click the **CALCULATE** pushbutton in the Edit Connectivity and Bonding control panel. Bonds are added or deleted so that they meet the criteria. Subsequent use of the cleaning function

(*Refining the conformation*) also uses the radii set with the Bond Calculation Preferences or Edit Elements control panel.

Hydrogen bonds

All or selected hydrogen bonds can be edited and deleted. Hydrogen bonds can also be calculated for all or selected atoms, based on distance and angle criteria.

Hydrogen bond criteria

When Cerius^2 decides which atom pairs to join by hydrogen bonds, it uses these criteria (Figure 1):

- The distance between a potential acceptor atom and a hydrogen atom is less than the distance criterion.
- The angle between a potential donor, a hydrogen, and a potential acceptor is greater than the angle criterion.

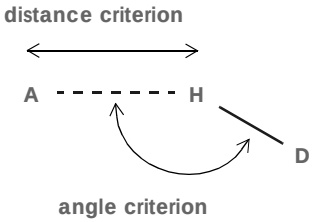


Figure 1. Hydrogen bond criteria

A = hydrogen-bond acceptor, D = hydrogen-bond donor.

Editing hydrogen bonds

Select the **Build/Edit H-Bonds...** menu item to access the Edit Hydrogen Bonding control panel.

With this control panel, you can calculate, delete, or make hydrogen bonds between all or selected atom pairs, as well as set the color in which hydrogen bonds are displayed in the model window. You can also enable automated recalculation of hydrogen bonds whenever, for example, the model's conformation changes.

Additional information

Please see the on-screen help for details on the functioning of each control in the Edit Hydrogen Bonding control panel.

Specifying how hydrogen bonds are calculated

To define the criteria by which hydrogen bonds are calculated, click the **Preferences...** pushbutton in the Edit Hydrogen Bonding control panel, to access the H-Bond Preferences control panel.

With this control panel, you can set the distance and angle criteria. You can also specify the hydrogen bonding nature of an element, i.e., whether it is a donor, an acceptor, either a donor or an acceptor, or neither a donor nor an acceptor. (The hydrogen-bonding nature of elements can also be changed with the Edit Elements control panel, see *Element properties*.)

When these criteria are altered, any existing hydrogen bonds that no longer meet the criteria are deleted when you click the **CALCULATE** pushbutton in the Edit Hydrogen Bonding control panel. Hydrogen bond recalculation occurs automatically if the **Enable automatic recalculation** check box in the Edit Hydrogen Bonding control panel is checked.

Additional information

Please see the on-screen help for details on the functioning of each control in the H-Bond Calculation Preferences control panel.

Calculating hydrogen bonds

To request hydrogen bond calculation between all or selected atom pairs that meet the criteria, click the **CALCULATE** pushbutton in the Edit Hydrogen Bonding control panel.

Introducing substitutional disorder

Uses of substitutional disorder

Substitutional disorder can be used whenever two elements need to be randomly replaced in a structure. For example, substitutional disorder is particularly useful in dealing with zeolites where you may want to randomly replace silicon atoms with aluminum.

How it works

Substitutional disorder randomly replaces a fraction of the atoms of one element type with atoms of another element type. Substitutional disorder can be applied to the whole model or to only a selected portion of the model. A target ratio is used to set the fraction of the atoms to be replaced.

Löwenstein's rule applies only to the substitution of aluminum. Generally, this rule is used in the random replacing of silicon by aluminum in zeolite structures. Application of Löwenstein's rule ensures that no two aluminum atoms share a common oxygen. This may mean that the target replacement ratio is not met. A message in the text window reports the actual ratio that is achieved.

Nonperiodic and periodic models

Substitutional disorder can be applied to nonperiodic models and to periodic models without symmetry.

Tip

To apply disorder to symmetric crystal structures, first convert the structure to a primitive superlattice (as described in the *Cerius^2 Builders* documentation) and then perform substitution.

Performing substitutional disorder

To introduce substitutional disorder into a model, select the **Build/ Disorder...** menu item to access the Disorder control panel. You can use this control panel to:

- Apply the substitution to the whole model or to selected atoms.
- Specify what element is to be replaced by what element and the target ratio to be achieved.

  For example, you can replace all silicon atoms in a model with aluminum by setting the target ratio to 0 or replace one-fourth of the silicons with aluminums by setting the ratio to 3.0.
- Apply Löwenstein's rule (if you are replacing silicon with aluminum).

Additional information

Please see the on-screen help for details on the functioning of each control in the Disorder control panel. After the substitution is performed, information on the number of atoms replaced, etc., is shown in the text window.

Introducing positional disorder

Uses of positional disorder

Positional disorder is a convenient way to move a model away from a local energy minimum. For example, you can apply positional disorder before cleaning a model (see *Refining the conformation*) or before performing an energy minimization (see the documentation for the Minimizer module in *Cerius^2 Simulation Tools*).

How it works

Positional disorder randomizes atomic positions—atoms are moved by the specified displacement in a random direction. Positional disorder can be applied to any model type. However, if an atom in a periodic structure is in a special symmetry position, it is not moved from that position, although it can be displaced in allowed directions. For example, if an atom lies on a symmetry

axis or plane, it (and all its symmetry copies) is moved only along that axis or within the plane, respectively. The distance the atom is moved is the component of the random displacement vector that lies on the symmetry axis or in the symmetry plane.

Performing positional disorder

To introduce positional disorder into a model, select the **Build/ Disorder...** menu item to access the Disorder control panel. You can use this control panel to:

- Apply the disordering to the whole model or to selected atoms.
- Specify the displacement distance (in angstroms) for each atom that is to be moved (in a random direction).

Additional information

Please see the on-screen help for details on the functioning of each control in the Disorder control panel.

Temperature factors

Finding information

If you need to know only how to work with temperature factors within the Cerius^2 interface, you may skip this theory section and go directly to:

Specifying temperature factors

Editing temperature factors

Loading and saving temperature factors

Related information

Representing the thermal motions of atoms graphically is discussed under *Thermal ellipsoids*.

Temperature factors and atomic vibrations

Atomic vibrations are described in the lowest order by their temperature factors. If the deviation of an atom from its equilibrium position is $\mathbf{r} = (x,y,z)$, the vibration is characterized by the matrix:

$$\mathbf{H} = \begin{bmatrix} \langle x^2 \rangle & \langle xy \rangle & \langle xz \rangle \\ \langle yx \rangle & \langle y^2 \rangle & \langle yz \rangle \\ \langle zx \rangle & \langle zy \rangle & \langle z^2 \rangle \end{bmatrix} \quad \text{Eq. 1}$$

Where $\langle xy \rangle$ represents the average over many vibrations.

Anisotropic and isotropic temperature factors

H is symmetric and contains six independent quantities, the anisotropic temperature factors U_{ij}. If the atomic vibration is isotropic, then **H** reduces to the form $\langle x^2 \rangle$ **I** and requires just one number (the isotropic temperature factor U_{iso}) to describe it:

$$\langle x^2 \rangle = \langle y^2 \rangle = \langle z^2 \rangle = \frac{\langle r^2 \rangle}{3} \qquad \text{Eq. 2}$$

Effects of vibration on X-ray scattering

Temperature factors are commonly used to describe the effect of vibration on X-ray, electron, and neutron scattering. For the first-order amplitude of scattering from an atom at $\mathbf{q} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$ in reciprocal space, the scattering amplitude is multiplied by:

$$e^{-2\pi \tilde{\mathbf{q}} \mathbf{H} \mathbf{q}} \quad \text{anisotropic}$$
$$e^{-2\pi \langle x^2 \rangle q^2} \quad \text{isotropic} \qquad \text{Eq. 3}$$

Conventions

Several different though equivalent ways of describing the temperature factors exist. (Cerius^2 can read temperature factors in several formats, see *Loading and saving temperature factors*.) Sometimes the vibration is described in terms of a crystal lattice coordinate system (a,b,c) rather than a Cartesian one.

Cartesian and crystal coordinate systems

If an atom has coordinates (x,y,z) with respect to the Cartesian axial system and (u,v,w) with respect to the lattice system so that:

$$x\hat{\mathbf{i}} + y\hat{\mathbf{j}} + z\hat{\mathbf{k}} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c} \qquad \text{Eq. 4}$$

then (x,y,z) and (u,v,w) can be interconverted by multiplying by a matrix **A** where $(x,y,z)^T = \mathbf{A}(u,v,w)^T$.

Table 3 shows the relationship between the different temperature factor forms and the way in which they modify the scattered amplitude.

Temperature factors in Cerius^2

Internally, Cerius^2 stores the atomic vibration matrix **H**. Cerius^2 stores isotropic and anisotropic temperature factors for every atom. You decide which of the two types to use for calculation or display.

For isotropic factors, the default format is U_{iso}. For anisotropic, the default format is U_{ij}.

Table 3. Forms of temperature factor terms

Form	Relationship to H or $\langle x^2 \rangle$	Scattering amplitude multiplied by
U_{iso}	$U_{iso} = \langle x^2 \rangle$	$T_{hkl} = e^{\frac{-8\pi^2 U_{iso} \sin^2\theta}{\lambda^2}}$
B_{iso}	$B_{iso} = 8\pi^2 \langle x^2 \rangle$	$T_{hkl} = e^{\frac{-B_{iso} \sin^2\theta}{\lambda^2}}$
U_{ij} [1]	$U_{ij} = (\mathbf{A}^{-1}\mathbf{H}\tilde{\mathbf{A}}^{-1})_{ij}$	$T_{hkl} = e^{-2\pi^2 U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{23}klb^*c^* + 2U_{13}hla^*c^*)}$
B_{ij} [2]	$B_{ij} = 8\pi^2(\mathbf{A}^{-1}\mathbf{H}\tilde{\mathbf{A}}^{-1})_{ij}$	$T_{hkl} = -\frac{1}{4}(B_{11}h^2a^{*2} + B_{22}k^2b^{*2} + B_{33}l^2c^{*2} + 2B_{12}hka^*b^* + 2B_{23}klb^*c^* + 2B_{13}hla^*c^*$
β_{ij} [2]	$\beta_{ij} = 2\pi^2(\mathbf{A}^{-1}\mathbf{H}\tilde{\mathbf{A}}^{-1})_{ij}\lvert\mathbf{a}_i^*\rvert\lvert\mathbf{a}_j^*\rvert$	$T_{hkl} = e^{-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{23}kl + 2\beta_{13}hl)}$

[1] $\mathbf{a}^* = (\mathbf{b} \wedge \mathbf{c})/(\mathbf{a} \cdot \mathbf{b} \wedge \mathbf{c})$, etc.
[2] For β, the factor of two on the cross terms is included in the term for some structure file formats (please see *File Formats* for more details).

Typical applications affected by temperature factors are X-ray, eletron, and neutron diffraction calculations (see separate documentation) and the display of thermal ellipsoids (*Thermal ellipsoids*).

Specifying temperature factors

Temperature factors can be specified when you add new atoms. Select the **Build/Add Atom...** menu item to access the Add Atom control panel. In this control panel, click the **Temperature Factors...** pushbutton to access the Added Atom Temperature Factors control panel.

With this control panel you can:

- Select **ISOTROPIC** or **ANISOTROPIC** to specify whether isotropic or anisotropic temperature factors will be used in any relevant calculation involving the atom to be added.
- Select the format to be used (i.e., B_{iso} or U_{iso} for isotropic temperature factors and U_{ij}, B_{ij}, or β_{ij} for anisotropic temperature factors; see Table 3).
- Enter the value of the isotropic temperature factor or the values for the anisotropic temperature factors.

  The six anisotropic temperature factors are entered as a matrix:

```
U11     U12     U13
        U22     U23
                U33
```

The selected specifications are applied when you add the atom with the Add Atom control panel (*Precise positioning of atoms during building*).

Command line

If you specify the anisotropic temperature factors from the command line, you should enter them in the order (1,1) (2,2) (3,3) (1,2) (2,3) (1,3).

Additional information

Please see the on-screen help for details on the functioning of each control in the Added Atom Temperature Factors control panel.

Editing temperature factors

The temperature factors of existing atoms can be edited. Select the **Build/Edit Atoms...** menu item to access the Edit Selected Atoms control panel. In this control panel, click the **Temperature Factors...** pushbutton to access the Edit Temperature Factors control panel. With this control panel you can:

- Select the format to be used (i.e., B_{iso} or U_{iso} for isotropic temperature factors and U_{ij}, B_{ij}, or β_{ij} for anisotropic temperature factors; see Table 3).
- Enter the value of the isotropic temperature factor or the values for the anisotropic temperature factors.

  The six anisotropic temperature factors are entered as a matrix:

```
U11     U12     U13
        U22     U23
                U33
```

- Click the **Use Isotropic** or **Use Anisotropic** action button to change the temperature factors of the atom to isotropic or anisotropic (using the format and value(s) specified).

Command line

If you specify the anisotropic temperature factors from the command line, you should enter them in the order (1,1) (2,2) (3,3) (1,2) (2,3) (1,3).

Additional information

Please see the on-screen help for details on the functioning of each control in the Added Atom Temperature Factors control panel.

Loading and saving temperature factors

As mentioned (*Conventions* and Table 3), several formats exist for describing temperature factors. When temperature factors are loaded from or saved in structure files, the factors are automatically converted to and from the Cerius^2 format.

The MSI, SHELX, CIF, ICSD, DBWS, and MolEN structure file formats can all be used to store isotropic and anisotropic temperature factors (please see *File Formats* for more details).

Isotropic temperature factors (but not anisotropic factors) are stored in both .xtl and .car / .mdf files.

Control of the model-cleaning function

The default mode of operation of the cleaning function is as described under *Refining the conformation*. However, you may want it to function differently.

You can specify the mode of operation of the cleaning function, the number of cycles performed (for one-shot cleaning), which atoms are to be cleaned, and which atoms are to be taken into account during the clean.

Specifying default behavior of the clean function

Click the **Preferences...** pushbutton near the bottom of the Sketcher control panel to access the Cleaner Controls control panel.

With this control panel you set preferences to:

- Optimize the positions of all atoms in a model during cleaning or only those of selected atoms.
- Take into account the interactions of all or selected atoms.
- Optimize for a specified number of cycles (“one-shot”) each time the **CLEAN** pushbutton in the Sketcher control panel is clicked or continue optimizing for as long as the mouse button is kept depressed after clicking the **CLEAN** pushbutton.
- Watch the progress during one-shot cleaning or update the view of the model only after cleaning is finished.
- Clean continuously (i.e., after every sketch operation) without needing to click the **CLEAN** pushbutton.

Additional information

Please see the on-screen help for details on the functioning of each control in the Cleaner Controls control panel.

Other builders

Tools designed to build more specialized models are available as separate modules and are accessed with the deck of cards menu. These include the Analog Builder, Crystal Builder, Surface Builder, Interface Builder, Polymer Builder, and Amorphous Builder. These modules are described in *Cerius^2 Builders*.

With these builders you can readily build series of analogous structures, crystals and other periodic structures, surfaces, interfaces, polymers, and amorphous structures.

Not all the Sketcher control panel functionality works with periodic systems. Those functions that *do* work include sketching bonds; changing the element, hybridization, or bond type; editing bond lengths, angles, and torsions; and deleting atoms or bonds.

6 Managing Models and Sessions

Among the many functions that you use the Visualizer to perform are management of the Cerius^2 session and of the models with which you work.

This section explains

This section tells you how to load and save structure files and how to manage Cerius^2 models and sessions:

Loading model structure files

Handling multiple models

Saving model structure files

Working with Cerius2 sessions

Table 4. Finding information about managing models and sessions

If you want to know about:	Read:
Controls in the model manager.	*The model manager*.
Finding files with file browsers in control panels.	*Loading model structure files*.
Mouse buttons and keyboard use.	*Mouse and Keyboard Actions*.
Model databases supplied by MSI.	*Models supplied by MSI*.
Building models.	*Building Models*.
Labeling and annotating models.	*Labeling and annotating models*.
Printing models.	*Printing models and graphs*.
Saving models.	*Saving individual models*.
Saving only part of a model.	*Saving part of a model*.
Saving all models in a Cerius^2 session.	*Saving the current session*.
Model data.	*What is saved as a model*.
File formats.	*File Formats*.
Making your own directories.	*Making custom directories*.
The current model.	*Specifying the current model*.

Table 4. Finding information about managing models and sessions

If you want to know about:	Read:
Model spaces, adding and removing.	*Creating, clearing, and deleting model spaces*.
Naming models.	*Renaming models*.
Model visibility.	*Controlling model visibility and the display mode*.
Displaying a model in the model window.	*Controlling model visibility and the display mode*.
Moving a model or part of a model between model spaces.	*Moving models between model spaces*.
Non-Cerius^2 applications.	*Copying models to and from other applications*.
Reinitializing Cerius^2.	*Starting a new session*.
Resuming a Cerius^2 session.	*Loading a previously saved session*.
Saving preferences.	*Using saved sessions as preferences settings*.
Customizing the Cerius^2 interface.	*Customizing the Interface*.
Running Cerius^2 from scripts contained in log files.	*Controlling Cerius2 from scripts*.

Loading model structure files

Why read this section

This section tells you how to bring one or more models that are stored on disk into your current Cerius^2 session. These can be models supplied with Cerius^2 by MSI (see *Models supplied by MSI*) or models that you or someone else built and saved earlier (*Saving individual models*).

Related information

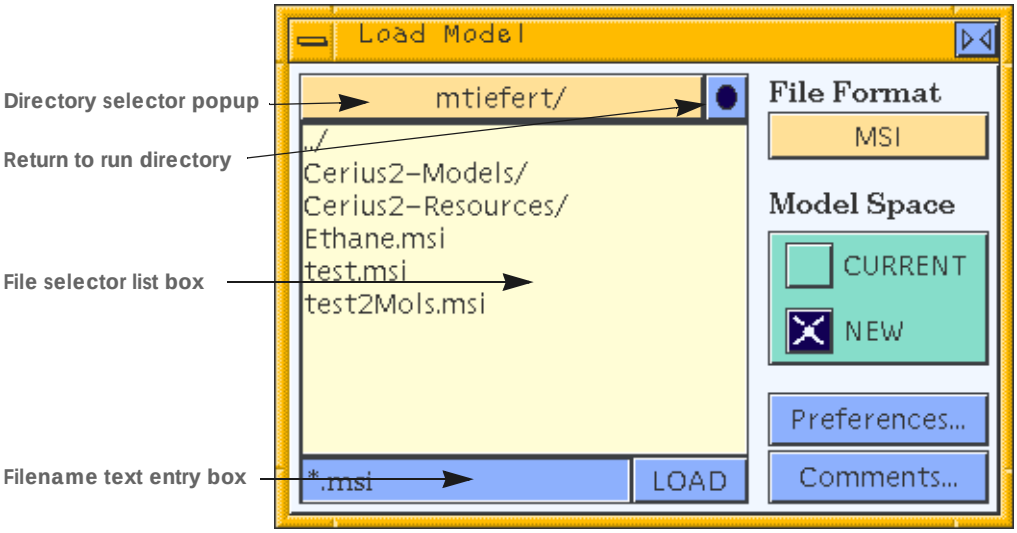
Building models is explained in *Building Models* and demonstrated in *Introducing Cerius2*. Saving models is discussed under *Saving model structure files*. File formats are presented in *File Formats*.

You should already know…

The basics of starting Cerius^2 and using its interface are demonstrated in *Introducing Cerius2* and described in *The Cerius2 Interface*.

Loading models

Select the **File/Load Model…** menu item (from the main control panel's menu bar) to access the Load Model control panel:



Finding model file(s)

Navigate the directory structure and find the desired file(s):

- To go to a higher-level directory, use the directory selector popup.

  The current directory is printed on the popup when it is in its inactive state.

- To return to the directory from which you started Cerius^2, click the small pushbutton next to the directory selector popup.

- To open a directory that's shown in the file selector list box (including the parent directory, indicated by **../**), double-click the directory name.

- To display the names of files having the desired format, set the **File Format** popup if necessary.

  For example, when the **File Format** popup is set to MSI, ***.msi** is listed in the filename text entry box (as a filename filter) and only filenames that end with .msi are shown in the file selector list box.

  You can also use the filename text entry box to specify a file, directory, or pathname or to set up your own filename filter. Valid UNIX wildcards and operators are allowed.

- If the list of file and subdirectory names is longer than the file selector list box, use the scroll bar on its right to move up and down the list.

Where to put the loaded model

To choose the target model space, set **Model Space** to **CURRENT** or **NEW** (see *Handling multiple models* for information on model spaces).

Note

If you load a model from a file into an already-occupied model space, all the contents of that model space are considered to be *one* model.

Loading the model file(s)

There are several ways of selecting and loading the desired file(s):

- To load a single model file, double-click its name in the file selector list box.

  or:

  Select its name file selector list box (the name becomes highlighted) and then click the **LOAD** button.

  or:

  Enter its name in the filename text entry box. (*Enter* means to type in the name and then press <Enter> or click the **LOAD** button.)

- To load several model files simultaneously, select their names in the file selector list box and then click the **LOAD** button.

  To select several model files, click the first filename and then drag to select several contiguous filenames, and / or <Shift> click to select a range of contiguous filenames, and / or <Ctrl> click to add a noncontiguous filename. Selected filenames are highlighted.

  To deselect filenames, <Ctrl> click to deselect individual filenames or simply click to start again with a single filename.

  The mouse / keyboard combinations for selecting and deselecting filenames (which are the same in any control panel that contains a file selector list box) are all described under *Mouse actions*.

Example

A tutorial example of loading models can be found in *Reading in additional models*.

Additional controls

You can change how files of a particular format are interpreted as they are read in. For example, whether to use any periodic information contained in the file, whether the number of hydrogen atoms is to be checked and corrected, whether and how to fill in possible missing bonds, etc.

To access these additional controls, click the **Preferences...** button in the Load Model control panel, which gives access to the Load Preferences control panel. The controls displayed in this panel depend on what the **File Format** popup in the Load Model control panel is set to.

Additional information

Please see the on-screen help for details on the functioning of each control in the Load Model control panel and the Load Preferences control panel.

Models supplied by MSI

Cerius^2 supplies databases for a wide range of types of molecules and materials. These databases are contained in subdirectories of the Cerius2-Models directory (accessible from your run directory during Cerius^2 sessions). These subdirectories include models of catalysts, ceramics, metals, minerals, molecular crystals, monomers, organics, polymers, sorbates, and others.

File formats

Many file formats besides the MSI format (see *File Formats*) can be imported if you need to use model files obtained from other programs or databases. However, transfer of all model data cannot be guaranteed when reading files that are not in MSI format.

Handling multiple models

Why read this section

Cerius^2 can hold many models at one time, each in its own *model space*. This section tells you how to work with several models that are present simultaneously in the same Cerius^2 session. The number of models allowed depends only on your computer's memory limitations.

Finding information

This section includes information on:

Basic model management tasks

Moving models between model spaces

Related information

Building models is explained in *Building Models* and demonstrated in *Introducing Cerius2*. Loading models is discussed under *Loading model structure files*.

You should already know...

The basics of starting Cerius^2 and using its interface are demonstrated in *Introducing Cerius2* and described in *The Cerius2 Interface*.

Basic model management tasks

Why read this section

When you have several models present simultaneously in the same Cerius^2 session, you need to know how to make a model be "current" so you can work with it. You may also want to know how to display one or more models, name models, open a new model space in order to load or build another model, etc.

Finding information

This section includes information on:

Creating, clearing, and deleting model spaces

Specifying the current model

Selecting model spaces

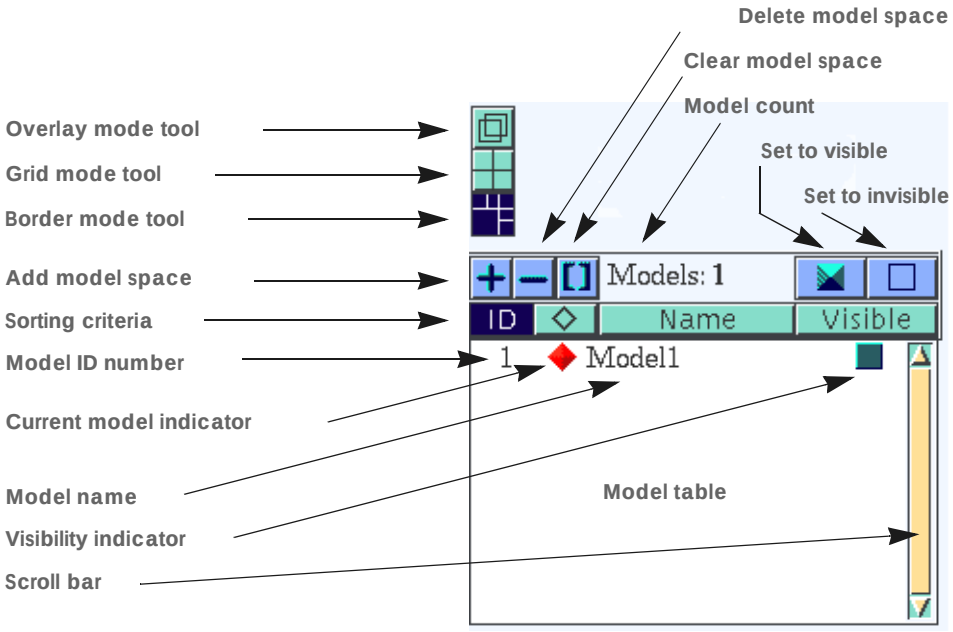
Controlling model visibility and the display mode

Renaming models

Sorting model table entries

The model manager

The model manager is part of the main control panel. When a Cerius^2 session is started with an empty model space (the usual default startup), the model manager looks like:



Additional information

Please see the on-screen help for details on the functioning of each control in the model manager.

Creating, clearing, and deleting model spaces

Model spaces are added automatically to accommodate models loaded from files or generated by application modules. For instance, when you use the Load Model control panel to read in a model from disk (*Loading model structure files*), the model is added by default to a newly created model space or (if it is completely empty) to the current model space.

When do you need to add model spaces?

However, for example, builders have no way of knowing when you may want to start a new model. They therefore assume that you want to continue modifying an existing model until you inform them otherwise.

Creating an empty model space

To add an empty model space, click the add model space tool in the model manager. The new model space's name is added at the bottom of the model table.

Clearing a model space

You may want to replace an existing model with a new one or perhaps realize you've built or loaded an incorrect model. Clearing a model space removes the model but allows its now-empty space to remain in the model manager.

To clear a model space, click the clear model space tool  in the model manager. If no model space(s) are selected (*Selecting model spaces*), the current (*Specifying the current model*) model space is cleared.

For many models, you can also select (*Selecting atoms and groups of atoms*) all the atoms of the current model and delete them (*Deleting atoms and bonds*) to clear the current model space. (Nonatomic information, if any, is not removed by this method.)

Deleting a model space

If you want to delete both the model and the space that contains it, click the delete model space tool  in the model manager. If no model space(s) are selected (*Selecting model spaces*), the current (*Specifying the current model*) model space is deleted. The last remaining model space cannot be deleted.

Example

A tutorial example of adding and deleting model spaces is found under *Managing multiple models*.

Specifying the current model

The *current* model is the one to which display, calculation, file, and other operations are applied.

Setting the current model

To specify that a certain model be current, click the current model indicator (diamond-shaped button) to the left of its name in the model table. The current model is identified by a red diamond; all other diamonds are greyed out.

Alternatively, you can press <Ctrl> on the keyboard and click any atom in the desired model with the left mouse button.

The current model is always visible in the model window, as the only model in the model window, in the lower left corner of a multi-paned model window displaying many models in grid or border mode (*Controlling model visibility and the display mode*), or as one of the models displayed in overlay mode (*Controlling model visibility and the display mode*).

Example

A tutorial example of handling multiple models is found under *Managing multiple models*.

Selecting model spaces

You can select one or more model spacess:

- On which to perform model management operations.
- To be used by various application modules.

Selecting models

To select model spaces, click the model ID number(s) in the model table, using the left mouse button. A single click selects only one model. You can select more than one model or change what is selected:

- To select several models, click the first model ID number and then drag to select several contiguous models, and / or <Shift> click to select a range of contiguous models, and / or <Ctrl> click to add a noncontiguous model name. Selected model rows are highlighted.
- To deselect models, <Ctrl> click to deselect individual models or simply click to start again with a single model.

The mouse button and keyboard combinations for selecting and deselecting model names (which are the same as for selecting file-names from file selector list boxes in control panels) are described under *Mouse actions*. Mouse operations are also described in the on-screen help (see *On-screen help*) for the model manager.

Controlling model visibility and the display mode

When you have several models in your Cerius^2 session, you may want to view only the current model, or you may also want to view one or more of the noncurrent models. You may display them in individual model window panes or overlay them all in the main model window.

Which models are visible

Use the visibility indicators (square buttons) to the right of the model names to control which models are visible.

- Click one or more of the visibility indicators to toggle the models between being visible (cyan, pyramidal visibility indicators) and hidden (empty visibility indicators).

You can also:

- Show all models, or all selected models, by clicking the set to visible button on the top row of the model manager.

  and / or:

- Hide all models (except the current model), or any selected models (except the current model), by clicking the set to invisible button.

The current model is always (implicitly) visible, and its colored visibility indicator looks flat by default. To make it remain explicitly visible even after some other model is made current, click its visibility indicator so that it appears pyramidal.

How they are displayed

The overlay mode, grid mode, and border mode display tools control how the model spaces are displayed in the model window:

- Border mode—To divide the model window into one large pane (located in the lower left corner, and which displays the current model) surrounded by a border of 5 smaller panes, select the border mode tool. If only the current model is visible, it fills the entire model window.

- Grid mode—To divide the model window into 4, 9, 16, … or 81 equal-sized panes (with the current model in the lower-left pane), select the grid mode tool. As many panes appear as are required to contain the visible models. If only the current model is visible, it fills the entire model window.

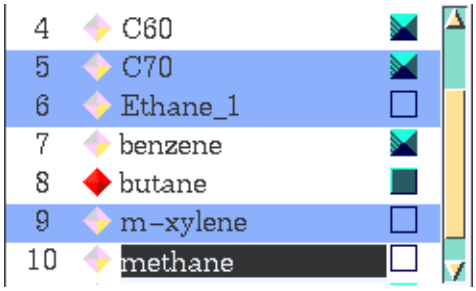
- Overlay mode—To display all visible models together in the same (large) model window, select the overlay mode tool. Although they are displayed together on the computer screen, the models still occupy separate model spaces.

Examples

A tutorial example of handling multiple models is found under *Managing multiple models*.

The following picture shows a model table with one current model that is implicitly visible (ID = 8), several visible models (IDs 4, 5, 7, 8), several invisible models (IDs 6, 9, 10), several selected model

spaces (IDs 5, 6, 9), and one model that is being renamed (ID = 10), with scrolling needed to see the whole list):



Renaming models

Newly created empty model spaces are given the name Model#, where # is the serial ID number of the model space. Models loaded from disk into an empty model space are given a name based on the structure file name. If a model has or is given the same name as an existing model, the name is suffixed with _1, _2, _3, etc.

You can rename models by clicking the existing name, then typing a new one and pressing <Enter> (or clicking somewhere else on a control panel).

Example

An example of renaming a model is given under *Reading in more models*.

Sorting model table entries

To assist you in browsing through the models stored in the model table, the model manager provides four sort-criteria controls. These controls enable you to sort model table entries according to model ID number, current model status, model name, or visibility.

Sorting criteria

To select the criteria by which models in the model table are sorted, select the appropriate control:

- The ID tool—Sort model table entries in ascending order according to the model ID number. These numbers are assigned serially as new model spaces are created. They cannot be reas-

signed during the current session and are not reused if a model space is deleted.

- The current (diamond) tool—Place the current model at the top of the model table and sort all other models in ascending order by model ID number.

- The name tool—Sort model table entries alphabetically by name.

- The visibility tool—Place all explicitly visible models at the top of the model table (sorted in ascending order by model ID number), followed by the current model (if it is not explicitly visible), followed by all invisible models (sorted in ascending order by model ID number).

Moving models between model spaces

Finding information

This section includes information on:

Copying whole models from one model space to another

Moving parts of models from one model space to another

Copying models to and from other applications

Copying whole models from one model space to another

You can copy the contents of some other model space to the current model space:

- You can copy a model into an empty current model space, for example, to use it as a base for additional building operations.
- You can also copy a model into a current space that already contains a model so as to build up a composite model. (The formerly separate models are now considered *one* model.)

Copying to the current model space

The simplest way to copy a whole model to a new model space is to make sure the desired model is current, then select (in order) the

Edit/Copy and **Edit/Paste** menu items. A new model space is created automatically.

If you have the display in border mode (*How they are displayed*) anyway, make sure the correct model is current (*Specifying the current model*). Then simply click in empty space within a border pane whose contents you want to copy and drag the cursor into the current model space's display pane (lower left of the model manager). (Clicking an atom in a border pane selects that atom, *Selecting atoms in several models*.)

You can also select all atoms in a model and use cut (or copy) and paste (*Moving parts of models from one model space to another*) to move entire sets of atoms from one space to another. (Nonatomic information, if any, is not copied by this method.)

Example

A tutorial example of copying model-space contents from one space to another can be found under *Copying models from one model space to another*.

Moving parts of models from one model space to another

You can also copy or move parts of models from one model space to another (or within the same model space) using atom selection (*Selecting atoms and groups of atoms*) and editing techniques (for how to specify the current model, see *Specifying the current model*):

- To remove selected atoms from the current model, select the **Edit/Cut** menu item or press <Alt> **x** on the keyboard. These atoms can then be pasted into the same or another model space.
- To make a copy of selected atoms from the current model, select the **Edit/Copy** menu item or press <Alt> **c** on the keyboard. These atoms can then be pasted into the same or another model space.
- To paste atoms (that were previously cut or copied from the same or a different model space) into the current model space, select the **Edit/Paste** menu item or press <Alt> **v** on the keyboard. If all the atoms to be pasted correspond to atoms in the current model, they are pasted to an offset position.

Important

In addition to the selected atoms, any bonds and hydrogen bonds between the selected atoms and linkages on selected atoms are copied into the paste buffer. Other information, such as monitors and subunit or chain information (if present) is not copied into the paste buffer.

Copying models to and from other applications

The cut- or copy-and-paste operations described in the previous section make use of your computer's clipboard. Thus, applications that can work with information stored in the system clipboard can make use of these structural elements (as does Cerius^2). This enables you to cut and paste structural elements back and forth between Cerius^2 and other applications such as Insight® II, ISIS™ / Draw, ChemDraw™, Catalyst®, and Open Inventor-based applications on SGI systems that have the Molecular Inventor Execution-Only Environment (molinv_eoe) installed. However, other applications may not be able to use all the information associated with Cerius^2 structural elements.

Timeout period

Transferring large models between Cerius^2 and other applications can take up to a minute or more. Cerius^2 is configured to wait up to 3 min for information pasted from other applications to complete transfer. However, transferring large models or structural elements from Cerius^2 to other applications may fail if the other application's timeout value is not increased. The default timeout period for most applications' paste operations is 5–30 s, depending on the operating system. If you have problems pasting large models from Cerius^2 to other compatible programs, you can usually increase the other application's timeout value by adding an entry to the .Xdefaults file in your home directory. For example, to increase the timeout value for SGI's InPerson application add the following entry:

```
InPerson*selectionTimeout:       180000
```

This changes the default selection timeout value to 180000 ms (3 min). The default value for Cerius^2 is 180000, but you can also change it in your .Xdefaults file, using this format:

```
Cerius2*selectionTImeout:       180000
```

Saving model structure files

Why read this section

This section tells you how to save one or more models that are in your current Cerius^2 session, to store them on disk. You will probably want to save models that you have built or modified and may want to use again. You should save your model before running any calculation or performing other activities that might change its conformation, if the original conformation of your model is important.

Finding information

This section includes information on:

Saving individual models

Saving all models

Related information

Building models is explained in *Building Models* and demonstrated in *Introducing Cerius2*. Loading models is discussed under *Loading model structure files*. File formats are presented in *File Formats*.

You should already know...

The basics of starting Cerius^2 and using its interface are demonstrated in *Introducing Cerius2* and described in *The Cerius2 Interface*.

Use of the file selection list box and other file selector controls to navigate the directory structure is presented in detail under *Finding model file(s)*.

How to make a model be the current one is described under *Basic model management tasks*.

Saving individual models

Making custom directories

You may want to create your own directories or subdirectories in which to save models. For example, you may want to save models relating to a specific project together or save related models as a database.

To do so, go to a UNIX shell window (not the one from which you are currently running Cerius^2), **cd** to the desired parent directory, and create your subdirectory with the UNIX **mkdir** command. (This can be done at any time.) For example:

```
> cd ~/CeriusRuns
```

```
> mkdir myModels
```

Alternatively, you can use the the text window and prefix a **!** to the UNIX commands (*Text window*).

Saving the current model

Select the **File/Save Model...** menu item (from the main control panel's menu bar) to access the Save Model control panel. This control panel is used to save the current (*Basic model management tasks*) model.

Use the file selector controls in the Save Model control panel to move through the file system to the directory in which you want to save the current model. (Newly created directories appear in the file selector list box when the appropriate parent directory is opened or reopened with the file selector controls or when the control panel is opened.)

After selecting the appropriate directory, specify a name for the structure file by typing that name in the file name entry box, then press <Enter> or click the **SAVE** button.

A warning helps prevent you from accidentally overwriting existing structure files. (You may choose and enter an existing filename if you want to overwrite an existing structure file.)

Example

A tutorial example of saving one model is given on *Saving a model*.

Additional controls

You can save files in a non-Cerius^2 format. Some formats allow a choice of formatting options. To set them, click the **Preferences...** pushbutton to accesses the Save Preferences control panel. The controls displayed in this panel depend on what the **Save format** popup in the Save Model control panel is set to.

Saving part of a model

If you want to save only part of a model, select the desired part (*Selecting atoms and groups of atoms*), cut or copy it and paste it into a new model space (*Moving parts of models from one model space to another*), and save the new model.

Additional information

Please see the on-screen help for details on the functioning of each control in the Save Model control panel and the Save Preferences control panel.

What is saved as a model

Model data that can be saved to file include atom coordinates (Cartesian, fractional, or internal), element type, charge, bonding connectivity, crystal unit cell, crystal symmetry, occupancy, and temperature factors. The exact combinations depend on the format

you select from the **Save Format** popup in the Save Model control panel. The default MSI file format holds *all* model data.

File formats

Cerius^2 has its own model-file format (.msi format) capable of storing every detail of any model in the Cerius^2 modeling environment. You should always store your model files using the .msi format unless you want to exchange them with databases, other molecular modeling applications, or your own programs.

Many file formats besides the .msi format (see *File Formats*) can be written if you need to transfer model files to other programs or databases. However, transfer of all model data cannot be guaranteed when writing files that are not in .msi format.

Saving all models

To conveniently save all models in the current session, save the session rather than its individual models (*Saving the current session*).

Working with Cerius^2 sessions

Why read this section

This section tells you what Cerius^2 sessions are and how to start, resume, and save them. It is useful if you, for example, want to:

- Resume a session that you had to interrupt earlier.
- Save all your models at once.
- Return Cerius^2 to its start-up state.
- Always start your sessions with Cerius^2 in a certain state.

Finding information

This section includes information on:

Starting a new session

Saving the current session

Loading a previously saved session

Using saved sessions as preferences settings

You should already know…

The basics of starting Cerius^2 and using its interface are demonstrated in *Introducing Cerius2* and described in *The Cerius2 Interface*.

Use of the file selection list box and other file selector controls to navigate the directory structure is presented in detail under *Finding model file(s)*.

What is a session?

A Cerius^2 *session* consists of all the models and data with which you are currently working, as well as application preferences that you have specified.

Starting a new session

Reinitializing Cerius^2

To start a new session, select the **File/New Session** menu item. Clicking **Confirm** in the message window that appears reinitializes Cerius^2, which is equivalent to quitting and restarting Cerius^2.

Important

All unsaved models and data are lost when you start a new session, and settings in control panels are returned to their defaults.

Saving the current session

You can save the current Cerius^2 session at any time. After you do so, you can then resume that session at some later time (as described under *Loading a previously saved session*), either later while you are still running Cerius^2 or after exiting and restarting Cerius^2.

Making custom directories

You may want to create your own directory or subdirectory in which to save your session.

To do so, go to a UNIX shell window (not the one from which you are currently running Cerius^2), **cd** to the desired parent directory, and create your subdirectory with the UNIX **mkdir** command. (This can be done at any time.) For example:

```
> cd ~/CeriusRuns
> mkdir tutorialSession
```

Saving the current session

Select the **File/Save Session...** menu item (from the main control panel's menu bar) to access the Save Session control panel. This control panel is used to save the current session.

Use the file selector controls in the Save Session control panel to move through the file system to the directory in which you want to save the current model. (Newly created directories appear in the file selector list box when the appropriate parent directory is opened or reopened with the file selector controls or when the control panel is opened.)

After selecting the appropriate directory, specify a name for the session file by typing that name in the file name text entry box, then press <Enter> or click the **SAVE** button.

A warning helps prevent you from accidentally overwriting existing session and model files. (You may choose and enter an existing filename if you want to overwrite an existing session file.)

What is saved as a session

A saved session consists of a session file (.mss file extension) and a set of standard MSI-format structure (model) files. When you save a session, one model is written in the specified directory for each occupied model space. The session file contains application preferences, customizations, any cross-model linkages, and references to the saved structure files.

Related information

Saving individual models is described in *Saving model structure files*.

Loading a previously saved session

You can resume a previously saved Cerius^2 session at any time.

What resuming a session does

When you load a saved session, the current session is reinitialized (i.e., unsaved models and data are lost and settings return to their defaults), all models referenced by the resumed-session file are loaded into model spaces, and application preferences are set to the values indicated in the resumed-session file.

Resuming a session

Select the **File/Load Session...** menu item (from the main control panel's menu bar) to access the Load Session control panel. This control panel is used to load the session you want to resume.

Use the file selector controls in the Load Session control panel to move through the directory system to find the session you want to resume.

Either double-click the name of the desired session file or select the desired session file and click the **LOAD** button. You can also enter its name in the session name text entry box.

Important

Any unsaved models and data in your current session are lost when you resume a saved session, and settings in control panels are returned to the values (if any) set in the resumed-session file or to their defaults.

What next?

You can now resume work from the point at which you saved the session you just loaded.

Related information

Loading individual models is described in *Loading model structure files*.

Using saved sessions as preferences settings

If you often need to change many settings before starting your work, you can load only the application preferences from a saved session file.

Saving preferences in a session file

Nondefault application settings are saved when you save a session (*What is saved as a session*). (However, not all applications save all nondefault control settings when a session is saved.)

You may want to start up one of your typical sessions by changing all settings as desired, in the absence of any models. Then you can save this “empty” session.

Although you can load only the preferences from any session file, saving an empty session may, depending on how you work, decrease disk space requirements.

Loading only preferences from a saved session

Before loading or building any models, load your preferences by:

- Loading (*Loading a previously saved session*) an empty session file.

  or:

- Checking the **Preferences Only** check box in the Load Session control panel and then loading any desired session file.

Warning

Loading an empty session file or loading only the preferences from any session file removes all models and associated data from your current session. Therefore, you need to load the session file *before* building or loading any models.

Related information

Information on controlling Cerius^2 from prerecorded command scripts is given in *Controlling Cerius2 from scripts.*

Other customization activities are covered in *Customizing the Interface.*

7 Geometry Analysis

The Visualizer's analysis and evaluation tools enable you to closely examine the three-dimensional structure of the models you are studying.

This section explains

This section contains information on:

Measuring models

Calculating close contacts

Model surfaces

Vector properties

Related information

Some other Cerius^2 application modules also contain various types of functionality for analyzing model geometry or calculating other types of surfaces. Information on using these tools is found in the specific documentation for the relevant application modules.

Table 5. Finding information about geometry analysis of models

If you want to know about:	Read:
Measuring distances, angles, torsions, and inversions of models.	*Measuring models*.
Examining and changing the model's geometry.	*Editing the structure*.
Refining the model's conformation.	*Refining the conformation*.
Close contacts between nonbonded atoms.	*Calculating close contacts*.
Solvent-accessible surfaces for models of a molecule, surface, or crystal.	*Model surfaces*.
van der Waals surfaces for models.	*Model surfaces*, *Atom and bond display styles*.
Displaying surfaces.	*Surfaces—style and transparency*.

You should already know…

The basics of starting Cerius^2 and using its interface are demonstrated in *Introducing Cerius2* and described in *The Cerius2 Interface*.

You need to know how to build (*Basic building*) and / or load (*Loading model structure files*) models and should know how to select atoms in model(s) (*Selecting atoms and groups of atoms*).

If your session contains several models, you should know how to specify the current model (*Specifying the current model*) or select atoms in more than one model simultaneously (*Selecting atoms in several models*).

Measuring models

Why read this section

You can measure distances, angles, planes, torsions, and inversions for the atoms in a model and display these measurements in the model window or the text window.

Finding information

This section includes information on measuring:

Distances

Angles

Planes

Torsions

Inversions

Accessing the tools

Access the Measurements control panel by selecting the **Geometry/Measurements…** menu item in the main control panel's menu bar.

Display of measurements

The calculated measurements are represented in the model window by lines and labels. These are automatically updated whenever the model is modified, enabling you to monitor the effects of manipulations as you perform them.

You can display all measurements in the text window by clicking the **List measurements** action button.

Removing displayed measurements

To remove all measurements from the display, click the **Delete measurements** action button. To temporarily hide the calculated

measurements (without deleting them), check the **Hide measurements** check box.

You can selectively delete measurements by selecting the appropriate measurement tool (see below) and then re-selecting the atoms that were picked to calculate those measurements.

Example

A tutorial example of using the Measurements control panel is found under *Measuring components of the model's geometry*.

Additional information

Please see the on-screen help for details on the functioning of each control in the Measurements control panel.

Distances

Measuring distances

To measure the distances between atoms, you use the **Distance** tool.

You can use it in two different ways:

- Select the **Distance** tool and then pick atom pairs whose distances you want to measure. These atoms need not be bonded to each other. The distance(s) in angstroms are indicated in the model window.

  or:

- Select any number of atoms and then double-click the **Distance** tool. The lengths (in angstroms) of each bond existing between selected atoms are indicated in the model window.

A dotted line indicates what distance was measured.

Related information

Information on examining and changing bond lengths is contained under *Examining and changing bond lengths*.

Angles

Measuring angles

To measure the angle involving any three atoms, you use the **Angle** tool.

You can use it in two different ways:

- Select the **Angle** tool and then pick atom triplets whose angles you want to measure. These atoms need not be bonded to one another. The angle(s) in degrees are indicated in the model window.

  or:

- Select any number of atoms and then double-click the **Angle** tool. The angles (in degrees) of each existing valence angle connecting three consecutively bonded, selected atoms are indicated in the model window.

Dotted lines indicate what angle was measured.

Related information

Information on examining and changing angles is contained under *Examining and changing angles*.

Planes

Measuring angles defined by two planes

To measure the angle between any two planes, you use the **Plane** tool.

You can:

- Select the **Plane** tool. Pick three atoms that define the first plane and then three that define the second plane.

  or:

- Select three atoms that define the first plane and then three that define the second plane. Then double-click the **Plane** tool.

The angle between the two planes (in degrees) is indicated in the model window, as well as dotted lines indicating what planes were used.

Torsions

Measuring torsions

To measure the torsion angle involving any four atoms, you use the **Torsion** tool.

You can use it in two different ways:

- Select the **Torsion** tool and then pick sets of four atoms whose dihedral angles you want to measure. These atoms need not be bonded to each other. The angle(s) in degrees are indicated in the model window.

  or:

- Select any number of atoms and then double-click the **Torsion** tool. The angles (in degrees) of each existing torsion among four consecutively bonded, selected atoms are indicated in the model window.

Dotted lines indicate what torsion was measured.

Related information

Information on examining and changing torsions is contained in *Examining and changing torsions.*

Inversions

Measuring inversions or out-of-plane angles

To measure the inversion or out-of-plane angle involving any four atoms, you use the **Inversion** tool. These atoms need not be bonded to each other. The vertex atom is the first one picked.

First set the definition according to which the inversion is calculated with the **Inversion** popup.

Then you can:

- Select the **Inversion** tool and then pick four atoms whose inversion (out-of-plane angle) you want to measure.

  or:

- Select the desired four atoms and then double-click the **Inversion** tool. These atoms need not be bonded to each other.

The out-of-plane angle in degrees is indicated in the model window, as well as dotted lines indicating what angle was measured.

Calculating close contacts

Displaying too-close contacts that may occur between atoms can be valuable for examining models resulting from simulations, preparing accurate models, or studying model–model interactions.

Accessing the tools

Access the Close Contacts control panel by selecting the **Geometry/Close Contacts...** menu item in the main control panel's menu bar. You use this control panel to calculate and display close contacts between all or selected atoms in one or more models.

Contact criteria

Two criteria are available for determining whether atoms are too close together:

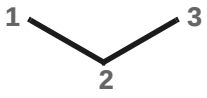
- If the distance between the atomic centers is less than a specified cutoff distance. Choose **DISTANCE** and enter the **Cut-off** in angstroms.
- If the distance between the atom centers is less than $\alpha (r_1 + r_2)$, where α is a specified ratio and r_1 and r_2 are the van der Waals radii of the two atoms. Choose **VDW RADIUS** and enter the **VDW Ratio** (α). A **1** means that close contacts are indicated whenever van der Waals spheres are just touching each other.

Exclusions

You may want to exclude certain atom pairs from the close contact calculation. You can exclude **BONDED** atoms or atoms in the same **GROUP**, **FRAGMENT**, or **MODEL**.

When excluding bonded atoms, you can specify a distance (in terms of number of bonds) within which atoms should be excluded. For example, a bond separation of 1 means to exclude only directly bonded atoms from the search. Choose **BONDED** and enter the **Separation**, in number of bonds.

For example (figure below), if the bond separation is 1, the distances between directly bonded atoms (1–2 and 2–3) are ignored. If the bond separation is 2, the distance between atoms 1 and 3 is also ignored:



Groups (*Defining and selecting groups*) are defined with the Groups control panel, which is accessed by clicking the **Define Groups...** pushbutton on the Close Contacts control panel or by selecting **Edit/Groups** from the menu bar.

A fragment includes all members of a bonded set of atoms. You would, for example, set the exclusion to **FRAGMENT** if you were examining the fit of a small molecule to a receptor or surface in the same model and wanted to ignore any close contacts within a fragment. However, if the small molecule and receptor were present as different models, you would set the exclusion to **MODEL**.

Calculating close contacts

Set the selection criteria and then click the **CALCULATE close-contacts** action button to calculate and display close contacts.

Display of close contacts

Once calculated, close contacts are continuously updated when fragments are moved, rotated, cleaned (*Refining the conformation*), etc. This enables you, for example, to position a fragment inside a larger structure while monitoring close contacts between the two or to monitor close contacts during minimization.

Additional information

Please see the on-screen help for details on the functioning of each control in the Close Contacts control panel.

Model surfaces

Connolly surfaces

You can use the Connolly (1983a, b) surface utility to probe a molecule, surface, or crystal to produce a dot display of the contact surface. You can use this utility, for example, to map out the internal channel structure of a crystal, find the solvent-accessible surface of a large model, or understand the topography of a 2D surface.

What is a Connolly surface?

You can use the Connolly surface utility to calculate and display a van der Waals or a Connolly surface for all or part of a model:

- A *Connolly surface* is the van der Waals surface of the model that is accessible to a solvent molecule having a nonzero radius. The surface is generated by rolling a spherical probe of a specified radius over the van der Waals surface of the model (Figure 2).

- A van der Waals surface is generated when the probe radius is zero.

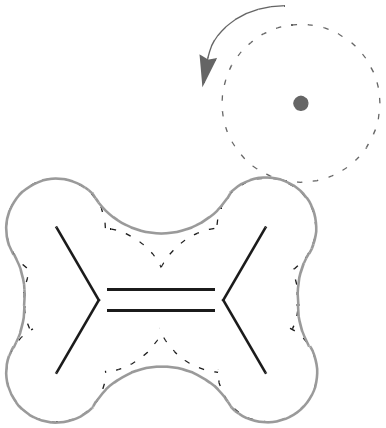


Figure 2. Generation of Connolly surfaces

Dotted lines represent the van der Waals surfaces of the model and the probe; the solid black line represents the Connolly surface. In this example, much of the Connolly surface is equivalent to the van der Waals surface.

Where the probe contacts only one atom of the model, the Connolly surface is equivalent to the van der Waals surface of the model. Where the probe contacts two or three atoms simultaneously, the Connolly surface is equivalent to the van der Waals surface of the probe (Figure 2). The resulting surface represents the solvent-accessible surface of the molecule (assuming that a molecule of solvent is a sphere with the same radius as the probe).

Accessing the tools

Access the Connolly Surfaces control panel by selecting the **Geometry/Connolly Surfaces…** menu item in the main control panel's menu bar. You use this control panel to calculate and display Connolly surfaces involving all or selected atoms in your model. You can:

- Calculate a surface for the entire model. Set both **Atoms to be surfaced** and **Atoms in calculation** to **ALL**.

- Calculate a surface that surrounds only selected atoms. Set both **Atoms to be surfaced** and **Atoms in calculation** to **SELECTED**.
- Calculate a partial surface. Set **Atoms to be surfaced** to **SELECTED** and **Atoms in calculation** to **ALL**.

Calculating Connolly surfaces

Set the **Calculation Preferences** controls in the Connolly Surfaces control panel as desired, then click the **CALCULATE** pushbutton to calculate and display a Connolly surface.

Displaying Connolly surfaces

Once you have calculated (and displayed) a surface for all or selected atoms in a model, you can toggle the display of that surface by using the **Hide** check box.

Tip

Surfaces can take up large amounts of memory. Therefore, it is a good idea to delete them when they are no longer required. Then recalculation (or reloading, if you saved the surface, see *Saving and loading Connolly surfaces*) is required to display them again.

A Connolly surface is not part of the fragment itself. So if you delete all or part of the fragment, the surface remains unchanged until you recalculate or delete it.

Before a new surface is calculated and displayed, the existing surface is deleted. If you want to view two different Connolly surfaces on a model, copy the model to a second model space (*Copying whole models from one model space to another*), generate the second surface for the copy, change its color, and then display both models together using the overlay display mode (*Controlling model visibility and the display mode*).

Saving and loading Connolly surfaces

Connolly surfaces can be saved and loaded using the **Save Surface...** and **Load Surface...** pushbuttons, respectively, on the Connolly Surfaces control panel. The file format is compatible with equivalent files generated in POLYGRAF and has a default extension of .dot. Note that the file saves only the position and color of the dots that make up the surface; the atomic positions are not saved in this file.

For operating the file selector control in the Load Connolly Surface and Save Connolly Surface control panels, please see *Finding model file(s)*.

Additional information

Please see the on-screen help for details on the functioning of each control in the Connolly Surfaces, Load Connolly Surface, and Save Connolly Surface control panels.

Vector properties

Vector attributes such as the force on an atom, its velocity, or its electron spin state can be displayed as arrows at all or selected atoms.

Calculating vector properties

Vector attributes are output by other Cerius^2 modules, such as the quantum chemistry modules, which are licensed and documented separately.

Accessing the tools

Access the Vector Properties control panel by selecting the **Geometry/Vector Properties...** menu item in the main control panel's menu bar. You use this control panel to display vector properties on all or selected atoms in your model.

Displaying vector properties

You can use the Vector Properties control panel to show, remove, or hide available vector properties. If you want to edit the style or size of the displayed vectors, click the **Preferences...** pushbutton to access the Vector Preferences control panel.

Additional information

Please see the on-screen help for details on the functioning of each control in the Vector Properties and Vector Preferences control panels.

8 Viewing and Displaying Models

The Cerius^2•Visualizer allows you to position models as desired, to move models relative to one another, and control how models are displayed and printed. You can also annotate them with labels and arrows, etc., and animate models according to the results of certain calculations.

This section explains

This section tells you how to accomplish:

Moving models on the screen

Animating models

Labeling and annotating models

Model display style

Resolution and graphical quality

Printing models and graphs

Table 6. Finding information about viewing models

If you want to know about:	Read:
Mouse buttons and keyboard use.	*Mouse and Keyboard Actions*.
Rotating, moving, and magnifying the model view.	*Moving models on the screen*.
Moving parts of models.	*Editing the structure*.
Transferring models or parts of models between model spaces.	*Moving models between model spaces*.
Docking models.	*Moving models relative to one another*.
Superimposing models (rms matching).	*Superimposing models*.
Continuous rotation or rocking of models.	*Changing the default mouse rotation action*.
Scaling the view.	*Changing the view magnification*.
Size of the model window.	*Maximum size*.

Table 6. Finding information about viewing models

If you want to know about:	Read:
Centering or resetting the model display.	*Setting position and orientation*.
Screen coordinates.	Figure 3. *Window axes in Cerius2 model window*.
Z-clipping.	*Cross sections of models*.
Kekule or resonant display of phenyl rings.	*Bond order display*.
Space-filling models.	*Atoms as balls*.
Structural display of charged inorganic systems.	*Cations as polyhedra*.
Thermal motion of atoms.	*Thermal ellipsoids*.
Adding lines, boxes, circles, etc. to display.	*Custom annotations*.
Labeling models with geometric measurements	*Measuring models*.
Viewing close contacts.	*Calculating close contacts*.
Controlling colors used in displaying models.	*Model display colors*.
Changing the display and print resolution.	*Resolution and graphical quality*.
Other advanced control of model rendering and lighting.	*Enhancing Model Display*.
Displaying Connolly surfaces.	*Model surfaces*.
Changing the display of model surfaces.	*Surfaces—style and transparency*.

You should already know…

The basics of starting Cerius^2 and using its interface are demonstrated in *Introducing Cerius2* and described in *The Cerius2 Interface*.

You need to know how to build (*Basic building*) and / or load (*Loading model structure files*) a model and should know how to select atoms in your model (*Selecting atoms and groups of atoms*).

If your session contains several models, you should know how to specify the current model (*Specifying the current model*). You may also want to know how to select atoms in several models (*Selecting atoms in several models*).

Moving models on the screen

Changing the position, viewing angle, and magnification of models in the model window aid in tasks such as accessing parts of the model, viewing small parts of the model in detail, understanding

the model's 3D structure, bringing related or complementary models together in space, optimizing displays for printout.

Finding information

This section includes information on:

Basic tasks and methods

Moving models relative to one another

Superimposing models

Storing and retrieving views

Related information

Moving parts of models is discussed under *Editing the structure*. Copying models or parts of models from one model space to another is discussed under *Moving models between model spaces*.

Basic tasks and methods

Basic model-viewing tasks can often be accomplished in several ways: by using the mouse in the model window, using tools in the toolbar of the Cerius^2•Visualizer's main control panel, using control panels accessed from menu items in the main control panel (mainly from the **View** menu), or using keyboard shortcuts. The various methods differ in convenience, quickness, and/or accuracy.

Note

The basic model viewing tools do not alter the original coordinates of the models. They affect only the view and appearance of models in the model window.

Finding information

Basic model-viewing tasks affect all models and include:

Translating models

Rotating models

Changing the view magnification

Setting position and orientation

Display axes

You rotate and translate models relative to the x, y, and z display (window) axes, which are *always* oriented as shown in Figure 3.

(These window axes are *not* the same as the model's viewing-angle axes, which are usually displayed in the lower right corner of the model window, see *Default annotation*.)

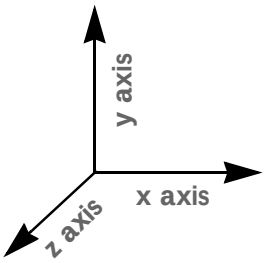


Figure 3. Window axes in Cerius^2 model window

The z axis points perpendicularly out of the computer screen.

Example

A tutorial example of basic model moving is found in *Moving a model*.

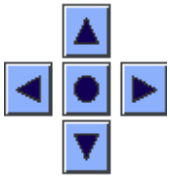
Translating models

Manual translation

To interactively translate models, place the cursor in the model window and then press the middle mouse button and drag the mouse in any direction within the xy plane.

Incremental translation

Select the **View/Dials...** menu item to access the Viewing Dials control panel.



To move the models in an x or y direction, use the arrow tools in the **Pan** controls.

To return the model to its original position, click the reset button (in the center of the arrow tools).

Additional information

Please see the on-screen help for details on the functioning of each control in the Viewing Dials control panel. Mouse functions and keyboard shortcuts are summarized in *Mouse and Keyboard Actions*.

Rotating models

Manual rotation

To interactively change the viewing angle of models, place the cursor in the model window and then:

- To rotate the models about the x axis, press the right mouse button and move the mouse vertically in the central area of the model window.
- To rotate the models about the y axis, press the right mouse button and move the mouse horizontally in the central area of the model window.
- To rotate the models about the y axis, press the right mouse button and move the mouse horizontally or vertically near an edge of the model window.

Tip

The default mouse behavior described here can be altered by changing the mouse rotation action from normal to continuous or rock (see *Changing the default mouse rotation action*).

Changing the default mouse rotation action

To change the default way in which mouse-driven rotations behave, select the **View/Options...** menu item to access the View Options control panel. Choose the desired function under **Mouse Rotate Action**. The available modes are:

- **NORMAL**—As described under *Manual rotation*.
- **CONTINUOUS**—As described under *Manual rotation*, except that rotation continues when you release the mouse button. To stop the movement, move the cursor out of the model window, press <Esc> on your keyboard, or click the right mouse button anywhere in the model window.
- **ROCK**—As for **CONTINUOUS**, except that rotation occurs only through the angle specified in the associated entry box. The direction of rotation alternates so that the model view rocks. To stop the movement, move the cursor out of the model window, press <Esc> on your keyboard, or click the right mouse button anywhere in the model window.

Large rotations

To quickly change the viewing angle in large steps, place the cursor in the model window and then:

- To rotate the models by 45° about the x axis, press the up or down arrows on an extended keyboard.

- To rotate the models by 45° about the y axis, press the right or left arrows on an extended keyboard.

Continuous rotation

Select the **View/Dials...** menu item to access the Viewing Dials control panel.

To continuously rotate the models about the x, y, or z axis, click and hold a slider or click and continuously drag a dial pointer.

Precise rotation

Select the **View/Dials...** menu item to access the Viewing Dials control panel.

To rotate the models to a specific angle about the x, y, or z axis, drag the sliders, click any point on the dials, and / or enter angles (in degrees) in the entry boxes. Dragging a slider is the least exact of these methods, and entering an angle, the most.

Orienting according to atom positions

You can orient the view so that selected atoms in the current model lie parallel or perpendicular to the computer screen.

To do this, select the **View/Orient...** menu item to access the Orient View control panel. Select the desired atoms. Click the **Parallel To Screen** or **Perpendicular To Screen** action button. (All visible models rotate in concert, around the same axis and by the same angle.)

The model view is reoriented so the best-fit plane through the selected atoms is lies in or perpendicular to the plane of the computer screen.

Additional information

Please see the on-screen help for details on the functioning of each control in the Viewing Dials, Orient View, and View Options control panels. Mouse functions and keyboard shortcuts are summarized in *Mouse and Keyboard Actions*.

Changing the view magnification

Manual zooming

To interactively change the view scaling of models, you can place the cursor in the model window and:

- Hold down the middle and right mouse buttons and drag the cursor in the model window.

  or:

- Hold down <Shift> plus the middle mouse button and drag the cursor in the model window.

Moving the cursor up and / or to the right increases the magnification; moving it down and / or to the left decreases magnification.

Filling the model window

To shrink or expand the view so that the models almost fill their model window pane(s), you can do any of:

- Select the **View/Fill Window** menu item in the main control panel.
- Press <End> on an extended keyboard.
- Press <Alt> **w** on your keyboard.
- Select the **View/Orient...** menu item to access the Orient View control panel. Click the **FILL WINDOW** pushbutton.

Maximum size

To obtain the largest viewing area possible, you can change the size of the model window.

To enlarge the model window so that it fills the computer screen, you can do any of:

- Press <F2> on your keyboard.
- Select the **View/Options...** menu item to access the View Options control panel. Click the **Set to Full Screen** action button.
- Grab a corner of the model window and pull it to the desired size.

Normal model window size

To return the model window to its usual size, you can:

- Press <F2> on your keyboard.

or:

- Click the **Reset to Default** action button in the View Options control panel.

Incremental zooming

To change the view scaling of the models in increments, you can place the cursor in the model window and:

- Press <+> or <–> on an extended keyboard.

or:

- Select the **View/Dials...** menu item to access the Viewing Dials control panel.

To zoom into or out of the models, use the arrow tools in the **Magnification** controls.

To return the models to their original magnification, click the reset button (between the arrow tools).

Continuous zooms

Select the **View/Dials...** menu item to access the Viewing Dials control panel.

Click and hold one of the **Magnification** arrow tools.

Precise magnification

Select the **View/Dials...** menu item to access the Viewing Dials control panel.

Enter a value in the **Magnification** entry box. Values greater than 1.0 enlarge the display. Values less than 1.0 shrink the display.

Additional information

Please see the on-screen help for details on the functioning of each control mentioned here. Mouse functions and keyboard shortcuts are summarized in *Mouse and Keyboard Actions*.

Setting position and orientation

Topics in this section include: resetting the view of the models to the default position, orientation, and magnification; centering the display (the differences between centering and resetting are presented in this section); and defining a center of rotation for the current model.

Resetting the view

Resetting changes the viewing angle so that the model's x, y, and z axes are coincident with the window x, y, and z axes. Any translations are reversed by returning the model to the origin, and the magnification is returned to unity.

To reset the view of the models, you can do any of:

- Click the reset tool on the toolbar.
- Select the **View/Reset View** menu item in the main control panel.
- Press <Alt> **r** on your keyboard.
- Press <Home> on an extended keyboard.

- Select the **View/Orient...** menu item to access the Orient View control panel. Click the **RESET VIEW** pushbutton.

Defining the center of rotation

The center of rotation of a model is the centroid of all or selected atoms. By default, all atoms are used. To redefine the center of rotation for the current model, select the desired atom(s). (Selecting no atoms is the same as selecting all atoms.) Then you can do any of:

- Select the **View/Set Origin** menu item in the main control panel.
- Press <Alt> **o** on your keyboard.
- Select the **View/Orient...** menu item to access the Orient View control panel. Click the **SET ORIGIN** pushbutton.

Centering the model

Centering a model translates it so that its center of rotation is in the center of the screen. Centering does not change the viewing angle or magnification. Centering immediately after defining the center of rotation (see *Defining the center of rotation*) affects only the current model. Centering after some other change in the model view moves all models in concert.

To center the model(s), you can do any of:

- Select the **View/Center** menu item in the main control panel.
- Press <Alt> **t** on your keyboard.
- Select the **View/Orient...** menu item to access the Orient View control panel. Click the **CENTER** pushbutton.

Any nondefault definition of the center of rotation is cancelled by such actions as resetting the view (*Resetting the view*) or filling the window (*Filling the model window*).

Additional information

Please see the on-screen help for details on the functioning of each control mentioned here. Mouse functions and keyboard shortcuts are summarized in *Mouse and Keyboard Actions*.

Moving models relative to one another

You can move one model relative to another, for example, to investigate how a ligand fits in a receptor site.

Although the models technically occupy separate model spaces, this functionality allows the models to behave *as if* they have been

redefined as submodels constituting one model in one model space.

Accessing the tools

Select the **Move/Model Move...** menu item to access the Model Space Transforms dcontrol panel. The current model is the one that is rotated and / or translated.

Alternatively, you can use mouse–keyboard combinations to control movement of the current model.

Bringing two models into one conjoined space

Simply make the desired models visible (*Controlling model visibility and the display mode*). Using the overlay display mode (*Controlling model visibility and the display mode*) and hiding any models you are not currently working with (*Controlling model visibility and the display mode*) should be most convenient; however, any display mode may be used.

Specifying the current model

Use any of the conventional means of defining a model as current (*Specifying the current model*).

Translating the current model

To translate the current model, you can:

- Press <Shift> and <Ctrl> on the keyboard and hold down the middle mouse button to move the cursor in the model window.

  or:

- Use the **Translate Model** controls in the Model Space Transforms control panel to translate the current model along the x, y, or z display axis or along a user-defined direction.

Specifying the translation axis

You can define a translation direction by entering a value in the **Translate/Rotate Axis** entry box or selecting some atoms and then clicking the associated **DEFINE** pushbutton in the Model Space Transforms control panel.

Rotating the current model

The rotation axes are the display axes, as shown in Figure 3.

To rotate the current model, you can:

- Press <Shift> and <Ctrl> on the keyboard and hold down the right mouse button to move the cursor in the model window. Move the cursor as described for simple rotation of all models (*Manual rotation*).

  or:

- Use the **Rotate Model** controls in the Model Space Transforms control panel to rotate the current model around the x, y, or z

display axis or around a user-defined center of rotation and axis.

Specifying the center of rotation

You can define the center of rotation and rotation axis by entering values in the **Rotation Center** and **Translate/Rotate Axis** entry boxes or selecting some atoms and then clicking the associated **DEFINE** pushbuttons in the Model Space Transforms control panel.

Saving the model with its transformed coordinates

When you save the model in .msi format (*Saving model structure files*), both its original coordinates and the transform for generating the transformed coordinates are automatically saved.

Additional information

Please see the on-screen help for details on the functioning of each control in the Model Space Transforms control panel. Mouse functions and keyboard shortcuts are summarized in *Mouse and Keyboard Actions*.

Superimposing models

You can superimpose (or "match") models by performing a least-squares fit between selected atoms. Whole (nonperiodic) models or the asymmetric unit of periodic models can be superimposed. One model is translated and rotated as a rigid unit to obtain the best rms fit of the selected atoms with those of a reference (or target) model. This is useful for comparing structures of all or parts of models.

Accessing the tools

Select the **Move/Atoms Match...** menu item to access the Match Models control panel.

Specifying the models

Specify which model is the reference model and which is the movable model by selecting them from the pulldowns or typing their model numbers or names in the text entry boxes.

Specifying the atoms to superimpose

The number of atoms specified in the reference model must be the same as the number in the moving model.

If you want to take all atoms into account during the fitting, the models must have the same number of atoms and they must be numbered identically (you can label a model according to atom numbers, see *Labels*). If this is true, you don't need to select atoms in order to specify them.

If you want or need to select the atoms to be matched, select them in the same order in both models. If atoms in the two models are numbered identically and you want to superimpose identically numbered atoms, you need select atoms only in one model.

Performing the superimposition

You can mass-weight the calculation (for example, if the positions of hydrogens are less important) by setting the **atom weighting** popup to **MASS**.

Be sure that all desired atoms are still selected, then click the **MATCH** pushbutton to superimpose the models and report the rms fit in the text window.

Additional information

Please see the on-screen help for details on the functioning of each control in the Match Atoms control panel. Selecting atoms in more than one model is discussed in *Selecting atoms in several models*.

Related information

The Cerius^2 • Align Molecules module (which is separately licensed and documented and is typically found in the DRUG DISCOVERY deck of cards) offers additional functionality for comparison of model structures.

Storing and retrieving views

You can save the current view (that is, the model and its viewing conditions such as orientation, location, magnification) in memory for later retrieval during the current session. Up to ten views can be saved and retrieved for later viewing within the current session.

Storing a view

To store a view, select the **View/Orient...** menu item to access the Orient View control panel. Set the **View A–J** popup as desired and click the **STORE** pushbutton.

Retrieving a view

To retrieve a view, select the **View/Orient...** menu item to access the Orient View control panel. Choose the desired view from the **View A–J** popup and click the **RETRIEVE** pushbutton.

Additional information

Please see the on-screen help for details on the functioning of each control in the Orient View control panel.

Animating models

The Visualizer animation facilities enable you to create an animation sequence from a trajectory file (such as that produced by the Cerius^2•Dynamics Simulation module), and then replay that sequence using VCR-style controls.

You should already know...

How to produce trajectory files is discussed in the documentation for the relevant application modules (which are purchased separately).

The animation process

Animating a model is a three-stage process. You first need to select a trajectory (.trj) file and load the information from it. Next you build an animation sequence. (Alternatively, check the **Automate Build** check box before loading the file.) Finally, the model is animated by "playing back" the animation sequence.

Accessing the tools

Select the **View/Animation...** menu item (on the main control panel's menu bar) to access the Animation control panel.

Loading a trajectory file

Use the file browser and selector tools to choose the trajectory file from which to construct the animation sequence. How to use these tools is detailed under *Loading model structure files*. (All file browsers work similarly.)

If the trajectory file you request appears to be associated with the current model, Cerius^2 asks if you want to use this model as the initial frame of the trajectory. Otherwise, Cerius^2 loads the associated MSI-format model file as the current model.

Building an animation sequence

To build an animation sequence that uses all frames from a trajectory file, simply check the **Automate Build** check box before selecting the trajectory file.

To use only selected frames from the selected trajectory file, click the **Frame Filter...** pushbutton to access the Frame Filter control panel. Use this control panel to select a subset of the frames: you can specify the starting and ending frame numbers and the frame increment. Then click the **BUILD FRAMES** pushbutton in the Animation control panel.

Animating the model

Once the desired frames have been built into an animation sequence, you can use the **Replay Animation** controls to animate

the model by replaying all or specified frames. These controls operate similarly to those on a tape recorder or VCR.

You can use other controls during or before the animation, for example, you can change the viewing angle (*Rotating models*), magnification (*Changing the view magnification*), or display style (*Atom and bond display styles*).

Clearing memory

Animation sequences consume a considerable amount of memory. When you have finished with a sequence, you should clear the memory buffer in which it is held, by clicking the **Clear All Frames** action button in the Animation control panel.

Additional information

Please see the on-screen help for details on the functioning of each control in the Animation and Frame Filter control panels.

Labeling and annotating models

Why read this section

Cerius^2 allows you to label atoms according to various properties such as element names, atom type, charge, temperature, hybridization, etc. You can also annotate models by adding text and graphical objects such as arrows and boxes. In addition, the default type of annotation that Cerius^2 always shows in the model window can be changed.

These functions are useful for understanding the displayed model and for enhancing the appearance of models for presentation and display purposes.

Finding information

This section includes information on:

Labels

Default annotation

Custom annotations

Related information

You can also enhance model displays by, for example, coloring atoms according to various properties (*Model display colors*) or color-mapping properties onto model surfaces (in, for example, the quantum chemical application modules, which have separate documentation).

Labels

Labels can be applied to entire models (when all or no atoms are selected) or to selected atoms within one or more models. Different labels may be used for different parts of a model.

The following label properties are available:

NO LABEL No labels

NUMBERS Atom serial numbers

SYM/NUM Crystal symmetry copy plus atom serial numbers

ELEMENTS Element types

CHARGES Atom partial charges

FORMAL CHARGE Atom formal charges

OCCUPANCY Atom site occupancies

ISOTROPIC Atom isotropic temperature factors

FFYTPE Forcefield atom types

HYBRID Atom hybridization

NAME Atom name

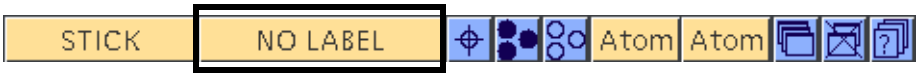
MASS Atom mass

CHIRALITY Atom chirality

Adding, changing, or removing labels on atoms

To add, change, or remove labels on all or selected atoms, you can:

- Set the label popup on the toolbar to the desired property (or to **NO LABEL**).



or:

- Select the **View/Display Attributes...** menu item to access the Display Attributes control panel. Set the **Label** popup under **All/Selected Atom Attributes** to the desired property.

Tip

You can interactively query the current properties of an atom by shift-clicking the atom with the right mouse button. A message box appears that lists the coordinates and properties of the atom.

Labeling bond attributes

Bonds can be labelled with their fractional bond orders.

To add or remove labels on all or selected bonds, you can:

- Select the **View/Display Attributes...** menu item to access the Display Attributes control panel. Set the **Label** popup under **All/Selected Bond Attributes** to the desired property.

Example

A tutorial example of labeling a model is found in *Labeling a model*.

Additional information

Please see the on-screen help for details on the functioning of each control in the Display Attributes control panel and in the toolbar.

Related information

Measuring distances, angles, planes, torsions, and inversions for the atoms in a model and displaying these measurements in the model window is discussed under *Measuring models*.

Default annotation

Basic information that is usually shown by default comprises the model name and model space number (in the lower left corner of the model window) and a small set of axes indicating the viewing angle (lower right corner). You may hide this information if you prefer.

In addition, you may want to show a scale bar and/or a large set of axes in the model window.

Accessing the tools

To change the default information shown in the model window, select the **View/Options...** menu item to access the View Options control panel. Check or uncheck the appropriate **View Annotation** check boxes.

Additional information

Please see the on-screen help for details on the functioning of each control in the View Options control panel.

Custom annotations

Accessing the annotation tools

Select the **Build/Annotation...** menu item to access the Annotation control panel.

Annotating your model

The Annotation control panel contains several types of tools to help you highlight and enhance your displayed model:

To add lines to the model display, you use the **Line** tool.

Select the **Line** tool, then click the left mouse button in the model window to place one end of the line. Without releasing the mouse button, drag the line out by moving the cursor, then release the mouse button to place the other end of the line.

The new line uses the currently set annotation color and line width (see *Editing the annotation objects*).

To add arrows to the model display, you use the **Arrow** tool.

Select the **Arrow** tool, then click the left mouse button in the model window to place the tail of the arrow. Without releasing the mouse button, drag the arrow out by moving the cursor, then release the mouse button to place the head of the arrow.

The new arrow uses the currently set annotation color and line width (see *Editing the annotation objects*).

To add rectangles or squares to the model display, you use the **Rectangle** tool.

Check the **Filled** check box if you want a filled rectangle; assure that it is unchecked if you want an outline rectangle.

Select the **Rectangle** tool, then click the left mouse button in the model window to place one corner of the rectangle. Drag the rectangle out by moving the cursor, then release the mouse button to place the opposite corner of the rectangle.

The new rectangle uses the currently set annotation color and line width (see *Editing the annotation objects*). For filled rectangles, the fill color is the same as the outline color.

To add circles to the model display, you use the **Circle** tool.

Check the **Filled** check box if you want a filled circle; assure that it is unchecked if you want an outline circle.

Select the **Circle** tool, then click the left mouse button in the model window to place the center of the circle. Drag the circle out by moving the cursor, then release the mouse button to place the circle.

The new circle uses the currently set annotation color and line width (see *Editing the annotation objects*). For filled circles, the fill color is the same as the outline color.

To add text to the model display, you use the **Text** tool.

Specify the text content by entering it in the entry box to the right of the **Text** tool. Then select the **Text** tool and click the left mouse button in the model window to place the text annotation.

The new text annotation object uses the currently set text content, annotation color, font, style, and size (see *Editing the annotation objects*).

Editing the annotation objects

You can use the annotation tools discussed in this section in two ways:

- To specify the defaults for new annotation objects, set the desired controls *before* placing the annotation object in the model window.

- To change the properties of existing annotation objects, use the selection tool to select one or more annotation objects and *then* set the desired controls.

To set or change the color of any annotation object, use the color popup (to the right of the **Line** tool in the control panel). Additional color controls can be accessed by clicking the **More Colors...** pushbutton. This brings up the Color Selected Objects control panel (see *Model display colors*).

To specify that rectangles or circles be drawn in filled or outline style, check or uncheck the **Filled** check box. The fill color is always the same as the outline color.

To set or change the line width of an annotation object (except for text), enter a number in the **Line Width** entry box.

To set or change the properties of text annotation objects:

- Use the entry box to the right of the **Text** tool to specify the text content.
- Set the font and style pulldowns as desired. These are located below the **Text** tool.

- Set the size by entering a font size in the size entry box or choosing a value from the associated popup.

Moving, resizing, and removing annotations

You can move, change the size of, delete, or hide annotation objects:

- To move an object, click the **Move** tool. Click an object with the left mouse button and drag in the model window to move it.

- To change the size of an object, click the **Resize** tool. Click the end, corner, or edge of an object with the left mouse button and drag in the model window to resize it). You can also change the shape of rectangles and the orientation of lines and arrows with this tool.

- To delete an object, click the **Delete** tool. Click the desired object(s) with the left mouse button to delete them.
- To hide all annotation objects, check the **Hide All** check box. To display them again, uncheck the **Hide All** check box.

- To delete all annotation objects, click the **Delete All** action button.

Recovering from mistakes

An **UNDO** pushbutton, provided at the top of the control panel, can be used to cancel one or a series of previous commands for many types of operations. The **UNDO** button is greyed out when there is nothing to cancel.

Help

Checking the **Guide?** check box gives you on-screen help (in the upper left corner of the model window) on the Annotation control panel functions.

Additional information

Please see the on-screen help for details on the functioning of each control in the Annotation control panel.

Model display style

Why read this section

You can change the model display to suit your needs. For example, you may want to display molecules in traditional stick style or with ellipsoids representing thermal movements of atoms, you may want to emphasize some atoms, or you may want to view a cross section of a model.

Finding information

This section includes information on:

Atom and bond display styles

Structure traces

Cross sections of models

Apparent depth effects

Related information

Labeling atoms according to various properties is discussed under *Labels*. Setting the graphical quality and screen resolution is discussed under *Resolution and graphical quality*.

You can also enhance model displays by, for example, coloring atoms according to various properties (*Model display colors*) or adding Connolly (*Model surfaces*) or other surfaces.

Atom and bond display styles

Display styles can be applied to entire models (when all or no atoms are selected) or to selected atoms within one or more models. Different display styles may be used for different parts of a model.

Finding information

This section includes information on displaying:

Bonds as sticks

Bond order display

Bonds as cylinders

Lone atoms

Atoms as balls

Ball and stick models

Cations as polyhedra

Thermal ellipsoids

Example

A tutorial example of changing model display styles is found under *Changing the display style*.

Additional information

Please see the on-screen help for details on the functioning of each control mentioned in this section.

Bonds as sticks

Understanding the display

The default is to display bonds as single, double, or triple lines. Atoms are not specifically shown, but are present at the ends of bonds. The bond colors represent the element types of the atoms at each end.

Specifying stick style

To reset stick display style, you can:

- Set the display style popup on the toolbar to **STICK**.

or:

- Select the **View/Display Attributes...** menu item to access the Display Attributes control panel. Set the **Style** popup to **STICK**.

Bond order display

Understanding the display

Multiple bonds can be shown as a set of parallel lines representing the bond order. Partial-double bonds in 6-membered ring systems can be represented as (both displayed and stored with the model as) Kekule or resonant bonds (Figure 4).

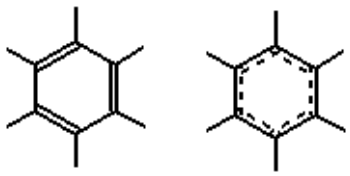


Figure 4. Representation of partial double bonds in 6-membered rings

Left: Kekule representation of benzene; right: resonant-bonds representation.

In addition, all bonds can be displayed as single lines regardless of the bond order (and without changing the actual bond order). This is useful, for example, for simplifying the display when viewing large models at small magnification. It does not change the actual bond type, which is stored with the model.

Specifying partial double bond style

To set the representation of partial double bonds to resonant (dashed lines) or Kekule (alternating single and double bonds), you can:

- Select the **Build/Edit Bonds...** menu item to access the Edit Connectivity and Bonding control panel. Set the bond-order

representation popup to **RESONANT** or **KEKULE**. Click the **Convert representation** action button.

or:

- Select the **Build/3D-Sketcher...** menu item to access the Sketcher control panel. Use the **Edit Bond** tool (*Changing the bond type*) to change the appropriate bonds from single or double to resonant (or vice versa).

Specifying multiple bond style

To display all bonds (in all models) as single lines (regardless of actual bond type), select the **View/Display Attributes...** menu item to access the Display Attributes control panel. Click the **Preferences...** pushbutton to access the Style Preferences control panel. Uncheck the **Highlight Multiple Bonds** check box.

To display the bond types again, simply check the **Highlight Multiple Bonds** check box.

Bonds as cylinders

Understanding the display

Cylinder style is similar to stick style, except that the bonds are represented by cylinders, providing a more three-dimensional representation. Atoms are not specifically shown, but are present at the ends of bonds. The bond colors represent the element types of the atoms at each end.

Specifying cylinder style

To display bonds in cylinder style, you can:

- Set the display style popup on the toolbar to **CYLINDER**.

or:

- Select the **View/Display Attributes...** menu item to access the Display Attributes control panel. Set the **Style** popup to **CYLINDER**.

Setting the radius

To set the radius of the cylinders, click the **Preferences...** button in the Display Attributes control panel to access the Style Preferences control panel. Enter the desired radius in the **Cylinder Radius** entry box.

Lone atoms

Understanding the display Lone (not bonded) atoms in a model can be represented as three-dimensional crosses, small spheres, or simple points or can be not displayed at all.

Specifying lone-atom style To change how lone atoms are displayed, select the **View/Display Attributes...** menu item to access the Display Attributes control panel. Click the **Preferences...** button to access the Style Preferences control panel. In the latter control panel, set **Lone Atom Style** to **CROSS**, **BALL**, **POINT**, or **NONE**.

Atoms as balls

Understanding the display Atoms can be represented by space-filling balls. If any bonds are visible between balls, they are represented as lines.

Specifying ball style To display atoms in ball style, you can:

- Set the display style popup on the toolbar to **BALL**.

  or:

- Select the **View/Display Attributes...** menu item to access the Display Attributes control panel. Set the **Style** popup to **BALL**.

Setting the radii The ball radii are proportional to the van der Waals radius of the respective atoms. To set the ratio of ball radius to van der Waals radius, click the **Preferences...** pushbutton in the Display Attributes control panel to access the Style Preferences control panel. Enter the desired proportion in the **Ball: Ball Size** entry box.

Ball and stick models

Understanding the display Ball and stick style represents atoms as van der Waals spheres and by bonds as cylinders.

Specifying ball-and-stick style

To display models in ball and stick style, you can:

- Set the display style popup on the toolbar to **BALL & STICK**.

  or:

- Select the **View/Display Attributes...** menu item to access the Display Attributes control panel. Set the **Style** popup to **BALL & STICK**.

Setting the ball radii

The ball radii are proportional to the van der Waals radius of the respective atoms. To set the ratio of ball radius to van der Waals radius, click the **Preferences...** pushbutton in the Display Attributes control panel to access the Style Preferences control panel. Enter the desired proportion in the **Ball & Stick: Ball Size** entry box.

Setting the stick radius

To set the radius of the sticks, click the **Preferences...** button in the Display Attributes control panel to access the Style Preferences control panel. Enter the desired radius in the **Stick Radius** entry box.

Cations as polyhedra

Understanding the display

Polyhedra are used to simplify structural display for inorganic systems that contain tetrahedrally, octahedrally, or square- planar coordinated units, for example, zeolites, the high Tc superconductors, and multi-molybdates.

Solid coordination polyhedra are drawn around cations, the number of corners indicating the coordination number as defined by bonding connectivity.

Specifying polyhedral style

To display cations as polyhedra, you can:

- Set the display style popup on the toolbar to **POLYHEDRA**.

  or:

- Select the **View/Display Attributes...** menu item to access the Display Attributes control panel. Set the **Style** popup to **POLYHEDRA**.

Displaying other atoms

Other atoms (non-cations) can be represented as crosses, small spheres, or single pixels or not drawn at all. To change how other atoms are displayed, click the **Preferences...** button in the Display Attributes control panel to access the Style Preferences control panel. Then set **Non-Polyhedral Style** to **CROSS**, **BALL**, **POINT**, or **NONE**.

Thermal ellipsoids

Understanding the display

Ellipsoid style represents a constant-probability surface for the thermal motion of the atoms. Atoms described by anisotropic temperature factors are represented by ellipsoids. (Atoms described by isotropic temperature factors are represented by spheres.) Lines representing bonds are drawn by default but can be removed. The orientation of the ellipsoid's principal axis may be displayed.

Spheres and ellipsoids are drawn only if the temperature factors describe a solid object. (In mathematical terms, the matrix must be positive definite.) If this is not true or if no temperature factor has been specified, atoms are represented by crosses.

Specifying ellipsoid style

To display atoms as thermal ellipsoids, you must first be sure that anisotropic temperature factors (see *Understanding the display* and *Temperature factors*) have been specified or loaded. Then you can:

- Set the display style popup on the toolbar to **ELLIPSOID**.

  or:

- Select the **View/Display Attributes...** menu item to access the Display Attributes control panel. Set the **Style** popup to **ELLIPSOID**.

Displaying bonds and ellipsoid axes

To show or hide the principal ellipsoid axis, click the **Preferences...** pushbutton in the Display Attributes control panel to access the Style Preferences control panel. Check or uncheck the **Show Principal Axes** check box.

Similarly, to show or hide bonds, check or uncheck the **Show Bonding** check box.

Size of ellipsoids

You can define a scaling factor for the display size of thermal ellipsoids. A value of 1.0 corresponds to an ellipsoid whose radius at any point on the surface is equal to the root mean square (rms) atomic vibration in that direction. At a scaling factor of 1.0, the

probability of the atom actually lying within the ellipsoid is low. Greater values produce greater probabilities, as shown in Table 7.

Table 7. Relation of thermal ellipsoid size to atom location

Scale factor	Probability of atom being within ellipsoid
1.54	50%
2.02	75%
2.50 (default)	90%
2.80	95%
3.37	99%

Setting the size

To set the scale factor for thermal ellipsoids, select the **View/Display Attributes...** menu item to access the Display Attributes control panel. Click the **Preferences...** pushbutton in the Display Attributes control panel to access the Style Preferences control panel. Enter the desired scale factor in the **Ellipsoid Size** entry box.

Structure traces

You can make only a structural trace of a model visible. This is done differently, depending on whether the model is a protein or any other kind of polymer.

Visibility of polymer backbones

To display only the backbone atoms of a polymer, select the **View/Atom Visibility...** menu item to access the Atom Visibility control panel. Click the **Hide Non-Backbone Atoms** action button. You must have previously defined some atoms as backbone atoms, using the Polymer Builder tools.

You can also use this control panel to hide hydrogen atoms or any selected atoms or to display all or selected atoms.

α-carbon trace of proteins

To display an alpha carbon trace of a protein model:

- Set the display style popup on the toolbar to **TRACE**.

  or:

- Select the **View/Display Attributes...** menu item to access the Display Attributes control panel. Set the **Style** popup to **TRACE**.

Additional information

Please see the on-screen help for details on the functioning of each control in the Atom Visibility and Display Attributes control panels.

Cross sections of models

You can control the apparent location of the viewing plane along a line perpendicular to the computer screen, as well as the plane's thickness, so as to view either the whole model or a cross section (slice or slab) through it. You do this by clipping the view between two coordinates of the screen z axis (that is, to set the apparent distance of the viewing plane from the computer screen).

Accessing the tools

To control and apply z-clipping, select the **View/Graphics/Z-Clipping...** menu item to access the Z-Clipping control panel. You can perform z-clipping in two ways:

- To position the front and back clipping planes independently, assure that the **Fixed Thickness Clipping** check box is unchecked and enter the positions of the back and front planes in the **Back** and **Front Z-Clip Plane** entry boxes by directly typing the values or by using the associated sliders. (The control panel does not allow you to enter unreasonable values.) Assure that the **Apply Z-Clipping** check box is checked.
- To specify a clipping slab (slice) of fixed thickness, check the **Fixed Thickness Clipping** check box and enter the thickness (in angstroms) in the **Z-Clip Range** entry box by directly typing the value or by using the associated slider. Assure that the **Apply Z-Clipping** check box is checked. You can adjust the position of the slice along the z axis by using the **Back** or **Front Z-Clip Plane** controls.

Additional information

Please see the on-screen help for details on the functioning of each control in the Z-Clipping control panel.

Apparent depth effects

Depth cueing

Depth cueing gives models an appearance of depth by displaying objects that are apparently closer to the surface of the computer screen in true color and mixing the color with the background color for objects that appear to be farther behind the surface of the computer screen. The extent of depth cueing can be changed.

Accessing the tools

Select the **View/Graphics/Depth Cueing...** menu item to access the Depth Cueing control panel.

Adjusting the perceived depth

To adjust the degree of depth cueing, use the **Depth Cue Factor** slider or its associated entry box. A value of 1 means that apparently near and far objects are all drawn with full color intensity; a value of 0 means that far objects disappear into the background.

To change the apparent distances at which objects are drawn with full or minimal color, adjust the **Near Distance** or **Far Distance** controls, respectively.

Additional information

Please see the on-screen help for details on the functioning of each control in the Depth Cueing control panel.

Projection

The projection method is another way of enhancing the appearance of depth in models. Two methods are available:

- In an orthographic projection, an object appears to be the same size at any apparent distance behind the surface of the computer screen. The observer is assumed to be infinitely distant, that is, the projection lines are parallel and normal to the screen.
- In a perspective projection, the object size diminishes with distance, so that (for example) parallel lines perpendicular to the computer screen would meet at some apparent distance behind the surface of the screen. The angle for perspective viewing can be set to produce narrow or wide (“fish-eye”) projections.

Accessing the tools

Select the **View/Graphics/Projection...** menu item to access the Projection control panel.

Adjusting the projection

Choose the desired projection method from the control panel. If you choose **PERSPECTIVE**, you can specify the projection angle by entering a number in the **Angle** entry box.

Alternatively, you can toggle the projection method by pressing <F3> on the keyboard. The perspective angle can be changed by dragging the mouse in the model window while holding down <Shift> and <Alt> and the middle mouse button.

Additional information

Please see the on-screen help for details on the functioning of each control in the Projection control panel.

Resolution and graphical quality

Object resolution

The balls, ellipsoids, and cylinders produced by the various display styles are represented on-screen as multifaceted polyhedral facets (for balls and ellipsoids) and prismoidal facets (for cylinders). A small number of facets used to draw an object results in a fast but coarse display. Large numbers of facets improve smoothness and specularity, but at the expense of drawing speed. The default value usually provides a reasonable compromise between display speed and resolution.

Although the actual number of facets used is determined by the size of the object being represented, you can adjust their relative number. To do so, select the **View/Display Attributes...** menu item to access the Display Attributes control panel. Click the **Preferences...** pushbutton to access the Style Preferences control panel. Adjust the **Resolution** sliders by dragging or directly enter values in the associated entry boxes for **Spheres**, **Cylinders**, and/or **Ellipsoids**.

Line widths for bonds

To change the line width used to draw (non-cylinder) bonds, select the **View/Display Attributes...** menu item to access the Display Attributes control panel. Click the **Preferences...** pushbutton to access the Style Preferences control panel. Adjust the **Line Width** slider by dragging or directly enter values in the associated entry box.

Graphics quality

Cerius^2 enables you to specify the quality of graphics displayed on the computer and written to vector PostScript files. Three quality settings are available: standard, better, and excellent. Higher qual-

ity settings reduce the golf-ball effect that results because X and vector PostScript triangles are flat-shaded instead of color-interpolated. However, each higher quality setting can also increase both the file size and the rendering time by a factor of four over the previous quality setting.

This quality setting is independent of the resolution settings for spheres, cylinders, and ellipsoids (*Object resolution*). This setting applies to the number of subdivisions made to simulate depth cueing of vectors, as well as to the number of subdivisions made to the triangles created during sphere, cylinder, ellipsoid, and surface tessellation.

To adjust the graphics quality, select the **View/Display Attributes...** menu item, then click the **Preferences...** button in the Display Attributes control panel. In the Style Preferences control panel that appears, set **X/PostScript Quality** to **STANDARD**, **BETTER**, or **EXCELLENT**. Each higher quality setting can increase both the file size and the rendering time by a factor of four over the next-lower quality setting.

Additional information

Please see the on-screen help for details on the functioning of each control in the Style Preferences control panel.

Printing models and graphs

Why read this section

This section includes information on:

- Printing models and graphs as hardcopy.

  You can print full-color, greyscale, or dithered black-and-white PostScript™ images.

- Converting model and graph displays to PostScript files.

  PostScript files can be printed later. You can transfer them to other applications to edit them. They can also be imported into other applications, such as desktop publishing packages, for use as illustrations,

Related information

Setting the print resolution is discussed in *Resolution and graphical quality*. Using PSYCHO within Cerius^2 for rendering models (and producing PostScript output) is discussed in *Rendering and ray-tracing*.

You should already know...

You need to know what UNIX print command (including command-line options) is usually used at your site for sending PostScript output from applications to a printer. Please ask an experienced user at your site, or your system administrator, if you do not know the command.

Accessing the tools

Select the **File/Print...** menu item to access the Print control panel. This contains the primary PostScript output controls and provides access to the Page Setup control panel, which contains supplementary controls.

Specifying what and how to print

Select the image source by setting **Image Capture** to **Model Window** or **Graph Window**. The size of the model window affects the image's detail when it is output as bitmap PostScript: the larger the window, the greater the detail. However, the size of the graph window does not affect the output detail.

Specify how you want the image to appear by setting **Color** to **Full Color**, **Grayscale**, or **Black & White**. Of course, your printer must be able to handle the selected color mapping.

Tell Cerius^2 to send the output to a printer or a file by choosing the relevant **PostScript Destination** radio button. You can enter a filename in the entry box to the right of the **FILE** button. Specify the UNIX print command (including pathname, if needed, and command-line options) by entering it in the **Command** entry box.

Additional controls

You can access some less frequently used controls by clicking the **Page Setup...** pushbutton in the Print control panel, which causes the Page Setup control panel to appear.

Options on the Page Setup control panel enable you to adjust the presentation of the PostScript image to be generated. You can also scale the image, add legends, and fine-tune the output for maximum clarity. The controls available in this panel depend on how controls in the Print control panel are set.

Vector or raster format for printing model windows

If you are printing the image in the model window, you can choose to output in vector PostScript or screen dump (raster) format. Vector PostScript images are device-independent, can be resized without loss of display quality, and can produce better quality output (colors, shapes, and so on) on a PostScript printer. Raster images, such as screen dump images, may become distorted when they are scaled.

A vector PostScript file is often smaller than a screen dump file and, as a result, prints faster. However, if the image in the model window is very complicated or the display quality is high, a vector PostScript file can be larger than a screen dump file and may take longer to print.

Bitmap resolution for printing graphs

You can specify the resolution (in dots per inch) for curves in graphs. Increasing this value allows improved definition of these images, although the resolution of the output device is always a limiting factor. Increasing the resolution results increases the PostScript image generation time, file size, and printing time.

Previewing the output

If you run Cerius^2 on an SGI platform, you can click the **PREVIEW** pushbutton in the Print control panel. This calls up SGI's xpsview utility, to preview your PostScript image before sending it to the printer or a file.

Printing or saving a PostScript file

Once all options have been set to your satisfaction, click the **PRINT** pushbutton in the Print control panel.

Example

A tutorial example of printing a model is found under *Printing a model*.

Additional information

Please see the on-screen help for details on the functioning of each control in the Print and Page Setup control panels. Changing the resolution with which graphics are displayed and written is covered under *Resolution and graphical quality*.

9 Enhancing Model Display

The Cerius^2•Visualizer includes many facilities for enhancing the display of your model, enabling you to interpret it better and to prepare effective graphical output.

This section explains

This section contains information on:

Model display colors

Customizing display colors

Surfaces — style and transparency

Lighting control

Rendering and ray-tracing

Stereo viewing

Important

To exploit Cerius^2's graphics functionalities to the full, you need to be running it on a machine with sufficient memory and graphics display capability. Some of the effects discussed in this section may appear less dramatic on lower-end machines.

Table 8. Finding information about enhancing model display

If you want to know about:	Read:
Changing color of selected atoms.	*Coloring selected objects*.
Changing color of all atoms of an element.	*Default element colors*.
Coloring atoms according to other characteristics.	*Coloring atoms by properties*.
Mapping atomic properties to colors.	*Property–color mapping*.
Changing the background color.	*Background color in model window*.

Table 8. Finding information about enhancing model display

If you want to know about:	Read:
Changes colors used by the Cerius^2 interface.	*Interface colors*.
Illuminating models from defined directions.	*Directional lights*.
Spotlighting parts of models.	*Spotlights*.
Labeling and annotating models.	*Labeling and annotating models*.
Changing the display resolution.	*Resolution and graphical quality*.
Printing models.	*Printing models and graphs*.
Exporting to non-Cerius^2 applications.	*Copying models to and from other applications*.
Saving preferences.	*Using saved sessions as preferences settings*.

You should already know…

The basics of starting Cerius^2 and using its interface are demonstrated in *Introducing Cerius2* and described in *The Cerius2 Interface*.

You need to know how to build (*Basic building*) and / or load (*Loading model structure files*) models. You should know how to select atoms in model(s) (*Selecting atoms and groups of atoms*) and how to position models on the screen (*Moving models on the screen*).

If your session contains several models, you should know how to specify the current model (*Specifying the current model*) or select atoms in more than one model simultaneously (*Selecting atoms in several models*).

Model display colors

Cerius^2 provides several methods of changing the colors of atoms according to their element type and other properties.

Finding information

This section includes information on:

Default element colors

Coloring selected objects

Coloring atoms by properties

Background color in model window

Related information

Displaying labels and other information about atoms in a model is presented under *Labels*.

Saving nondefault settings for later use is described under *Working with Cerius2 sessions*.

Default element colors

To help in understanding models, atoms are colored according to their element, For example, carbon is dark grey, hydrogen is white, and oxygen is red. You may want to change these colors, for instance if you change the background color of the model display window (*Background color in model window*).

Accessing the tools

Select the **Build/Element Defaults...** menu item from the main Visualizer control panel to access the Edit Elements control panel. If desired, access the Periodic Table window by clicking the periodic table tool in the upper right of this control panel.

Changing element default colors

Enter the desired element in the **Current Element** entry box, either by typing it in or by choosing it from the Periodic Table window.

Choose the desired color from the **Display Color** popup in the Edit Elements control panel. This is now the new default color for that element for the remainder of your current Cerius^2 session or until you change it again.

Example

A tutorial example of using the Edit Elements control panel to change default element colors is found under *Changing atom colors*.

Additional information

Please see the on-screen help for details on the functioning of each control in the Edit Elements control panel.

Coloring selected objects

You can specifically color selected atoms and other objects (such as annotations, see *Custom annotations*) by one of several coloring methods.

Predefined "pen" colors

To color selected atom(s) or other object(s) with a predefined color, you can:

- Select the **View/Colors...** menu item to access the Color Selected Objects control panel, then choose a color from the **Pen**

popup. (You can also access this control panel from the **More Colors...** pushbutton on the Annotation control panel, next paragraph.)

or:

- Select the **Build/Annotation...** menu item to access the Annotation control panel, then choose a color from the colors popup (to the right of the **Line** tool).

You can edit the pen colors to make your own set of predefined colors (see *Drawing colors*).

Mixing your own colors

To mix your own colors for selected atom(s) or other object(s), select the **View/Colors...** menu item to access the Color Selected Objects control panel.

Use the red, green, and blue sliders (or the entry boxes below them) to set the proportions of red, green, and blue in the final color.

Choosing colors from a color range

To choose colors for selected atom(s) or other object(s) from a range of colors, select the **View/Colors...** menu item to access the Color Selected Objects control panel. Click the **Color Ranges...** pushbutton to access the Color by Range control panel.

Choose any range from the list and check the **Show Color Range** check box if you want to display the color range (with color numbers) in the model display window.

Then enter the number of the desired color in the **Use color number** entry box.

You can edit color ranges to change them or create additional color ranges (see *Color ranges*).

Reverting to default colors

To set selected atom(s) or object(s) back to their default colors, select the **View/Colors...** menu item to access the Color Selected Objects control panel.

Set the **Pen** popup to **DEFAULT**.

Tip

You can also access the Color Selected Objects control panel by selecting the **Build/Annotations...** menu item to access the Annotation control panel, then clicking the **More Colors...** pushbutton.

Additional information

Please see the on-screen help for details on the functioning of each control in the Color Selected Objects control panel.

Coloring atoms by properties

Cerius^2 enables you to color atoms according to *properties* such as charge, whether atoms are fixed or moveable, mass, radius, etc., as another aid to abstracting information from your model.

Accessing the tools

Select the **View/Colors...** menu item on the main Visualizer control panel to access the Color Selected Objects control panel. This control panel can also be accessed by selecting the **Build/Annotation...** menu item and then clicking the **More Colors...** pushbutton in the Annotation control panel.

Coloring atoms according to a property

To color atoms according to a property, simply select them and choose the desired property from the **Color by a Property** list in the Color Selected Objects control panel.

You can create your own color maps for additional properties (see *Property–color mapping*).

Coloring a model according to multiple maps

To color selected atoms according to a cascading series of property color maps, click the **Multiple Mappings...** pushbutton in the Color Selected Objects control panel to access the Multiple Color Mappings control panel.

Use the arrows in this control panel to move selected maps between the **Available Mappings** and **Selected Mappings** lists and to change the priority of map application within the **Selected Mappings** list. Then click the **APPLY** pushbutton.

Any atoms that are not colored by the first map in the list (because they do not have the relevant property or because "as-is" coloring is specified for the relevant map value, *Creating and editing a binary property color map*) are colored according to the second map in the list, and so on in sequence down the list.

Returning to default atom coloring scheme

To return selected atoms to their default element colors, click the **Reset selected object colors to default** action button in the Color Selected Objects control panel. You also can set the **Pen** popup to **DEFAULT** (or click this popup if it is already set to **DEFAULT**).

Example

A tutorial example of using the Color Selected Objects control panel to color atoms according to a property is found in *Coloring atoms according to a property*.

Additional information

Please see the on-screen help for details on the functioning of each control in the Color Selected Objects control panel.

Background color in model window

You may want to change the background color in the model window to enhance the appearance of the model or because you may require a light background.

Accessing the tools

To change the color of the model window background from the default black to something else, select the **Utilities/Customize/ Pen Colors...** menu item to access the Pen Colors control panel.

Changing the background color

To change the background to white, black, or one of two shades of grey, choose the desired color from the **Background** popup.

To change the background to any color, either set the **Pen** popup to **BACKGROUND** or set the **Background** popup to **OTHER**. Then use the red, green, and blue sliders (or the entry boxes below them) to set the proportions of red, green, and blue desired in the background color.

Tip

To improve the appearance of your model after you change the background color or to, for example, enable hydrogens to be seen against a white background, you can use the lighting controls (*Lighting control*) and / or change selected object colors (*Coloring selected objects*) or default element colors (*Default element colors*).

Additional information

Please see the on-screen help for details on the functioning of each control in the Pen Colors control panel.

Customizing display colors

Cerius^2 provides several ways of customizing the use of colors in the model window.

Finding information

This section includes information on:

Drawing colors

Color ranges

Property–color mapping

Drawing colors

Cerius^2 enables you to customize the drawing colors ("pen colors") used in the model window and the graphs window (see *Working with Graphs*). You do so by adjusting the relative red, green, and blue (RGB) color values of one or more of the 16 standard pen colors.

Accessing the tools

Select the **Utilities/Customize/Pen Colors...** menu item on the main Visualizer control panel to access the Pen Colors control panel.

Examining the currently defined colors

To display a window showing all currently defined standard colors, click the **Show Current Pens** action button. A Cerius2 Graphs window appears, showing all 16 pen colors.

Alternatively, you can show the pen colors as a color range within the model window by checking the **Show Color Range** check box in any control panel in which it appears (e.g., *Property–color mapping*) and selecting PEN_COLORS as the range to display.

The appropriate color changes when you redefine a color (next paragraph).

Changing the standard colors

To change one of the predefined colors, choose its name from the **Pen** popup in the Pen Colors control panel and use the red, green, and blue sliders (or the entry boxes below them) to set the proportions of red, green, and blue in the final color. (You cannot, however, change the name used for that color.)

Returning to the preset default colors

To return a single pen color to its default value, choose its name from the **Pen** popup and click the **Reset Pen to Default** action button.

To return all pen colors to their defaults, click the **Reset all to Default** action button.

Tip

You can also define a new set of pen colors in the same way as color ranges are created (*Color ranges*).

Additional information

Please see the on-screen help for details on the functioning of each control in the Pen Colors control panel.

Color ranges

A *color range* is a set of colors that you apply or that Cerius^2 automatically applies to various properties and data values. You can create and edit color ranges.

Uses of color ranges

Customized color ranges are useful for tasks such as:

- Highlighting an important point on a graph.
- Using a colored contour line within a greyscale diffraction pattern to highlight an interesting point.
- Appropriately changing all the colors used in a model to improve its visibility after the background color of the model window is changed.
- Changing a greyscale plot to a monochromatic colored plot.

You can edit all the color ranges that are supplied with Cerius^2 (Table 9), as well as create your own color ranges.

Table 9. Some color ranges supplied in Cerius^2 and their typical uses

Color range	Some uses
pen colors	Structure displays in model window; simple line graphs; filled-circle plots.
color wheel	Mass cloud plots (Sorption module); probe surfaces for field calculations.
greyscale	HRTEM simulations; diffraction patterns, graphs.
electrostatic	Graphs (difference colors).
spectrum	Graphs (“color” colors).

Finding information

This section includes information on:

Creating and editing a new color range

Editing a color range

Concepts

To facilitate editing color ranges or constructing your own color ranges, several concepts need to be defined:

- *Critical entries* are points within a color range for which relative red, green, and blue color values are specifically defined and between which Cerius^2 automatically interpolates colors.

  Each color range must contain at least two critical entries, defining the ends of the range (for example, only the two end values of the greyscale color range are defined).

  A color range may contain more than two critical entries (the two endpoints and one or more points in between), as well as interpolated colors (for example, the electrostatic, color wheel, and spectrum color ranges have many critical entries).

  A color range may be composed of only critical entries (for example, the pen colors color range).

- *Noncritical entries* are the automatically interpolated colors that lie between critical entries.

- The *number of entries* means the number of noncritical entries. The greater the number of entries, the smoother the color interpolation in the color range.

In editing or constructing color ranges, you can change the color definition of each critical entry, the number of critical entries, the position within the range of each critical entry, and the number of noncritical entries between each two sequential critical entries.

Viewing color ranges

You can display a color range in the model window by selecting the **Utilities/Customize/Color Ranges...** menu item from the main Visualizer control panel to access the Edit Color Ranges control panel. Then choose a color range from the **Color Range** popup and check the **Show Color Range** check box.

Identifying critical and noncritical entries

The numbers of the critical entries are displayed alongside the critical entries in the displayed range, facilitating their identification.

The numbers of the critical entries are displayed in a list box under **Edit Critical Color Entries** in the Edit Color Ranges control panel (whether or not you display a color range).

Selecting colors from ranges

To apply a color from a range to an object in the model window, see *Choosing colors from a color range*. (You can select a color from a color range by specifying the number of the entry (whether critical or noncritical) that corresponds to the position of the color in the range.)

Creating and editing a new color range

Accessing the tools

Select the **Utilities/Customize/Color Ranges…** menu item from the main Visualizer control panel to access the Edit Color Ranges control panel. Alternatively, if you have the Color Selected Objects control panel open (*Accessing the tools*), you can click its **Color Ranges…** pushbutton to access the Color by Range control panel and then click the **Edit Ranges…** pushbutton to access the Edit Color Ranges control panel.

Naming the color range

Type a name in the **New** entry box. Enter it by pressing <Enter> on the keyboard or clicking elsewhere in the control panel. Default values appear for the number of colors in the range and the numbers of the critical entries.

Defining the color range

Choose the number of color entries from the **Number of colors in range** pulldown. More numbers give you smoother color gradations, but you shouldn't set the number so high that it's beyond of your computer's graphics capability.

Set the colors of the critical entries at either end of the range by using the red, green, and blue sliders (or the entry boxes below them) to set the proportions of red, green, and blue in the color.

Tip

You can display your new color range at any time (see *Viewing color ranges*), to help in defining it. The display is updated as you change the definition of the color range.

Add an additional critical color, if desired, by entering its position in the entry box for **Add a new critical color** and then defining the color by using the sliders. If you subsequently decide to increase the number of entries in the range, critical colors in the interior of the range maintain their approximate relative positions (for exam-

ple, a critical entry at position 7 in a 16-color range becomes position 14 if you increase the number of entries to 32).

To change the position of a critical color (other than one of the end colors), enter a new position number in the entry box for **Move selected critical color**.

Saving a color range

You can save a custom color range by saving the current Cerius^2 session (see *Saving the current session*).

Additional information

Please see the on-screen help for details on the functioning of each control in the Edit Color Ranges control panel.

Editing a color range

Caution

You should edit only color ranges that you create. You should never delete or rename the color ranges that are supplied with Cerius^2, because many automatic Cerius^2 functions require the supplied ranges to be present and have the correct name. However, you may change the colors that are used in the supplied color ranges.

Accessing the tools

Select the **Utilities/Customize/Color Ranges...** menu item from the main Visualizer control panel to access the Edit Color Ranges control panel. Alternatively, if you have the Color Selected Objects control panel open (*Accessing the tools*), you can click its **Color Ranges...** pushbutton to access the Color by Range control panel and then click the **Edit Ranges...** pushbutton to access the Edit Color Ranges control panel.

Selecting the color range

Choose the name of the range you want to edit from the **Color Range** popup. The current values for the number of colors in the range and the numbers of the critical entries appear. The color definitions appear in the sliders when you choose a critical entry from the **Edit Critical Color Entries** list.

If you saved the custom color range during some earlier Cerius^2 session (*Saving a color range*), you have to load that session to access that color range (see *Loading a previously saved session*).

Editing the color range

Edit the color entries by the same procedure as used in creating a color range (*Creating and editing a new color range*).

You can also use the Edit Color Ranges control panel to delete or rename an entire color range or to remove a selected critical color. (You should *not* delete either of the end colors.)

Additional information

Please see the on-screen help for details on the functioning of each control in the Edit Color Ranges control panel.

Property–color mapping

A *color map* is a definition of how a quantitative (continuous, numerical) property maps to a specified color range or how a qualitative (binary, on / off) property maps to a set of two colors.

Uses of color maps

Customized color maps are useful for tasks such as:

- Coloring atoms according to their size or mass.
- Highlighting the backbone atoms of a polymeric model.
- Coloring atoms according to their isotropic temperature factors.

Finding information

This section includes information on:

Creating and editing a binary property color map

Creating and editing a continuous property color map

Editing a property color map

Related information

Labeling atoms according to various properties is discussed under *Labels*.

You should already know…

Color mapping makes use of color ranges, so you should have some familiarity with them (*Color ranges*). In addition, you may want to define custom color ranges to use in your maps (*Creating and editing a new color range*).

Tip

You can display a color range at any time, to help in applying it to a map, by checking the **Show Range** check box in the Edit Color Mappings or the **Show Color Range** check box in any of the control panels in which this control appears.

Creating and editing a binary property color map

Accessing the tools

Select the **Utilities/Customize/Color Mappings...** menu item from the main Visualizer control panel to access the Edit Color Mappings control panel. Alternatively, if you have the Color Selected Objects control panel open (*Accessing the tools*), you can click its **Edit Mappings...** pushbutton to access the Edit Color Mappings control panel.

Naming your color map

Type a name in the **New Map** entry box. Enter it by pressing <Enter> on the keyboard or clicking elsewhere in the control panel.

What type of property is to be mapped?

Identify what type of property is to be mapped, by choosing an item from the **Attribute** popup in the Edit Color Mappings control panel.

Specify that the property to be mapped will use just two (on / off) colors, by setting the **Type** popup to **BINARY**.

The contents of the bottom of the Edit Color Mappings control panel depend on the value of the **Type** popup.

Setting the "on" and "off" colors

Set the color popups to the desired colors for the "on" and "off" values. You can also choose to color *only* the "on" or "off" value by setting the other to **Use As-is**.

To apply the map to your model, select the desired atoms and choose your new map's name in the **Color by a Property** list in the Color Selected Objects control panel (*Coloring atoms according to a property*).

If the map is already applied to your model, any changes you make to the on and off colors appears immediately in the displayed model.

More colors

If you want some color that's not available in the popups, click the **More On Colors...** or **More Off Colors...** pushbutton to access the On Color Selection or Off Color Selection control panels, respectively.

In addition to controls that are also available in the Edit Color Mappings control panel, these control panels allow you to:

- Define a custom color by using the red, green, and blue sliders (or the entry boxes below them) to set the proportions of red, green, and blue in the color.

- Select any color entry number from any already-defined color range.

Saving a color map

You can save a custom color map by saving the current Cerius^2 session (see *Saving the current session*).

Additional information

Please see the on-screen help for details on the functioning of each control in the control panels mentioned in this section.

Creating and editing a continuous property color map

Accessing the tools

Select the **Utilities/Customize/Color Mappings...** menu item from the main Visualizer control panel to access the Edit Color Mappings control panel. Alternatively, if you have the Color Selected Objects control panel open (*Accessing the tools*), you can click its **Edit Mappings...** pushbutton to access the Edit Color Mappings control panel.

Naming your color map

Type a name in the **New Map** entry box. Enter it by pressing <Enter> on the keyboard or clicking elsewhere in the control panel.

What type of property is to be mapped?

Identify what type of property is to be mapped, by choosing an item from the **Attribute** popup in the Edit Color Mappings control panel.

Specify that the property to be mapped will use a color range, by setting the **Type** popup to **CONTINUOUS**.

The contents of the bottom of the Edit Color Mappings control panel depend on the value of the **Type** popup.

Setting the range of property values

Set the **Min**imum and **Max**imum **Attribute Values** between which the color map's range is to extend.

Tip

For properties that have integer or close-to-integer values (such as the atomic mass), set the minimum and maximum values so that they fall about halfway *between* expected values. For example, you might set the minimum mass to 0.5 and the maximum to 40.5 if you are modeling a biochemical molecule.

Coloring the values within the range

Decide what part of what color range to apply to the range of mapped property values by choosing the range's name from the **Use Range** popup and entering the **Min**imum and **Max**imum range-color entry numbers (in the **Color Scheme** section of the

control panel). If you want to use the color range in reverse order, make the "maximum" smaller than the "minimum".

More colors

If you want, for example, to create a ternary mapping scheme rather than a full-color range or to highlight the outliers but *not* the intermediate values, click the **More Colors...** pushbutton to access the Range Mapping Color Selection control panel. In addition to controls that are also in the **Color Scheme** section of the Edit Color Mappings control panel, the Range Mapping Color Selection control panel allows you to:

- Set the intermediate values (i.e., those that are not outliers) to a constant color (with the **Use Pen** or **Use RGB Color** controls).
- Not apply any color to the intermediate values (**Use As-is** control).

How to handle outliers

Use the **Outlier...** buttons to access Outlier Handling control panels that govern how values beyond the minimum and maximum values are displayed.

You can handle outliers in any of several ways:

- Set outliers to a constant color (with the **Pin to**, **Use Pen**, or **Use RGB Color** controls).
- Set outliers to a constant color chosen from the same or a different color range (**Use Color Range** and **Use entry number** controls).
- Continue the color range beyond the maximum or minimum values (**Wraparound** control—the color range continues beyond the outlier, in head-to-head order, i.e., the order of the colors is not reversed).
- Do not apply any color to outliers (**Use As-is** control).

Saving a color map

You can save a custom color map by saving the current Cerius^2 session (see *Saving the current session*).

Example

A tutorial example of using the Edit Color Mappings control panel to create a color map of atomic mass is found in *Coloring atoms according to a property*.

Additional information

Please see the on-screen help for details on the functioning of each control in the control panels mentioned in this section.

Editing a property color map

Accessing the tools	Select the **Utilities/Customize/Color Mappings...** menu item from the main Visualizer control panel to access the Edit Color Mappings control panel. Alternatively, if you have the Color Selected Objects control panel open (*Accessing the tools*), you can click its **Edit Mappings...** pushbutton to access the Edit Color Mappings control panel.
Selecting the color map	Choose the name of the map you want to edit from the **Mapping** popup. Its current defining parameters appear in the control panel. If you saved a custom color map during some earlier Cerius^2 session (*Saving a color map*), you have to load that session to access that color map (see *Loading a previously saved session*).
Editing the color map	Edit the map definitions by the same procedure as used in creating a color map (*Property–color mapping*). You can also use the Edit Color Mappings control panel to delete or rename a color map.
Additional information	Please see the on-screen help for details on the functioning of each control in the Edit Color Mappings control panel.

Surfaces—style and transparency

Various Cerius^2 application modules (for example, Receptor, CASTEP UI, Gaussian UI, and MOPAC UI) enable you to generate surfaces and then adjust their transparency.

You should already know...	How to create surfaces is found in the documentation for the relevant application modules.
Accessing the tools	To set the style with which surfaces are made transparent, select the **View/Display Attributes...** menu item to access the Display Attributes control panel.
Setting the transparency style	Cerius^2 provides two methods for applying transparency to surfaces. Set the **Transparency Method** popup to **PATTERN** or **BLEND**.

Blend transparency can be compared to looking at the model through a surface made of fine silk cloth.

Pattern transparency gives a screened effect, where the overall transparency is an average of a net of opaque and transparent areas on the surface.

Additional information

Please see the on-screen help for details on the functioning of each control in the Display Attributes control panel.

Lighting control

Cerius^2 has enhanced lighting capability that also can aid in understanding your model's 3D structure and in spotlighting certain features.

Important

You must be running Cerius^2 in OpenGL mode in order to use all the lighting controls documented in this section. On Silicon Graphics machines, OpenGL mode is used by default or is available for Indy machines, those with XL or Impact graphics, and all with R5K and above processors. If some of the color controls do not work, you could try issuing this command:

```
> setenv FORCEOPENGL 1
```

before starting Cerius^2. Please see the *Installation and Administration Guide* for additional information.

If you prefer to learn by doing, you can skip the following discussion of concepts and proceed to *Accessing the tools*.

Finding information

This section includes information on:

Adjusting global light settings

Defining discrete light sources

Related information

Setting the graphical quality and screen resolution is discussed under *Resolution and graphical quality*. The screen coordinate axes are shown in Figure 3.

Concepts

An understanding of the following concepts can help you use the lighting controls effectively:

- The global *ambient light* (as controlled directly on the Lighting control panel) is general lighting in the scene that does not appear to come from any particular source.
- The *ambient light component* of defined lights is light that is scattered so much, by reflection from the "walls" enclosing the virtual scene and from objects within the scene, that there is no way to determine its original direction. Ambient light tends to take on the primary color of the surroundings and is most apparent in parts of the object that do not receive direct illumination.
- *Diffuse* light is scattered from an object in all directions; *specular* light appears as highlights on spherical or cylindrical objects. Matte surfaces are simulated by a high proportion of diffuse scattering; shiny surfaces by a high proportion of specular reflections. Diffuse light takes on (and in essence, defines) the perceived color of the object; specular light is usually the same color as the light as it leaves the light source.
- A *directional* light is located infinitely far away from the scene; consequently, its light rays are parallel.
- A *positional* light is located at some exact position within the scene. A positional light radiates light in all directions from the source unless it is defined as a spotlight.
- A *spotlight* is a positional light whose light output is restricted to a cone. The *cutoff* determines the width of the cone, and the *falloff* determines its concentration, that is, the light intensity across a plane that intersects the cone at right angles to its axis (Figure 5)..
- *Latitude* and *longitude* are defined as for the earth. Values towards the "north" and "east" are positive; those towards the "south" and "west" are negative. The *radius* is defined from the center of the viewing sphere.
- Real light is *attenuated*, meaning that its intensity decreases as the distance from the light source increases. Light attenuation is

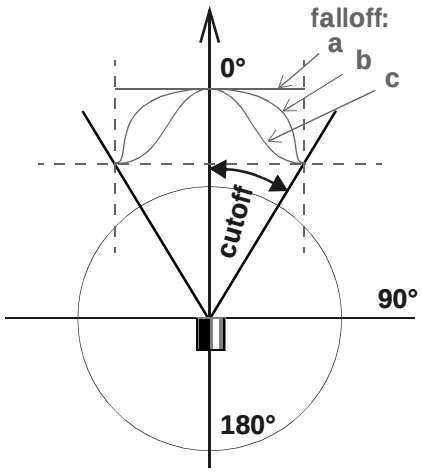


Figure 5. Cutoff and falloff in spotlights

Looking down from above a plane containing the spotlight and the center of its light beam. The spotlight is located at the origin and the beam points directly upwards. The *cutoff* is the half-angle of the cone of light, in degrees. Line c shows the light intensity vs. distance from the beam's center with a higher *falloff* value than used for line b. Line a shows zero falloff, i.e., the intensity is the same across the beam of light.

simulated by multiplying the intensity of light from a given source by an attenuation factor:

$$\text{attenuation factor} = \frac{1}{k_c + k_l d + l_q d^2}$$

where d = distance between the light and the object, k_c = a constant, k_l = the linear attenuation factor, and k_q = the quadratic attenuation factor.

Attenuation applies only to positional lights, since they are located at a defined distance from the scene.

Additional information

The book by Neider et al. (1993) contains a good discussion of lighting that can help in understanding and using the Cerius^2 lighting controls.

Accessing the tools

Select the **View/Graphics/Lighting...** menu item to access the Lighting control panel. Unless you also have a solid surface displayed, make sure your model is displayed in some style other than stick or trace (*Atom and bond display styles*), since lighting has no effect on lines or points.

Tip

It is often helpful turn off all other lights when you are defining a light. You can turn off global ambient lighting by setting **Gray** to 0.0 in the Lighting control panel. You can turn off any numbered light by choosing it from the **Light** popup in the Lighting control panel and unchecking the **Enabled** check box.

Example

A tutorial example of using the lighting controls to illuminate a model is found under *Lighting your model*.

Additional information

Please see the on-screen help for details on the functioning of each control in the control panels mentioned in this section.

Adjusting global light settings

Two-sided lighting

To light both the inside and outside of models displayed in cylinder style (*Bonds as cylinders*) or both sides of solid surfaces (e.g., such as those produced with one of the quantum chemistry modules), check the **Two Sided Lighting** check box. (This control has no effect with ball or ball-and-stick display styles.)

Viewing position

To change your virtual viewing position, check or uncheck the **Local Viewer** check box. Depending on the type of model, display style, and light position(s), the model may or may not look better with local viewing. However, graphics speed can be noticeably slower with **Local Viewer** enabled.

Ambient light

To change the brightness of the ambient light, adjust the **Gray** control. This affects only the global ambient light, which does not have any discrete light source.

To use a colored ambient light, use the red, green, and blue sliders (or the entry boxes below them) to set the proportions of red, green, and blue.

To return to a neutral-colored ambient light, click or adjust the **Gray** control.

Defining discrete light sources

You can illuminate your model with one or more discrete light sources, to spotlight various features and to dramatize its appearance.

Preliminary activities

First, choose which light source to define or redefine from the **Light** popup on the Lighting control panel (see *Accessing the tools*) and check the **Enabled** check box to turn it on. Turn off other lights (see *Tip*), if you want to see the effects of only the light you are defining.

Finding information

This section includes information on:

Color and components

Directional lights

Positional lights

Spotlights

Light attenuation

Color and components

Adjusting the ambient, diffuse, and specular components of a light source affects the perceived color of an object and makes it appear shiny or matte (*Concepts*).

Accessing the tools

Click the **Color...** pushbutton on the Lighting control panel to access the Lightsource Colors control panel.

Brightness and color of ambient, diffuse, and specular components

To change the brightness of the **Ambient**, **Diffuse**, and **Specular** components of your light source, adjust the appropriate **Gray** control in the Lightsource Colors control panel.

To adjust the colors of the **Ambient**, **Diffuse**, and **Specular** components of your light source, use the appropriate red, green, and blue sliders (or the entry boxes below them) to set the proportions of red, green, and blue.

To return the **Ambient**, **Diffuse**, and **Specular** components of your light source to a neutral color, click or adjust the appropriate **Gray** control.

How it works

In general, the ambient component affects the contrast (how flat or 3D the model appears), and the relative amounts of the specular (highlighting) and diffuse components affect how shiny or matte the object appears (see *Concepts* for more details).

Directional lights

Directional lights give overall illumination of a scene from a particular direction (*Concepts*).

Accessing the tools

To set up a directional light (located at infinity), click the **Position...** pushbutton in the Lighting control panel to access the Lightsource Position control panel.

Select the **Light is Directional** control.

Changing the direction of illumination

You can change the *direction* from which the light illuminates the model by using any combination of the **X**, **Y**, **Z**, **Latitude**, and **Longitude** controls (the **Radius** control is ignored, since the a directional light is, by definition, located at infinity).

How it works

For example, you can:

- Illuminate from directly in front of the computer screen by setting the **X** and **Y** directions to 0 and the **Z** direction to any positive number.

  This is equivalent to setting the **Latitude** and **Longitude** both to 0.0°.

- Illuminate from the lower right front by setting the **X** and **Z** directions to positive values and the **Y** direction to a negative number.

  The absolute values of these numbers are unimportant since you are a defining only a direction, not a position; however, their ratios do affect the direction.

- Move the light source upwards by increasing the value of the **Latitude**.

- Swing it around to the left by decreasing the **Longitude**.

- Illuminate from directly behind your model by setting the **X** and **Y** directions to 0 and the **Z** direction to a negative number.

  This is equivalent to setting the **Latitude** to 0.0° and the **Longitude** to 180°.

Positional lights

Positional lights can often be used to increase the perceived three-dimensionality of a scene (*Concepts*). In addition, they can be converted to spotlights (*Spotlights*).

Accessing the tools

To set up a positional light (located within the scene), click the **Position...** pushbutton in the Lighting control panel to access the Lightsource Position control panel.

Select the **Light is Positional** control.

Changing the location of the light

You can change the light's *location* by using any combination of the **X**, **Y**, **Z**, **Latitude**, **Longitude** and **Radius** controls.

How it works

You can, for example:

- Illuminate from a light positioned directly to the right of your model by setting **Y** and **Z** to 0.0 and **X** to a number (in angstroms) beyond the right side of your model (say, 10 Å for a small-molecule model).

  This is equivalent to setting **Latitude** to 0.0°, **Longitude** to 90°, and the **Radius** (in angstroms) to the value used for **X**.

- Position the light in the lower right forward quadrant of the scene by setting **Latitude** to about -30°, **Longitude** to about 80°, and **Radius** as needed to produce the desired effect (perhaps 10 Å for a small-molecule model).

- Provide backlighting by increasing the absolute **Longitude** beyond 90° (or -90°) or by using a negative value for Z.

- Illuminate at the position of an atom by pressing <Shift> on the keyboard and clicking the atom with the right mouse button to obtain an information window that includes its Cartesian coordinates (this information is also printed in the text window). Enter these values as the **X**, **Y**, and **Z** values. You can then pull the light away from the model by increasing the **Radius**.

Tip

To help in assessing the size of your viewing area, you can select the **View/Options...** menu item to show a scale bar in the model window.

Spotlights

Positional lights can be made into spotlights, which can highlight various features by illuminating only a small part of your model with a cone of light. (Directional lights cannot become spotlights, since they are located at infinity and their rays are therefore parallel—*Concepts*.)

Accessing the tools

To convert a positional light (*Positional lights*) into a spotlight and adjust the spotlight, click the **Spotlight...** pushbutton in the Lighting control panel to access the Spotlight Settings control panel.

Width of the spotlight

To control the width of the spotlight, adjust the **Cutoff** control. A value of 180° means the positional light is not a spotlight, and only cutoff values between 0° and 90° have any meaning (see Figure 5).

Tip

It can be helpful to use a very wide beam at first (**Cutoff** set to 90°), adjust the spotlight direction (*Aiming the spotlight*), and then narrow the beam. Otherwise, you can narrow the beam so much that none of its light hits the model.

Aiming the spotlight

To illuminate the model, a spotlight not only has to be located at the desired position (as defined and displayed in the Lightsource Position control panel, *Positional lights*) but also needs to be pointed in the correct direction.

To adjust the direction in which the spotlight shines, use the **Spotlight Direction** controls in the Spotlight Settings control panel. You would generally want the direction to proceed from the position of the spotlight towards the model.

You might want to start your adjustments by setting the spotlight's latitude to the negative of its positional latitude and the spotlight's longitude to its positional longitude plus 180° (subtract the resulting longitude from 360 if it is greater than 180, since the value entered must be < |180|). You may also want to increase the **Radius** of the spotlight's position (using the Lightsource Position control panel) to illuminate the entire model.

Final adjustments

Then you can narrow the cutoff, and iterate using the **Cutoff** and **Spotlight Direction** controls (in the Spotlight Settings control panel), as well as the position controls (in the Lightsource Position control panel), until the light shines exactly where you want it.

To make the illuminated area gradually fade into the nonilluminated area of your model, you can increase the **Falloff** value. Larger values make the light relatively more intense near the center of the light cone and smooth the transition from the light to the dark area.

Related information

If the edges of the illuminated area appear too jagged, you can increase the display resolution (see *Object resolution*).

Light attenuation

Positional lights (*Positional lights*) (whether or not they are also spotlights, *Spotlights*) can be *attenuated* to make objects that are closer to the light source appear brighter than those farther away (*Concepts*).

Accessing the tools

Click the **Attenuation...** pushbutton in the Lighting control panel to access the Lightsource Attenuation control panel.

Adjusting the attenuation

To make the relative brightness a linear function of the distance of an object from the light source, enter a nonzero value for the **Linear** factor.

To make the relative brightness a square function of the distance of an object from the light source, enter a nonzero value for the **Quadratic** factor.

To uniformly make the illumination dimmer or brighter, adjust the **Constant** control.

Rendering and ray-tracing

Cerius^2 provides a rendering facilities that enable you to produce high-quality 3D images of specified models and atoms. Two rendering facilities are provided: RayTrace and PSYCHO (PostScript utilitY for Color Hardcopy Output).

How RayTrace works

Regardless of the display style that you have selected, RayTrace uses the ball display style (*Atoms as balls*) and the currently defined default element colors to render atoms as van der Waals spheres. The lighting controls (*Lighting control*) do not affect ray tracing at this time.

The rendered image appears in a separate Cerius^2 window called the Cerius2 Ray Tracing window. The bitmapped image displayed in this window cannot be manipulated or printed. However, you can use a third-party screen-capture utility or print utility to capture or print the rendered image. You can also save the intermediate files that are used in producing the ray-traced image.

How PSYCHO works

PSYCHO produces an encapsulated PostScript file and enables more flexibility than RayTrace in defining the output. PSYCHO reads atom and bond information and can generate color or gray-scale images of spheres, cylinders, and polyhedra and can label atoms with any text strings. PSYCHO also plots any isosurfaces that are present on the model (such as orbitals), although this creates significantly larger output files.

The final PSYCHO image is generally similar to the image in the Cerius^2 model window, although it does not include (for example), bond orders, hydrogen bonds, custom pen colors, or custom lighting effects.

When you render a PSYCHO image, Cerius^2 creates a PSYCHO input file (default name = C2Psycho.dat) and then runs PSYCHO with appropriate options. PSYCHO reads the input file and creates a PostScript file (default name = C2Psycho.eps or C2Psycho.ps), which by default is automatically previewed on your machine's PostScript previewer. If you like what you see, you can then send the PostScript file to your PostScript printer, through your previewier or via the Cerius^2 **File/Print...** menu item (*Printing models and graphs*).

The Cerius^2 PSYCHO control panels also give you access to the PSYCHO input file and options so that you can experiment with more complex PSYCHO renderings.

Accessing the tools

Select the **View/Rendering...** menu item to access the Render Models control panel. Click the **Preferences...** pushbuttons on that control panel to access the Psycho Preferences and Raytrace Preferences control panels.

Rendering models

Use the Render Models control panel to specify the model(s) and atoms that you want to be rendered, as well as the rendering method.

For raytracing, you may want to change how shiny or dull the atoms appear and how jagged or fuzzy the image appears by

using controls in the Raytrace Preferences control panel. You can also use this control panel to specify that the intermediate files be saved and to give them a common root name.

For PSYCHO, you can use the Psycho Preferences and More Psycho Options control panels to set many available options.

Click the **RENDER** pushbutton in the Render Models control panel to start the rendering process.

Depending on your computing power, the rendering process may take some time. (There may also be a delay before the model reappears, if you move the Cerius2 Ray Tracing window.)

To close the Cerius2 Ray Tracing window, click anywhere in it.

Additional information

Please see the on-screen help for details on the functioning of each control in the Render Models, Raytrace Preferences, Psycho Preferences, and More Psycho Options control panels.

Stereo viewing

In stereoscopic viewing mode, an impression of three-dimensionality can be achieved by using an appropriate stereo viewer or (if you can manage it) by crossing your eyes.

Accessing the tools

Select the **View/Graphics/Stereo...** menu item to access the Stereo control panel.

Specifying stereo display

Two stereo viewing methods are available, each producing dual images of the current model (or models, if in overlay mode, see *Controlling model visibility and the display mode*) in a slightly different orientation:

- To use the Crystaleyes stereo hardware and glasses from StereoGraphics Corporation (marketed by Silicon Graphics, Inc. as Stereo View), set the **STEREO CONTROLS** to **CRYSTALEYES** and select **STEREO**.
- To use an ordinary stereo viewer or view in stereo by crossing your eyes, set the **STEREO CONTROLS** to **STEREO-PAIR** and select **STEREO**.

  For viewing with a stereo viewer, set the popup to **DISTAL**.

For viewing cross-eyed, set the popup to **DISTAL** or **PROXIMAL**, whichever works for you. (In distal mode, the left-eye image is on the left side of the screen and the right-eye image on the right; in proximal mode, the images are reversed.)

Adjust the **Stereo Separation** control to optimize your comfort and ease in interpreting the model. The separation affects the apparent flatness or three-dimensionality of the model.

To return to mono display, select **MONO** on the Stereo control panel or press <F4> on the keyboard.

Keyboard shortcuts

To toggle between mono and stereo display, press <F4>.

To toggle between Crystaleyes and stereo-pair modes, press <F5>.

To adjust the separation, drag the mouse in the model window while holding down <Shift> and <Alt> and the right mouse button.

Note

Use of the left mouse button for selection is disabled during full-screen stereo viewing.

Related information

You may find that the stereo option works better for you if you view the model in perspective projection (*Projection*).

Additional information

Please see the on-screen help for details on the functioning of each control in the Stereo control panel. Mouse functions and keyboard shortcuts are summarized in *Mouse and Keyboard Actions*.

10 Working with Graphs

Graphical output is generated by a wide variety of Cerius^2 application modules. This information is automatically formatted and displayed as a graph. The controls in the Graphs module allow you to save and reload graphs and also give you great freedom to manipulate the appearance of the graphs. For example, you can scale and annotate graphs, as well as change the color ranges used, to highlight important areas for presentation.

This section explains

This section contains information on:

Creating graphs

Displaying and editing graphs

Managing graphs

Table 10. Finding information about graphs

If you want to know about:	Read:
Finding the Graphs module.	*Accessing the tools*.
Types of graphs.	*Concepts*.
Displaying or hiding individual graphs.	*Selecting graphs to display*.
Generating series of graphs.	*Preventing replacement of old graphs*.
Plotting values from a table.	*Graphing table information*.
Starting to edit graphs.	*Selecting graphs for editing*.
Editing graph appearance.	*Changing plotting style and color*.
Adding labels, arrows, etc.	*Labeling and annotating graphs*.
Editing graph axes.	*Changing graph axes and scale*.
Shifting, scrolling, or zooming an axis.	*Changing graph axes and scale*.
Mouse buttons and keyboard use.	*Mouse and Keyboard Actions*.
Starting to edit how data sets are displayed.	*Selecting a data set*.

Table 10. Finding information about graphs

If you want to know about:	Read:
Displaying or hiding data sets.	*Selecting a data set*.
Color ranges in 2D graphs.	*Specifying color use in 2D graphs*.
Changing color ranges used in graphs.	*Color ranges*.
Setting graph preferences.	*Controlling default display format*.
Printing graphs.	*Printing models and graphs*.
Saving files containing graphs.	*Saving graphs*, *Saving individual models*.
Saving graph and other preferences.	*Using saved sessions as preferences settings*.
Loading files containing graphs.	*Loading graphs*, *Loading model structure files*.
Finding files with file browsers in control panels.	*Loading model structure files*.
Formats of graph files.	*File Formats*.
Freeing memory and clearing the graph display.	*Removing graphs and data from a Cerius2 session*.

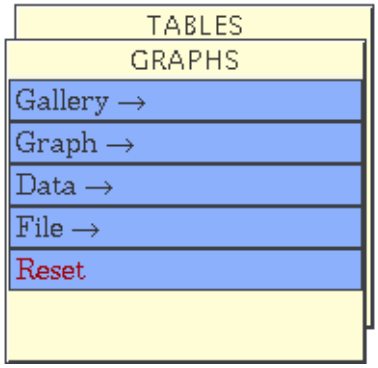
You should already know…

The basics of starting Cerius^2 and using its interface are demonstrated in *Introducing Cerius2* and described in *The Cerius2 Interface*.

Graphs in Cerius^2 are produced as output from calculations in various other application modules. How to set up and run the appropriate calculations are discussed in the documentation for the relevant application modules.

Accessing the tools

The tools for handling graphs are accessed from one of the decks of cards in the main Visualizer control panel. To access the Graphs module, click the deck selector (see also *Access to application modules*) and choose **TABLES & GRAPHS** from the list that appears. Then click the title of the **GRAPHS** card to bring it to the front. The deck of cards menu area should now look like this



Additional information

Please see the on-screen help for details on the functioning of each control on the **GRAPHS** card.

Creating graphs

Why read this section

Ordinarily, graphs are created and displayed automatically as the result of some calculation in a Cerius^2 application module. If you are dealing with such graphs, you do not need to read this section.

However, you may want to create a graph from a blank "user graph" and selected data. Or you may want to import and graph data from a file output by an Insight II module.

Finding information

This section includes information on:

Starting a new, empty graph

Specifying the type of graph

Selecting data to plot

Loading graphs

Related information

Controlling which one(s) of several plots (which are held in computer memory during a Cerius^2 session) are displayed in the Cerius2 Graphs window is discussed under *Selecting and displaying graphs*.

You should already know…

How to access the Graphs module is described under *Accessing the tools*.

Starting a new, empty graph

Accessing the tools

Select the **Gallery/Manager** menu item from the **GRAPHS** card to access the Gallery Manager control panel.

Creating a new graph

To create a new graph, check a check box in the **Display** column, to the left of the blank line below the last name, if any, in the list of graph names in the Gallery Manager control panel.

Check the **Edit** check box to the right of the name (User Graph v#) of the new graph. Make sure all other **Edit** check boxes are unchecked.

Additional information

Please see the on-screen help for details on the functioning of each control in the Gallery Manager control panel.

Specifying the type of graph

When you create a new graph, you need to specify whether the graph should be an x–y graph, a 2D Cartesian graph, or a 2D polar graph. (For automatically created graphs, the type of data determines what type of graph is used to display it.)

Concepts

An x–y data set is an ordered series of independent coordinates in a plane. The data points in a set may be connected by lines or displayed in styles such as histogram, points, or delta lines.

A 2D Cartesian data set is a regular grid of points in a plane, sometimes with symmetry properties. Each point is associated with a real value, such as an intensity or an energy. Different real values are usually color-coded to differentiate them.

A 2D polar data set is similar to a 2D Cartesian data set, except that it is mapped in polar coordinates.

A special type of 2D data set is used to display LEED/RHEED reflections and single-fiber diffraction patterns. These are called x–y–z plots, where circles whose radii represent the value of the z coordinate are drawn in the xy plane. This is different from a 2D contour plot in the delta style. The latter draws circles on a regular grid, whereas the x–y–z plot places circles only as prescribed by the x,y coordinates.

Accessing the tools

If you already have the Gallery Manager control panel open (*Accessing the tools*), click the **Graph Manager...** pushbutton in the Gallery Manager control panel to access the Graph Manager control panel.

Alternatively, select the **Graph/Manager** menu item from the **GRAPHS** card to access the Graph Manager control panel.

Specifying the type of graph

Set the **Type** popup to the desired graph type.

Additional information

Please see the on-screen help for details on the functioning of each control in the Graph Manager control panel.

Selecting data to plot

Any Cerius^2 data set(s) currently in the computer memory can be selected and plotted in a new graph. However, the data set must be compatible with the type (see *Specifying the type of graph*) of graph specified. In addition, only Cerius^2 data sets can be plotted in newly created Cerius^2 graphs.

Related information

Loading graphs containing data sets is discussed in *Loading graphs*. Generating data for graphs is discussed in the documentation for the relevant application modules.

Accessing the tools

If you already have the Gallery Manager control panel open (*Accessing the tools*), click the **Graph Manager...** pushbutton in the Gallery Manager control panel to access the Graph Manager control panel.

Alternatively, select the **Graph/Manager** menu item from the **GRAPHS** card to access the Graph Manager control panel.

Selecting the data

To add a data set to the new graph, check the **Display** check box(es) next to the names of the data sets that you want to display in the currently editable graph. (The name of this graph appears

near the top of the Graph Manager control panel.) You can only select data sets that are of the appropriate type (*Specifying the type of graph*).

Additional information

Please see the on-screen help for details on the functioning of each control in the Graph Manager control panel.

Tip

You may need to scale the graph (*Changing graph axes and scale*) for the data set(s) to appear in it.

Loading graphs

Graphs that have been created and saved to a file (*Saving graphs*) can be loaded into a subsequent Cerius^2 session, to compare results or to print the graphs.

Once a graph file has been loaded, each graph and its data sets can be manipulated in exactly the same way as those newly created by Cerius^2 (see, for example, *Displaying and editing graphs*). Old and new graphs can be displayed side by side in the Cerius2 Graphs window, or old and new data sets can be displayed together in a single graph. However, Insight and Cerius^2 data cannot be mixed in one graph.

Accessing the tools

To load graphs saved from Cerius^2, select the **File/Load Graphs** menu item from the **GRAPHS** card to access the Load Graphs control panel.

To load graphs saved from Insight II, select the **File/Import Insight TBL** menu item from the **GRAPHS** card to access the Import TBL File control panel.

Finding and loading graph files

Using the file browser in the control panel to navigate the directory structure is fairly intuitive. The procedure is described under *Loading model structure files*.

If the name of the file you want to load does not end in .grf (Cerius^2) or .tbl (Insight), change the name in the filename text entry box as desired (see *File formats*).

For Cerius^2 graphs, loading the graph also loads its included data sets.

However, since Insight graphs contain multiple data sets, you need to first select the graph and then choose the desired types of data to be plotted. Then click the **PLOT** pushbutton to load the graph and the desired data sets.

Additional information

Please see the on-screen help for details on the functioning of each control in the Load Graphs and Import TBL File control panels.

File formats

Because all Cerius^2 graphs are saved in the .grf format, most graphs loaded in are also in this format. However, the Cerius^2 graph system recognizes and correctly loads graphs in the .xy and .con formats used by CERIUS prior to version 3.1.

Cerius^2 can also read in graphs that were saved in the Insight II program's .tbl format. (Cerius^2 .tbl files are *not* the same format as Insight .tbl files.)

Cerius^2 recognizes graph files according to their format, so it is not strictly necessary to save them with the standard filename extensions. However, it is generally less confusing and more convenient to do so.

For detailed information about Cerius^2 file formats, please see *File Formats*. Insight files are described in separate file formats documentation.

Displaying and editing graphs

Why read this section

When a graph is output by an application, it automatically appears in a separate *Cerius2 Graphs window* (sometimes called a *gallery*). You may want to change such things as:

- How many graphs are currently displayed in the window.
- The range of data points that are visible.
- The text that accompanies a graph.

Finding information

This section includes information on:

Selecting and displaying graphs

Selecting which data sets to display and edit

Labeling and annotating graphs

Changing graph axes and scale

Changing plotting style and color

Related information

How to print the contents of the Cerius2 Graphs window is explained under *Printing models and graphs*.

You should already know...

How to access the Graphs module is described under *Accessing the tools*. How to load graphs from files is described under *Loading graphs*.

Selecting and displaying graphs

To display or edit graphs, you need to select them.

Accessing the tools

Select the **Gallery/Manager** menu item from the **GRAPHS** card to access the Gallery Manager control panel. (The graph window is also referred to as the gallery.)

Selecting graphs to display

To display or hide particular graphs, check or uncheck the appropriate check boxes in the **Display** column to the left of the list of graph names in the Gallery Manager control panel.

For changes in the graphs displayed to occur immediately, make sure the **Auto** check box is checked. If the **Auto** check box is unchecked, you need to click the **SHOW** pushbutton to update the graph window. Turning off automatic updating can be faster if you are dealing with graphs containing many data points, which may therefore be slow to update.

Accommodating graphs within the graph window

You can allow Cerius^2 to set the graph window width and height automatically by setting both the **Gallery Width** and **Gallery Height** popups to **AUTO**.

If you prefer some other width and/or height, set the **Gallery Width** and **Gallery Height** to the desired numbers of columns and rows (respectively) of graphs to display.

Tip

You can find the coordinates of any point on any type of graph by pressing <Ctrl> on the keyboard and left-clicking a point in the graph. The information is displayed in the text window.

Selecting graphs for editing

To enable graphs to be edited, check or uncheck the appropriate check boxes in the **Edit** column to the right of the list of graph names in the Gallery Manager control panel.

Only graphs of the same type (*Specifying the type of graph*) can be edited simultaneously.

Additional information

Please see the on-screen help for details on the functioning of each control in the Gallery Manager control panel.

Selecting which data sets to display and edit

If you do not want all data sets in a selected graph to displayed, or if you want them to be displayed in different styles, you need to select the data set.

Related information

How to select a graph for display and editing is discussed under *Selecting and displaying graphs*.

Accessing the tools

If you already have the Gallery Manager control panel open (*Accessing the tools*), click the **Graph Manager…** pushbutton in the Gallery Manager control panel to access the Graph Manager control panel.

Alternatively, select the **Graph/Manager** menu item from the **GRAPHS** card to access the Graph Manager control panel.

Selecting a data set

To display or hide particular data sets, check or uncheck the appropriate check boxes in the **Display** column to the left of the list of data set names in the Graph Manager control panel.

To enable the display style (etc.) of data sets to be edited, check or uncheck the appropriate check boxes in the **Edit** column to the right of the list of data set names in the Graph Manager control panel.

Additional information

Please see the on-screen help for details on the functioning of each control in the Graph Manager control panel.

Labeling and annotating graphs

You can change labels for graph axes and data-set keys and enter text for a graph title. You can also specify whether to display the axis labels, the title (above the graph), the color-code key to the

data sets, the axis lines and numbers, or lines indicating cells (data-set boundaries) in 2D graphs that contain periodically repeated data.

Related information

Selecting graphs (*Selecting and displaying graphs*) and data sets (*Selecting which data sets to display and edit*) for editing are discussed above. Specifying immediate or delayed updates of the graph display is presented under *Selecting graphs to display*.

Accessing the tools

To change the text of data-set keys, select the **Data/Plotting Attributes** menu item from the **GRAPHS** card to access the Plotting Attributes control panel. Alternatively, click the **Plotting Attributes...** pushbutton in the Graph Manager control panel to access the Plotting Attributes control panel.

The controls that are included in this control panel depend on what type of graph is being edited.

To perform any other function listed under *Labeling and annotating graphs*, select the **Graph/Annotation** menu item from the **GRAPHS** card to access the Graph Annotation control panel. Alternatively, click the **Graph Annotation...** pushbutton in the Graph Manager control panel to access the Graph Annotation control card.

Changing text annotations

To change the text of the x- or y -axis label, enter the text in the **x Axis Label** or **y Axis Label** entry boxes in the Graph Annotation control panel.

To change the text of the graph's title, enter the text in the **Graph Title** entry boxes in the Graph Annotation control panel. Several entry boxes are available, so you can use multi-line titles.

To change the text of data-set color-code keys, select one (only) data set and enter the text in the **Label** entry box in the Plotting Attributes control panel.

To display or hide hkl labels next to data circles on x–y–z graphs, check or uncheck the **Include hkl Labels** check box in the Plotting Attributes control panel.

Displaying annotations

To display or hide axes, axis labels, the title, all the data-set keys, or cell indications, set the appropriate **Annotation Options** pop-ups in the Graph Annotation control panel. (A **-->** popup label means that several graphs are selected for editing and that the

annotation options differ for those graphs, or that no graph is selected.)

Additional information

Please see the on-screen help for details on the functioning of each control in the Graph Annotation and Plotting Attributes control panels.

Changing graph axes and scale

You can scale selected graphs in several ways, to aid in viewing their data. For example, you can change the ranges of the x and y axes, scroll along an axis, and change the proportions of a graph.

Related information

Selecting graphs (*Selecting and displaying graphs*) and data sets (*Selecting which data sets to display and edit*) for editing are discussed above. Specifying immediate or delayed updates of the graph display is presented under *Selecting graphs to display*.

Accessing the tools

To shift only selected data set(s) along the y axis, select the **Data/Plotting Attributes** menu item from the **GRAPHS** card to access the Plotting Attributes control panel. Alternatively, click the **Plotting Attributes…** pushbutton in the Graph Manager control panel to access the Plotting Attributes control panel.

To change the proportions of the graph window, select the **Gallery/Manager** menu item from the **GRAPHS** card to access the Gallery Manager control panel.

For all other scaling or axis-shifting tasks, select the **Graph/Scaling** menu item from the **GRAPHS** card to access the Graph Scaling control panel. Alternatively, click the **Graph Scaling…** pushbutton in the Graph Manager control panel to access the Graph Scaling control panel. The controls available in this control panel depend on the type of graph you have selected for editing. (The name of this graph appears near the top of the Graph Scaling control panel.)

Changing x and y axes

The x- and y-axis ranges can be changed for x–y and 2D Cartesian graphs. The angle between the axes can be changed for 2D Cartesian graphs.

To explicitly set the range of values covered by the x and y axes, enter values in the **Min x**, **Max x**, **Min y**, and **Max y** entry boxes of

the Graph Scaling control panel. For 2D Cartesian graphs, you can also set the range values relative to the width of the data set.

For x–y graphs, you can also choose among several options for automatic axis scaling, by choosing from the **Axis Scaling** popup in the Graph Scaling control panel.

To force the axes in a 2D Cartesian graph to be drawn perpendicularly, check the **Force Rectangular Axes** check box in the Graph Scaling control panel. For example, check this box when viewing HRTEM output for nonorthogonal periodic cells, to view the graph as a rectangle rather than a parallelogram.

Changing angles in polar graphs

To set the minimum and maximum displayed angles in 2D polar graphs, use the **Min Angle** and **Max Angle** entry boxes in the Graph Scaling control panel. The angles are defined clockwise (in degrees) from north (up).

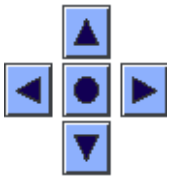
To set the displayed radius in 2D polar graphs, use the **Max Radius** entry box in the Graph Scaling control panel.

Shifting a data set along the y axis

To shift a curve or other representation of a data set up or down the y axis of an x–y graph, enter a value in the **Y Offset** entry box of the Plotting Attributes control panel. This does not change the actual data points.

Scrolling a graph

X–y graphs can be scrolled along either axis.



To scroll the graph along the x or y axis, use the arrow tools in the **Scroll** controls of the Graph Scaling control panel.

To return the view to its original position (that is, centered on the same area as before you began scrolling), click the reset button (in the center of the arrow tools) or press <Home> on the keyboard.

You can also scroll graphs interactively, by placing the cursor within a graph, depressing the middle mouse button, and dragging the mouse in any direction within the xy plane.

Changing size or proportions of a graph display

The proportions (rectangular or square) of all types graphs can be changed. In addition, the x and y axes of x–y graphs can be expanded or contracted (zoomed, see *Expanding or shrinking an axis*).

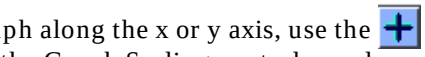
To change the proportions of the Cerius2 Graphs window and any graph(s) it contains, grab a corner of the window with the cursor

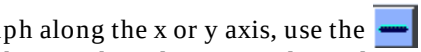
and drag it. Changing the graph window's width and height (*Accommodating graphs within the graph window*) also affects the proportions of the displayed graphs.

Alternatively, you can set the window proportions by entering a number in the **Aspect ratio** entry box in the Gallery Manager control panel.

Expanding or shrinking an axis

To zoom in on a specific part of the displayed graph, hold down <Alt> and the middle mouse button and drag out a rectangle over the desired part of the graph.

To expand the graph along the x or y axis, use the  tools in the **Zoom** controls of the Graph Scaling control panel.

To contract the graph along the x or y axis, use the  tools in the **Zoom** controls of the Graph Scaling control panel.

To return the view to its original position (that is, to the same magnification as before you began zooming), click the reset button (in the center of the **Zoom** tools) or press <Home> on the keyboard.

You can also zoom graphs interactively, by placing the cursor within a graph and:

- Holding down the middle and right mouse buttons and dragging the cursor in the model window.

  or:

- Holding down <Shift> plus the middle mouse button and dragging the cursor in the model window.

Moving the cursor up and / or to the right increases the magnification along the y and / or x axes, respectively; moving it down and / or to the left decreases the magnification.

Additional information

Please see the on-screen help for details on the functioning of each control in the control panels mentioned in this section. Mouse functions and keyboard shortcuts are summarized in *Mouse and Keyboard Actions*.

Changing plotting style and color

You can change features of the graph appearance such as style and color. For 2D graphs, you can also set whether data values are dif-

ferentiated by lines of constant value (contours) or by spots or areas of color and also specify how colors are applied.

Related information

Selecting graphs (*Selecting and displaying graphs*) and data sets (*Selecting which data sets to display and edit*) for editing are discussed above. Specifying immediate or delayed updates of the graph display is presented under *Selecting graphs to display*.

You can also edit the color ranges (see *Color ranges*) that are used to color-code values shown in graphs.

Accessing the tools

Select the **Data/Plotting Attributes** menu item from the **GRAPHS** card to access the Plotting Attributes control panel. Alternatively, click the **Plotting Attributes...** pushbutton in the Graph Manager control panel to access the Plotting Attributes control panel. The controls available in this control panel depend on the type of graph you have selected for editing.

Changing line style and color in x–y graphs

To change the plot style used for selected data sets in x–y graphs, set the **Style** popup.

To change the line style (when the plot style is line, histogram, or delta) used to plot selected data sets in x–y graphs, set the **Lines** popup. Styles other than **SOLID** work best when data points are spaced relatively far apart.

To change the color used for selected data sets in x–y graphs, select a color from the **Color** popup.

Changing the style of 2D graphs

To change the style (contour lines, continuous shading, or delta) used to differentiate ranges of values in 2D Cartesian and 2D polar graphs, set the **Style** popup.

Specifying color use in 2D graphs

For 2D Cartesian and 2D polar graphs, as well as x–y–z graphs, you can specify:

- The color range (*Color ranges*) that is used.
- The direction in which the color range is used for the contour and continuous styles of 2D graphs (that is, which color represents a high value and which low).
- Whether the color scale is applied in a linear or log way.
- The number of contours used in contour-style 2D graphs (fewer contours means faster redrawing when you make changes).

- How smooth is the color shading for continuous-style 2D graphs.
- The range of values that are mapped to colors.
- The exposure, brightness, and contrast of the displayed colors.

Additional information

Please see the on-screen help for details on the functioning of each control in the Plotting Attributes control panel.

Managing graphs

Why read this section

You may be running an application that produces many graphs. However, you can, for example, control how new graphs are added to the graphing system and remove graphs from the gallery manager.

Finding information

This section includes information on:

Controlling default display format

Preventing replacement of old graphs

Removing graphs and data from a Cerius2 session

Saving graphs

Related information

Controlling which one(s) of several plots (which are held in computer memory during a Cerius^2 session) are displayed in the Cerius2 Graphs window is discussed under *Selecting and displaying graphs*.

Saving preferences is discussed under *Using saved sessions as preferences settings*.

You should already know…

How to access the Graphs module is described under *Accessing the tools*.

Controlling default display format

When a graph is created by a Cerius^2 application module, the "best" graph axes, annotations, and plot attributes are set automatically. When a graph is loaded from file, the format that was

saved with the file is used. However, you can set your own preferences.

Controlling formats in generated graphs...

For example, in doing a series of Rietveld refinements, you may be most interested in a particular data range. After the graph from the first refinement appears, you can zoom in on the desired data range and then set these graph axes as your preferences. When graphs that are output from subsequent refinement are sent to the graph window, the graph axes remain in your region of interest and do not revert to showing the entire data set.

... and in graphs loaded from files

By default, when a graph file is loaded, it uses the same axis scales, types of annotations, and other settings that were in effect when the file was saved. However, you can override some of these settings before loading the graph file.

Accessing the tools

Select the **Gallery/Expert Functions** menu item from the **GRAPHS** card to access the Graphs Expert Functions control panel. Alternatively, click the **Expert Functions...** pushbutton in the Gallery Manager control panel to access the Graphs Expert Functions control panel.

Resetting the default graph format

To retain current graph format settings in future graphs (in the current Cerius^2 session), after the first graph is output from an application module, format it as desired (see *Displaying and editing graphs*). For example, display only the "interesting" data points by scrolling along the x and / or y axes (*Scrolling a graph*) and / or by expanding or contracting one or both axes (*Expanding or shrinking an axis*), then make sure that the **Axis Scaling** popup in the Graph Scaling control panel is set to **FIXED**.

In the Graphs Expert Functions control panel, check the desired **Keep Same** check boxes to apply features of the current graph's format to future graphs:

- **Gallery Content**—To regenerate only graphs having the same name(s) as currently displayed graphs.
- **Graph Axes**—To retain the same axis scale (*Expanding or shrinking an axis*) and labels (*Changing text annotations*).
- **Graph Content**—To display only data sets having the same name(s) and to maintain the same plotting order.
- **Plot Attributes**—To use the same style and color (*Changing line style and color in x–y graphs*), y-axis offset (*Shifting a data set along*

the y axis), and key (*Changing text annotations*) for data sets (having the same names) as in the previous graph.

When a new graph is generated by your application module, it is displayed in the same format. It can be reformatted, if necessary, as described under *Displaying and editing graphs*.

Additional information

Please see the on-screen help for details on the functioning of each control in the Graphs Expert Functions control panel.

Preventing replacement of old graphs

Some Cerius^2 modules can produce a series of similar graphs, overwriting the previous graph with the new one. In addition, when you load a graph from file, it usually replaces those displayed in the graph window.

Controlling graph replacement when many graphs are generated...

For example, a graph of energy vs. minimization step can be produced by the Minimizer module each time a minimization is run; and in the Rietveld module, each refinement produces a new diffraction data set. The graph and data set(s) from the preceding run are lost when this happens.

The default is to overwrite any old version of these graphs with the newest one. This prevents many versions of obsolete graphs from accumulating in the graph window *and in computer memory.* However, if you want to retain old versions of graphs along with the new ones, you can:

- Place the new graph in the graph window next to the old graph.

  or:

- Place the new data set in the same graph along with the old data set.

...and when graphs are loaded from files

As another example, when a graph file is loaded, the graphs in the file usually replace those currently shown in the graph window (although the previous graphs and their data sets are still present in memory). However, you can load a graph file without displaying its graph(s) immediately.

Accessing the tools

Select the **Gallery/Expert Functions** menu item from the **GRAPHS** card to access the Graphs Expert Functions control panel. Alternatively, click the **Expert Functions...** pushbutton in

the Gallery Manager control panel to access the Graphs Expert Functions control panel.

Preventing old graphs from being overwritten

After the first graph is output from an application module, set the **Data Placement** popup in the Graphs Expert Functions control panel to **ADDITIONAL GRAPH**.

When a new graph is generated by your application module, both it and the older graph are displayed in the graph window.

Adding new data to an existing graph

After the first graph is output from an application module, set the **Data Placement** popup in the Graphs Expert Functions control panel to **COMBINE WITH EXISTING**.

When a new graph is generated by your application module, the new data set is displayed in the older graph that is already displayed in the graph window.

Additional information

Please see the on-screen help for details on the functioning of each control in the Graphs Expert Functions control panel.

Removing graphs and data from a Cerius^2 session

You can remove all graphs and their data sets from the graph window and computer memory, or you can remove all except those that are currently displayed.

Related information

You can completely reinitialize Cerius^2 by starting a new session (*Starting a new session*).

Selecting graphs (*Selecting and displaying graphs*) and data sets (*Selecting which data sets to display and edit*) for display are discussed above.

Accessing the tools

Select the **Gallery/Expert Functions** menu item from the **GRAPHS** card to access the Graphs Expert Functions control panel. Alternatively, click the **Expert Functions...** pushbutton in the Gallery Manager control panel to access the Graphs Expert Functions control panel.

Deleting all invisible graphs and data sets

First make sure that all graphs (*Selecting and displaying graphs*) and data sets (*Selecting which data sets to display and edit*) that you want to keep are currently displayed in the Cerius2 Graphs window.

To remove all undisplayed graphs and data sets, click the **CLEAN** pushbutton in the Graphs Expert Functions control panel.

Deleting all graphs and data sets

To delete *all* graphs and their data sets from both display and memory, click the **Reset** menu item on the **GRAPHS** card.

Additional information

Please see the on-screen help for details on the functioning of each control in the Graphs Expert Functions control panel.

Saving graphs

Saving graphs produced by Cerius^2 modules enables you to keep a record of your results. Saved graphs can be loaded back into a Cerius^2 session (*Loading graphs*) for printing or for comparison with other graphs.

A saved graph file contains all graphs and data sets just as they appear in the current graph window.

Important

Unless a graph and its desired data set(s) are actually displayed in the graph window, the graph is not saved, even if it is currently in computer memory.

Related information

Creating your own directories or subdirectories is described under *Making custom directories*.

Accessing the tools

To save graphs from the current Cerius^2 session, select the **File/ Save Graphs** menu item from the **GRAPHS** card to access the Save Graphs control panel.

Saving graphs to a file

Once you have located the directory in which you want to store your graph, click the **SAVE** pushbutton. (Use of the file selection list box and other file selector controls to navigate the directory structure is presented in detail under *Finding model file(s)*.)

Additional information

Please see the on-screen help for details on the functioning of each control in the Save Graphs control panel.

File formats

Cerius^2 saves graphs in .grf format and automatically adds .grf to the filename if you have not specified some other extension.

11 Working with Tables

In Cerius^2 you can create your own tables containing both data and models and can modify tables created by Cerius^2 application module. This section provides basic information on working with Cerius^2 tables.

This section explains

Following an introduction to Cerius^2 tables (*Introduction to Cerius2 tables*), this section contains information on:

Managing and editing tables

Table style and display

Values and mathematical expressions

Models in tables

Grouping table information

Searching for information in a table

Viewing subsets of a table

Sorting table information

Graphing table information

Exporting table information

Table 11. Finding information about tables

If you want to know about:	Read:
Finding the Tables module.	*Accessing the tools*.
Parts of the table window.	*The table window*.
Making a table current.	*Specifying the current table*.
Attaching control panels to tables.	*Keeping track of the current table*.
Moving the cursor in a table.	*Selecting a cell*.

Table 11. Finding information about tables

If you want to know about:	Read:
Cursor wrapping.	*Table expansion and cursor control*.
The current cell.	*Understanding cell values, types, and formats*.
Default cell format.	*Understanding cell values, types, and formats*.
Data type and display format.	*Assigning data types*, *Technical notes*, *Setting display formats*.
Entering data into or editing a cell.	*Editing cell contents*.
Recording your edits.	*Entering your changes*.
Cutting and pasting values.	*Copying, moving, and clearing information*.
Working with rows and columns.	*Selecting rows and columns*.
Applying equations to cells and columns.	*Entering mathematical expressions*.
Relation between values and expressions.	*Concepts*.
Components to include in expressions.	*Operators*.
Getting models into a table.	*Copying models into columns*.
Referring to other cells in expressions.	*Cross references*.
Refering to models in expressions.	*Calculations on models*, *Setting up calculations on models*.
Displaying atom–atom distances and other measurements.	*Measuring models*.
Displaying vector properties.	*Vector properties*.
Updating calculations.	*Recalculating table values*.
Column width and row height.	*Changing row, column, and heading sizes*.
Aligning cell contents.	*Aligning information within columns*.
Adding and removing rows and columns.	*Inserting and deleting entire rows or columns*, *Table expansion and cursor control*.
Saving tables to files.	*Saving a table*.
Saving models with tables.	*Saving tables containing models*.
What kinds of data are associated with models.	*What is saved as a model*.
Formatting ASCII files as tables.	*Importing an ASCII text file into a new table*.
Mouse buttons and keyboard use.	*Mouse and Keyboard Actions*.

Uses of tables

You can use Cerius^2 tables to display and manipulate tabular information generated by Cerius^2 application modules. Unlike many dedicated spreadsheet programs, the Cerius^2 table facility understands and can make calculations that refer to (molecular)

models. However, the Cerius^2 table facility does not have all the features of a typical dedicated spreadsheet program. Therefore, you can export Cerius^2 tables for further study to programs such as Microsoft® Excel. You can also import tabular data from ASCII files into a Cerius^2 table for further manipulation and display.

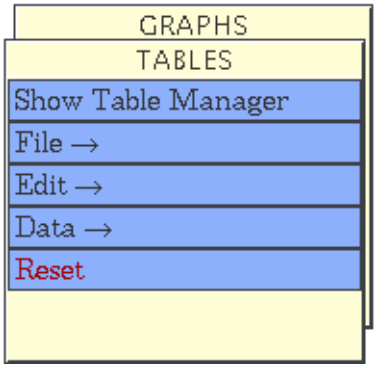
You should already know...

The basics of starting Cerius^2 and using its interface are demonstrated in *Introducing Cerius2* and described in *The Cerius2 Interface*.

Tables in Cerius^2 are produced as output from calculations in various other application modules. How to set up and run the appropriate calculations are discussed in the documentation for the relevant application modules.

Accessing the tools

The tools for handling tables are accessed from one of the decks of cards in the main Visualizer control panel. To access the Tables module, click the deck selector (see also *Access to application modules*) and choose **TABLES & GRAPHS** from the list that appears. If the **TABLES** card is not already in front of the **GRAPHS** card, click the title of the **TABLES** card. The deck of cards menu area should look like:



Additional information

Please see the on-screen help for details on the functioning of each control on the **TABLES** card.

Introduction to Cerius^2 tables

Why read this section

This section introduces basic features of the Table Manager window, which controls the display of tables. Since each part of this window is presented where relevant in the task-oriented sections that follow (*Managing and editing tables*), this section is mainly useful as an overview or if you don't have a table displayed on your screen.

Finding information

This section includes information on:

The table window

Keeping track of the current table

You should already know...

How to access the Tables module is described under *Accessing the tools*). Mouse functions and keyboard shortcuts are summarized in *Mouse and Keyboard Actions*.

Additional information

Please see the on-screen help for details on the functioning of each control in the Table Manager window.

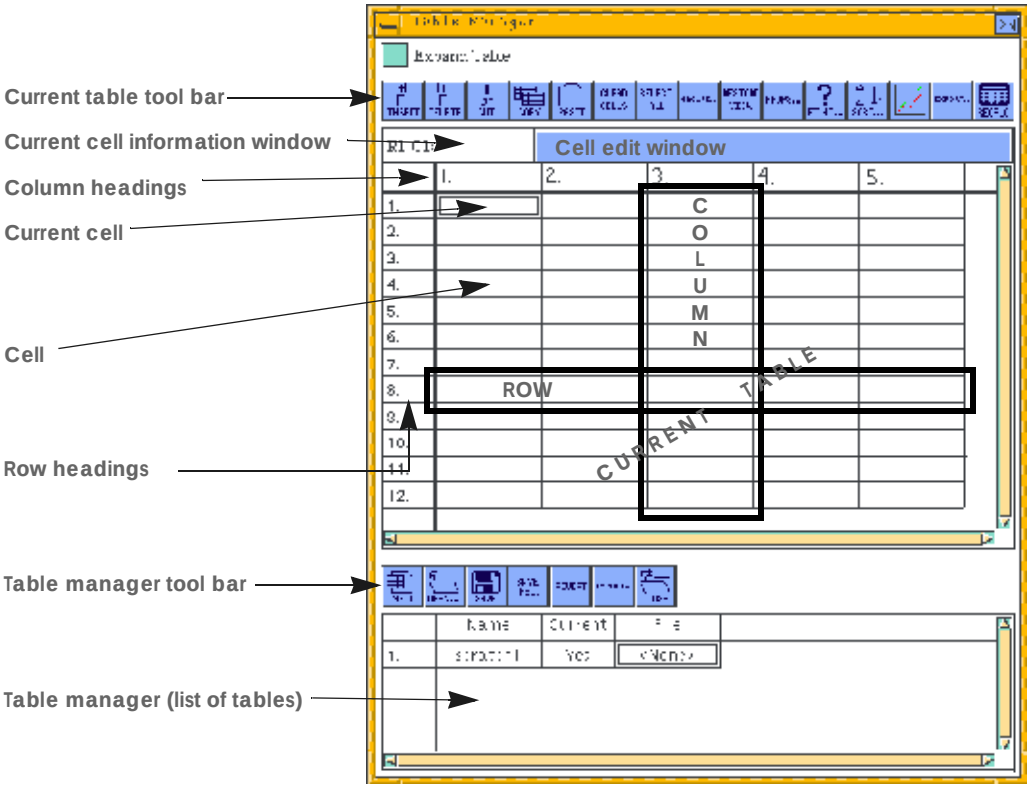
The table window

How it works

Any of several tables that are present in computer memory can be displayed, one at a time, in the table window. The *current table* is selected with the *table manager*, which is located near the bottom of the table window. The current table then appears in the current table area of the table window, where it may be edited and formatted, etc.

Accessing the tools

Click the **Show Table Manager** menu item on the **TABLES** card to display the Table Manager (or *table*) window. A new, empty table window appears:



Sections of the table window

The two major sections of the table window are the upper (main) table section, which displays the contents of the current table, and the lower table manager section, which lists all tables currently in computer memory *and* under the control of the Table Manager window. (This table manager does *not* necessarily keep track of tables created by other Cerius^2 applications, for example, the C^2•QSAR+ module's Study Table.)

The tools in the *current table tool bar* affect only the current table (see *Specifying the current table*) and can be used to change parts of the table. Examples include specifying alignment, grid type, and numeric properties; formatting; and activities like cutting, copying, and pasting values.

The tools in the *table manager tool bar* operate on tables as a whole. Examples include creating a new table and opening an existing

table, as well as saving and closing a table. You do not need to select any portion of the table to perform these types of activities.

Keeping track of the current table

How it works

The table manager has several control panels that can be open at the same time. Each control panel keeps track of the current table and updates its display to reflect the current conditions for the active table.

Precautions

When using control panels accessed from the Table Manager window or the **TABLES** card, you need to be sure of which table the panel is "attached" to, that is, which table is affected by using the tools in the control panel.

Note that the table window includes two tabular displays that contain a current cell: the current table in the main table section, and the list of tables in the table manager section. Therefore:

Caution

When you are working in a control panel, make sure its **Table** entry box contains **main_table**. Otherwise, changes you make may be applied to the list of tables rather than the current table.

In addition, you may have several table windows open simultaneously, which may be associated with different Cerius^2 modules. If so, control panels need to be attached to *both* the correct table and the correct table window (many table-related control panels can operate on *any* displayed table, even if the Table Manager window does not know about that table). Therefore:

Tip

If you have several table windows open, it is good practice to click once in the table window with which you are working *before* using tools in a control panel. This assures that the control panel's **Table** entry box refers to the correct current table.

Managing and editing tables

Why read this section

If you run calculations in any application modules that output tables, you need to know at least how to load, save, and close

tables and how to specify the current table in the table manager window.

The other information in this section is useful if you want to create tables by hand or from an imported text file, to edit any table, or to move around in tables that are larger than the current table display area in the table window.

Finding information

This section includes information on:

Creating a new table

Loading and reloading tables

Importing an ASCII text file into a new table

Specifying the current table

Entering values and editing individual cells

Copying, moving, and clearing information

Inserting and deleting entire rows or columns

Table expansion and cursor control

Saving a table

Closing a table

Related information

Table style and format is presented under *Table style and display*.

You should already know...

How to access the Tables module is described under *Accessing the tools*. How to display a table window is shown under *Accessing the tools*.

Concepts

Table management tasks are those that apply to tables as a whole rather than to the rows and columns of a table. In the Cerius^2 Tables module, table management functions are accomplished in the table manager section of the Table Manager window.

Creating a new table

You can create a new, empty table and fill it in by hand (this section), or you can create a Cerius^2 table from an ASCII text file (*Importing an ASCII text file into a new table*).

Creating a new empty table

To create a new, empty table, either:

- Click the **NEW** tool in the table manager tool bar (for illustration, see *Accessing the tools*) of the table window.

  or:

- Select the **File/New** menu item from the **TABLES** card.

The new, empty table appears (as the current table) in the main section of the table window.

Loading and reloading tables

Tables that have been created and saved to a file (*Saving a table*) can be loaded into a subsequent Cerius^2 session.

In addition, you can revert to the previously saved version of a table file if you want to discard changes that you made since the last time you saved the table.

Loading saved table files

To load a table, you need to access the Open Table control panel:

- Click the **OPEN** tool in the table manager tool bar.

  or:

- Select the **File/Open** menu item from the **TABLES** card.

Using the file browser in the control panel to navigate the directory structure is fairly intuitive. The procedure is described under *Loading model structure files*.

Reloading the current table

To revert to the previously saved version of the current table:

- Click the **REVERT** tool in the table manager tool bar.

  or:

- Select the **File/Revert** menu item from the **TABLES** card.

Any changes you made since you last saved the table are lost when the table file is reloaded.

Additional information

Please see the on-screen help for details on the functioning of each control in the Open Table control panel.

File formats

Note that two different filetypes end in .tbl: those produced by Cerius^2 are table files, but those produced by Insight II are graphs.

Importing an ASCII text file into a new table

You can create a table by importing appropriately formatted data from an ASCII text file.

File format

To be imported into the Cerius^2 Tables module, the file must be as ASCII text file and meet these requirements:

- Columns of numerical or text data must be separated by a specific separator character. The same character must separate each column.
- If a column contains text and at least one entry in that column consists of more than one word, each entry in the text column must be enclosed in a specific delimiter character.

For example:

```
"Sample"    "X1"  "X2"   "X3"   "X4"
"A 17"      7     26     6      60
"B 16"      12    9      15     52
"C"         11    56     8      20
"D 118"     11    31     8      47
"A 12"      7     52     6      33
```

Accessing the tools

To access the Import Table control panel:

- Click the **IMPORT...** tool in the table manager tool bar.

  or:

- Select the **File/Import** menu item from the **TABLES** card.

Finding the file

Using the file browser in the control panel to navigate the directory structure is fairly intuitive. The procedure is described under *Loading model structure files*.

The file extension .dat is present in the filename entry box by default, but you may use any extension. Enter the name of the file containing tabular data.

Interpreting the file contents

Since Cerius^2 has no way of automatically knowing how the data is presented in the file, you need to specify whether the file contains row and/or column headings (labels) and what characters are used in the files to indicate new lines within text strings, to delimit text strings, and to separate columns.

If you are not sure of the file's format, you can examine it with any text editor. Alternatively, you can load the file with the Import Table control panel (*Importing the data*), examine the loaded table in the table window, and then if necessary, close the table (*Closing a table*) without saving any changes and then re-import it with different specifications.

Importing the data

Double-click the name of the desired file or select it and click the **IMPORT** pushbutton in the Import Table control panel. Cerius^2 creates a new table from the imported data, adding an untitled entry to the list of tables

Additional information

Please see the on-screen help for details on the functioning of each control in the Import Table control panel.

Specifying the current table

To edit, format, or perform other tasks that work on the contents of one table, you need to select the desired table to make it *current*. The contents of the current table are displayed in the upper section of the table window.

Making a table current

To specify a table as current, click any cell in its row (or its row heading) in the list of tables that appears in the lower (table manager) section of the table window.

Entering values and editing individual cells

Understanding cell values, types, and formats

You can generally override table-, column-, and row-wide default values for any individual cell. However, you cannot override the data type for strongly typed cells (see *Assigning data types*).

You can enter or change values only in the *current cell*. The current cell is highlighted with a rectangle, its contents appear in the cell edit window, and the cell's location and additional information about its contents appear in the current cell information window (for illustration, see *Accessing the tools*). The additional information consists of:

- The word **Derived** if the value of the current cell is derived from a calculation (see *Values and mathematical expressions*).
- The words **Read Only** if the cell cannot be modified.
- An asterisk (*****) if the cell is strongly typed and can thus contain data only of a certain type (see *Assigning data types*)

For empty cells, the default numeric data type is double (an eight-byte real number), and the default cell format is a floating point number with two decimal places. If you enter a number with more decimal places, the displayed value is rounded to two places, but the value is stored in the cell the way you enter it. You can change the format and other properties of your entries, as described under *Table style and display*.

Related information

Formatting and naming rows and columns are presented under *Table style and display*. Applying mathematical expressions to columns is discussed under *Values and mathematical expressions*.

Selecting a cell

Make the desired cell current by clicking it with the mouse or moving the cursor to that cell with the arrow, <Tab>, or <Enter> keys.

Editing cell contents

To replace the current cell's content with new content, you can simply start typing while the cursor is anywhere in the table window.

To edit or replace the current cell's content, select the cell edit window by clicking it or by pressing <Shift> <Tab> on the keyboard. Then position the cursor as desired within the content of the cell edit window (by clicking and / or using the arrow keys) and type the desired cell contents. Until you *enter* the new content (*Entering your changes*), you can edit it in the cell edit window.

Entering your changes

To *enter* your changes, do one of:

- Press <Enter> or <Tab> on the keyboard. (<Enter> makes the next cell in the column current; <Tab> makes the next cell in the row current.)

- Click another cell to make it current.

Cancelling an edit

To cancel an edit, press <Esc> on the keyboard. The previously entered value (if any) is restored.

Additional information

Mouse functions and keyboard shortcuts are summarized in *Mouse and Keyboard Actions*.

Copying, moving, and clearing information

You can copy or move values from one cell, row, or column to another. You can also clear the contents of the current cell or of selected row(s) or column(s) without removing the emptied cell(s) from the table.

Selecting rows and columns

To work with cells, columns, and rows, you generally need to select them first.

You explicitly select (and highlight) a row or column by clicking a row or column heading (for illustration, see *Accessing the tools*). For some purposes, implicit selection of a row or column is sufficient: the row and column containing the current cell (see *Selecting a cell*) are implicitly selected.

To select a continuous range of rows or columns, click the first row or column heading, then <Shift> click the last row or column heading in the range. <Shift> click to select additional contiguous rows or columns.

To select several noncontiguous rows or columns, click the first row or column heading, then <Ctrl> click each additional row or column heading that you want to select. Your final selection may contain both rows and columns.

To select all cells in the current table, do one of the following:

- Click the **SELECT ALL** tool in the current table tool bar.
- Click the top left cell in the table.
- Select the **Edit/Select All** menu item from the **TABLES** card.

Copying one or more cells

To copy the contents of selected row(s) or column(s) or the current cell to the system clipboard for later pasting to a row, column, or cell (respectively):

♦ Click the **COPY** tool in the current table tool bar.

See *Pasting a column or row* for pasting the copied information into a new location.

Moving (cutting) one or more cells

To clear (cut) the contents from selected row(s) or column(s) or the current cell and place them in the system clipboard for later pasting to a row, column, or cell (respectively):

♦ Click the **CUT** tool in the current table tool bar.

See *Pasting a column or row* for pasting the copied information into a new location.

Pasting a column or row

To paste the contents of the paste buffer (clipboard) into selected row(s) or column(s) or the current cell:

♦ Click the **PASTE** tool in the current table tool bar.

See *Copying one or more cells* and *Moving (cutting) one or more cells* for copying or cutting information into the clipboard.

Technical notes on copying, cutting, and pasting

The Cerius^2 table clipboard holds the contents of only the one most recent copy or cut operation.

Pasted rows and columns are always inserted into the table; the pasted information does not replace the contents of any selected row(s) or column(s).

If both rows and columns are selected for the copy or cut operation, Cerius^2 asks you before pasting whether you want to past the rows or the columns into the current selection. (The results are more intuitively predictable if only contiguous columns or only contiguous rows are selected during copying or cutting.)

If no region is selected before pasting, or if the selected region is differently shaped than the contents of the clipboard, the paste operation fills down and to the right starting from the top cell in the selected column, the left-most cell in the selected row, or (if no row or column is selected) the current cell.

You can use this feature to copy or move a column or row to a different part of the target column or row. For example, you can copy

rows 1–4 of a column to rows 5–8 of the target column. You do this by clicking row 5 of the target column before pasting. You can offset the pasted-in information by making some cell other than the first one in row 5 current and *not* selecting the entire row.

It makes no difference if the target region is larger than the region contained in the clipboard. The pasted-in material either (if it is from one cell) replaces the contents of the current cell or (if it is a row or column) is inserted into the current table, displacing the selected area down or to the right (see *Inserting and deleting entire rows or columns* for information on inserting columns and rows).

Clearing one or more cells

To clear the values in the selected row(s) or column(s) or of the current cell (clearing does not remove mathematical expressions, see *Deleting expressions*):

- Click the **CLEAR CELLS** tool in the current table tool bar.

  or:

- Select the **Edit/Clear** menu item from the **TABLES** card.

Technical notes on cutting, deleting, and clearing

You can cut or clear the contents of rows, columns, or cells (*Moving (cutting) one or more cells* and *Clearing one or more cells*), and you can delete entire rows or columns (*Deleting columns and rows*). The differences between these superficially similar operations are:

- *Clearing* removes the information from the cell(s) and leaves the empty cells in the current table.
- *Cutting* removes the information from the cell(s), places the information in the clipboard, and either leaves the empty cell in the table (if only the current cell was cut) or removes the now-empty cells from the current table (if entire rows or columns were cut).
- *Deleting* applies only to entire rows or columns. It removes both the information and the row or column from the current table.

Inserting and deleting entire rows or columns

You can insert or delete entire rows or columns.

Related information

Selecting columns, rows, and cells is presented in *Selecting rows and columns*. The differences between cutting, clearing, and deleting are summarized under *Technical notes on copying, cutting, and pasting*.

Inserting columns and rows

To insert a new, empty column to the left of the selected column or current cell or to insert a new, empty row above the selected row or current cell:

- Click the **INSERT** tool in the current table tool bar.

  or:

- Select the **Edit/Insert** menu item from the **TABLES** card.

If you selected only a cell, choose **Row** or **Column** in the message window that appears.

Tip

Select two (or three, four, or more) rows or columns if you want two (or three, four, or more, respectively) new, empty rows or columns to be inserted.

To insert a new column on the far right side of the table or a new row at the bottom of the table, please see *Table expansion and cursor control*.

Deleting columns and rows

To delete the selected column(s) or row(s) or the column or row containing the current cell:

- Click the **DELETE** tool in the current table tool bar.

  or:

- Select the **Edit/Delete** menu item from the **TABLES** card.

If you selected only a cell, choose **Row** or **Column** in the message window that appears.

Caution

Cerius^2 does not ask you to confirm a row or column deletion. The information contained in these columns or rows is lost when they are deleted (unless you previously saved the table to a file).

Table expansion and cursor control

Tables opened from a file, and certain tables generated by Cerius^2 modules, have an initially fixed number of rows and columns. You may want to allow the current table to automatically expand when you use the arrow, <Tab>, or <Enter> keys.

Enabling table expansion

To enable the current table to automatically expand beyond its fixed size when you use the arrow, <Tab>, or <Enter> keys, check the **Expand Table** check box in the table window.

Enabling cursor wrap

To enable the cursor to wrap to the next column or row when you get to the end of a preceding column or row by using the arrow, <Tab>, or <Enter> keys, uncheck the **Expand Table** check box in the table window.

Saving a table

Saving and naming a table file

To save a table file for the first time (when you need to give it a name and specify a directory in which to save it) or to save a file under a different name (or in a different directory) from the previous version, you need to use the Save Table control panel:

- Click the **SAVE AS...** tool in the table manager tool bar.

  or:

- Select the **File/Save As** menu item from the **TABLES** card.

Enter a filename in the entry box and click the **SAVE** pushbutton to save your file.

Use of the file selection list box and other file selector controls to navigate the directory structure is presented in detail under *Finding model file(s)*. Creating your own directories or subdirectories is described in *Making custom directories*.

Resaving a table file

A file that has been saved previously can be saved again without using the Save Table control panel.

To resave a file in the same directory and with the same filename as before:

- Click the **SAVE** tool in the table manager tool bar.

  or:

- Select the **File/Save** menu item from the **TABLES** card.

If the current table has previously been saved to a file, it is resaved as the same file, overwriting the previous version.

If the file has never been saved before, the Save Table control panel (*Saving and naming a table file*) appears so that you can name the file and specify a directory in which to place it.

Saving only part of a table

If you want to save only part of a table in MSI format, you need to "export" the table (*Exporting table information*).

Additional information

Please see the on-screen help for details on the functioning of each control in the Save Table control panel.

File formats

Cerius^2 saves tables in MSI .tbl format and automatically adds .tbl to the filename if you have not specified some other extension.

Closing a table

You may remove any unwanted tables from the current Cerius^2 session at any time by closing them.

Closing a table

To close the current table, you can:

- Click the **CLOSE** tool in the table manager tool bar.

  or:

- Select the **File/Close** menu item from the **TABLES** card.

Table style and display

When you create a new table or when a Cerius^2 application generates a table, the cells have a default set of properties. Many table properties can be modified to meet your specific requirements for how your data is displayed. You can modify the properties of all cells in a table, of the cells in the current selection, or of the cells in a named group.

Finding information

This section includes information on:

Aligning information within columns

Assigning data types

Setting display formats

Specifying headings and banners

Changing row, column, and heading sizes

You should already know...

How to access the Tables module is described under *Accessing the tools*. How to select a table for display and editing is discussed under *Specifying the current table*. How to select columns (*Selecting rows and columns*) and make a cell current (*Selecting a cell*) are described above.

Aligning information within columns

You can align cell content in selected column(s) or the current cell both vertically and horizontally. As with many functions in the Table Properties control panel, alignment does not work on selected rows—if you select a row, only the current cell in that row is aligned as specified.

Accessing the tools

To modify any table properties, you need to access the Table Properties control panel:

- Click the **PROPS...** tool in the table manager tool bar.

  or:

- Select the **Data/Properties** menu item from the **TABLES** card.

To align the contents of selected columns or of the whole table, access the Alignment pane of the Table Properties control panel by setting the **Properties** popup to **Alignment**.

Aligning selected columns or the current cell

Assure that the **Selection** control is selected, select the desired **Horizontal** and **Vertical** alignments, and click the **APPLY TO** pushbutton. The contents of the selected column(s) or of the current cell (if no column is selected) are aligned as specified.

Aligning the entire table

Assure that the **Entire Table** control is selected, select the desired **Horizontal** and **Vertical** alignments, and click the **APPLY TO** pushbutton. The contents of all columns in the table are aligned as specified.

Aligning named groups

Columns within named groups (*Grouping table information*) can similarly be alligned, by selecting the **Group** command and choosing the desired group from the **Group** pulldown.

Additional information

Please see the on-screen help for details on the functioning of each control in the Table Properties control panel.

Assigning data types

You can assign or reassign data types to selected column(s) or the current cell. The *data type* determines whether content that is subsequently entered in that cell or column is interpreted as real numbers, Booleans, text, etc. The type interacts with the cell format (*Setting display formats*) to affect how the cell content is displayed.

For example, when **false** is entered into a (weakly typed) character or real-number type cell, it is displayed and interpreted merely as text (and therefore evaluates to **True** if the format is subsequently changed to **True/False**, since it is true that the cell *has* content). However, when **false** is entered into a Boolean type cell, it is interpreted and displayed as **0.00** if the format is set to a floating-point real number or as **False** if the format is set to **True/False**.

Note

If a table generated by a Cerius^2 application module contains strongly typed cells, you cannot change the data type for those cells.

Accessing the tools

To assign or reassign data types, access the Table Properties control panel as above (see *Accessing the tools*) and set the **Properties** popup to **Datatype** to access the Datatype controls.

Assigning data types

To assign a data type to the selected column(s), the current cell (if no column is selected), or the entire table, choose the desired data type from the **Column/Cell Data Type** list box. Assure that **Selection**, **Entire Table**, or **Group** is set as desired, then click the **APPLY TO** pushbutton.

Additional information

Please see the on-screen help for details on the functioning of each control in the Table Properties control panel.

Setting display formats

You can assign a display format to selected column(s) containing numeric, Boolean, text, or model data. (You can also assign a display format to the current cell or the entire table.) These formats affect only how numbers are displayed—the full number is retained in computer memory and stored with the table.

Accessing the tools

To assign or reassign display formats for numeric, Boolean, or model data, access the Table Properties control panel as above (see *Accessing the tools*) and set the **Properties** popup to **Format** to access the Format controls.

To assign a display format to the selected column(s), the current cell (if no column is selected), or the entire table, choose the desired format (see below) from the list box. Assure that **Selection**, **Entire Table**, or **Group** is set as desired, then click the **APPLY TO** pushbutton.

Changing the display format for integers and real numbers

You can display numbers as integers (real numbers are rounded to the nearest integer), as floating-point real numbers, or as real numbers in scientific notation.

For either real-number format, you can enter the number of decimal places to display in the **Decimal Places** entry box.

Changing the display format for Booleans

Cell contents can be displayed in Boolean format as either **Yes/No** or **True/False** alternatives. A value of zero or an expression that evaluates to "False" is displayed as **No** or **False**, any other value is displayed as **Yes** or **True**, and empty cells remain empty.

Mapping numbers to categories

You can display numerical data as a limited set of text items called *categories*. Real numbers are rounded to the nearest integer for this purpose. Values that round to 1 (not zero) are assigned the first item in the set.

For example, you might want to display the values 1, 2, 3, etc. as the color names red, orange, yellow, etc. To do this, you select **Category** from the list box in the Table Properties control panel and then enter **red,orange,yellow,green,blue,violet** in the Categories entry box. Numbers that round to 1, 2, 3, 4, 5, or 6 are displayed as

red, **orange**, **yellow** (etc.), respectively. Numbers outside this range are displayed as **<Unknown>**.

Changing the display of text

You can change the display of text from native (i.e., the text as entered) to all uppercase or all lowercase letters (and can return to the "native" format).

Changing the display format of model data

Model data can be displayed as small 2D structure diagrams or as the chemical formula, chemical name, or the internal Cerius^2 identification number for that model.

Additional information

Please see the on-screen help for details on the functioning of each control in the Table Properties control panel.

Specifying headings and banners

You can enter text into the row and column headings and choose to display the headings *or* the row or column numbers (or both headings and numbers). You can also prevent a row or column from scrolling when you scroll the rest of the table, making it, in effect, an additional heading or banner row or column.

Accessing the tools

To label selected rows or columns (that is, enter some text to be displayed in the row or column headings) or to lock the scroll function for selected rows or columns, access the Table Properties control panel as above (see *Accessing the tools*) and set the **Properties** popup to **Row** or **Column**, respectively. The resulting control panel is referred to as the Row or Column pane of the Table Properties control panel.

To specify whether to show row or column headings, access the Table Properties control panel as above (see *Accessing the tools*) and set the **Properties** popup to **Heading**. The resulting control panel is referred to as the Heading pane of the Table Properties control panel.

Entering and displaying row headings

In the Row pane of the Table Properties control panel, enter the heading text for the selected row(s) in the **Row Name** entry box and assure that the **Row Name** check box is checked. Click the **APPLY TO** pushbutton.

Next, in the Heading pane of the Table Properties control panel, check either or both the **Show Row Names** and **Show Row Numbers** check boxes. Click the **APPLY TO** pushbutton.

You may want to change the width of the heading column (*Changing heading sizes*).

Entering and displaying column headings

In the Column pane of the Table Properties control panel, enter the heading text for the selected column(s) in the **Column Name** entry box and assure that the **Column Name** check box is checked.

If you want a second line of heading (often used to specify the units for the data, e.g., kcal or angstroms), enter the text in the **Column Units** entry box and assure that the **Column Units** check box is checked. Click the **APPLY TO** pushbutton.

Next, in the Heading pane of the Table Properties control panel, check one or more of the **Show Column Names**, **Show Column Numbers**, and **Show Column Units** check boxes. Click the **APPLY TO** pushbutton.

To display two lines of heading, you probably need to increase the height of the heading row (*Changing heading sizes*).

Specifying banners

To prevent a row or column from scrolling off the screen when the rest of a large table is scrolled, use the Row or Column pane (respectively) of the Table Properties control panel. Check the **Lock Row Scroll** or **Lock Column Scroll** check box (respectively) and click the **APPLY TO** pushbutton.

Additional information

Please see the on-screen help for details on the functioning of each control in the Table Properties control panel.

Changing row, column, and heading sizes

You can change the width of any column, including the column containing the row headings, and can change the height of any row, including the row containing the column headings.

Changing column width and row height

To resize a column, drag the line to the right of a column in the column heading area of the current table display. The cursor changes to red double arrows to indicate it is over the line.

Alternatively, access the Table Properties control panel as above (see *Accessing the tools*) and set the **Properties** popup to **Column**. Enter the desired width in the **Column Width** entry box and click the **APPLY TO** pushbutton.

To resize a row, drag the line below a row in the row heading area of the current table display. The cursor changes to red double arrows to indicate it is over the line.

Alternatively, access the Table Properties control panel as above (see *Accessing the tools*) and set the **Properties** popup to **Row**. Enter the desired height in the **Row Height** entry box and click the **APPLY TO** pushbutton. Rows may not be less than 0.25 inches high.

If more than one row or column is selected, all are resized equally.

Changing heading sizes

To change the depth of column headings, access the Table Properties control panel as above (see *Accessing the tools*) and set the **Properties** popup to **Heading**. Enter the desired value in the **Column Heading Height** entry box and click the **APPLY TO** pushbutton. Column heading rows may not be less than 0.25 inches high.

To change the width of row headings, access the Table Properties control panel as above (see *Accessing the tools*) and set the **Properties** popup to **Heading**. Enter the desired value in the **Row Heading Width** entry box and click the **APPLY TO** pushbutton.

Using grid lines

To change how cells are delineated, access the Table Properties control panel as above (see *Accessing the tools*) and set the **Properties** popup to **Grid**. Set the **Horizontal Lines** and **Vertical Lines** as desired and click the **APPLY TO** pushbutton.

Additional information

Please see the on-screen help for details on the functioning of each control in the Table Properties control panel.

Values and mathematical expressions

A mathematical expression can be applied to a cell or column. The cell displays the value derived from the expression, *not* the expression itself. The expression may contain scientific constants, binary math and text operators, built-in operators, unary math and text operators, trigonometric operators, statistical operators and transformations, binary and unary molecule operators, and command operators. The expression can return (that is, generate) numbers, text, or models.

Finding information

This section includes information on:

Applying mathematical expressions to cells or columns

Entering mathematical expressions

Recalculating table values

You should already know...

How to access the Tables module is described under *Accessing the tools.* How to select a table for display and editing is discussed in *Specifying the current table.* How to select columns (*Selecting rows and columns*) and make a cell current (*Selecting a cell*) are described above.

Applying mathematical expressions to cells or columns

Concepts

The following terms define the relationship between values and mathematical expressions ("derivations") in Cerius^2 tables:

- *Value*—The information displayed in any cell. A cell can contain numerical, text, or model data.
- *Derived value*—The value displayed in a cell that results from the evaluation of an expression.
- *Derived cell*—A cell whose contents are derived from an expression applied only to that cell.
- *Derived column*—A column in which all cells display values derived from an expression applied to the entire column.
- *Label*—A text description you can apply to a row or column as a whole. Columns and rows can be referenced by their labels in expressions. For example: **column "velocity" * column "time"**.
- *Index*—The sequence number of a row or column, assigned by Cerius^2. Columns or rows can be referenced by their index numbers in mathematical expressions. For example: **column 2 * column 3**. To reference the current row or column in an expression, use **row#** and **col#**.

Technical notes

The type of data that cells can contain is generally assigned to all cells in a column. Cells in tables generated by Cerius^2 application modules may be weakly or strongly typed:

- Weekly typed columns—Regardless of the data type specified for a column, its cells can contain data of any type.

- Strongly typed columns—Some Cerius^2 application modules create strongly typed columns. Cells in these columns can contain *only* the type of data specified for the column.

  Generally, you cannot enter data of another type into a strongly typed cell. For example, if a strongly typed cell is assigned the character data type, you cannot enter numbers into the cell. However, Cerius^2 can convert some data into the appropriate type. For example, if a strongly typed cell is assigned the integer data type and you enter a value of 2.2, Cerius^2 rounds the value to 2 and stores it as an integer.

  How to change the data type (where possible) is presented on (*Assigning data types*).

Accessing the tools

To enter a mathematical expression into the current cell or a selected column, you can type the expression in the cell edit window (illustrated under *Accessing the tools*) and then press <Enter> or <Tab> or click some other cell to *enter* the expression.

Alternatively, you can use the Table Properties control panel. The Table Properties control panel allows you to, in addition, enter mathematical expressions into the entire table, selected columns, or the columns in a named (*Specifying headings and banners*) group.

To access the Table Properties control panel.

- Click the **PROPS…** tool in the table manager tool bar.

  or:

- Select the **Data/Properties** menu item from the **TABLES** card.

In the Table Properties control panel, set the **Properties** popup to **Derivation** to access the Derivation controls, then enter your mathematical expression in the **Enter Cell Derivation** entry box.

Entering mathematical expressions

The exact procedure, including the character(s) with which your mathematical expressions begin, differ depending on what tool you are using and whether you are applying the expression to the current cell or one or more selected columns:

- To enter an expression in the current cell using the cell edit window in the table window, start your expression with an equals sign (=). The rest of the expression is made up of one or more of the operators described under *Entering mathematical expres-*

sions. Press <Enter> or <Tab> or click some other cell to *enter* the expression.

- To enter an expression in every cell of a column using the cell edit window in the table window, select the column or any cell in it and start your expression with *two* equals signs (==). The rest of the expression is made up of one or more of the operators described under *Entering mathematical expressions*. Press <Enter> or <Tab> or click some other cell to *enter* the expression.
- To enter an expression in every cell of selected column(s) or the current cell using the Table Properties control panel, assure that the **Selection** control is selected and simply enter your expression in the **Enter Column Derivation** entry box, using one or more of the operators described under *Entering mathematical expressions*. Do *not* begin the expression with an equals sign. Click the **APPLY TO** pushbutton.
- To enter an expression in every cell of the current table, use the Table Properties control panel and select the **Entire Table** control. Enter your expression in the **Enter Column Derivation** entry box, using one or more of the operators described under *Entering mathematical expressions*. Do *not* begin the expression with an equals sign. Click the **APPLY TO** pushbutton.
- To enter an expression in every cell of a named group (*Grouping table information*), use the Table Properties control panel, select the **Group** control, and choose the desired group from the **Group** pulldown. Enter your expression in the **Enter Cell Derivation** entry box, using one or more of the operators described under *Entering mathematical expressions*. Do *not* begin the expression with an equals sign. Click the **APPLY TO** pushbutton.
- To apply an expression only once to a cell or column(s), so that the results are calculated and displayed but the expression is not retained, use the Table Properties control panel as above, except check the **Apply Derivation Only Once** check box.

Important

Applying an expression only once can save time later, since these expressions are not recalculated when the table is recalculated (*Recalculating table values*). However, you *should not* refer to other parts of the table (*Cross references*) in these expressions, since these unretained expressions cannot be recalculated if you change values in any of the columns, cells, etc. that are referred to.

Deleting expressions

To remove an expression from the current cell or a selected column (without deleting the calculated value), enter an expression containing only two quotes (that is, =”” or ==””) in the cell edit window.

Additional information

Please see the on-screen help for details on the functioning of each control in the Table Properties control panel.

Entering mathematical expressions

Finding information

This section includes information on:

Using numbers

Cross references

Calculations on models

Manipulating text

Table and command operations

Operators

Available components that may be included in expressions are:

- *Unary math operators*
- *Binary math operators*
- *Statistical operators*
- *Statistical transformations*
- *Trigonometric operators*
- *Cross references*
- *Constants*
- *Unary model operators*

- *Binary model operators*
- *Unary text operators*
- *Binary text operators*
- *Table operators*
- *Command operators*

Using numbers

Unary math operators

Unary math operators (Table 12) take one argument that must evaluate to a number.

Examples of expressions including unary mathematical operators are:

```
abs (col 5)
sqrt (abs (col 5 * col 6))
rand (20)
```

The column references (see *To columns…*) in this example all evaluate to numbers.

Table 12. Unary math operators in Cerius^2 table expressions

Operator	Returns	Description
–	number	Negation.
abs	number	Absolute value.
ceil	number	Return the largest integer not less than *x*.
cbrt	number	Cube root.
exp	number	Exponentiation (inverse of log).
fact	number	Factorial (*x*!).
floor	number	Return the largest integer not greater than *x*.
frac	number	Return the fractional part of *x*.
ln	number	Natural log.
log	number	Natural log.
log10	number	Log base 10.

Table 12. Unary math operators in Cerius^2 table expressions

Operator	Returns	Description
neg	number	Negation.
rand	number	Random number between zero and *x*.
sign	number	Return 1 if $x > 0.0$, return 0 if $x = 0$, return -1 if $x < 0$.
spline	number	Return *x* if $x \geq 0.0$; otherwise return zero.
sqrt	number	Square root.

Binary math operators

Binary mathematical operators (Table 13) are placed between two values, both of which must be or evaluate to numbers.

Mathematical operations using binary mathematical operators are evaluated using algebraic logic in the standard order of precedence. You can use parentheses to alter the order of precedence.

Examples of expressions including binary mathematical operators are:

```
12 + 3
4 * col 6
7 * col Concentration +2
7 * (col Concentration + 2)
```

The column references (see *To columns…*) in this example all evaluate to numbers.

If division by zero is attempted, an error message shows the row and column where the error occurred, and the cell is set to null.

Table 13. Binary math operators in Cerius^2 table expressions

Operator	Description
+	Addition.
–	Subtraction.

Table 13. Binary math operators in Cerius^2 table expressions

Operator	Description
*	Multiplication.
/	Division.
%	Modulus.
mod	Modulus.
^	Exponentiation.

Statistical operators

Statistical operators (Table 14) take one argument. This argument must refer to a collection of numeric data, such as a column, a row, or a group consisting of numeric cells. Statistical operators return null if anything else is specified.

Examples of expressions including statistical operators are:

```
mean (col 1)
max (row TG)
sum (group "query results")
```

In general, statistical operators should be used only in cell expressions, not column expressions. The column, row, and group referred to (*Cross references*) in this example all contain numerical values.

Table 14. Statistical operators in Cerius^2 table expressions

Operator	Returns	Description
avg	number	Numeric mean.
mean	number	Numeric mean (same as avg).
median	number	Median value.
sum	number	Sum of all values.
min	number	Minimum value.
max	number	Maximum value.
range	number	Numeric range (abs (max – min)).

Table 14. Statistical operators in Cerius^2 table expressions

Operator	Returns	Description
count	number	Number of non-null values in the data set.
stdev	number	Standard deviation of the population (*n*).
var	number	Variance of the population (*n*).
skew	number	Skewness.
kurtosis	number	Kurtosis.

Statistical transformations

Statistical transformations (Table 15) take one argument that must refer to a column of numeric values. They return null if anything else is specified.

Examples of expressions including statistical transformations are:

```
normalize (col 1)
scale (col TG)
```

Statistical transformations should be used only in column expressions, not cell expressions. The columns referred to (see *To columns*...) in this example all contain numerical values.

Table 15. Statistical transformations in Cerius^2 table expressions

Operator	Returns	Description
meancenter	number	Transform a data set so that its mean is 0.0.
normalize	number	Transform a data set so that its mean is 0.0 and its standard deviation is 1.0.
scale	number	Uniformly map a data set onto the range 0.0 to 1.0.

Trigonometric operators

Trigonometric operators (Table 16) take one argument that must evaluate to a number.

Examples of expressions including trigonometric operators are:

```
sind (col 5)
tan (sqrt (abs (col 5 * col 6)))
```

The column references (see *To columns…*) in this example all evaluate to numbers.

Table 16. Trigonometric operators in Cerius^2 table expressions

Operator	Returns	Description
sin	number	Sine (radians).
cos	number	Cosine (radians).
tan	number	Tangent (radians).
asin	number	Arcsine (radians).
acos	number	Arccosine (radians).
atan	number	Arctangent (radians).
sind	number	Sine (degrees).
cosd	number	Cosine (degrees).
tand	number	Tangent (degrees).
asind	number	Arcsine (degrees).
acosd	number	Arccosine (degrees).
atand	number	Arctangent (degrees).

Constants

In addition to numbers that you type in, you can use any of the physical constants shown in Table 17:

Table 17. Physical constants in Cerius^2 table expressions

Constant	Description
e	Base of the natural logarithm (2.71828).
h	Planck's constant (9.53709 E-14 kcal sec mol^{-1}).
k	Boltzmann's constant (3.2998 E-27 kcal mol^{-1} deg^{-1}).
n	Avogadro's number (6.02204 E+23 particles mol^{-1}).
pi	Pi (3.14159).
r	Gas constant (1.98717 E-3 kcal mol^{-1} deg^{-1}).

SMARTS table derivations

The following derivations can be entered as column headers in the QSAR study table:

```
==daysss(Structure, ) and

==daysss_unique(Structure, )
```

For example:

```
==daysss(Structure, “c1ccccc1”)

==daysss_unique(Structure, “[C;H1]NOH”)
```

Cross references

In writing expressions, you can refer to columns, rows, groups, or cells in the current table and to columns, rows, groups, or cells in other tables. These references are evaluated as numbers, text, or models, depending on the content of the items that are referred to.

Examples of expressions including cross references are:

```
sqrt (col 4)
sqrt (column 4)
sqrt (col Concentration)
sqrt (Concentration)
sqrt (col "H2SO4 Conc")
mean (row 6)
mean (row TG)
sum (group "query results") * 5
```

To columns...

You can refer to a column in any expression. The syntax for column cross references is any of:

```
col index
col name
column index
column name
name
```

The column *name* (*Setting display formats*) must be enclosed in quotes (") if it contains spaces.

rows...

You can refer to rows only within statistical operators (*Statistical operators*). The syntax for row cross references is any of:

```
row index
row name
```

The row *name* (*Setting display formats*) must be enclosed in quotes (") if it contains spaces.

groups...

You can refer to groups (*Grouping table information*) only within statistical operators (*Statistical operators*). The syntax for group cross references is:

```
group name
```

The group *name* (*Creating a named group*) must be enclosed in quotes (") if it contains spaces.

cells...

You can refer to a named cell in any expression. The syntax for cell cross references is:

```
cell name
```

You cannot name cells, but some application modules may name certain cells. The cell *name* must be enclosed in quotes (") if it contains spaces.

...and other tables

You can refer to named columns, rows, groups, or cells that are contained in other tables. The syntax for table cross references is any of:

```
col table_name::col_name
row table_name::row_name
group table_name::group_name
cell table_name::cell_name
```

The *table_name* is the name of the table in which the named entry is found. All names that contain spaces must be enclosed in quotes (").

Calculations on models

Columns in Cerius^2 tables may contain chemical models (*Models in tables*), and calculations may be performed using these models.

Unary model operators

Unary model operators (Table 18) take one argument, which must evaluate to a cell of type molecular. The operators return null if anything else is specified.

Examples of unary model operators are:

```
mw (col Structure)
atoms (col 1) / bonds (col 1)
```

Table 18. Unary model operators in Cerius^2 table expressions

Operator	Returns	Description
atoms	number	Number of atoms.
bonds	number	Number of bonds.
idtomol	chemical data	Convert a model ID number (assigned in the model table) into a model.
inttomol	chemical data	Convert an integer into a Cerius^2 model if that integer references an entire model.
inttooid	chemical data	Convert an integer into a Cerius^2 model component (for example, an atom, a bond, or an entire model).
isvisible	number	Return 1 if the model is visible and 0 (zero) if the model is invisible.
makecurrent	0 (zero)	Make the referenced model the current model.
mf	text	Molecular formula.
mw	number	Molecular weight.
numchildren	number	The number of dependent objects contained in the parent object. For a model, this includes the total number of atoms and bonds, along with any other objects included in the model.
thename	text	Object name.

Binary model operators

Binary model operators (Table 19) take two arguments. The first argument must evaluate to a cell of type molecular. The operators return null if anything else is specified.

Several of these operators use atom names to specify the second argument. Atom names can be separated by commas or hyphens if more than one atom name is required. (Hyphens work exactly like columns in these table expressions; hyphens do *not* indicate ranges of atoms.)

The following examples assume that column one contains molecular type data:

```
distance (col Structure, "CA-CB")
charge (col 1, "CA") / bonds (col 1)
```

Tip

Some expressions involving models can be complicated to set up manually. Provided you have the desired model present in the model window, Cerius^2 can calculate certain properties and automatically insert them in a table column (for details, see *Setting up calculations on models*).

Table 19. Binary model operators in Cerius^2 table expressions

Operator	Returns	Description
angle	number	Bond angle in degrees (atoms referenced using a named triple). Usage: angle (col structure, "C1,C2,C3")
anglebyname	number	Bond angle in degrees (atoms referenced using a user-assigned name). Usage: angle (col structure, "CA,CB,CC")
charge	number	Partial atomic charge of a named atom. Usage: charge (col structure, "C1")
chargebyname	number	Partial atomic charge of an atom referenced using a user-assigned name. Usage: charge (col structure, "CA")
distance	number	Interatomic distance (atoms referenced using a named pair). Usage: distance (col structure, "C1,C2")
distancebyname	number	Interatomic distance (atoms referenced using a user-assigned name). Usage: distance (col structure, "CA,CB")
ecount	number	Count the number of occurrences of a specified element. Usage: ecount (col structure, "C")
exact	number	Perform an exact search for an object and count the number of occurrences found. Hydrogens are *not* ignored. Usage: exact (col structure, cell frag_tbl::CO)
smol	number	Calculate various steric properties of a molecule. No coordinate transformations are made as part of this calculation. Thus, the result of this calculation changes as the molecule is reoriented. Properties are: RX—Range of x coordinate values RY—Range of y coordinate values RZ—Range of z coordinate values MINX—Smallest x coordinate value MINY—Smallest y coordinate value MINZ—Smallest z coordinate value MAXX—Largest x coordinate value MAXY—Largest y coordinate value MAXZ—Largest z coordinate value VOLUME—Volume of the box in which the molecule is contained Usage: smol (col structure, "RX")
sss	number	Perform a substructure search for an object and count the number of occurrences found. Hydrogens are ignored. Usage: sss (col structure, cell frag_tbl::CO)

Table 19. Binary model operators in Cerius^2 table expressions

Operator	Returns	Description
torsion	number	Torsion angle (atoms referenced using a named quad). Usage: torsion (col structure, "C1,C2,C3,C4")
torsionbyname	number	Torsion angle (atoms referenced using a user-assigned name). Usage: torsion (col structure, "CA,CB,CC,CD")
userdata	text	Return the named user data from the object (if the field exists). Array-based user data fields are not supported. Usage: userdata (col structure, "Rotatable_Torsions")

Additional information

Please see the on-screen help for details on the functioning of each control in the Tabulate Atom Properties control panel.

Manipulating text

Unary text operators

Unary text operators (Table 20) take one argument that must evaluate to characters. This argument either controls the operation of the function or is the text to be operated upon.

Table 20. Unary text operators in Cerius^2 table expressions

Operator	Returns	Description
cdate	text	Return time and date based on the input argument: TODAY—Today's date. NOW—Today's date and time. YEAR—Current year. MONTH—Current month. DAY—Current day. DOW—Current day of the week. TIME—Current time.
ctext	text	Convert an entity to a text string.
reverse	text	Reverse the order of characters in a string.
strlen	number	Return the length of a string.
tolower	text	Convert text to lower case.
toupper	text	Convert text to upper case.

Binary text operators

Binary text operators (Table 21) are placed between two values, both of which must evaluate to characters.

Table 21. Binary text operators in Cerius^2 table expressions

Operator	Returns	Description
+	text	Concatenate text strings (for example, "A" + "B" produces "AB").
cattonumber	number	Convert a category[1] to its corresponding ordinal.
format	text	Format an entity based on a C-style format string in the second argument, e.g.: format (col Activity, "%8.3f").
numbertocat	text	Convert an ordinal number to the corresponding category[1].

[1] Categories are described under *Mapping numbers to categories*.

Table and command operations

Table operators

Table operators (Table 22) take no arguments. They return the row or column number of the current cell.

Table 22. Table operators in Cerius^2 table expressions

Operator	Returns	Description
row#	number	Current row index.
col#	number	Current column index.

Command operators

Command operators (Table 23) enable you to run Cerius^2 command scripts and / or evaluate Tcl (Tool Command Language) expressions and return the results to table cells. These operators take a single argument that must evaluate to one or more Cerius^2 commands or one or more legal Tcl commands. For more information about Cerius^2 and Tcl commands, refer to *Cerius^2 Command Script Guide*.

Table 23. Command operators in Cerius^2 table expressions

Operator	Returns	Description
eval	any	Evaluate a Cerius^2 or Tcl command and return the result.
source	any	Open the file named in the argument, evaluate each Cerius^2 or Tcl command in that file, and return the result.

Recalculating table values

How it works

When you type in or edit an expression for a column or cell using the cell edit window in the table window, Cerius^2 calculates and displays the value of the derivation as soon as you enter the derivation by pressing <Enter> (*Entering mathematical expressions*).

If you use the Derivation pane of the Table Properties control panel (*Entering mathematical expressions*) to enter or edit an expression, Cerius^2 calculates and displays the value of the derivation as soon as you click the **APPLY TO** pushbutton.

If you change the values in a column, row, group, or cell that is referred to in another cell or column's expression, the values in that cell or column are *not* recalculated until you request that the table be recalculated.

Recalculating table values

To recalculate all the expressions in the current table:

- Click the **RECALC** tool in the table manager tool bar.

  or:

- Select the **Data/Recalculate** menu item from the **TABLES** card.

To select a cell, column, or row and also send to Cerius^2 any command that has been associated with that cell, column, or row by a module, double-click the cell or the column or row heading.

Models in tables

Cerius^2 tables can store model information in table cells and can display this information in several formats (*Setting display formats*). You can also store atoms, bonds, and several other types of chemical data in the columns and cells of Cerius^2 tables.

Uses of model data in tables

You can perform certain model-specific operations on model columns and can include model operators in mathematical expressions (*Values and mathematical expressions*) in other columns that refer to a cell containing a model.

Finding information

This section includes information on:

Copying models into columns

Setting up calculations on models

Saving tables containing models

You should already know...

How to access the Tables module is described under *Accessing the tools*. How to select a table for display and editing (*Specifying the current table*) and how to make sure control panels are connected to the desired table window (*Keeping track of the current table*) are discussed above. How to select columns (*Selecting rows and columns*) and make a cell current (*Selecting a cell*) are described above.

Copying models into columns

Tables generated and presented by other Cerius^2 modules, such as QSAR+, may contain models in columns.

You cannot copy models from the model window to a model data type column in a table. However, you can copy a model column from a table generated by another Cerius^2 module, such as QSAR+, into some other table.

Copying models from other tables

Copying columns from one table to another is essentially the same as copying columns from one part of a table to another part of the same table (*Copying, moving, and clearing information*).

The tables need not be displayed in the same table window. However, if they are being handled by the same table manager, the table whose column(s) are being copied needs to be displayed as the current table (*Specifying the current table*), and then the other table needs to be made current in order to paste the column(s) into it.

The data type of the newly pasted column (*Assigning data types*) is automatically set to the model type.

Setting up calculations on models

Since it can be tedious to set up mathematical expressions including model references by hand (*Binary model operators*), Cerius^2 can calculate certain properties and automatically insert them in a table column. The models you are working with must be present in computer memory and at least one of them must be displayed in the model window.

Accessing the tools

Select the **Data/Atomistic Properties** menu item from the **TABLE** card to access the Tabulate Atom Properties control panel.

Automated model calculations

If the table contains more than one model column, specify which one you want to refer to by choosing its name or number from the **Molecule Column** pulldown in the Tabulate Atom Properties control panel.

Several types of calculations are facilitated:

- To calculate the charge on atoms, select the **Charge** tool and click an atom in a representative model in the model window.

- To calculate the distance between pairs of atoms, select the **Distance** tool and click two atoms in a representative model in the model window.

- To calculate the angle between three atoms, select the **Angle** tool and click three atoms in a representative model in the model window.

- To calculate the dihedral angle relating four atoms, select the **Dihedral** tool and click four atoms in a representative model in the model window.

The correct mathematical expression is generated automatically and placed in an empty column in the table (on its right side). The calculated charge, distance, etc., is displayed in that column.

The term “representative model” (above) assumes that all the models in the column have some structural moiety in common. If, for example, you request the distance between atoms C1 and C2 and all models in the model column contain atoms labeled C1 and C2, then calculated values are displayed in all cells of the column containing the expression. If, however, you request the distance between C12 and C16, and these atoms are *not* present in all the models, calculated values are displayed only for those models that do have these atoms.

Tip

To input expressions into several columns simultaneously, you can select more than the number of atoms specified above and then double-click the desired tool. This method does not, for example, calculate all distances among the set of atoms selected, but the pairwise distances in the order in which atom pairs were selected.

To recalculate model expressions after changing the models (for example, after optimizing their structures), click the **RECALC** button in the current table tool bar.

Help

Checking the **Guide?** check box gives you on-screen help (in the upper left corner of the model window) on using the Tabulate Atom Properties control panel.

Additional information

Please see the on-screen help for details on the functioning of each control in the Tabulate Atom Properties control panel.

Saving tables containing models

Saving a table (*Saving a table*) that contains models saves only the model ID with the table. Structural data are not saved; therefore, structures are not displayed if you open that table file in a future

Cerius^2 session. If you want to also save the models, you need to save the session (*Saving the current session*).

Grouping table information

You can define any subset of columns and/or rows as a *group* and give that group a name. Named groups are stored in the table file when you save the table to disk.

Finding information

This section includes information on:

Creating a named group

Editing a group definition

Selecting named groups

Deleting a group definition

Uses of named groups

Groups can be used in several ways in the Cerius^2 table window. You can:

- Refer to a named group of numeric cells in statistical expressions (*Statistical operators*).
- View only a named group by collapsing the display of the table (*Viewing subsets of a table*).
- Plot the data in a named group (*Graphing table information*).
- Restrict a search to a named group (*Searching for information in a table*).
- Sort the rows in a named group made up of rows (*Sorting table information*).
- Export a named group (as a subset of the table) to a new file (*Exporting table information*).

You should already know...

How to access the Tables module is described under *Accessing the tools*. How to select a table for display and editing (*Specifying the current table*) and how to make sure control panels are connected to the desired table window (*Keeping track of the current table*) are discussed above. Selecting columns and rows is discussed under *Selecting rows and columns*.

Creating a named group

You can create a named group from a selection of rows or columns, by saving the results of a search (*Searching for information in a table*) as a group, or by duplicating an existing group.

Creating a named group from a selection

To create a named group from selected rows and / or columns, you need to access the Table Groups control panel:

- Click the **GROUPS...** tool in the table manager tool bar.

  or:

- Select the **Data/Groups** menu item from the **TABLES** card.

Assure that the **Selection** tool is selected, enter a name in the **Group Name** entry box, then click the **CREATE** pushbutton. All currently selected rows and / or columns are included in the newly defined group. (The columns and / or rows need not be contiguous.)

Defining the entire table as a named group

First defining a table as a group could be a convenient way of selecting or displaying the original table after you have added columns or rows to that table.

To create a group from the entire table, access the Table Groups control panel as under *Creating a named group from a selection*. Select the **Entire Table** tool, enter a name in the **Group Name** entry box, then click the **CREATE** pushbutton.

Creating a named group from search results

To create a named group from the results of a search, you can specify that the search results be output as a group. Before starting the search (*Searching for information in a table*), check the **Save Results** check box in the Find Cells control panel and enter a name in the associated **Group** entry box. After the search is complete, the results are defined as a named group.

Duplicating an existing group

To use an existing group as the basis for starting to define a new group, you can duplicate the original group.

To make a copy of an existing group, access the Table Groups control panel as under *Creating a named group from a selection*. Select the **Group** tool and enter the name of the group to be duplicated in the **Group** entry box by choosing its name from the associated popup.

Enter a name for the new group (the copy) in the **Group Name** entry box, then click the **CREATE** pushbutton.

Additional information

Please see the on-screen help for details on the functioning of each control in the Table Groups and Find Cells control panels.

Editing a group definition

You can add more rows and / or columns to an existing named group, merge two groups, and remove rows and / or columns from an existing group.

Adding rows or columns to a named group

To add selected rows and / or columns to an existing group, access the Table Groups control panel as under *Creating a named group from a selection*. Select the name of that group by clicking its name in the **Groups In Table** list box. Assure that the **Selection** tool is selected and click the **MERGE** pushbutton.

Merging existing groups

To merge two or more existing groups into a new, larger group, access the Table Groups control panel as under *Creating a named group from a selection*. Enter a name for the new group in the **Group Name** entry box. Select the **Group** tool and enter the name of the first group to be merged in the **Group** entry box by choosing its name from the associated popup. Click the **CREATE** pushbutton.

The new group's name appears in the **Groups In Table** list box and should be highlighted. Enter the name of the second group to be merged in the **Group** entry box by choosing its name from the associated popup and click the **MERGE** pushbutton. Repeat for any additional groups that you want to include in the new group.

To simply merge the contents of two or more existing groups without creating a new group, access the Table Groups control panel as under *Creating a named group from a selection*. Select the name of the group that you want to add material to by clicking its name in the **Groups In Table** list box. Select the **Group** tool and enter the name of the group to be merged in the **Group** entry box by choosing its name from the associated popup. Click the **MERGE** pushbutton. Repeat for any additional groups that you want to include in the enlarged group.

Removing rows or columns from a group

To remove selected rows and / or columns from an existing group, access the Table Groups control panel as under *Creating a named group from a selection*. Select the name of that group by clicking its

name in the **Groups In Table** list box. Assure that the **Selection** tool is selected and click the **REMOVE** pushbutton.

Additional information Please see the on-screen help for details on the functioning of each control in the Table Groups control panel.

Selecting named groups

You can select a group, either to use it in some task or as a way of viewing its contents.

Selecting groups To select (and highlight) an existing group, access the Table Groups control panel as under *Creating a named group from a selection*. Select the name of that group by clicking its name in the **Groups In Table** list box. Click the **SELECT** pushbutton.

Related information If you want *only* the desired named group to be visible in the table window, please see *Viewing named groups.*

Additional information Please see the on-screen help for details on the functioning of each control in the Table Groups control panel.

Deleting a group definition

You can delete a group definition from the current table. This deletes only the definition, *not* the rows and/or columns themselves, which remain in the table.

Removing named groups To remove the definition of an existing group, access the Table Groups control panel as under *Creating a named group from a selection*. Select the name of that group by clicking its name in the **Groups In Table** list box. Click the **DELETE** pushbutton.

Removing all groups To remove all group definitions from the table, click the **Delete All Groups** action button in the Table Groups control panel.

Additional information Please see the on-screen help for details on the functioning of each control in the Table Groups control panel.

Searching for information in a table

Why read this section

You can use a search facility to locate cells containing information of interest. You can specify relational operators and perform comparison operations and can save the result of the query as a table group or view the results as a subset view. You can also replace found values with new values that you specify.

You should already know...

How to access the Tables module is described under *Accessing the tools*. How to select a table for display and editing (*Specifying the current table*) and how to make sure control panels are connected to the desired table window (*Keeping track of the current table*) are discussed above. Selecting columns and rows is discussed under *Selecting rows and columns*.

Accessing the tools

To search selected rows and / or columns or the entire table, you need to access the Find Cells control panel:

- Click the **FIND...** tool in the current table tool bar.

  or:

- Select the **Data/Find** menu item from the **TABLES** card.

Where to search

You can search all or part of the current table:

- To search the whole table, set the **Find Within** option to **Entire Table**.
- To search within selected rows and / or columns, set the **Find Within** option to **Selection**.
- To search within groups (if any are defined in the current table, *Grouping table information*), set the **Find Within** option to **Group** and choose the desired group from the **Group** pulldown.

What to look for

To find any string of alphanumeric characters, enter what you want to look for in the **Find** entry box. The associated popup must be set to **Text**.

To search for exact matches to your entered characters, assure that the **Where Cells Are** popup is set to an equals sign (**=**). (To search for values that are greater than or less than (etc.) your entered characters, see *What constitutes a find*.)

Potential text matches are compared with your entered characters as text strings. Case is ignored in character matches unless you check the **Case Sensitive** check box. Potential numeric matches are compared with your entered characters as numbers, unless you check the **Compare Numbers as Text** check box.

To search for all empty cells, set the **Find** popup to **Null Cells**.

What constitutes a find

To perform tests other than exact matches between the potential matches and your entered characters, change the **Where Cells Are** popup from an equals sign (**=**) to some other criterion (Table 24).

Text comparisons are done alphabetically. For example, searching for cells containing values greater than **m** would match toluene and xylene, but not acetate.

Table 24. Comparison criteria in Cerius^2 table searches

Relational operator	Description
=	Search cells for an exact match to the entered characters[1].
~	Search cells for an approximate match to the entered characters, using a tolerance value specified in the **Tolerance** entry box.
!=	Search cells for items that do *not* match the entered characters.
>	Search cells for items that are greater than the entered characters.
>=	Search cells for items that are greater than or equal to the entered characters.
<	Search cells for items that are less than the entered characters.
<=	Search cells for items that are less than or equal to the entered characters.
in	For text comparisons, search cells to determine whether the entered characters is contained within a cell value. In a replace operation, *only* the *matching* content of the found cell(s) is replaced with the specified replacement characters. For example, suppose the entered characters[1] **bcd** is to be replaced with the value **BCD**. If the string **AbcdEF** is found, it is replaced with **ABCDEF** (not simply BCD).
!in	For text comparisons, search cells to determine whether the entered characters are *not* contained within a cell value.

[1]That is, the characters you entered in the **Find** entry box.

Changing the contents of "found" cells

To replace found material with something else, enter the replacement characters in the **Replace** entry box and assure that the associated popup is set to **Text**.

To delete found material from the cells containing them, set the **Replace** popup to **Null Cells**.

(Then initiate the search by clicking the **FIND & REPLACE** pushbutton, see *Initiating the search*.)

Where to put the results

Ordinarily, "found" cells are just highlighted after the search is complete. However, you may also:

- View only the rows and columns that contain the found cells by checking the **View Results** check box. Additional information on viewing subsets of a table starts under *Viewing subsets of a table*.

  and / or:

- Define the rows and columns that contain the found cells as a group by checking the **Save Results** check box and entering a group name in the associated **Group** entry box. Additional information on groups in tables is in *Grouping table information*.

Initiating the search

To simply search for the desired information, click the **FIND** pushbutton in the Find Cells control panel.

To search for information and replace it with the specified text, click the **FIND & REPLACE** pushbutton in the Find Cells control panel.

Additional information

Please see the on-screen help for details on the functioning of each control in the Find Cells control panel.

Viewing subsets of a table

You can collapse the view of a table so that only a designated set of rows or columns is displayed. You can toggle between viewing the full table and viewing the designated subset.

Finding information

This section includes information on:

Viewing named groups

Viewing search results

You should already know...

How to access the Tables module is described under *Accessing the tools*. How to select a table for display and editing (*Specifying the current table*) and how to make sure control panels are connected to the desired table window (*Keeping track of the current table*) are discussed above.

Viewing named groups

Accessing the tools

To view only a named group, you need to access the Table Groups control panel:

- Click the **GROUPS...** tool in the table manager tool bar.

  or:

- Select the **Data/Groups** menu item from the **TABLES** card.

Viewing named groups

To view only an existing group, select the name of that group by clicking its name in the **Groups In Table** list box in the Table Groups control panel. Click the **VIEW** pushbutton.

Viewing the whole table

To view the entire table, do one of thee:

- Click the **RESTORE VIEW** pushbutton in the Table Groups control panel.

- Click the **RESTORE VIEW** tool in the table manager tool bar.
- Select the **Data/Restore View** menu item from the **TABLES** card.

Related information

Creation of named groups is discussed under *Grouping table information*. If you just want to highlight the desired named group (without hiding columns or rows that are not in the group), please see *Selecting named groups*.

Additional information

Please see the on-screen help for details on the functioning of each control in the Table Groups control panel.

Viewing search results

Accessing the tools

To view only the results of a search, you need to request this while setting up the search criteria with the Find Cells control panel:

- Click the **FIND...** tool in the table manager tool bar.

  or:

- Select the **Data/Find** menu item from the **TABLES** card.

Viewing only search results

You can specify that only the search results be displayed after a search. Before starting the search (*Searching for information in a table*), check the **View Results** check box in the Find Cells control panel. After the search is complete, only the results are visible in the current table.

Viewing the whole table

To view the entire table, click the **RESTORE VIEW** tool in the table manager tool bar or select the **Data/Restore View** menu item from the **TABLES** card. (The **RESTORE VIEW** pushbutton in the Table Groups control panel also works.)

Related information

Conducting searches is discussed under *Searching for information in a table*.

Additional information

Please see the on-screen help for details on the functioning of each control in the Find Cells control panel.

Sorting table information

You can reorganize a table by sorting its rows on the basis of the contents of up to three columns.

You should already know...

How to access the Tables module is described under *Accessing the tools*. How to select a table for display and editing (*Specifying the current table*) and how to make sure control panels are connected to the desired table window (*Keeping track of the current table*) are discussed above. Selecting columns and rows is discussed under *Selecting rows and columns*.

Accessing the tools

To sort all or part of a table, you need to access the Sort Table control panel:

- Click the **SORT...** tool in the current table tool bar.

  or:

- Select the **Data/Sort** menu item from the **TABLES** card.

Specifying sort criteria

To specify the primary sort criterion (that is, the column whose contents are used first for ordering the table), enter the column name or number in the **Sort First By** entry box by:

- Selecting the column (or a cell in it) in the table window.

  or:

- Choosing its name from the **Sort First By** popup in the Sort Table control panel.

For situations in which more than one row contains identical values in the column containing the primary sort criterion, you can use one or two additional sort criteria. Enter these columns' names or numbers in the **Then By** entry boxes (as described above for the first criterion).

Tip

You can set the first (and second and third) sort criteria by simply selecting the column(s) in that order. Those column names or numbers automatically appear in the correct entry boxes in the Sort Table control panel.

You cannot use columns containing model data (*Models in tables*) as sort criteria unless the column contents are displayed as object IDs. However, you can use a binary (*Binary model operators*) or unary (*Unary model operators*) model operator in an expression in some other column and use *that* column as a sort criterion.

Specifying sort order

Specify whether the sort order for each criterion is to be **Ascending** or **Descending** by setting the popups under each of the criterion entry boxes.

How many rows to sort

You can specify whether all or only part of the table is sorted:

- To sort the entire table, select the **All Rows** control.
- To sort only selected rows, select the **Selected Rows** control. (You usually have to specify search criteria from the **Sort First**

By and **Then By** popups instead of by selecting columns if you use this option.)

- To sort only rows contained within a group (if any exist in the table, see *Grouping table information*), select the **Group** control and specify the group by choosing its name from the associated popup.

All nonsorted rows remain in their original positions within the table.

Starting the sort

When you have specified all your desired options, click the **SORT** pushbutton to initiate the sort.

Additional information

Please see the on-screen help for details on the functioning of each control in the Sort Table control panel.

Graphing table information

You can plot selected columns or rows as line graphs, scatter plots, or histograms. (Values in columns are plotted vs. corresponding values in other columns, or values in rows vs. values in rows.)

Related information

Editing (*Displaying and editing graphs*) and managing (*Managing graphs*) graphs are discussed in *Working with Graphs*.

You should already know...

How to access the Tables module is described under *Accessing the tools*. How to select a table for display and editing (*Specifying the current table*) and how to make sure control panels are connected to the desired table window (*Keeping track of the current table*) are discussed above. Selecting columns and rows is discussed under *Selecting rows and columns*.

Accessing the tools

To graph table contents, you need to access the Plot Table control panel:

- Click the graph tool in the current table tool bar.

  or:

- Select the **Data/Graph** menu item from the **TABLES** card.

Specifying the data to plot on the y axis

Ordinarily, related data are contained in columns, and the **Y Axis** popup should remain set as **Columns**.

To plot all data contained in one or more columns, select the column(s) whose values you want to plot on the y axis and assure that the **Selection** control on the left is selected.

You can plot every column in the table by selecting the **Entire Table** control on the left side of the control panel.

If groups are present (*Grouping table information*), you can plot only columns contained in a group by selecting **Group** (on the left) and choosing the group name from the associated popup.

The procedure is analogous if you set the **Y Axis** popup to **Rows**.

Specifying the x axis

To specify the data to be used as the x axis, choose a column name or number from the **X Axis** popup.

To plot all values in the table, select the **Entire Table** control on the right side of the control panel.

You can restrict the x axis to a part of the specified column by selecting the desired rows and selecting the **Selection** control on the right side of the control panel or by selecting **Group** (on the right) and choosing a group name (*Grouping table information*) from the associated popup.

You could, for example, plot all columns within a restricted range of values along the x axis by selecting **Entire Table** on the left and **Selection** on the right.

Note

If the x axis is anything other than the row index numbers, you probably want to sort (*Sorting table information*) the table using the column that you will use as the x axis as the primary sort criterion.

The procedure is analogous if you set the **Y Axis** popup to **Rows**. In this case only rows appear in the **X Axis** popup.

Specifying the type of graph

To specify the type of graph, choose **Line**, **ScatterPlot**, or **Histogram** from the **Type** popup.

Titles and labels

If you want a title for your graph, enter it in the **Title** entry box.

You can enter axis labels for the x and y axes in the **Axis Label** entry boxes on the right and left sides (respectively) of the control panel.

Generating the graph

Finally, click the **PLOT** pushbutton in the Plot Table control panel.

Additional control over graph style, range, labels, annotations, etc. is available in the Graph module of Cerius^2 (*Working with Graphs*) and can be used to modify graphs after they are generated by the Table module and to control, for example, whether new graphs replace or are added to previous graphs displayed in the graph window.

Note

The graph in the graph window is not automatically updated if you change the data in the table or decide you want a different type of graph. You must click the **PLOT** pushbutton to regenerate a graph.

Additional information

Please see the on-screen help for details on the functioning of each control in the Plot Table control panel.

Exporting table information

You can export all or part of the current table to disk in a variety of formats for later importation into an external program such as a spreadsheet.

Related information

The usual procedure for saving a table in the default MSI table format is discussed in *Saving a table*. However, if you want to save only part of a table in MSI format, you need to use the procedure described here.

You should already know...

How to access the Tables module is described under *Accessing the tools*. How to select a table for display and editing (*Specifying the current table*) and how to make sure control panels are connected to the desired table window (*Keeping track of the current table*) are discussed above. Selecting columns and rows is discussed under *Selecting rows and columns*.

Accessing the tools

To export table contents, you need to access the Export Table control panel:

- Click the **EXPORT...** tool in the current table tool bar.

  or:

- Select the **File/Export** menu item from the **TABLES** card.

Exporting table information

To select the file format in which to save the current table, set the **Format** popup as desired.

To save the entire table, select the **Entire Table** control. Columns containing model data (*Models in tables*) cannot be saved in any format other than MSI. However, you may save other columns in your table in any available format, by selecting only part of the table:

To save selected row(s) and / or column(s), select the **Selection** control. To save a group (if present in the table, see *Grouping table information*), select the **Group** control and choose a group name from the associated popup.

To set any additional options you want to use, set the appropriate controls in the area of the control panel below the **Format** popup. (The controls that are available in this section depend on which format you choose.)

Enter a filename in the entry box and click the **EXPORT** pushbutton to save your file.

Use of the file selection list box and other file selector controls to navigate the directory structure is presented in detail under *Finding model file(s)*. Creating your own directories or subdirectories is described under *Making custom directories*.

Additional information

Please see the on-screen help for details on the functioning of each control in the Export Table control panel.

11. Working with Tables

12 Working with Isosurfaces

Grid properties are generated by a number of Cerius^2 application modules (e.g., ADF, MOPAC, DMOL3, Free_Volume), as well as many third party applications. A grid specifies a volumetric property as a three dimensional array encompassing a molecular model. Typical grid properties are molecular orbitals, electron density, electrostatic potential, and molecule accessible surface. The Isosurfaces application provides generic capabilities for the analysis of such grids via the construction of either a 3D isosurface or a 2D slice plane. Isosurface imports only .grd and .mbk format files, so data from non-Cerius^2 applications must be converted to these formats. It is most convenient to convert to ASCII .grd format when necessary.

While most applications in Cerius^2 have customized panels for grid manipulations, Isosurfaces offers a wider range of options. It makes it convenient to manipulate a large number of surfaces; it allows stepwise progress through a range of isocontour values, and it lets you use grid files created with external applications.

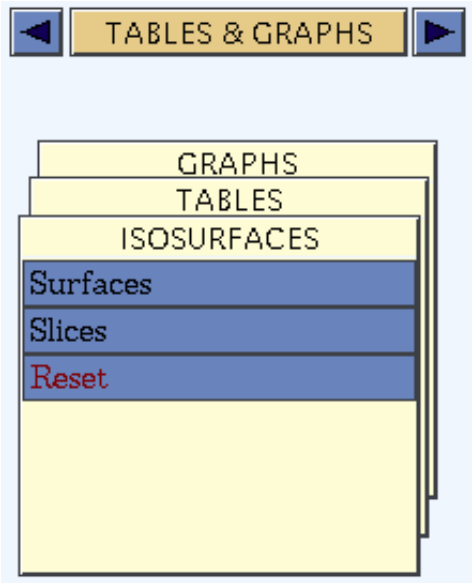
You should already know...

The basics of starting Cerius^2 and using its interface are demonstrated in *Introducing Cerius2* and described in *The Cerius2 Interface*.

Grids in Cerius^2 are produced as output from calculations in various other application modules. How to set up and run the appropriate calculations are discussed in the documentation for the relevant application modules.

Accessing the tools

The tools for handling isosurfaces are accessed from one of the decks of cards in the main Visualizer control panel. To access the **TABLES & GRAPHS** module, click the deck selector and choose **TABLES & GRAPHS** from the list that appears. Then click the title of the **ISOSURFACES** card to bring it to the front. The deck of cards menu area should now look like this:



Analyzing 3D grid properties

Three dimensional grid properties such as orbitals, densities, and potentials are scalar functions that are defined in the continuous 3D space surrounding the model. In practice, they are evaluated on a fine grid of points that completely encompass the model. This produces a large amount of information, which is typically visualized as an isosurface; that is, the constant-value points surrounding the model are connected so as to form a surface. The data can also be visualized as slices showing the values of the function on a 2D plane cutting through the model.

The Isosurfaces feature can read both .grd and .mbk file formats.

For detailed information about Cerius^2 file formats, please see File Formats. Insight files are described in separate file formats documentation.

To display the orbitals, electron density, or potential for your model as a surface or to change the display of an existing surface, use the Isosurfaces control panel, which is accessed by selecting the **Surfaces** menu item on the **ISOSURFACES** card.

Finding your surfacing files

If you want to display a currently undisplayed surface, use the **Files...** pushbutton to access the Isosurfacing Files control panel. Select the desired .grd or .mbk file and click the **LOAD** button. You can use the browser popup to access directories other than the current one.

Surface specification and display

Once you have a surfacing file loaded and if the default settings in the Isosurfaces control panel are satisfactory, you can click the **Create New Surface** action button (on the Isosurfaces control panel) to create and display that surface on your model. Make sure that none of the surfaces in the list box is selected if you want to create and display a new surface in addition to those already displayed.

You can edit surfaces in several ways:

- Change the value in the **Isosurface Value Range** entry box to change which iso-value points within the grid are displayed when the **Create New Surface** action button is clicked again.
- Check or uncheck the **Show Surface** check box to display selected surface(s) or not.
- Click the **Delete Surface** action button to delete selected surface(s) from the display and the **Edit Surface** list.
- Change the transparency and color of surfaces with the relevant controls at the bottom of the Isosurfaces control panel.

Additional information

Please see the on-screen help for details on the functioning of each control.

Mapping a property onto a surface

How maps on surfaces function

An isosurface connects points in space that have the same value of some parameter. However, you can add an additional dimension to a surface, by making a property map, which displays the values of another property as different colors on an existing displayed surface.

To do this, use the Property Maps control panel, which is accessed by selecting the **Property Maps...** button on the Isosurfaces control panel.

Finding your property files

Specify a property to be mapped by choosing the desired .grd or .mbk file from the list box and clicking the LOAD pushbutton. You can use the browser popup to access directories other than the current one.

Map specification and display

If more than one surface is displayed or has been loaded, you may need to select the one on which to map the property, using the list box on the Isosurfaces control panel.

Click the **Add Property** action button on the Property Maps control panel to display the property map.

You can vary the transparency of the displayed property map with the **Transparency (%)** entry box.

You can change the range and color spectrum with which to display the property map by clicking the **Preferences...** pushbutton to access the Property Maps Preferences control panel.

Additional information

Please see the on-screen help for details on the functioning of each control.

Editing and displaying slices

To edit and display a 2D slice through the 3D grid of orbitals, density, or potential for your model, use the Slices control panel, which is accessed by clicking the **Slices** menu item on the ISOSURFACES card.

Finding your surfacing files

If necessary, choose the grid file to be analyzed by clicking the **Files...** pushbutton to access the Isosurfacing Files control panel. Select the desired .grd or .mbk file from the list box and click the **LOAD** pushbutton. You can use the browser popup to access directories other than the current one.

Slice specification and display

Once you have loaded a file and if the default settings in the Slices control panel are satisfactory, click the **Create New Slice** action button (on the Slices control panel) to create and display a selected slice for your model. You may want to edit the slice now (e.g., by changing the transparency value and redisplaying).

The **Edit Slice** list box shows the slice(s) that are currently displayed. You can select one by clicking its name in the list box. Make sure that none of them is selected if you want to create and display a new slice in addition to those already displayed.

Check or uncheck the **Show Slice** check box to indicate whether to display the selected slice. Click the **Delete Slice** action button to delete the selected slice from the display and the list.

You can change the transparency in the **Transparency** entry box near the bottom of the Slices control panel.

Positioning the slice plane

A slice is defined by its position and direction. The default position and direction are chosen so that the slice passes through the best-fit plane to the whole model or any selected atoms. A slice is created with a default position and direction and can be returned to the default position or direction by clicking the appropriate reset action button.

To change the position through which the slice plane slices the grid, use the **Position** arrows to move the slice up or down the perpendicular to the slice plane. The numbers show the position that the slice plane passes through. They change as you click the arrows, or you can edit them directly.

To change the direction of the line perpendicular to the slice plane (up and down which the plane can be moved), edit the numbers in the **Direction** entry box.

Other controls

Clicking the **Preferences...** pushbutton gives you access to the Slice Preferences control panel, which contains additional controls that affect slices.

Plot the plane's values

To create a 2D contour graph corresponding to a selected slice plane, click the Create Slice Plot in Graph Window action button in the Slices control panel.

Additional information

Please see the on-screen help for details on the functioning of each control.

13 Scripts and Licensing

All Cerius^2 applications, including the Visualizer, are command driven. The graphical interface takes your input (mouse clicks and drags, etc.), continuously translates it into commands, records the commands into logs, and passes the commands to the programs themselves.

Although many users generally need to know nothing about this process, you may want to learn about creating and using Cerius^2 commands, to facilitate performing a series of related or identical tasks in an automated way.

You may also want to know about Cerius^2's facilities for running application modules on remote machines and for managing licenses.

This section explains

This section contains information on:

Command logging and scripting

Controlling Cerius2 from scripts

Managing licenses

Running application modules externally

Table 25. Finding information about scripts and licensing

If you want to know about:	Read:
Initialization (startup) scripts.	*Starting Cerius2 with a command script file*.
Performing repetitive or routine tasks.	*Playing back scripts and log files*, *Starting Cerius2 with a command script file*.
Recording aall or part of a Cerius^2 session.	*Recording commands*.

Table 25. Finding information about scripts and licensing

If you want to know about:	Read:
Starting and saving Cerius^2 sessions.	*Working with Cerius2 sessions.*
Other ways of setting preferences and customizations.	*Using saved sessions as preferences settings*, *Customizing the Interface*.
Running Cerius^2 without its graphics.	*Starting Cerius2 with a command script file*.

You should already know…

The basics of starting Cerius^2 and using its interface are demonstrated in *Introducing Cerius2* and described in *The Cerius2 Interface*.

Command logging and scripting

Command logging and scripting utilities enable you to record Cerius^2 commands into script files and play them back (*Playing back scripts and log files*) at a later time.

Finding information

This section includes information on:

Recording commands

Command tracing

Recording commands

If you want to understand the course of all or part of a Cerius^2 session, you can examine files containing logged commands. These files form basic *command scripts*.

Command scripts can be played back later (*Playing back scripts and log files*) unmodified, to repeat a previous session. Alternatively, you can supplement a command script with Tool Command Language (Tcl) statements to produce responsive, program-like scripts that can be used to drive Cerius^2 and its applications.

Related information

To learn more about using Tcl to enhance script files, see *Cerius^2 Command Script Guide*, as well as information in the documentation and support areas of our website

http://www.msi.com/doc/

http://www.msi.com/support/

How it works

During every Cerius^2 session, generated commands are continuously logged to a file named RUN.LOG. This continuous log file provides a record of the modeling activity that took place in a Cerius^2 session.

The RUN.LOG file is normally overwritten when a new Cerius^2 session is started; however, the contents of the current RUN.LOG file (that is, the session log) can be saved under another filename at any time. Such files provide a snapshot of the session at a particular time.

You can also open a supplementary log file, called a *segment log file*, into which all generated commands are logged until this file is closed. A segment log file enables you to create a log of only part of a session (for example, only that part of a session from which you want to create a command script). Command logging to RUN.LOG also continues, regardless of whether a segment log file is open.

Accessing the tools

Select the **Utilities/Record Commands...** menu item in the main Visualizer control panel to access the Record Commands control panel.

Recording commands

To copy all the current contents of the RUN.LOG file to a file with a different name, change the filename in the entry box near the top of the Record Commands control panel (if desired) and click the **Dump current Log contents** action button.

To start copying commands into a supplementary log file, check the **Echo commands into file** check box. All subsequent commands appear in both the RUN.LOG file and the segment log file.

To discontinue copying commands into the supplementary log file, uncheck the **Echo commands into file** check box. If you want to record more commands into the same file later in your session, simply check the **Echo commands into file** check box again.

To enter a comment in the current RUN.LOG file (and the current segment log file, if one is open), enter the desired text into the **Enter Comment into Log File** entry box.

Managing command logs

To empty and restart the current RUN.LOG file from the current point in your Cerius^2 session, click the **Empty Log File contents**

action button in the Record Commands control panel. This action does *not* reinitialize the Cerius^2 session (*Starting a new session*), it merely restarts the log file.

Additional information

Please see the on-screen help for details on the functioning of each control in the Record Commands control panel.

Command tracing

Command tracing enables you to view and store various levels of Cerius^2 command output. You can also display the commands in the text window as they are generated. This output can be useful for monitoring the commands generated during a Cerius^2 session, especially if you are logging commands for use in a script.

Levels of commands

Three levels of commands are generated by the graphical interface and application modules:

- Primary—Generated by primary command generators, such as the graphical interface or a script file, or by your direct entry of commands in the text window.
- Secondary—Generated directly or indirectly by application modules as a result of processing a primary command.
- Utility—Generated internally within Cerius^2, for defining the environment in which Cerius^2 and its application modules are to run (for example, the commands generated when command tracing is turned on or off).

Accessing the tools

Select the **Utilities/Command Tracing...** menu item in the main Visualizer control panel to access the Command Tracing control panel.

What level of commands to trace

To specify the level (see *Levels of commands*) of commands to trace, check one or more of the **Activate Command Tracing** check boxes.

Tip

To turn on or off tracing of primary commands, you can also check the **Activate command tracing** check box in the Customize Environment control panel (*Accessing the tools*). The commands are sent to the text window and/or a file, as specified in the Command Tracing control panel (see *Where to send the commands*).

Where to send the commands

To display the traced commands in the text window, check the **Text Window** check box.

To log the traced commands in a file, check the **Trace File** check box and (if desired) enter a filename in the **Trace File** entry box.

Changing command tracing

To stop command tracing or change the level of commands to trace, uncheck the relevant check boxes in the Command Tracing control panel.

Examining most recent commands

To print the most recent primary and utility commands in the text window, enter the command **history** in the text window.

Additional information

Please see the on-screen help for details on the functioning of each control in the Command Tracing control panel.

Some additional control over command logging and history is accessible via the Customize Environment control panel (*Accessing the tools*).

Controlling Cerius^2 from scripts

Cerius^2 enables you to play back command scripts containing command strings, control syntax, and, optionally, additional Tcl commands. The commands in the script are processed as though they were being generated in real time by the Cerius^2 interface, triggering the appropriate actions.

Command logging and scripting utilities enable you to record Cerius^2 commands (*Recording commands*) into script files and play them back at a later time.

Command scripts are often based on Cerius^2 log files, which can be used unmodified, to repeat a previous session. Alternatively, you can supplement a log file with Tool Command Language (Tcl) statements to produce responsive, program-like command scripts that can be used to drive Cerius^2 and its applications. In addition, you can write command scripts completely from scratch.

Finding information

This section includes information on:

Playing back scripts and log files

Starting Cerius2 with a command script file

Related information

To learn more about using Tcl to enhance script files, see *Cerius^2 Command Script Guide*.

You should already know…

Recording commands is discussed under *Command logging and scripting*.

Playing back scripts and log files

If you have certain tasks that you nearly always perform during a Cerius^2 session, you can record them in a command script file, and then have Cerius^2 automatically perform these tasks from the script, either immediately (*Starting Cerius2 with a command script file*) or when you request it (this section). Then you can proceed with additional tasks using the graphical interface.

Accessing the tools

Select the **Utilities/Playback Script…** menu item in the main Visualizer control panel to access the Playback Script control panel.

Finding the script file

Use the file browser and selector tools to find and choose the desired script file. How to use these tools is detailed under *Finding model file(s)*. (All file browsers work similarly.)

Playing back Cerius^2 scripts

You can play back the script file in several ways:

- To simply run the script now, click the **RUN** pushbutton in the Playback Script control panel.
- To reinitialize the session (*Starting a new session*) before running the script, check the **Re-initialize** check box and then click the **RUN** pushbutton.
- To run the script repeatedly (reinitializing the session before each pass through the script), check the **Run Script Repeatedly** check box and then click the **RUN** pushbutton.

Additional information

Please see the on-screen help for details on the functioning of each control in the Playback Script control panel.

Starting Cerius^2 with a command script file

Ordinarily, the **cerius2** script (*Starting Cerius2*) starts a regular Cerius^2 session that takes its input by means of your interaction with the graphical interface.

Cerius^2 can also be run from a recorded script, either with or without the graphical interface. You can manually specify the script when you start Cerius^2 or have Cerius^2 always process a certain script automatically without your needing to specify it.

Ways of automating Cerius^2

You can run Cerius^2 from a command script in several ways:

- With the graphical interface—automatically process the commands immediately when Cerius^2 starts, then await your additional input (see *Starting Cerius2 with an automatic script* and *Starting Cerius2 with a specified script*).
- With the graphical interface—process the commands when you request it, then await your additional input (see *Playing back scripts and log files*).
- Without the graphical interface—as a foreground job, process the commands automatically, then exit (see *Running Cerius2 without the graphical interface*).
- Without the graphical interface—as a background job, process the commands automatically, then exit (see *Running Cerius2 without the graphical interface*).

Uses of start-up command scripts

If you have certain tasks that you always or often perform when you start a Cerius^2 session, you can record them in a command script file, and then have Cerius^2 automatically perform these tasks from the script, either immediately (this section) or when you request it (*Playing back scripts and log files*). Then you can proceed with additional tasks using the graphical interface.

If you have repetitive, routine calculations or other tasks that can be performed without the graphical interface, you can record these tasks in a command script file. Then you can run Cerius^2 in a completely automated way, in either the foreground or background, without your interacting with the graphical interface at all.

Starting Cerius^2 with an automatic script

To run Cerius^2 from a command script with the graphical interface and have it immediately and automatically process a certain command script, move (cd) to a directory containing an *initialization script*, then simply start Cerius^2 as usual.

An initialization script is simply an ordinary command script file that you have saved with the filename cerius2.ini (see *Recording commands*).

To set up different initialization scripts for use when you run Cerius^2 for different purposes or projects, simply create separate directories, each containing a different cerius2.ini file. If Cerius^2 does not find a cerius2.ini file in the directory in which you start it, it looks for a cerius2.ini file in your home directory.

After the initialization file's command script terminates, Cerius^2 enters interactive mode, awaiting your input.

Starting Cerius^2 with a specified script

To run Cerius^2 from a command script with the graphical interface and have it immediately process a specified command script, start Cerius^2 by entering at the system prompt:

```
> cerius2 scriptfile
```

where *scriptfile* is the name of your command script file. Any text output is sent (as usual) to the text window.

To run Cerius^2 from a command script with the graphical interface, have it immediately process a specified command script, and have it send any text output to a file instead of to the text window, start Cerius^2 by entering at the system prompt:

```
> cerius2 -o outputfile scriptfile
```

where *outputfile* is the name of the file that you want to send any text output to, and *scriptfile* is the name of your command script file.

In either case, graphics are displayed in normal fashion in the model window. After the command script terminates, Cerius^2 enters interactive mode, awaiting your input.

Running Cerius^2 without the graphical interface

To run Cerius^2 without the graphical interface in background mode, enter at the system prompt:

```
> cerius2 -b outputfile scriptfile
```

where *outputfile* is the name of the file that you want to send any text output to, and *scriptfile* is the name of your command script file.

To run Cerius^2 without the graphical interface in foreground mode, enter at the system prompt:

```
> cerius2 -n -o outputfile scriptfile
```

where *outputfile* is the name of the file that you want to send any text output to, and *scriptfile* is the name of your command script file.

To run Cerius^2 without the graphical interface in foreground mode and send any text output to the shell window rather than to a file, enter at the system prompt:

```
> cerius2 -n scriptfile
```

where *scriptfile* is the name of your command script file.

Managing licenses

As an end user, you rarely need to be concerned about license management, since it is handled automatically after the Cerius^2 software has been installed.

When to manage licenses

Some situations exist in which you may want to manage licenses interactively, for example:

- Suppose your site has a limited number of licenses and they are all being used by other people. If you need a license, you may want to determine who the other users are. Then you can ask one of them to replace (that is, check in) the license so that you can work.
- If you plan to run a long command script, you may want to reserve (that is, check out) enough licenses to assure that they are available when needed.

Important

If you want to run Cerius^2 applications in parallel, please see the *Cerius^2 Installation and Administration Guide.*

Accessing the tools

Select the **Utilities/Application Licensing…** menu item in the main Visualizer control panel to access the License Management control panel.

For all of the functions below, select the name of the desired module in the **Available Licenses** list box. This list box shows the names of modules that require licenses and for which you have purchased licenses.

What licenses are available?

The **Available Licenses** list box shows the names of modules that require licenses and for which you have purchased licenses.

The total number of supported floating licenses (i.e., module-specific licenses that your site has purchased) for a selected module appears near the bottom of the License Management control panel.

The total number of people currently using floating licenses for that module is listed in the line below the total number supported.

Who are using other licenses?

The login name(s) of the people using floating licenses for the selected module are shown in the **Checked out to** list box.

For token licenses, this user list appears only if you currently have the selected feature checked out via token licensing. This list of users includes the total number of tokens each person has checked out (in parentheses after their name). However, it does not indicate which people have a particular feature checked out. When you check out a feature, the indicated total number of tokens by your name is increased.

Reserving licenses

To manually reserve (check out) one floating licence for the selected module, click the name of the selected module in the **Available Licenses** list box or click the **CHECK OUT** pushbutton.

To manually reserve several token licenses for a specific feature, user, or machine, please see the *Cerius^2 Installation and Administration Guide* on using an options file.

Releasing licenses

To return (check in) a license that you have checked out manually for a selected module but are finished using, click the name of the selected module in the **Available Licenses** list box or click the **CHECK IN** pushbutton.

Additional information

Please see the on-screen help for details on the functioning of each control in the License Management control panel.

For additional information about a particular license (i.e., when it expires and what machine is serving it), click the **License** pushbutton.

For more information about licensing (including the differences between token and floating licenses and between features and modules) and license management, please refer to the *Cerius^2 Installation and Administration Guide*.

Running application modules externally

External application facilities enable you to manage Cerius^2 application modules running on external servers.

Cerius^2 applications are implemented as modules that plug into the modeling environment provided by the Visualizer. Most Cerius^2 application modules function (either individually or grouped with related modules) as independent processes. As a result, these application modules can be run on your local machine or externally on a remote host (of the same or different type) anywhere on your network.

Uses of remote servers

This implementation method has several advantages, including:

- You can start and run only the application module(s) that you want to use, thereby saving memory and reducing overhead.
- You can purchase licenses to run application modules only on certain machines and still control those modules from any other machine on your network.
- You can run application modules that perform complex, computationally intensive calculations on remote servers, which may be more powerful than your own (local) machine.

How it works

To run application modules externally, you use the controls on the Process Management control panel to select the appropriate application module, process, remote host, and executable program, to modify any of your selections (if necessary), and to specify that the module should be started either immediately or when the module is accessed from a menu card. Once you have started an application module on a remote host, you can also use the Process Management control panel to stop that module's process.

Tip

To always run an application module externally under the conditions you set with the Process Management control panel, you need to save the current session (*Saving the current session*). Otherwise, your settings are saved only for the current Cerius^2 session.

Cerius^2 and independent processes

Some application modules (for example, those on the **QUANTUM** cards) are actually used only to set up and act as interfaces to cal-

culations that are run by essentially separate programs that are independent of the Cerius^2 interface. Such modules offer their own job-control options that affect the separate (usually computationally intensive) program. These controls are accessed from the application module itself and are documented in the user guide for the relevant module.

The Process Management control panel affects *only* those processes that are under the direct control of the Cerius^2 interface, *not* independent processes that are spawned by applications such as the quantum modules.

For example, the MOPAC interface application (control panels, etc.) is controlled by the Process Management control panel, but the MOPAC program itself (the calculation job) is managed by MOPAC Job Control control panel.

Accessing the tools

Select the **Utilities/External Processes...** menu item in the main Visualizer control panel to access the Process Management control panel.

Specifying processing conditions

To specify what process you want to start or stop, select its name from the **Application** list box in the Process Management control panel. The name of the relevant process appears in the **Process** list box.

Tip

If you are unsure of the application name assigned to a module, go to the module, open any of its control panels, and use the right mouse button to request help. The first line of the help window that appears contains the application name.

The names of machines on your network appear in the **Host** list box. Select the one that you want to send the process to. (The machine you are running Cerius^2 on is called *localhost*.) If a machine's name is not on that list but you know it is accessible from your machine, you can enter its name in the **Remote Host** entry box.

If you need a password in order to use the specified machine, enter it in the **Password** entry box.

Tip

To determine whether you must enter a password, enter the command **rsh *hostname*** in a separate shell window. If you are not prompted for a password to log on to the specified remote host, a password is not required here.

To specify your working directory on the specified host, if it does not appear automatically, enter the name of your working directory in the **Working Directory** entry box. This directory must already exist.

If more than one executable can run on the chosen machine, select the name of the desired executable in the **Executable** list box. You can also enter the complete path and file name of the executable in the **Executable** entry box.

(The registry information contained the list boxes in this control panel can become outdated if changes are made after Cerius^2 was installed at your site. To update this information, your installation administrator needs to edit the applcomm.db file. For additional information on this file, please see the *Cerius^2 Installation and Administration Guide*.)

Starting an external process

You can start the specified Cerius^2 process on an external host in two ways:

- To save the settings for use later in the current session, so that the process is started as instructed only when you access the application module from its menu card, click the **Save Selection** action button.
- To start the process immediately, click the **Start** action button. The process starts, but does not do anything other than wait for your additional input from the application module's menu card.

Ending an external process

To stop running the selected Cerius^2 process on the specified host, click the **Kill** action button. You would typically use this button if you want to restart the selected process on another host.

Additional information

Please see the on-screen help for details on the functioning of each control in the Process Management control panel.

Related information

Executing Cerius^2 on one machine while displaying its interface on another is discussed in the *Cerius^2 Installation and Administration Guide*.

13. Scripts and Licensing

14 Customizing the Interface

You may want to rearrange the Cerius^2 decks of cards, specify that certain control panels be open or easily accessible when Cerius^2 starts, change the interface colors, or set various other environment-customization options.

This section explains

This section contains information on:

Interface configuration

Interface look and feel

Table 26. Finding information about customizing Cerius^2

If you want to know about:	Read:
Creating and adding cards to card decks.	*Deck of cards menu configuration*.
Using configuration files.	*How it works*.
Displaying, closing, reorganizing control panels on the screen.	*Control panel management*.
Starting Cerius^2 with open control panels.	*Control panel management*.
Customizing Cerius^2 control colors.	*Interface colors*.
Launching Cerius^2 from the desktop.	*Cerius2 as a desktop icon*.
Pitch and volume of the bell.	*Adjusting the beeper*.
Customizing color use in the model and graph display windows.	*Model display colors*, *Customizing display colors*.
Customizing Cerius^2 by means of command scripts.	*Starting Cerius2 with a command script file*.
Customizing Cerius^2 by means of session preferences.	*Using saved sessions as preferences settings*.

You should already know…

The basics of starting Cerius^2 and using its interface are demonstrated in *Introducing Cerius2* and described in *The Cerius2 Interface*.

Interface configuration

Visualizer customization options enable you to change various aspects of the Cerius^2 graphical interface to suit your unique requirements.

Finding information

This section includes information on:

Deck of cards menu configuration

Control panel management

Related information

Setting other Cerius^2 preferences and performing certain functions automatically are covered under *Working with Cerius2 sessions* and *Controlling Cerius2 from scripts*.

See the following section, *Interface look and feel* for information on changing control panel colors and some aspects of how Cerius^2 runs.

Deck of cards menu configuration

Cerius^2 enables you to change the configuration of the deck of cards menus. You can:

- Add cards to or remove cards from existing decks.
- Change the order of cards in existing decks.
- Create new decks and rename or remove others.
- Save your deck configuration for future Cerius^2 sessions.

Accessing the tools

Select the **Utilities/Customize/Menu Deck...** menu item in the main Visualizer control panel to access the Customize Menu Deck control panel.

All menu cards that are available at your site are listed in the **Licensed Cards** list box. Select one or more of the menu cards by clicking its name in this list. Selected card names become highlighted. (Deselect a card by clicking a highlighted name again.)

Creating and renaming card decks

To create a new card deck, click the **ADD NEW DECK** pushbutton in the Customize Menu Deck control panel.

To rename any card deck, choose the deck from the deck selector popup (above the list box toward the right side of the Customize Menu Deck control panel). Enter the new name in the **Rename Deck** entry box.

To delete a selected deck, click the **DELETE DECK** pushbutton. The cards that were in that deck are still available in the **Licensed Cards** list box for inclusion in other decks, if desired.

Editing deck contents

To change what cards are in a deck or the order in which they appear, choose the deck you want to edit from the deck selector popup (above the list box toward the right side of the Customize Menu Deck control panel). The menu cards currently included in this deck are shown in the list box below its name, in the (virtual) top-to-bottom order in which they appear in the deck when it is first opened in the Visualizer main control panel.

To add selected cards from the **Licensed Cards** list box to the current menu deck (up to a maximum of five in a deck) click the right-pointing arrow. The same card may appear in more than one deck.


To change the order of cards in the deck, click a card name in the right-hand list box and click the up- or down-pointing arrow.

To remove a card from the deck, click the card's name in the right-hand list box and click the **REMOVE** pushbutton. The card is still available in the **Licensed Cards** list box for inclusion in other decks, if desired.

Saving the new deck configuration

Any card deck configuration changes you make are immediately reflected in the deck-of-cards area of the main control panel. Your changes remain throughout the current Cerius^2 session.

To save your changes so that Cerius^2 always starts up with your custom configuration, click the **SAVE CONFIGURATION** pushbutton in the Customize Menu Deck control panel.

How it works

When you click the **SAVE CONFIGURATION** pushbutton, the current configuration of the deck of cards menus is saved to a file named decks in an .MSIguirc subdirectory in your home directory. This file is automatically read whenever you start Cerius^2.

To set up different deck of cards configurations for use when you run Cerius^2 for different purposes or projects, simply create separate directories and copy the ~/.MSIguirc subdirectory and its contents to the new directory. Then change the decks file as described in *Saving the new deck configuration*.

If Cerius^2 does not find an .MSIguirc subdirectory in the directory in which you start it, it looks for an .MSIguirc subdirectory in your home directory.

Additional information

Please see the on-screen help for details on the functioning of each control in the Customize Menu Deck control panel.

Control panel management

In addition to basic control-panel management as presented under *Managing control panels*, Cerius^2 offers additional functions for displaying, closing, and reorganizing open control panels.

You can also specify that certain panels be displayed automatically whenever you start Cerius^2.

Accessing the tools

Select the **Utilities/Panel Manager...** menu item in the main Visualizer control panel to access the Panel Manager control panel.

All control panels that are currently open or were open at some time during the current Cerius^2 run are considered *active*. In addition, selected control panels can be marked so as to be considered active in subsequent Cerius^2 sessions (even without being manually opened first—see *Saving control panel configuration*). Their names appear in the **Active Control Panels** list box.

To perform one of the tasks listed here, select one or more of the active control panels by clicking its name in this list. Selected control panel names become highlighted. (Deselect a control panel by clicking a highlighted name again.)

Reopening control panels

To open or reopen selected active control panel(s), click the **DISPLAY** pushbutton in the Panel Manager control panel.

Closing control panels

To close all open control panels, click the **HIDE** pushbutton that is located in the **All Visible Control Panels** area of the Panel Manager control panel (near the top).

To close only selected open control panels, click the **HIDE** pushbutton that is located in the **Selected Panels** area of the Panel Manager control panel.

Alternatively, to close all open control panels, click the clear panels tool  on the toolbar of the Visualizer main panel.

Deactivating control panels

To remove a selected control panel's name from the **Active Control Panels** list, click the **REMOVE** pushbutton. (This action does not hide the panel if it is open.)

To add a control panel's name to the **Active Control Panels** list, close it if it is open (by clicking that panel's close box ), and then open it by using the usual menu bar or card menu item.

Cascading control panels

To group all open control panels into an orderly cascade, click the **CASCADE** pushbutton in the Panel Manager control panel.

Alternatively, to cascade all open control panels, click the cascade panels tool  on the toolbar of the Visualizer main panel.

Automatic panel display

If you commonly use the same control panels during a Cerius^2 session, you may find it useful to save the list of active control panels to a file that is read at startup time for subsequent sessions.

To cause certain control panels to be automatically opened whenever you start Cerius^2, open the desired control panel(s) if they are not in the **Active Control Panels** list in the Panel Manager control panel, select their name(s) in that list, click the **Toggle startup flag** action button so that an asterisk appears next to each desired name in the list, and then click the **SAVE CONFIGURATION** pushbutton (see *How it works* for additional information).

Cancelling automatic panel display

To specify that a control panel no longer be displayed automatically upon startup, select its name in the **Active Control Panels** list, click the **Toggle startup flag** action button so that the asterisk next to its name disappears, and click the **SAVE CONFIGURATION** pushbutton.

Saving control panel configuration

To save the current list of active control panels (along with the specifications as to which ones are and are not displayed automatically upon startup, see *Automatic panel display*), click the **SAVE CONFIGURATION** pushbutton in the Panel Manager control panel.

How it works

When you click the **SAVE CONFIGURATION** pushbutton, the list of active and automatically displayed control panels is saved

to a file named panels in an .MSIguirc subdirectory in your home directory. This file is automatically read whenever you start Cerius^2.

To set up different lists of active and displayed control panels for use when you run Cerius^2 for different purposes or projects, simply create separate directories and copy the ~/.MSIguirc subdirectory and its contents to the new directory. Then change the panels file as described in *Saving control panel configuration*.

If Cerius^2 does not find an .MSIguirc subdirectory in the directory in which you start it, it looks for an .MSIguirc subdirectory in your home directory.

Additional information

Please see the on-screen help for details on the functioning of each control in the Panel Manager control panel.

Additional ways of setting Cerius^2 preferences and/or performing certain functions automatically are covered under *Working with Cerius2 sessions* and *Controlling Cerius2 from scripts*.

Interface look and feel

Visualizer customization options enable you to change part of the "look and feel" of the Cerius^2 interface to suit your preferences.

Finding information

This section includes information on:

Interface colors

Miscellaneous environment customizations

Interface colors

Cerius^2 enables you to customize the colors used in the graphical user interface (GUI). These customizations affect all control panels and all controls within them. Color-coding of controls according to their function remains consistent.

Related information

Please see *Enhancing Model Display* for customization of colors used for objects in the model and graph display windows.

Accessing the tools

Select the **Utilities/Customize/GUI Colors...** menu item in the main Visualizer control panel to access the Customize GUI Colors control panel.

Examining the color-coding system

The color codes listed in the **Functional color groups** list box each affect a certain type of item in the interface. To examine what items any color code affects, click its name in the **Functional color groups** list box in the Customize GUI Colors control panel and hold down the left mouse button over the **Show Scope** action button. All items affected by that color code are highlighted for as long as you hold down the mouse button.

Changing the interface colors

To color related groups of interface items according to your own color scheme, select the name of the color code you want to change from the **Functional color groups** list box. Then use the red, green, and blue sliders (or the entry boxes below them) to set the proportions of red, green, and blue in the final color.

You can reset all or selected color codes to default values by using the appropriate **Reset** action buttons in the control panel.

Color changes take place immediately and remain in force for the duration of the current Cerius^2 session.

Saving the interface colors

To save your customized color-coding of the graphical interface for use in future Cerius^2 sessions, click the **SAVE CONFIGURATION** pushbutton in the Customize GUI colors control panel.

How it works

When you click the **SAVE CONFIGURATION** pushbutton, the current interface colors are saved to a file named gui_colors in an .MSIguirc subdirectory in your home directory. This file is automatically read whenever you start Cerius^2.

If you create separate directories and copy the ~/.MSIguirc subdirectory and its contents to the new directory for other purposes (*How it works*, *How it works*), the copied gui_colors file should not be removed from this new directory. Although you would probably not want to change the gui_colors file for different projects, Cerius^2 does *not* look for another .MSIguirc subdirectory in your home directory if it finds an .MSIguirc subdirectory in the directory in which you start it.

Additional information

Please see the on-screen help for details on the functioning of each control in the Customize GUI Colors control panel.

Miscellaneous environment customizations

Related information

See *Interface configuration* for information on changing the content of deck of card menus.

Running Cerius^2 on one machine while displaying and interacting with its interface on another is discussed in the *Cerius^2 Installation and Administration Guide*.

Accessing the tools

Select the **Utilities/Customize/Environment...** menu item in the main Visualizer control panel to access the Customize Environment control panel. This control panel is used in many of the tasks mentioned in this section.

Cerius^2 as a desktop icon

Most window managers allow frequently used applications to be configured as desktop or tool box icons or as popup menu items for easy launching.

If you want to use one of these methods, you need to configure the launch action so that the **cerius2** script is invoked from a shell window. The startup shell window becomes the text window to which Cerius^2 sends certain information.

To learn the application-launching shortcuts supported by your window manager and how to configure them, please refer to that window manager's documentation.

Starting with no banner

You can suppress the display of the Cerius^2 startup banner (also called a splash screen) if you want, by using the **nobanner** option when you start Cerius^2, for example:

```
> cerius2 -nobanner
```

Running in OpenGL mode

Generally, Cerius^2 runs by default in either OpenGL or GL graphics mode, as appropriate to your machine. If your machine is capable of running in either mode and you want to force it to run in the nondefault mode, you can set the FORCEOPENGL or FORCEGL env to any value before starting Cerius^2. For example:

```
> setenv FORCEOPENGL 1
```

or:

```
> setenv FORCEGL 1
```

	Please see the *Installation and Administration Guide* for additional information.
Balloon help	To enable or disable display of small explanatory boxes whenever the cursor lingers over certain controls (for example, many of the tools in the Visualizer's main control panel), check or uncheck the **Activate balloon help** check box in the Customize Environment control panel.
Adjusting the beeper	You can adjust the pitch and volume of the beeper (bell) with the **Tone** and **Volume** controls (respectively) in the Customize Environment control panel.
Finding atom information	You can choose to have brief information on atom properties sent to the text window whenever you click an atom. To do this, check the **Echo object reference on pick** check box in the Customize Environment control panel. Uncheck the box to turn this feature off.
Additional information	Please see the on-screen help for details on the functioning of each control in the Customize Environment control panel.

14. Customizing the Interface

A References

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A. References

B Definitions

Models, fragments, and templates

Why read this section

It is easy to get the terms fragment, model, template, and molecule confused. We have tried to be consistent in this documentation.

Definitions

- A *fragment* is a set of covalently bonded atoms.
- A *model* is the entire contents of a Cerius^2 model space. The visible part(s) of a model may include:

  A single atom.

  One fragment, for example, a model of caffeine.

  Several fragments that interact by noncovalent bonds or that do not interact, for example, a large solute fragment and many small solvent fragments.

  A protein consisting of many residues and one or more subunits.

  A receptor–ligand complex.

  A 1D periodic structure such as polyethylene or DNA.

  A 2D periodic structure such as a regular surface.

  A 3D periodic structure such as a crystal.
- A *template* is a model or fragment that is used in building models.
- Strictly speaking, *molecules* exist only in the real world, not in the simulated world of computational chemical modeling.

Glossary

Some other words that have specific meanings within Cerius^2 are listed below:

word	meaning	additional information
ambient light	Light impinging on a scene from all directions.	*Concepts*
balloon help	Small explanatory text boxes displayed when the cursor lingers over a control.	*Balloon help*
bitmap resolution	Number of dots per inch (used in printing graphs).	*Bitmap resolution for printing graphs*
bond type	Associated with the nature and number of shared electrons between atoms (e.g., single, double, partial bond types).	*Changing the bond type*
charge	The overall partial charge on an atom.	—
cleaning a model	Optimizing the model conformation.	*Refining the conformation*
color map	Defined correlation of properties with a color range.	*Editing a property color map*
color range	Defined sets of colors.	*Creating and editing a new color range*
command script	A file of Cerius^2 commands that can be used to control future Cerius^2 sessions.	*Recording commands*
data set	A set of related points in a graph, for example, all the points belong to one curve.	*Selecting data to plot*
data type	Real numbers, Booleans, text, etc., in a table.	*Assigning data types*
depth cueing	Representation of aerial perspective.	*Apparent depth effects*
derivation	Mathematical expression in table cells.	*Applying mathematical expressions to cells or columns*
diffuse lighe	Light scattered from an object in all directions.	*Concepts*
display style	Display of atoms and/or bonds as sticks, balls, etc.	*Ball and stick models*
dummy atoms	Nonstandard “elements” with defined properties.	*Dummy atoms*
enter	Type some characters, then press <Enter> or click anywhere else in the control panel.	*Type a C in the sketch...*

word	meaning	additional information
formal charge	The difference between the number of electrons possessed by the neutral isolated atom and that formally possessed by the atom within the molecule, assuming that electrons in covalent bonds are shared equally between participating atoms and that no sharing of core and lone pair electrons occurs.	—
fractional bond order	A quantitative measure of the order of a bond, which may, for example, be related to overlap integrals in the molecular-orbital description of the system.	—
gallery	The graph window.	*Displaying and editing graphs*
graphics quality	Related to the color interpolation between facets used to draw curved surfaces.	*Graphics quality*
graphics resolution	Related to the number of facets used to draw curved surfaces.	*Object resolution*
group	A named set of atoms.	*Defining and selecting groups*
group	A named set of table cells.	*Grouping table information*
initialization script	A command script that is run automatically when Cerius^2 is started.	*Starting Cerius2 with an automatic script*
mixture elements	Special "elements" whose properties are definable as proportional mixtures of those of real elements.	*"Mixture" elements*
model manager	Set of tools in the main control panel for managing models and model spaces.	*Using the main control panel*
model space	A virtual "space" in the model manager environment that may or may not contain a model.	*Creating, clearing, and deleting model spaces*
pen colors	Individually defined drawing colors.	*Creating and editing a new color range*
projection	Representation of linear perspective.	*Superimposing models*
rendering	The production of high-quality 3D images.	*Rendering and ray-tracing*
residue ID	Alphanumeric representation of the location of a residue within a sequence.	—
residue type	Standard chemical name for an amino acid residue.	—
session	Lasts from when you start or reinitialize Cerius^2 until you quit or reinitialize Cerius^2.	*Working with Cerius2 sessions*

word	meaning	additional information
specular light	Highlights reflected from an object.	*Concepts*
temperature factors	Used to describe the effect of thermal vibration on crystal structures.	*Temperature factors*
thermal ellipsoids	Used to represent the thermal motion of atoms.	*Thermal ellipsoids*
value	The information actually displayed in a table cell.	*Applying mathematical expressions to cells or columns*
Visualizer	The core components and main control panel of Cerius^2.	*The Cerius2 Interface*

B. Definitions

C Mouse and Keyboard Actions

This section summarizes mouse and keyboard actions, organized according to what part of the Cerius^2 interface the cursor is over. To find mouse and keyboard actions organized according to what tasks you want to perform, please see the relevant sections of this documentation.

This section includes

This section summarizes:

Mouse actions

Keyboard shortcuts

Additional information

A graphical table of mouse actions in the model window can be accessed by selecting the **Help/Topics/Mouse Operations...** menu item in the main control panel to access the Model Window Mouse Operations control panel.

A table of keyboard shortcuts that apply to the model window can be accessed by selecting the **Help/Topics/Keyboard Operations...** menu item in the main control panel to access the Model Window Keyboard Operations control panel.

Mouse actions

This section summarizes what mouse button (and simultaneously pressed key on the keyboard, if any) to press and what mouse action to take in order to perform various activities when the cursor is over:

Control panels

Graph window

Model window

Table window

This section summarizes mouse activities only when the cursor is *in selection mode* (see *Selecting and deselecting individual atoms*). (Equivalent information for other modes, such as various measuring modes, is contained in the relevant sections of this documentation, since other modes are generally specific to certain types of tasks.)

Control panels

Any control

Table 27. Mouse actions that work when cursor over almost any control

Button[1]			Key	Operation	Action
				wait	Allow balloon help to appear.
✓				click	Activate or operate a control.
		✓		click	Obtain help on a control.

[1]The check mark indicates which mouse button to press.

File browser

Table 28. Selecting files in file browser (in any control panel containing one)

Button[1]			Key	Operation	Action
✓				click	Select only one file.
✓				drag	Select only a range of files.
✓				double click	Load the file.
✓			<Shift>	click	Select from the last selection through the file clicked upon.
✓			<Ctrl>	click	Select/deselect the clicked file; no change to other selections.
✓			<Ctrl>	drag	Select a range of files; no change to other selections.

[1]The check mark indicates which mouse button to press.

Model table

Table 29. Selecting models in main control panel's model table

Button[1]			Key	Operation	Action
✓				click	Select only one model (*Controlling model visibility and the display mode*).
✓				drag	Select only a range of models.
✓				double click	Select all models.
✓			<Shift>	click	Select from the last selection through the model clicked upon.
✓			<Ctrl>	click	Select/deselect the clicked model; no change to other selections.
✓			<Ctrl>	drag	Select a range of models; no change to other selections.
✓			<Ctrl>	double click	Deselect all models.

[1]The check mark indicates which mouse button to press.

Graph window

Table 30. Manipulating graph in graph window with mouse

Button[1]			Key	Operation	Action
✓			<Ctrl>	click	Identify coordinates and data points in graph.
	✓			drag horizontally	Scroll along the x axis.
	✓			drag vertically	Scroll along the y axis.
	✓		<Shift>	drag	Zoom in or out on graph.
	✓		<Alt>	drag	Zoom in on area within the dragged-out rectangle (*Changing graph axes and scale*).
	✓	✓		drag	Zoom in or out on graph (*Changing graph axes and scale*).

[1]The check mark indicates which mouse button to press.

Model window

Table 31. Manipulating model in model window with mouse

Button[1]			Key	Operation	Action
✓				click	Select an atom (click empty spot to deselect all atoms).
✓				drag	Select atoms enclosed by dragged-out rectangle.
✓			<Shift>	click	Select or unselect additional atom (*Selecting and deselecting individual atoms*).
✓			<Shift>	drag	Select more atoms enclosed by dragged-out rectangle.
✓			<Ctrl>	click	Make a model current (*Specifying the current model*).
	✓			drag	Translate all models in xy plane (*Translating models*).
	✓		<Shift>	drag	Change magnification of model view (*Changing the view magnification*).
	✓		<Shift><Ctrl>	drag	Translate current model in xy plane (*Translating the current model*).
	✓		<Shift><Alt>	drag	Change perspective angle (*Superimposing models*).
	✓		<Ctrl>	drag	Translate selected atoms as group in xy plane (*Translating and rotating atoms*).
	✓		<Ctrl><Alt>	drag	Translate selected atoms as a group along z axis.
		✓		drag horizontally	Rotate all models about y axis (*Rotating models*).
		✓		drag vertically	Rotate all models about x axis.
		✓		drag near edge	Rotate all models about z axis.
		✓	<Shift>	click	Obtain information about atom properties (*Tip*).
		✓	<Shift><Ctrl>	drag horizontally	Rotate current model about y axis (*Rotating the current model*).
		✓	<Shift><Ctrl>	drag vertically	Rotate current model about x axis.
		✓	<Shift><Ctrl>	drag near edge	Rotate current model about z axis.
		✓	<Shift><Alt>	drag	Change stereo separation (*Stereo viewing*).
		✓	<Ctrl>	drag horizontally	Rotate selected atoms as group about y axis (*Translating and rotating atoms*).
		✓	<Ctrl>	drag vertically	Rotate selected atoms as a group about x axis.
		✓	<Ctrl>	drag near edge	Rotate selected atoms as a group about z axis.
	✓	✓		drag	Change magnification of model view (*Changing the view magnification*).

[1]The check mark indicates which mouse button to press.

Table window

Cursor over individual cell

Table 32. Mouse actions when cursor is over a cell

Button[1]			Key	Operation	Action
✓				click	Make that cell (and also its row and column) current.
✓				double click	Same as click *and* send command (if any) to Cerius[2] (*Recalculating table values*).

[1]The check mark indicates which mouse button to press.

Cursor over row or column heading

Table 33. Mouse actions when cursor is over a row or column heading

Button[1]			Key	Operation	Action
✓				click	Select the entire row or column.
✓				drag line	Change row height or column width (*Changing row, column, and heading sizes*).
✓				double click	Same as click *and* send commands (if any) to Cerius[2] (*Recalculating table values*).
✓			<Shift>	click	Select from the last selection through the item clicked upon.
✓			<Ctrl>	click	Select an additional row or column.

[1]The check mark indicates which mouse button to press.

Keyboard shortcuts

This section summarizes what keys to press on your keyboard in order to perform various activities when the cursor is over:

Graph window

Model window

Table window

Graph window

Table 34. Manipulating graph in graph window with keyboard

Keys	Action
<Home>	Return magnification or scrolling to its original value.

Model window

Table 35. Key combinations that mimic menu items in main control panel

Keys	Menu item
<Ctrl> <Delete>	**Edit/Delete**
<Alt> a	**Edit/Select All**
<Alt> c	**Edit/Copy**
<Alt> l	**Edit/Duplicate**
<Alt> o	**View/Set Origin**
<Alt> r	**View/Reset View**
<Alt> t	**View/Center**
<Alt> v	**Edit/Paste**
<Alt> w	**View/Fill Window**
<Alt> x	**Edit/Cut**

Table window

Table 36. Manipulating model in model window with keyboard

Use keys on an extended keyboard, not on a numeric keypad.

Keys	Action
<F1>	Display function key help.
<F2>	Toggle between full screen and normal model display.
<F3>	Toggle between orthographic and perspective display projection (*Projection*).
<F4>	Toggle between full-screen stereo and normal model display.
<F5>	In stereo mode, toggle between Crystaleyes and stereo-pair mode (*Stereo viewing*).
<F10>	On 8-bit machines, toggle between single- and double-buffer graphics mode.
<->	Decrease magnification of model view (zoom out).
<+>	Increase magnification of model view (zoom in).
<Home>	Reset model view.
<End>	Fill window.
<↑>	Rotate model up by 45°.
<←>	Rotate model left by 45°.
<↓>	Rotate model down by 45°.
<→>	Rotate model right by 45°.

Table 37. Moving cursor in table window with keyboard

Use keys on an extended keyboard, not on a numeric keypad.

Keys	Action
<Esc>	Cancel and undo editing.
<Tab>	Enter value (if any) and move to the cell to the right of the current cell (*Entering your changes*).
<Tab><Shift>	Activate the cell edit window (*Editing cell contents*).
<Enter>	Enter value (if any) and move to the cell below the current cell.

Table 37. Moving cursor in table window with keyboard

Use keys on an extended keyboard, not on a numeric keypad.

Keys	Action
<↑>	Move to the cell above the current cell.
<←>	Move to the cell to the left of the current cell; in cell edit window, move one character to the left.
<↓>	Move to the cell below the current cell.
<→>	Move to the cell to the right of the current cell; in cell edit window, move one character to the right.
any other	Activate the cell edit window and start entering characters.

D File Formats

Cerius^2 supports the import and export of a wide range of common file formats for the storage of atomic coordinates and associated data. This facility enables you to interface with other molecular modeling and computational chemistry programs, including procedures you have written yourself.

This section briefly describes the file formats supported in Cerius^2:

MSI-format structure files

MSI — Molecular Simulations native Cerius^2 format

CAR, MDF, ARC, COR — Molecular Simulations native Insight II formats. Documentation can be found elsewhere in: http://www.msi.com/doc/

MSF — Molecular Simulations QUANTA® structure file format

BGF — Molecular Simulations BIOGRAF™ file format

Other-format structure files

CAMBRIDGE (read only) — Cambridge Crystallographic Database FDAT format

CIF (read only) — Crystallographic Information File

CSSR — SERC Daresbury Laboratory's Cambridge Structure Search and Retrieval file format.2

ICSD (read only) — Inorganic Crystal Structure Database

MACCS/Molfile— MDL's MACCS file format

MolEN — Enraf–Nonius' MolEN file format

MOPAC — MOPAC/AMPAC file format

PDB — Brookhaven Protein Data Bank format

SHELX — SHELX structure file format

Temperature factors in files

Information on storing temperature-factor information in structure files of various formats:*Loading and saving temperature factors in structure files.*

Graph files

.Grf— Molecular Simulations native Cerius^2 format for graphs

TBL — Molecular Simulations native Insight II format for graphs. Documentation can be found elsewhere in:http://www.msi.com/support/

.Xy and .con files — Molecular Simulations old format for graphs

Note

The format descriptions in this appendix detail only what Cerius^2 actually loads or saves, which may not be all types of data stored in nonMSI files.

Structure files

MSI

The MSI Cerius^2 native file format, the default for loading and saving in the Cerius^2 environment, is extremely flexible. This format (default extension .msi) can hold all the information in the Cerius^2 data model necessary to describe the attributes of a model.

The MSI file format is not designed to allow easy manual creation or editing. However, you can easily read it, if required. An example file for an methane model is (comments in bracketed *italic type* are *not* part of the file):

```
# MSI CERIUS2 DataModel File Version 2 0
(1 Model [1 is the object ID, Model is the object type and delimits model data]
 (A C Label methane) [A = attribute tag, C = string-type attribute]
 (2 Atom [2 is the object ID, Atom is the object type and delimits data for first atom]
  (A I ACL "1 H") [A = attribute tag, I = integer-type attribute]
  (A F Charge 0.028) [F = floating-point type attrubute, Charge is the nameof the attribute,
            the following number is the attribute's value]
  (A C Label H1)
 )
 (3 Atom
  (A I ACL "6 C")
  (A F Charge -0.11)
  (A D XYZ (1.087 0 0)) [D = double-precision type attribute, the three values are an array]
  (A C Label C2)
 )
 (4 Atom
  (A I ACL "1 H")
  (A F Charge 0.028)
  (A D XYZ (1.4493 1.02483 0))
  (A C Label H3)
 )
 (5 Atom
  (A I ACL "1 H")
  (A F Charge 0.028)
  (A D XYZ (1.44936 -0.51245 -0.88749))
  (A C Label H4)
 )
 (6 Atom
  (A I ACL "1 H")
  (A F Charge 0.028)
```

```
  (A D XYZ (1.44934 -0.51236 0.88756))
  (A C Label H5)
 )
 (7 Bond  [Bond is the object type and delimits data for first bond]
  (A O Atom1 2)  [O = object-OD type attribute]
  (A O Atom2 3)
 )
 (8 Bond
  (A O Atom1 3)
  (A O Atom2 4)
 )
 (9 Bond
  (A O Atom1 3)
  (A O Atom2 5)
 )
 (10 Bond
  (A O Atom1 3)
  (A O Atom2 6)
 )
)
```

Allowable attribute types are: B (byte), C (string), D (double-precision number), F (floating-point number), I (integer), O (object ID), S (short), T (table).

Allowable object types include ACL, Atom, Bond, Group, SCL, Sequence, Subunit, *string*.

Allowable values are scalars (number or quoted string), arrays (values in parentheses, separated by white space), tabular data.

MSF

The Molecular Simulations File (MSF) format enables you to communicate with the QUANTA / CHARMm software. MSF files (default extension .msf) store element types, coordinates, connectivity, crystal cell parameters, symmetry information, and charges. Symmetry information is written out and read in as General Positions. MSF files are suitable for crystal and nonperiodic structures.

Note

MSF files are not written in ASCII format; you cannot edit them.

BGF

The Molecular Simulations BIOGRAF (BGF) format allows communication with the BIOGRAF, POLYGRAF, and NMRgraf programs. BGF files (default file extensions .bgf or .xtl) are suitable for periodic and nonperiodic structures, storing element types, coordinates, connectivity data, and charges. For periodic structures, space group and space group table number are also stored.

Cerius^2 reads in POLYGRAF monomers (with H atoms labeled as Head and Tail), and substitutes Cerius^2 Head and Tail atoms. When saving Cerius^2 monomers in the BGF format, POLYGRAF Heads and Tails are substituted for their Cerius^2 equivalents.

Cerius^2 crystals are written as periodic POLYGRAF BGF files. On importing, crystal details from these periodic files are read into the Cerius^2 data structures, although the crystal cell is not automatically reconstructed.

The significant records recognized by Cerius^2 are described in terms of FORTRAN edit descriptors in the following table:

Record	Format	Storage
(1) FILTYP	(A6,I5)	File Header – 'BIOGRF' or 'XTLGRF' (for periodic files), version number of software in which file format was last changed (for example, 300 for version 3.0 of POLYGRAF).
(2) DESCRP	('DESCRP',1X,A8)	Descriptor – 'DESCRP', a short descriptor for the file (can contain upper/lower cases and spaces).
(3) REMARK	('REMARK',1X,A)	File Description – 'REMARK', descriptive information about the file.
(4) FORCEFIELD	('FORCEFIELD', 1X,A8)	ASCII force field name – 'FORCEFIELD', name of the force field.
(5) PERIOD (periodic files only)	('PERIOD',1X,3I1)	Periodicity in x, y, and z – 'PERIOD', 0 | 1, 0 | 1, 0 | 1 (flags indicate whether periodic in x, y, and z). Ignored on reading, set to '111' when writing crystals.
(6) AXES (periodic files only)	('AXES',3X,A)	Axis order – 'AXES', order of axes (for example, 'zyx'). Ignored on reading, set to 'zyx' when writing crystals.

Record	Format	Storage
(7) SGNAME (periodic files only)	('SGNAME',1X, A8,1X,A8,2I5)	Space group information – 'SGNAME', space group name, Schönflies symbol for the space group, space group number, case number. A case number is only used for space groups where there is a choice of unique axis, cell origin, or axis geometry. Note: Ignored on reading because all atoms (including symmetry copies) are contained in atom records.
(8) CRYSTX (periodic files only)	('CRYSTX',1X, 6F11.5)	Cell parameters – 'CRYSTX', Specification of unit cell parameters, lengths of axes (a,b,c) in Å and angles (alpha, beta, gamma) in degrees.
(9) CELLS (periodic files only)	('CELLS',1X,6I5)	Cell extension limits – 'CELLS', Min a, Max a, Min b, Max b, Min c, Max c (the number of rows of cells to be added in negative and positive directions along the a, b, and c axes). Ignored on reading. On writing, min set to -1, max to +1. This ensures that model is extended in POLYGRAF, ensuring any crystal bonding is not lost.
The following five record classes are present only in periodic files.		
(10) XTLUNQ (files with structures generated by POLYGRAF Crystal Builder only)	('XTLUNQ',I5,1X, A5,1X,A3,1X,A1, 1X,3F9.6,1X,A5, 1X,2I3,F8.4,I2, F6.2	Fractional coordinates and designator information – 'XTLUNQ', atom number, atom label, residue name, chain designator (must be upper case or blank), residue number, fractional x, y, and z coordinates, atom type, max. number of covalent bonds, no. of lone pairs, atomic charge, atom symbol code (1=dots, 2=tetrahedron, 3=octahedron, 4=6-point jack, 5=12-point jack, 6=18-point jack), atom symbol size (in Å), atom symbol color (hue value in range 0-360).
(11) FORMAT ATOM	'FORMAT ATOM', 3X, A	ATOM/HETATM record format specification (if not present, the default format is used) – 'FORMAT ATOM', format specification for ATOM/HETATM records.
(12) ATOM or HETATM	('ATOM' | 'HETATM', 1X,I5,1X,A5,1X, A3,1X,A1,1X,A5, 3F10.5,1X,A5,I3, I2,1X,F8.5)	Atomic coordinate and force field records for standard groups – 'ATOM' or 'HETATM', atom number, atom label, residue name, chain designator (must be in upper case or blank, residue number, x, y, z coordinates (in Å), atom type, max. no. of covalent bonds, no. lone pairs, atomic charge. Note: Only atom number, label (HX, TX label monomer heads and tails), coordinates, types, and charges are relevant in Cerius^2. The other variables are XXXGraf entities.
(13) FORMAT CONECT	('FORMAT CONECT', 1X,A	CONECT record format specification (if not present, the default format is used) – 'FORMAT CONECT', format specification for CONECT records.
(14) CONECT	('CONECT', 12I6)	Connectivity list – 'CONECT', number of central atom, atom numbers of atoms bonded to central atom.

Record	Format	Storage
(15) ORDER	('ORDER'),1X,12I6)	Bond order records – 'ORDER', number of central atom, bond orders for atoms bonded to central atoms (0/1=single, 2=double, 3=triple bond).
The atom numbers in CONECT records represent the atom numbers of the equivalent unit cell atoms. The following three records specify whether the central atom is bonded to an atom in the same cell or a neighboring cell. These record classes are present only in periodic files, where there are one or more connections to a neighboring cell.		
(16) DISPX	('DISPX',1X,12I6)	X cell displacement record – 'DISPX', number of central atom, x differences in cells of the two connected atoms. Values correspond to equivalent numbers in 'CONECT' list. Possible values are -1, 0, and 1.
(17) DISPY	('DISPY',1X,12I6)	Y cell displacement record – 'DISPY', number of central atom, y differences in cells of the two connected atoms. Values correspond to equivalent numbers in 'CONECT' list. Possible values are -1, 0, and 1.
(18) DISPZ	('DISPZ',1X,12I6)	Z cell displacement record – 'DISPZ', number of central atom, z differences in cells of the two connected atoms. Values correspond to equivalent numbers in 'CONECT' list. Possible values are -1, 0, and 1.
(19) END	('END')	End of file marker – 'END'.

CAMBRIDGE (read only)

Cerius^2 provides read only support for Cambridge Crystallographic Database FDAT format files (default file extension .fdat).

Cerius^2 reads only atom coordinates, element types, crystal cell parameters, symmetry operators, and bonding connectivity from FDAT files.

For more information about the FDAT format, contact the Cambridge Crystallographic Database.

CIF (read only)

Cerius^2 provides read only support for Crystallographic Information File (CIF) format files. Beginning with version 3.0 Cerius^2 could read CIF files generated by the Cambridge Structural Database to their specification. Beginning with version 3.7 Cerius^2 includes a reader that supports more generic CIF files, i.e., files

specified to the minimum requirement for submission to the journal *Acta Cryst C* by the International Union of Crystallography.

At a minimum the file must contain either:

- unit cell parameters or
- atom coordinates (Cartesian) and atom types (or atom labels).

To utilize space group information the file must include:

- symmetry positions and
- either International Tables (IT) number OR cell setting.

If space group information is not used, the file must include both:

- cell setting and
- space group name

so that the lattice type and the lattice centering can be found.

Cerius^2 reads:

cell setting

space group name

symmetry positions

unit cell parameters

atom labels

atom types (if present -- if not, get from atom labels and _atom_type_symbol, if present)

atom coordinates (fractional)

occupancies

isotropic temperature factors

isotropic / anisotropic flag

anisotropic temperature factors

connectivity

CSSR

SERC Daresbury Laboratory's Cambridge Structure Search and Retrieval (CSSR) files contain information very similar to CAMBRIDGE files, but were developed to be easier to create, read, and edit manually.

Suitable for storing nonperiodic, 2D, and 3D structures, CSSR files can store Cartesian or fractional coordinates of atoms and their element types. Optionally, bonding connectivity (higher-order bonds), crystal unit cell parameters, space group, and atomic charge information can also be stored. The default file extension for CSSR files is .cssr, although for 3D structures, .fcssr is sometimes used to indicate that fractional coordinates have been used.

CSSR files consist of four standard records plus one for each atom. These records are described in terms of FORTRAN edit descriptors in the table below.

Record	Format	Stores
1	38X, 3F8.3	Cell dimensions – Contains the length of the three cell parameters (a, b, and c) in angstroms.
2	21X, 3F8.3, 4X, 'SPGR =', I3, 1X, A11	Cell angles and space group – Cell angles, a, b, g in degrees, space group number, space group name.
3	2I4, 1X, A60	Title, number of atoms and coordinate system – Number of atoms stored, coordinate system flag (0=fractional coordinates, 1=orthogonal coordinates in Å), first title.
4	A53	Second title – A line of text that can be used to describe the file; read on input but otherwise unused.
5 on... (one per atom)	I4, 1X, A4, 2X, 3(F9.5.1X), 8I4, 1X, F7.3	Atom specific information – Atom serial number, atom name, x, y, z coordinates, bonding connectivities (max 8), charge. Note: The atom name is a concatenation of the element symbol and the atom serial number.

ICSD (read only)

Cerius^2 provides read-only support for Inorganic Crystal Structure Database ICSD format files (default file extension .icsd).

Cerius^2 reads element types, bonding, atom coordinates, and crystal unit cell parameters. Symmetry information is loaded as space groups unless the information is nonstandard, in which case special position information is provided. For details, refer to the *ICSD User Manual* (1991), Section 9.

MACCS/Molfile

MDL's MACCS file format is widely recognized by modeling programs and chemical information systems. MACCS files (default file extension .mol) are similar to CSSR files but are not suitable for periodic models, as they do not store unit cell parameters or fractional coordinates. Bond order information is stored but not used by Cerius^2.

MACCS files consist of four standard records plus one record for each atom and each bond. These records are described in terms of FORTRAN edit descriptors in the table below:

Record	Format	Stores
1	A	Title – A line of text description for the file
2	20X, A2	Dimensionality – The dimensionality of coordinates; this is always '3D' for MACCS files output by Cerius^2
3		Unused
4	2I3	Number of atoms and bonds – Total number of atoms and total number of bonds in the file
5 onwards (one for each atom)	3F10.5, 1X, A2	Atom coordinates and elements – X,Y,Z coordinates, (each atom), element type
(then for each bond)	3I3	Bonding – The serial numbers of the two bonded atoms and the order of the bond between them

MolEN

Support for the Enraf–Nonius' MolEN file format (default file extension .xyz) is provided for editing existing MolEN files. Only users of MolEN can load and save files of this type.

The files atoms.xyz and master.par must be present in the directory where the files are stored. Any .xyz files may be loaded into Cerius^2, but MolEN files saved by Cerius^2 are named cerius.xyz. Only atom information can be saved from Cerius^2; changes in symmetry or crystal cell dimensions cannot be saved.

MOPAC

The MOPAC / AMPAC Z-matrix file format is the data input standard for the MOPAC and AMPAC quantum mechanical programs. The default file extension for MOPAC files is .pac.

Model structures are stored as internal coordinates using Z-matrix format (that is, bond lengths, bond angles, and torsion angles), rather than Cartesian coordinates (that is, x y z positions). Although certain connectivity information is included, MOPAC files do not store true bonding data. If required after loading, bonding can be recalculated using the **Bond Calculation** controls in the Edit Connectivity and Bonding control panel. Atomic charges are optionally stored. Because no crystal or surface information is stored, MOPAC files are suitable for storing only nonperiodic structures.

The principal advantage of the internal coordinates system over a Cartesian structure description is the ease of creating structures from known bond length, angle, and torsion data.

The first three records are text: Record 1 is reserved for MOPAC key words, and records 2 and 3 are text lines that can be used for whatever purpose you want. (Cerius^2 leaves them blank.) These are followed by records that define element type, bond length, bond angle, torsion angle, connectivity, and charge for each atom.

The three geometry parameters (bond length, angle, and torsion angle) are followed by a flag that can be 0 or 1. If the flag is 0, the geometric variable is fixed; if 1, it will be optimized.

MOPAC files consist of three standard records plus one record for each atom. These records are described in terms of FORTRAN edit descriptors in the following table:

Record	Format	Storage
1	Free format space separated text	Keywords – Reserved for MOPAC or AMPAC keywords
2	A (free format text)	Title 1 – A line of optional, user-specified text
3	A (free format text)	Title 2 – A further line of optional, user-specified text
4 on... (one per atom)	A, F, I, F, I, F, I, 3I, F	Element type, (in free format) length, flag, angle, flag, torsion angle, flag, connectivity atom numbers, charge

Bond lengths are specified in angstroms and angles in degrees. Flags in record 4 onwards can take values of 0 or 1:

- **0** — The preceding geometric variable is fixed.
- **1** — The preceding geometric variable will be optimized.

PDB

The Brookhaven Protein Data Bank (PDB) structure file format can be used to save both 3D and nonperiodic structures and is widely recognized by molecular modeling software. Brookhaven PDB files (default file extension .pdb) store Cartesian coordinates and element types of atoms. Bonding connectivity and crystal unit cell parameters can also optionally be stored (although crystal cells are not automatically reconstructed upon reloading into Cerius^2).

PDB files consist of 80-character records, each with a left-justified keyword of as many as six characters that indicates its record format type. Records can be in any order, with at least one ATOM record present. Of the many PDB record types in the complete specification, only the following are supported in Cerius^2:

- ATOM
- CRYST1
- HETATM

- CONECT
- END

Others are ignored on input and blank on output.

For a full description of the PDB format, refer to *Atomic Coordinate and Bibliographic Entry Format Description* (1985).

SHELX

The SHELX structure file format (default file extension .res) allows communication with the SHELXTL program, the standard for X-ray single-crystal structure determination.

It stores element types, coordinates, connectivity, isotropic and anisotropic temperature factors, occupancies, crystal cell parameters, and symmetry. Symmetry is written out and read in as General Positions.

Loading and saving temperature factors in structure files

The MSI, SHELX, ICSD, DBWS, and MolEN structure file formats can all be used to store isotropic and anisotropic temperature factors (*Temperature factors*). The DBWS file format can be saved and read only by using the Rietveld (DBWS) menu card, *not* by using the Visualizer.

The conversions made between the stored file format and the Cerius^2 format use the assumptions described below:

MSI

The MSI structure file format:

- Uses U_{iso} and U_{ij} formats
- Order is U_{11}, U_{22}, U_{33}, U_{12}, U_{23}, U_{13}

SHELX

The SHELX (Siemens 1990) structure file format:

- Uses U_{iso} and U_{ij} formats
- Order is U_{11}, U_{22}, U_{33}, U_{23}, U_{13}, U_{12}

ICSD

The ICSD (Fachinformationszentrum 1991) structure file format:

- Uses U_{iso} and B_{iso}
- Uses U_{ij}, β_{ij}, and β_{ij}
- Order is U_{11}, U_{22}, U_{33}, U_{12}, U_{13}, U_{23}
- β cross terms include a factor of two in the term

DBWS

The DBWS (1991) structure file format:

- Uses B_{iso} and β_{ij}
- Order is β_{11}, β_{22}, β_{33}, β_{12}, β_{13}, β_{23}
- β cross terms do *not* include a factor of two

MolEN

The MolEN (Enraf-Nonius 1990) structure file format:

- Uses B_{iso} and β_{ij}
- Order is β_{11}, β_{22}, β_{33}, β_{12}, β_{13}, β_{23}
- β cross terms include a factor of two in the term

.Grf

Files for graphical data in Cerius^2 should be stored in files with the extension .grf. Cerius^2 .grf files can describe any state of the GRAPHS data structure. Some example files are stored in the Cerius2-Resources/EXAMPLES/data directory.

The file format consists of a header record, followed by any number of Object Definition Blocks (ODB), followed by a termination record.

Header record

A header must be the first record of the file. It is of the form:

```
CERIUS Grapher File
```

Comments

Any subsequent line of the file can be a comment line, in which the first character must be an exclamation point (!). Such lines are ignored by the file parser.

Object definition blocks

Each ODB is an independent unit, although it may be referenced from other ODBs. A single ODB may define a single:

- Data set
- Set of plotting attributes — This references one data set ODB
- Graph — This references any number of data set ODBs
- Gallery — This references any number of graph ODBs

Any record that begins with a greater-than symbol (that is, >) is considered to mark the beginning of an ODB and the end of any previous ODB.

Subsequent records of the ODB are single-record token descriptors in the form of a token (in capital letters) followed by a value. The only exceptions to this are graph-title descriptors and data-value descriptors, both of which occupy multiple records.

In the following description, terms enclosed in brackets ([ ]) are values / strings extracted from the file by Cerius^2. Where such values have been expressed in capitals, these represent the range of accepted values.

All token descriptors within an ODB are optional and can appear in any sequence. When Cerius^2 expects a token descriptor in an ODB and does not find one, a default value is used for the associated attribute.

X–Y data set ODB

Initiation record

```
>PLOT XY DATA: "[name]" [version]
```

`[name]` This is the character name by which the data set can be referenced.

`[version]` This optional integer can be used to distinguish different versions of data sets that share the same name. When loaded, the sequence of these numbers among the data sets is preserved.

Descriptors

Descriptors are any number of records, each containing two blank-delimited real numbers. They define the x and y ordinates of each point in the data set.

2D data set ODB

Initiation record

```
>PLOT 2D DATA: "[name]" [version]
```

`[name]` This is the character name by which the data set can be referenced.

`[version]` This optional integer can be used to distinguish different versions of data sets that share the same name. When loaded, the sequence of these numbers among the data sets is preserved.

Descriptors

`SYSTEM [POLAR/CARTESIAN]` The coordinate system of the data set. This must match the SYSTEM of any graph referencing the data set.

`SYMMETRY [NONE/LATTICE/XREFLECT/YREFLECT/XYREFLECT/QUADRANT]` LATTICE means regular unit-cell repeats and is for Cartesian systems only. XREFLECT, YREFLECT, and XYREFLECT are for Cartesian systems only. QUADRANT is for polar systems.

`XMIN [ordinate/angle in degrees]` In Cartesian graphs, this is the center of the first pixel.

`XMAX [ordinate/angle in degrees]` This equals xmin + width * (ordinates per pixel).

`YMIN [ordinate]` In Cartesian graphs, this is the center of first pixel.

`YMAX [ordinate/radius]` This equals ymin + height * (ordinates per pixel).

`XSIZE [width]` This is the number of data points in each row.

`YSIZE [height]` This is the number of rows of data.

DATAPOINTS [points] This must be the last record of the ODB. It is followed by [points] = [width] * [height] blank-delimited real values.

X–Y plotting attribute ODB

Initiation record

```
>PLOT XY METHOD: "[name]" [version]
```

[name] and [version] These refer to an X–Y data set ODB within the file.

Descriptors

COLOUR [color] One of the Cerius^2 colors (for example, RED, PIN, YEL etc.). The default is WHI (white).

STYLE [LINE/POINT/HISTOGRAM/DELTA/DELTA-TIC] The default is POINT.

YOFFSET [ordinate] The default is 0.0.

LABEL [string] This is the label to appear on the key. The default is the string “Undefined”.

2D plotting attribute ODB

Initiation record

```
>PLOT 2D METHOD: "[name]" [version]
```

[name] and [version] These refer to a 2D data set ODB within the file.

Descriptors

STYLE [CONTINUOUS/CONTOUR/DELTA] Data representation, the default is CONTINUOUS.

CONTOURS [contours] A positive integer.

COLOUR [GREY-SCALE/COLOR/DIFFERENCE] Color-map. The default is GREY-SCALE.

CONVERSION [LINEAR/LOG] Mapping function. The default is LINEAR.

INTERP [NEAREST/LINEAR] Interpolation system. The default is NEAREST.

POLARITY [POSITIVE/NEGATIVE] The default is POSITIVE.

LOWEST [data-value] A real number. This is the lowest color-mapping value.

`HIGHEST [data-value]` A real number. This is the highest color-mapping value.

`EXPOSURE [exposure]` A real number. The default is 1.0.

`BRIGHTNESS [brightness]` A real number. The default is 1.0.

`CONTRAST [contrast]` A real number. The default is 1.0.

X–Y graph ODB

Initiation record

`>GRAPH XY METHOD: "[name]" [version]`

`[name] and [version]` Unique to this Graph. These are very similar to data set name and version number.

Descriptors

`SCALE [FIXED/AUTO-XY/NICE-XY/AUTO-Y/NICE-Y]` The default is FIXED; the specified range is used.

`XMIN [ordinate]` Not needed for AUTO-XY or NICE-XY.

`XMAX [ordinate]` Not needed for AUTO-XY or NICE-XY.

`YMIN [ordinate]` Not needed for AUTO-XY, NICE-XY, AUTO-Y, or NICE-Y.

`YMAX [ordinate]` Not needed for AUTO-XY, NICE-XY, AUTO-Y, or NICE-Y.

`XLABEL [string]` Text for the X axis label.

`YLABEL [string]` Text for the Y axis label.

`TITLE [lines]` The number of title lines on records to follow.

`SCALES [ON/OFF]` Axis box numbering; the default is ON.

`KEY [ON/OFF]` The default is ON.

`PLOT "[name]" [version]` An x–y data set ODB within the file. These may occur any number of times, for different data sets, within the ODB. Sequenced in plotting order (that is, in reverse precedence).

2D graph ODB

Initiation record

`>GRAPH 2D METHOD: "[name]" [version]`

`[name] and [version]` Unique to this graph. These are very similar to data set name and version number.

Descriptors

`SYSTEM [POLAR/CARTESIAN]`

`XMIN [ordinate/angle in degrees]`

`XMAX [ordinate/angle in degrees]`

`YMIN [ordinate]` Not needed in polar system.

`YMAX [ordinate/radius]`

`AXES [RECTANGULAR/OBLIQUE]` Cartesian system only. The default is OBLIQUE.

`XYANGLE [angle in radians]` Cartesian system only. Angle between axes.

`ASPECT [aspect ratio]` Cartesian system only. y:x. The default is 1.0.

`XLABEL [string]` Text for the x axis label.

`YLABEL [string]` Text for the y axis label.

`TITLE [lines]` The number of title-lines on records to follow.

`SCALES [ON/OFF]` Axis box, numbering. The default is ON.

`KEY [ON/OFF]` The default is ON.

`PLOT "[name]" [version]` A 2D data set ODB within the file. These may occur any number of times, for different data sets, within the ODB. Sequenced in plotting order (that is, in reverse precedence).

Gallery ODB

Initiation record

`>GALLERY METHOD:`

Descriptors

`GRAPH "[name]" [version]` Any graph ODB within the file. These may occur any number of times, for different graphs, within the ODB. Sequenced in plotting order (from top-left, row by row).

Termination record

This is normally the last record of the file. It is of the form:

`>END`

.Xy and .con files

Versions of CERIUS prior to CERIUS3.2 used different file formats for one and two dimensional data:

- XY file (extension .xy) for 1D data. Stores xy graph data in a sequence list of x and y values.
- CON file (extension .con) for 2D data. Stores data points as a function of two fixed range and interval variables, x and y.

These two formats can be loaded into Cerius^2, but files cannot be saved in this format. All graphs are saved in the current .grf format.

File documentation at our website

The formats of these files are documented at our website, in http://www.msi.com/doc/

- .car, .mdf, .arc,. cor
- .tbl

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