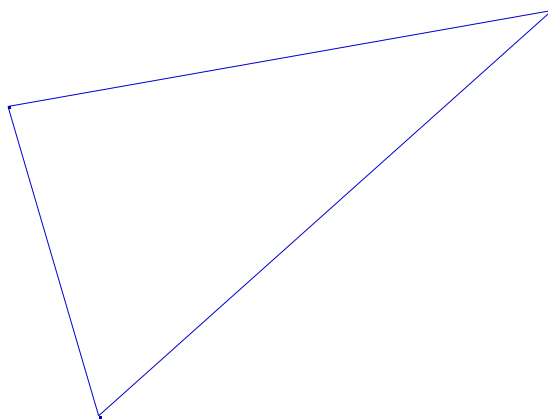


CrystalDesigner User's Guide



Crystal Structure Design AS

Crystal Structure Design AS License Agreement

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1. Welcome

About CrystalDesigner

CrystalDesigner is a computer program available on the Macintosh platform. The program is a complete tool for building, studying and visualising all kinds of inorganic crystal structures. CrystalDesigner is intended to be used by students and teachers at colleges and universities and by scientists at universities and in the industry.

From an educational point of view, CrystalDesigner will make the learning of crystallography more interesting and will provide a faster way of understanding crystal structures in general. This is possible through the easy-to-use graphical user interface to CrystalDesigner.

From a scientist point of view, CrystalDesigner is a lighting fast way of creating all kinds of graphical representations of inorganic crystal structures.

Main features of CrystalDesigner:

All kind of crystal structures can be build by knowing the crystal system, space group, lattice parameters and atom positions. The program generates symmetry elements and atom positions based on the input.

Viewing the crystal structure can be done in three different ways: i) as unit cells or multiples of it, ii) as a plane with a user defined thickness or iii) by coordination around a selected atom within a user defined ratio.

The atoms may alternatively by viewed as points, circles or spheres. Bonds between atoms can be created and be viewed as lines, cylinders or cones. Groups of atoms can alternatively be viewed as polyhedra.

The crystal structure may be rotated in any direction or around a fixed axis. Distance and angle between atoms can be measured.

CrystalDesigner is a multiple document window application. Each document window contains all the necessary the information about a crystal structure and for each document the program can create multiple windows visualising the crystal structure.

Different versions

Three different versions of CrystalDesigner have been made in order to take advantage of the different processor configurations: They are named CrystalDesigner DR4, 68k-version, CrystalDesigner DR4, FPU-version and CrystalDesigner DR4, PCC-version. There is also a fourth version named CrystalDesigner DR4 68k + PPC-version that consist of both CrystalDesigner DR4 68k-version and the CrystalDesigner DR4 PCC-version. You do not need

to worry about which version to use. The CrystalDesigner installer program on Disk #1 does the job for you.

CrystalDesigner DR4 68k-version runs on all Macintosh computers with a 68020 CPU or higher. CrystalDesigner DR4 FPU-version require a Macintosh with a 68020, 68030 or a 68040 CPU with a math coprocessor installed to run, and CrystalDesigner DR4 PPC-version require a Power Macintosh to run.

What You Need

CrystalDesigner runs on all Macintosh computers with a 68020 CPU or higher. This includes all Macintosh models except Macintosh 128, 512, Plus, SE, Portable, Classic and PowerBook 100.

In addition, CrystalDesigner requires that you have a hard drive, System 7 or higher and at least 2.5 MB of available memory to run. When you install CrystalDesigner on your startup disk, it takes up about 4-5 MB of your disk space.

About this documentation

This user's guide contain the necessary information to use CrystalDesigner. The guide consist of four parts: Welcome, Installation, Tutorial and finally a part that describes the Menus and floating Windows.

Welcome

This is the part you are reading now. It gives you a general introduction about CrystalDesigner and the necessary requirements to be able to use the program. You will also get information about how to get support and how to get the latest news about CrystalDesigner.

Installation

The installation part tells you how to install CrystalDesigner. Be sure to read the installation instructions before you install CrystalDesigner.

Tutorial

The tutorial part gives you an introduction to the basics of CrystalDesigner. You will learn how to build a crystal structure and how to create different graph views of a crystal structure. It will take you about half an hour to complete the tutorial. If you do not normally read manuals, please at least scan through the tutorial.

Menus and floating windows

Here all the CrystalDesigner menu commands will be described. A description of the floating windows visible when a graph window is active is also present.

Naming Conventions

Names of menus, buttons, commands and icons are in **boldface**.

A crystal structure project is defined as the document window containing the crystal structure data and all the graph windows representing the crystal structure. Figure 1.1 shows you a graphical illustration of the definition of a crystal structure project.

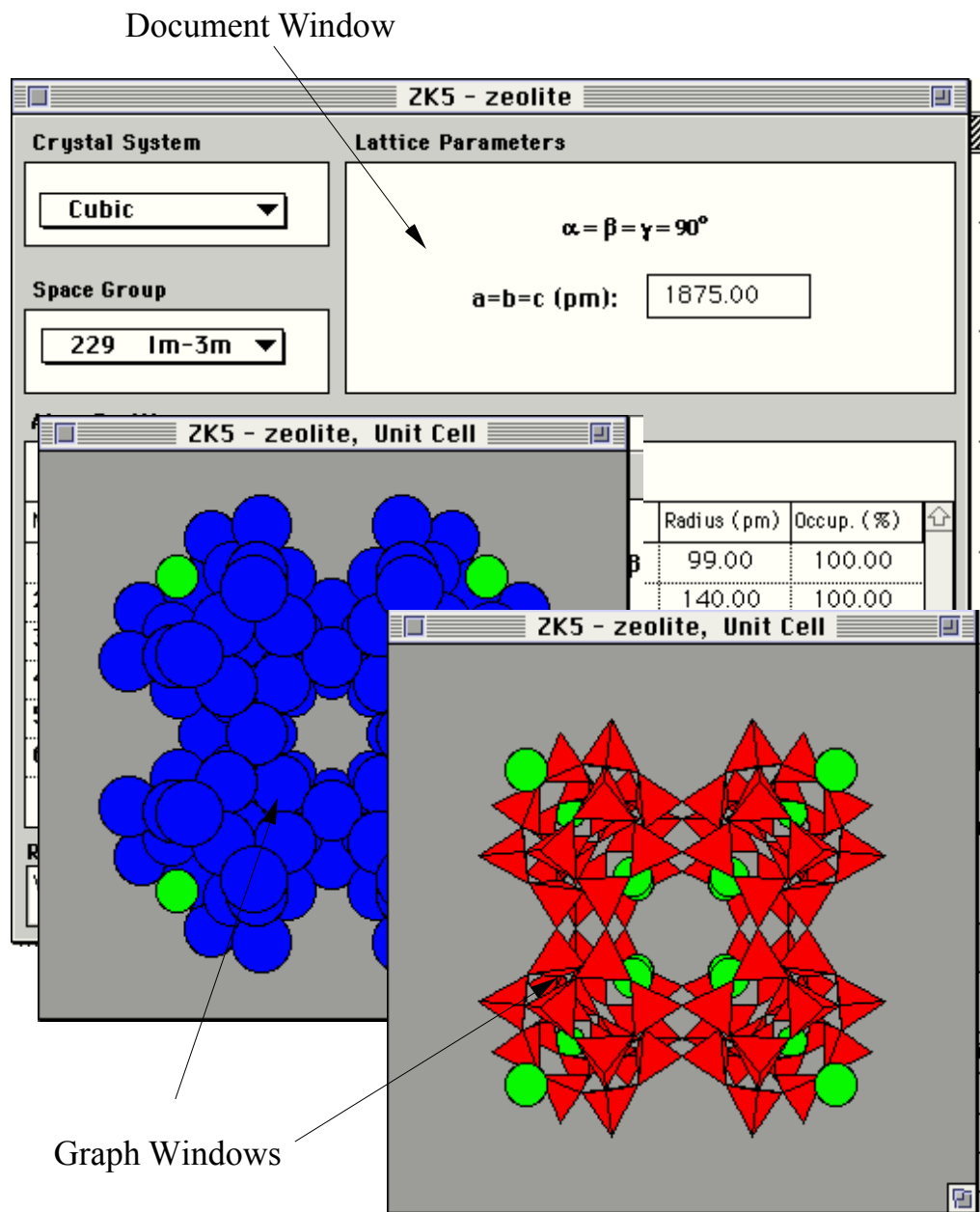


Figure 1.1 A crystal structure project is defined as the document window containing the crystal structure plus all the graph view belonging to the corresponding crystal structure.

Support and info

All customers of CrystalDesigner will receive free support through Internet by sending <mailto:support@crystaldesigner.no>. We will reply to all questions about CrystalDesigner within 24 hours. Please, send also general feedback about CrystalDesigner. We will try to incorporate as many as possible of the suggested features in upcoming versions of CrystalDesigner.

Information about CrystalDesigner is also available via WWW on the Internet. Here you can find the latest news, example files, order and contact information, feature list, company information and demo versions of the CrystalDesigner. The address is:

<http://www.oslonett.no/CrystalD/index.html>.

You can also download demo versions by using ftp. The address is <ftp://ftp.oslonett.no/Software/Mac/omp/crystald/>

Release Schedule

Crystal Structure Design AS plans to release new versions of CrystalDesigner with a four month interval. The next two releases will be CrystalDesigner DR5 scheduled for Mars 1996 and CrystalDesigner DR6 scheduled for August 1996.

Please note that all current customers will receive free updates of both CrystalDesigner DR5 and DR6. The updates will be sent to you free of charge by Air mail when they are available.

Our goals for the next two releases:

- Import of crystal structure data from text files. (CIF format , +++))
- Support for coordination polyhedra around atoms that have coordination twelve or less
- Support for occupancy lower than 100 %
- Improved documentation
- Full support of QuickDraw 3D

References to text books

This manual assumes you are familiar with or are in the process of learning Crystallography, the science concerned with the study of crystal structures. Supplementary readings are available. Check out

"International Tables for Crystallography", Volume A, Edited by Theo Hahn, Kluwer Academic

Publishers, Dordrecht, 1992, ISBN 0-7923-1678-9

"Fundamentals of Crystallography", Edited by C. Giacovazzo, Oxford University Press, Oxford, 1992, ISBN 0-19-855579-2

"Solid State Chemistry and its Applications", Written by A. R. West, John Wiley & Sons, New York, 1987, ISBN 0-471-90377-9



Figure 1.2 A screen capture of the Home Page of CrystalDesigner on Internet

2. Installation

Before you install CrystalDesigner DR4, be certain that you have enough space on your startup disk. The installation will require about 4-5 MB of disk space. If you have a math processor emulator (SoftwareFPU) installed on your computer, turn it off before you install CrystalDesigner DR4.

To install CrystalDesigner, insert Disk #1 and double-click the file CrystalDesigner Installer. You will see a dialog like the one in figure 2.1.



Figure 2.1 Welcome to the Installer for CrystalDesigner

Click **continue** and a dialog like the one in figure 2.2 appears on the screen.

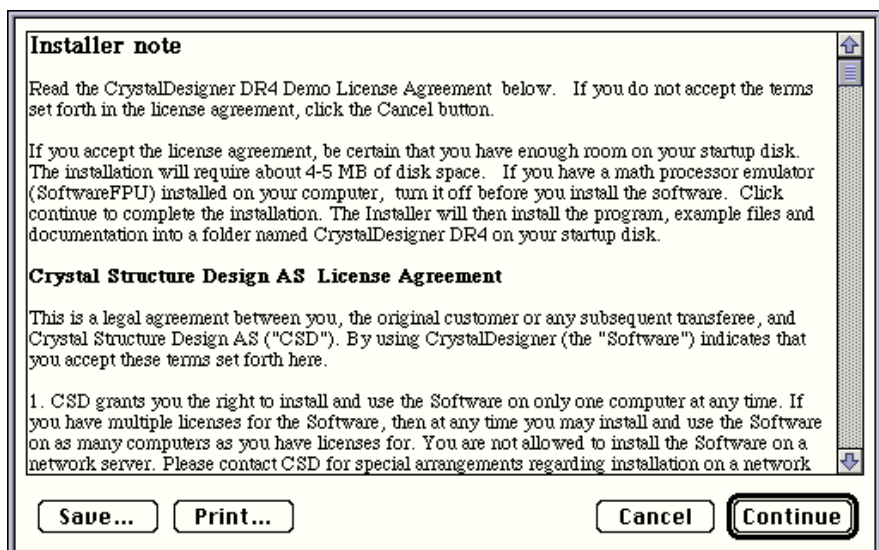


Figure 2.2 Installer note dialog.

If you accept the Crystal Structure Design AS License Agreement, Click **Continue** to complete the installation. The Installer now installs the program, example files and documentation into a folder named CrystalDesigner DR4 on your startup disk. When the installation is completed the following dialog box appears.



Figure 2.3 A dialog that confirms that installation was successful.

3. Tutorial: CaTiO₃

This tutorial will give you an introduction to CrystalDesigner. As an example through the tutorial, the cubic perovskite CaTiO₃ will be used (high temperature phase). You will be guided through four sections. The first section describes how to enter the crystal structure data, while the last three sections describe how to create different graph views of the crystal structure entered.

The first graph view section you will learn how to create a unit cell from the crystal structure data entered. You will also learn how to insert bonds and how to define polyhedra around atoms. In addition a description on how to measure distances and angles between atoms is also present.

In the second graph view section you will learn to create a graphical representation of a plane through the crystal structure. It will also be shown how to add thickness to the plane and how to shift distance from origin. At the end of this tutorial you will learn how to make a graph view of the coordination around a atom.

Entering the Crystal Structure Data

Document window

When you start CrystalDesigner a new untitled window appears on screen, shown in figure 3.1.

The image shows a software window titled "Untitled 1" with a light gray border and standard window controls. The window is divided into several sections for data entry:

- Crystal System:** A dropdown menu currently showing "None".
- Space Group:** An empty text input field.
- Lattice Parameters:** A large empty rectangular area for entering lattice parameters.
- Atom Positions:** A large empty rectangular area for entering atom positions.
- Reference:** A single-line empty text input field.

Figure 3.1 A new untitled document window. No data has yet been entered.

This window is called the document window. The document window contains the data of the crystal structure. The window consists of five regions; the crystal system, the space group, the lattice parameters, the atom positions and the reference region. From the data entered in these regions you can create as many graph windows as you like representing different views of the crystal structure. Let us start by entering the crystal structure data of CaTiO_3 into the document window.

Crystal system

The first thing you need to do is to select the crystal system from the popup menu in the document window. Choose the **Cubic** crystal system as shown in figure 3.2.

Lattice parameters

After choosing the cubic crystal system, enter CaTiO_3 crystal structure lattice parameter into the edit box in the lattice parameter region, $a = b = c = 380$ pm. Enter the lattice parameter. Only numbers and the decimal separator character are accepted. Please note that CrystalDesigner uses the decimal separator character defined by your system software. End the input with pressing the tab key.

Space group

Cubic perovskite has space group symmetry $\text{Pm}\bar{3}\text{m}$ (221). Choose this entry from the **Space Group** popup menu.

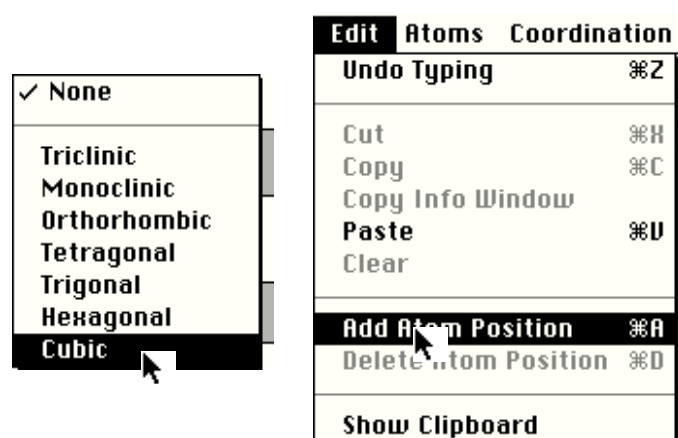


Figure 3.2 This figure shows a popup menu for choosing a crystal system. The second menu is the **Edit** menu. Here, the user is adding an atom position to the atom position table.

Atom positions

Cubic perovskite (CaTiO_3) contains three atom positions. Only one atom position is currently defined. Add therefore two new atom

positions by choosing **Add Atom Position** two times from the **Edit** menu, as shown in figure 3.2.

Select the first cell in the element column in the atom position table. The first atom position to enter is calcium. You can either type in the symbol, the element number or choose the element from the arrow

popup menu located on the right side of the input field. Figure 3.3 shows the document window at this stage when the popup menu are pulled down.

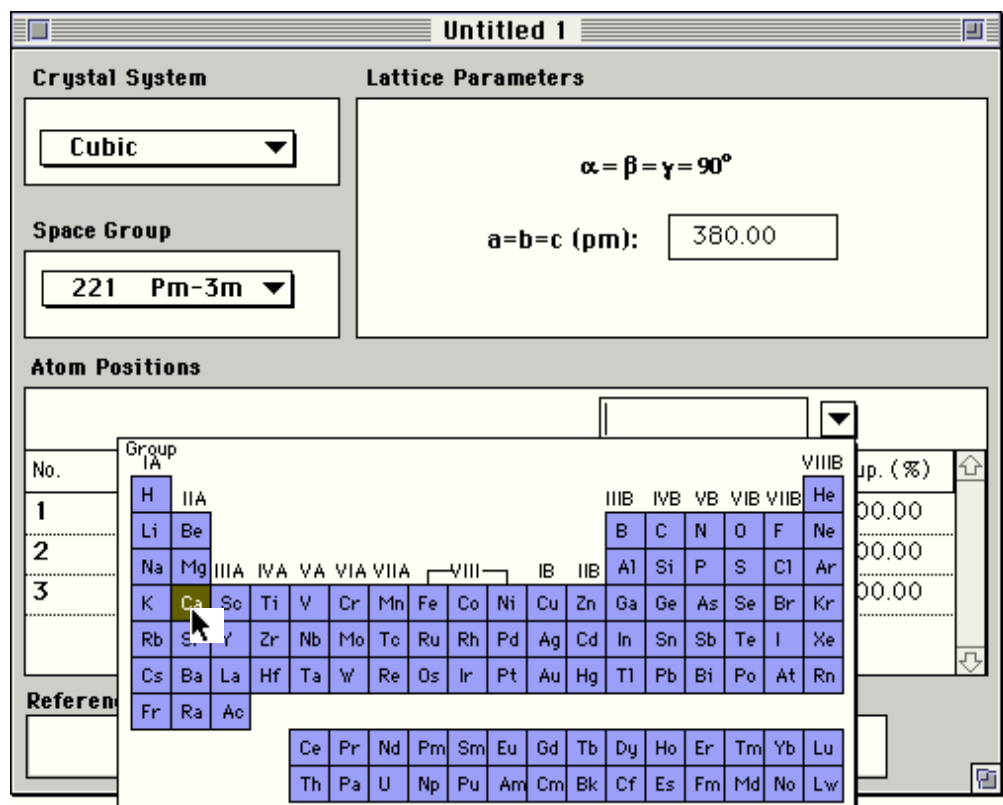


Figure 3.3. The document window with the element popup menu pulled down.

Calcium is located in the origin of the unit cell, (0 0 0). Enter the coordinates. You can navigate between the different cells by using the tab or arrows keys or you can just click in the cell that you want to change or enter a new value.

Radius Lookup Table

Current element : Ca ▼

Select a Radius to Use :

Metalic (pm): 197,00

Covalent (pm): 174,00

Ionic (pm): 134,00

Number	Oxid. State	CN	Spin	Radius (pm)
3	2	8		112,00
4	2	9		118,00
5	2	10		123,00
6	2	12		134,00

Degree of Covalence: 0 % ▼

Figure 3.4. Radius lookup table dialog window.

To complete the entering of the atom position of calcium, you also need to enter the radius of the element. You can enter the radius directly or you can let CrystalDesigner suggest a radius by opening the lookup table by clicking **Look Up** button on the left side of the input field. Figure 3.4 shows the Radius Lookup Table Dialog.

CaTiO₃ is an ionic crystal structure and the calcium atoms have oxidation state two and they are twelve coordinated. You can select the correct radius by clicking on the specific row. To return to the document window, click **OK**. Press tab key to confirm the radius you just selected.

Currently only occupancy equal to 100% is accepted as input in CrystalDesigner DR4. Complete the rest of the atom positions by inserting the values given in figure 3.5. Remember to confirm the last cell you enter.

Reference

The reference field at the bottom of the document window is a place where you can store the reference to the crystal structure data. The crystal structure data in this example has been taken from "Barth, Norsk Geologisk Tidsskrift, 8 (1925) p 201".

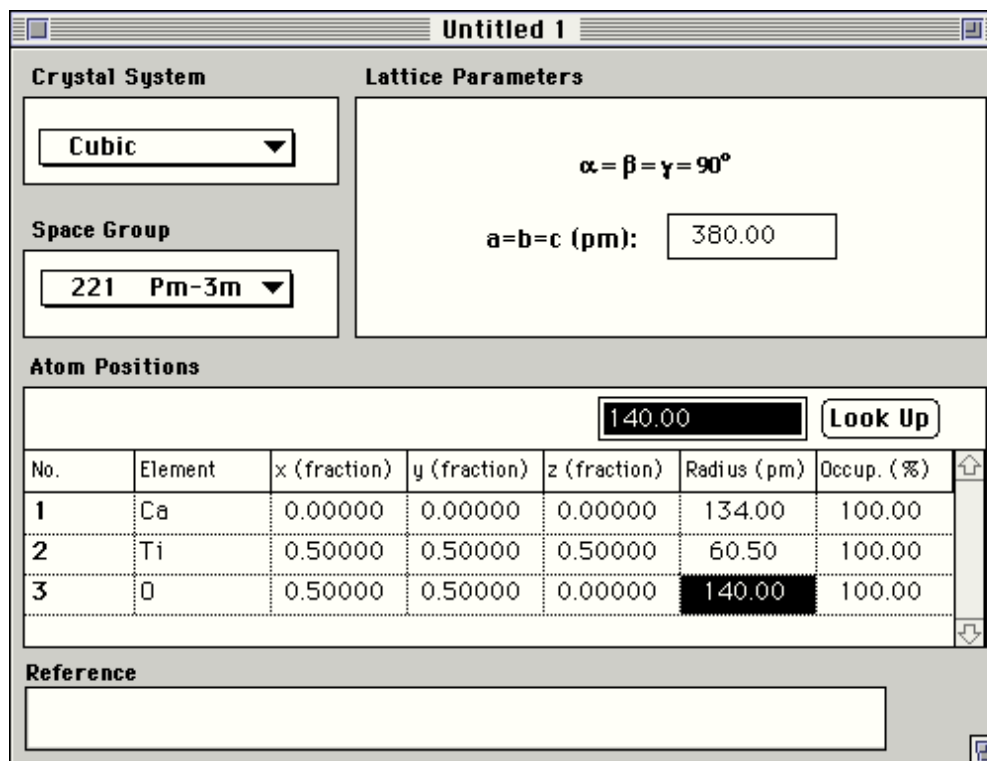


Figure 3.5 The document window when all crystal structure data are entered. Please note that CrystalDesigner uses the decimal separator character defined by your system software.

Save data

It is time for saving the data. Choose **Save Crystal Structure** from the **File** menu (not possible in the demo version). You may name the file Perovskite. The dialog should then look like figure 3.6 when you save the data. Click **Save**.

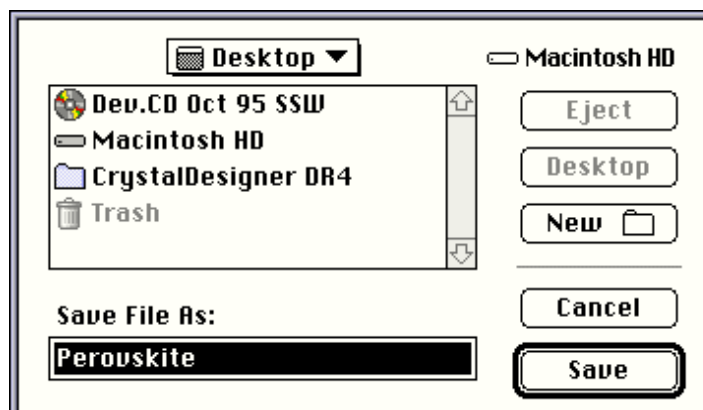


Figure 3.6 An example of a standard file dialog box.

Creating a unit cell drawing

A unit cell drawing can be created by choosing **New Unit Cell View** from the **Windows** menu as shown in figure 3.7. The unit cell window, also shown in figure 3.7, will then be created.

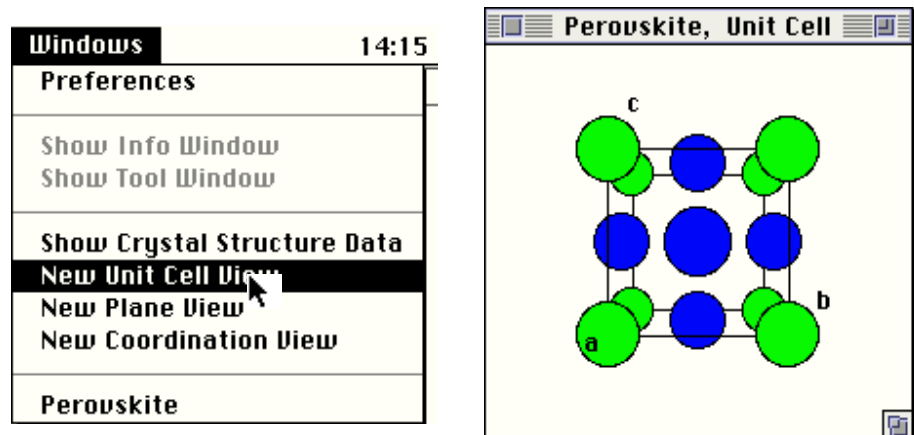


Figure 3.7 The **Windows** menu and a graph window displaying a unit cell.

In addition, two floating windows are also shown when the unit cell window is in front. These windows are shown in figure 3.8 and they are only visible when a graph window is in front. By activating the document window containing the crystal structure data the floating windows will disappear again. To bring the unit cell window in front again choose **Perovskite, Unit Cell** from the **Windows** menu.

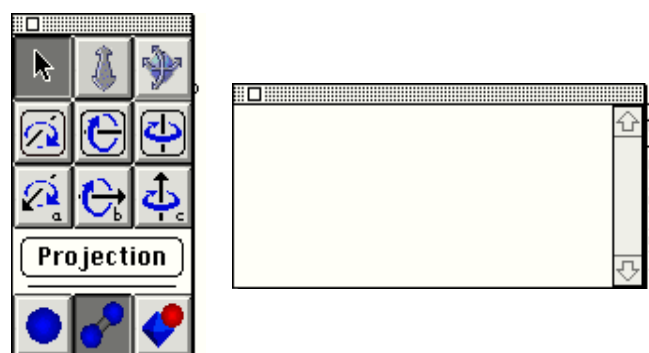


Figure 3.8. Floating windows. The empty window is the **Info Window**. The window containing the icons is the **Tool Window**.

Distances and angles between atoms



The arrow icon shown in the margin is called the **Selection Tool**. With this tool selected you can select different atoms in the drawing.

When an atom is selected the information about the atom is shown in the info window. By shift clicking you can select up to three

different atoms. The info window will then display additional information

about the distances and angles between the atoms selected. You can deselect the atoms by clicking somewhere else in the drawing.

Rotation of the drawing



The globe icon is called the **Free Rotation Tool**. With this tool selected you can rotate the unit cell in space by mouse dragging.

Try to rotate your unit cell. A circle in the drawing is shown when a rotation task is performed. The circle symbolise a silhouette of a sphere. It will help you to make the rotation easier. It is also possible to rotate the drawing by using the arrow keys.

Flickering

When you are rotating the unit cell the window flickers. To avoid the flickering, you can turn on the off screen buffering. This can be done by choosing **BitMap Buffering** from the **Render** menu.

Graph modes

The three icons in the bottom of the tool window symbolise three different modes of the drawing. The different modes are:



Atoms Only Mode. Only atoms are drawn.



Atoms and Bonds Mode. In this mode bonds and atoms are drawn and it is possible to create or modify coordination bonds between elements.



Atoms and Polyhedra Mode. Polyhedra and atoms are drawn and it is possible to create new coordination polyhedra around an element.

Inserting bonds

To define coordination bonds, choose **Insert/ Modify Bonds** from the **Coordination** menu. This entry is only enabled if you are in **Atoms and Bonds Mode**. Insert bonds between the titanium atoms and the oxygen atoms. After you have selected the atoms involved in the bonds, click the **Add** button. Your dialog at this stage should look like the dialog in figure 3.9.

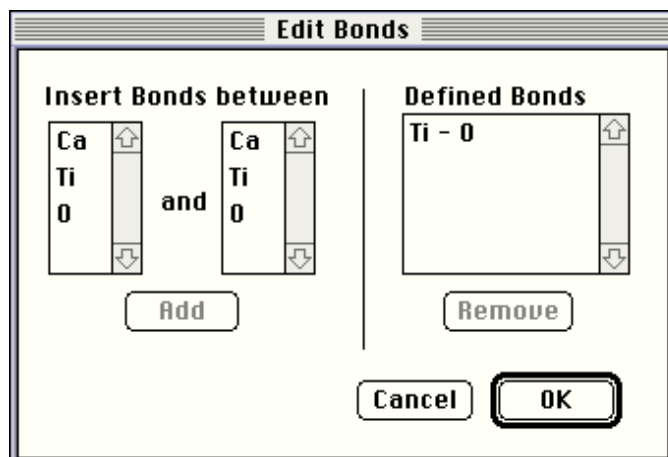


Figure 3.9. The edit bonds dialog.

Click **OK**. The drawing now displays the coordination bonds between oxygen atoms and titanium atoms. Figure 3.10 shows the graph window when the bonds have been inserted. Your graph window may have been rotated differently.

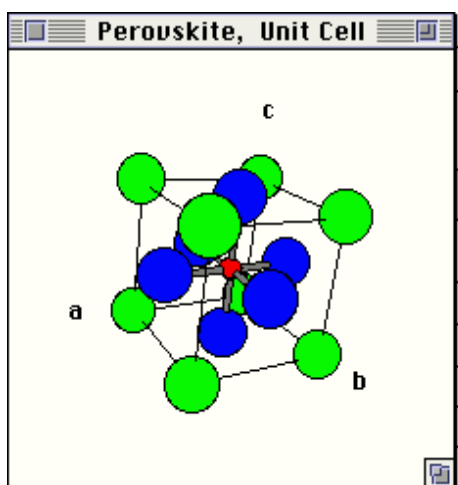


Figure 3.10 A graph window displaying a unit cell of CaTiO_3 with coordination bonds defined between oxygen and titanium atoms.

Inserting polyhedra

Select the **Atoms and Polyhedra Mode** icon. The bonds that we have created are now hidden. To insert a polyhedron around the titanium atom, choose **Insert Polyhedra Around** and the sub entry **Titanium** from the **Coordination** menu as shown in figure 3.11.

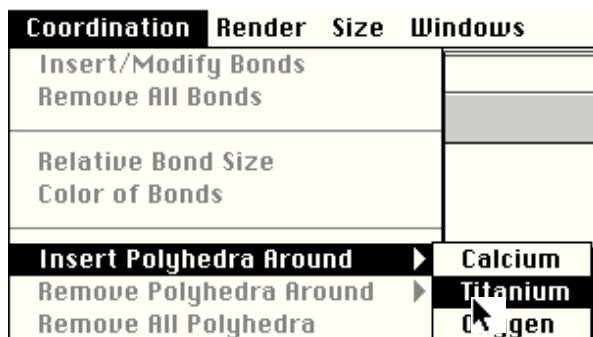


Figure 3.11. The **Coordination** menu. The user is inserting polyhedra around titanium atoms.

As you can see on your screen or in figure 3.12, CrystalDesigner automatically calculates the coordination polyhedra around titanium, which in this case is an octahedron. Figure 3.12 also includes a graph window where eight unit cells are displayed. Choose **(2x2x2) Units** from the **Size** menu to view these eight unit cells.

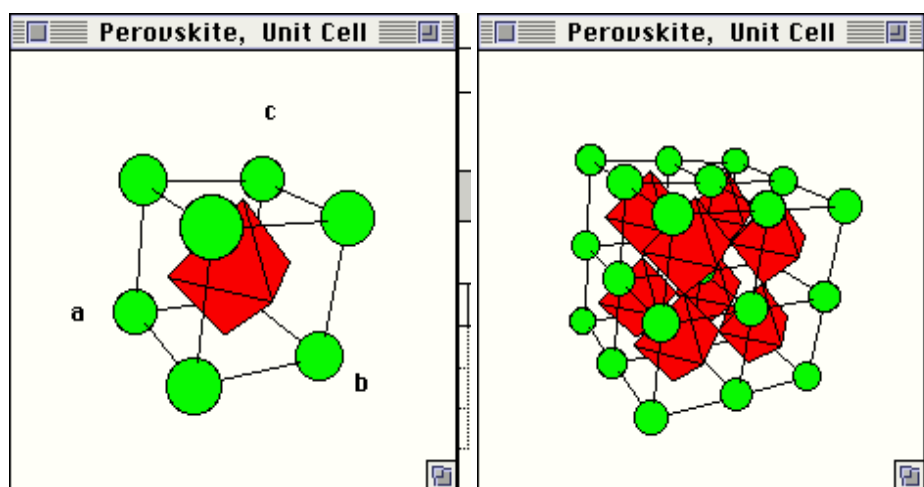


Figure 3.12. A graph window displaying a unit cell of CaTiO_3 with coordination polyhedra defined between around the titanium atoms.

Choose **Save Crystal Structure** from the **File** menu to save your current work. If you want to save your unit cell graph to a PICT file, you can choose **Save Graphics** from the **File** menu to save the drawing to a file.

Viewing a plane in the crystal structure

In this section you will learn how to create a graphical representation of a plane through the crystal structure. It will also be shown how to add thickness to the plane and how to shift distance from origin.

Defining a plane

To create a new plane view, choose **New Plane View** from the **Windows** menu as shown in figure 3.13.

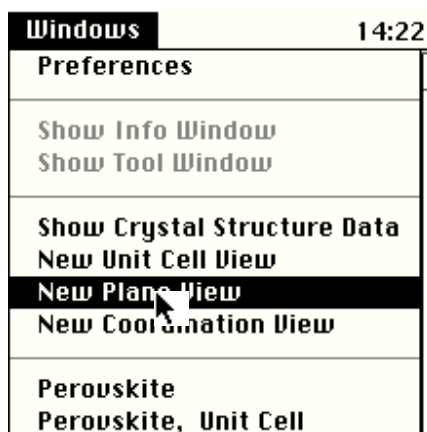


Figure 3.13. The window menu. The user is creating a new plane view.

A dialog box appears on the screen. In this dialog box you can select the hkl plane you want to view. In this tutorial, select the (111) plane. This can be done by entering the numbers or by choosing the plane from popup menu named **Predefined**. At this stage your dialog should look like figure 3.14.

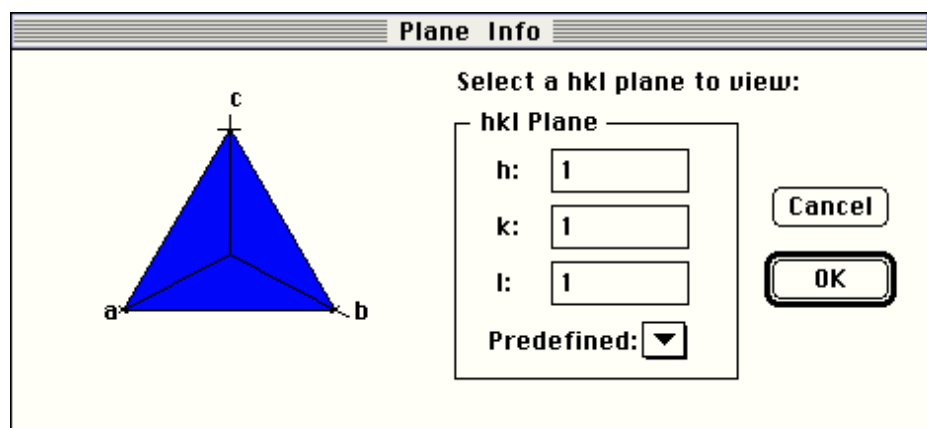


Figure 3.14. The plane info dialog box. The user has selected the (111) plane.

Click **OK** and a new graph view window appears named Perovskite, (111) plane.

Moving the plane away from origin

The boundary of the plane displayed is defined by the first octant. In the case where one of the crystallographic axes is parallel to the plane, you can define how many unit cells that should be included in the specific direction. In our case none of the axes are parallel to the displayed plane.

The current plane is at a distance d from origin. To incorporate more atoms in the drawing you can transfer the defined plane away from origin by an integer multiply of d . This is possible by choosing a sub entry of the menu item **Distance from Origin** from the **Size** menu. Choose **7d** as shown in figure 3.15.

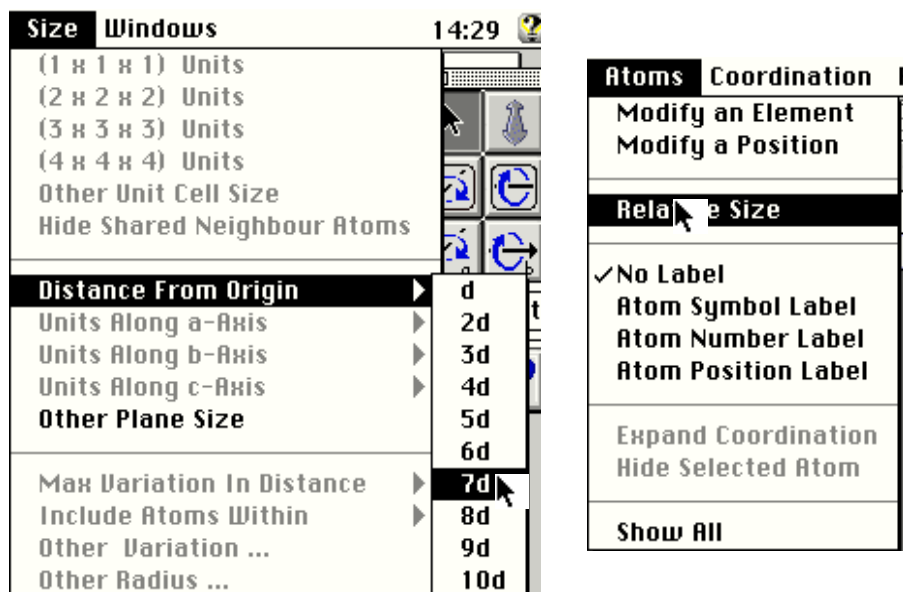


Figure 3.15 The **Size** and **Atoms** menus. In the **Size** menu the user transfers a plane to a distance $7d$ from origin. In the **Atoms** menu the user selects an entry to change the relative atom radius.

To see the close-packing of this layer, change the relative size of the atoms to 100%. Choose **Relative Size** from the **Atoms** menu. Enter the value 100 and click **OK**. Your graph window should now look like figure 3.16.

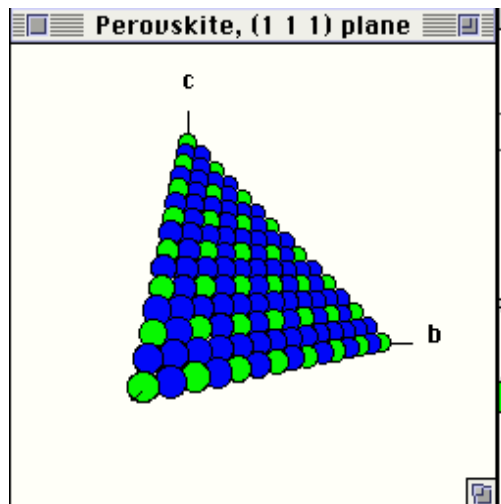


Figure 3.16. A graphical representation of the (111)plane at a distance of $7d$ from origin. The relative size of the atoms is set to 100%.

Adding thickness to a plane

Often it is interesting to see the packing of the layers of a crystal structure. This can be done by adding a thickness to a plane. To add thickness to the plane, choose **Other Plane Size** from the **Size** menu. A dialog as shown in figure 3.17 appears. Change the thickness above the plane to 1000 pm and click **OK**.

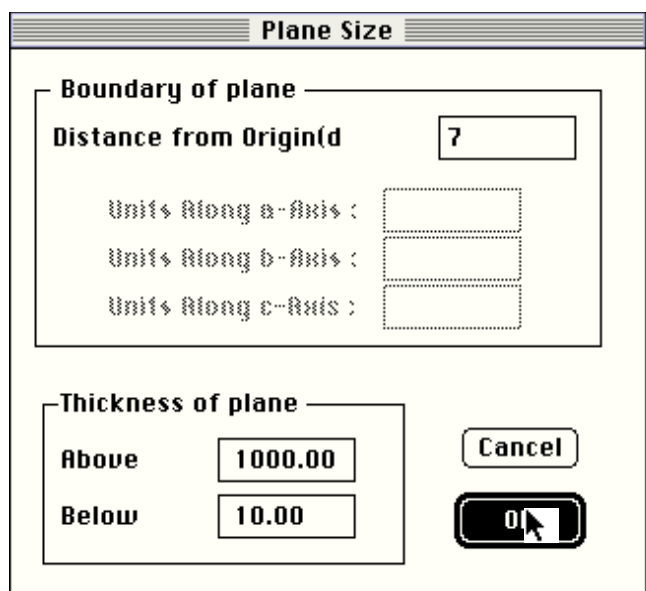


Figure 3.17. A plane size dialog box. A thickness of 1000 pm above the plane has been entered.

After a rotation the plane the drawing of the plane may look something like figure 3.18.

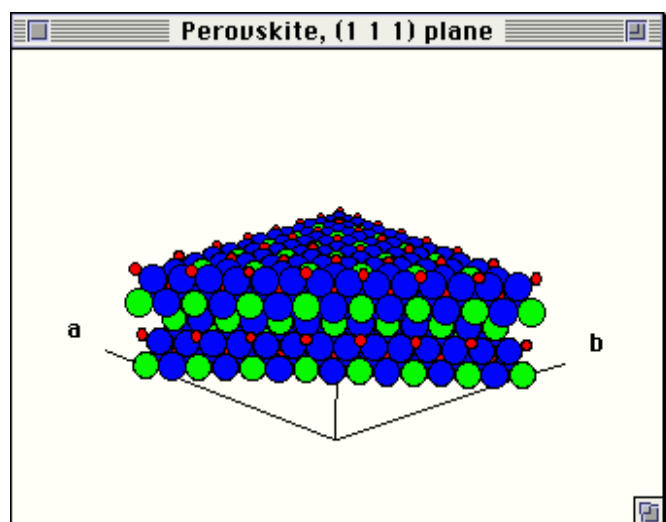


Figure 3.18. A graphical representation of the (111) plane in a distance $7d$ from origin. The relative size of the atoms is set to 100% and the thickness above the plane is set to 1000 pm.

Viewing a coordination around a atom

To view the coordination around a atom, choose **New Coordination View** from the **Windows** menu. Select the calcium atom as shown in figure 3.19 and click **OK**.

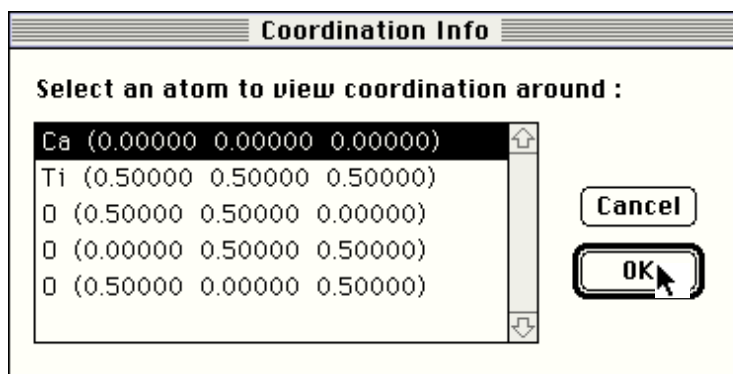


Figure 3.19. A dialog where the user can select an atom to view coordination around. Calcium (0,0,0) has been selected.

A new window viewing the coordination of calcium then appears. Atoms within a given radius are included in this drawing. The given radius (R) is calculated by the equation

$$R = r_0 + \delta$$

where r_0 is the distance to the nearest neighbour and δ is the acceptable variation in distance from the core atom between the neighbouring atoms. The default value of δ is 20 pm.

You can change the values of R and δ . To change R directly, choose **Other Radius ...** from the **Size** menu. To Change δ , choose **Other Variation ...** from the **Size** menu. Try to experiment with different values. Figure 3.20 gives you an example of this view.

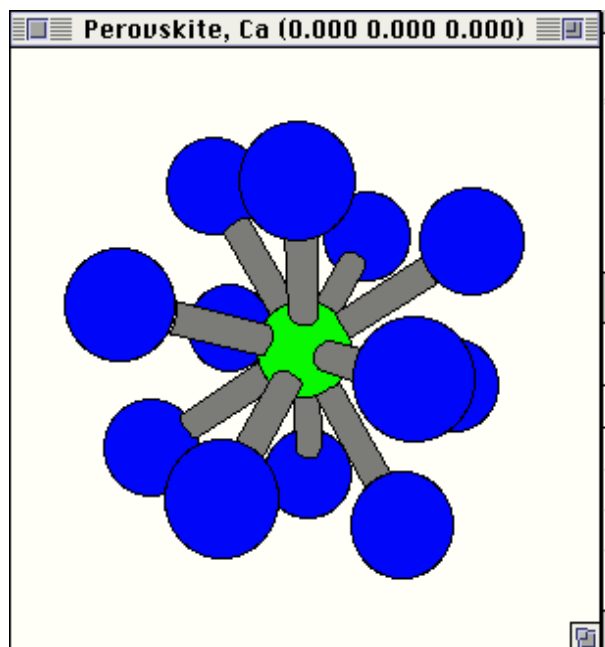


Figure 3.20. A graphical representation of the coordination around the calcium atom. The maximum variation in distance between neighbouring atoms to the core atom is set to 50 pm. Bonds have been inserted between calcium and oxygen atoms. From the **Render** menu **Hide Reference Framework** have been chosen.

4. Menus and Floating Windows

This chapter describes each of the CrystalDesigner menu commands. It is organised by menu, from left to right along the menu bar. Within each menu commands are described in the order in which they appear in the menu.

The Apple Menu

The menu entry **About CrystalDesigner ...** tells you what version of CrystalDesigner you are using and how to get in contact with Crystal Structure Design AS.

The File Menu

Use the **File** menu commands to work with files that you open and edit. The menu also lets you save graphics and text to files. Figure 4.1 shows you the file menu.



Figure 4.1 File menu

New Crystal Structure

The **New Crystal Structure** opens a new untitled document window. You can have as many document windows open simultaneously as you like. The maximum number of windows are only limited by the application memory.

Open Crystal Structure

The **Open Crystal Structure** command displays a dialog that lets you select from existing crystal structure files on disk and open one for editing and displaying. A crystal structure file contains the data and all the graph windows created or modified last time the user saved the crystal structure.

Close Crystal Structure

This command has the same effect as clicking in the active document window's close box. A dialog box asks if you want to save the changes, discard them, or cancel the **Close** command. When you closes the crystal structure document window all the graph windows that belong to that crystal structure will also be closed.

Close

If a crystal structure document window is active, the **Close** command has the same effect as the **Close Crystal Structure** command. The document window plus all its graph windows will be saved and closed. If a graph window is active, a dialog box will appear and you you must confirm that you want to remove this graph view from your crystal structure project. The confirmation dialog is shown in figure 4.2.

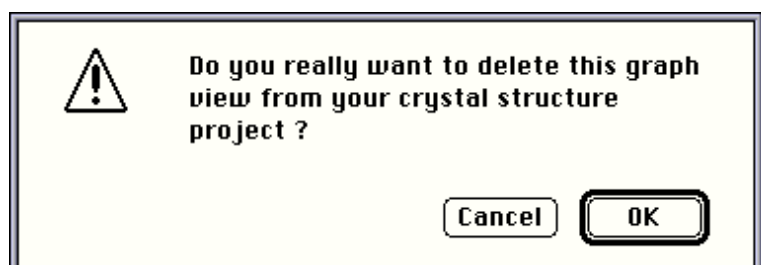


Figure 4.2 A dialog box asking you if you really want to delete the active graph window.

If you confirm the command the graph window will be closed and all the information stored will be lost. Sometimes you want to active a window that is not visible. Instead of closing graph windows or moving windows until you can click on a part of a window you want to activate, you can select the window from the **Windows** menu. All displayed windows are listed in this menu.

Save

This command saves the all the windows belonging to the active crystal structure project. A crystal structure project consist of a document window containing the crystal structure data and all the graph views representing the particular crystal structure. When you perform the **Save** command all windows are stored to file. In other words when you open your crystal structure project next time the windows will appear in the same order, position and size and they will contain the same information as last time you saved the crystal structure project.

Save As ...

This command allows you to save the active crystal structure project under an other name. The active project is the same project the the front most window on screen belongs to. If you have made edits in the current session, they are saved under the new name. The original project remain unchanged.

Revert to Saved

This command restores the last saved version of the current active project and discard any edits made since the last save.

Save Graphics

The **Save Graphics** command allows you to save the active graph view to file. The drawing will be saved as a PICT file. The resolution of the saved drawing is dependent on wether you us **BitMap Buffering** or not. You can check what kind of buffering using by examine the **Render** menu. If **BitMap Buffering** is on the resolution is the same as the screen resolution, else the resolution is device dependent. If you want to print the file, the resolution of the drawing is the same as the resolution of the printer.

Save Text

This command saves the text in the crystal structure data window.

Page Setup

This command displays the standard Page Setup dialog that lets you specify the size of the paper you are printing on, and whether the file should be printed upright on the page(tall orientation) or sideways(wide orientations).

Print

This commands opens a dialog thatlets you print the contents of the active graph window. The resolution of the output of the graph views are dependent on if you are using BitMap buffering or not. If the **BitMap Buffering** in the **Render** menu is checked the resolution on the output will be the same as the screen resolution, else the resolution of the drawing will be the same as the resolution of the printer you are using.

Quit

This command exits CrystalDesigner program. If you have any open crystal structure projects you will be asked if you want to save the changes for each one of the projects.

The Edit Menu

The **Edit** menu contains the standard Macintosh editing commands: **Cut**, **Copy**, **Paste** as well as the commands editing the crystal structure data. Figure 4.3 shows the menu.

Undo

The **Undo** command reverses the last edit operation. The name of this command changes to reflect the operation you are undoing. After a paste, for instance, this command changes to **Undo Paste**. Once you have undone something, the name of this command changes to Redo. If nothing exist to undo, this command is dimmed.

Cut

This command removes selected text and places it in the Clipboard. It replaces the current contents of the Clipboard. Use the Paste command to insert text from the Clipboard into your file at the insertion point.

Edit	Atoms	Coordination
Undo		⌘Z
Cut		⌘H
Copy		⌘C
Copy Info Window		
Paste		⌘V
Clear		
Add Atom Position		⌘A
Delete Atom Position		⌘D
Show Clipboard		

Figure 4.3. **Edit** menu

Copy

This command copies the selected text or graph view and place it in the Clipboard. Note that if a graph window is active, the name of this menu command changes to **Copy Graph View**. The copy, containing text or graphics, can now be pasted somewhere else using the **Paste** command.

Copy Info Window

This command lets you copy the content of the Info Window. The copy can now be pasted somewhere else using the **Paste** Command.

Paste

This command copies the contents of the Clipboard into the text field being edit at the insertion point. Please note that CrystalDesigner currently do not letsyou paste row or columns or both into the atom position table in crystal structure data window.

Clear

This command clears the selected text, but the cleared text is not placed in the Clipboard.

Add Atom Position

This command lets you add a new atom position row to the atom position table. The command is only active if a document window is active. The atom position table can contain up to 32767 positions. By the introduction CrystalDesigner DR5 you will be able to import data from text files (CIF -format).

Delete Atom Position

This command allows you to delete the selected row in the atom position table. You can select a row by clicking in its row first cell. The last position in the atom position table is not possible to delete. If no row is selected this command is dimmed.

Show Clipboard

This command opens a window that displays the content of the Clipboard.

The Atoms Menu

The **Atoms** menu contains commands for editing the atoms in a drawing. You are able to change the relative size, the colour and the appearance of the atoms. Figure 4.4 shows the Atoms menu.

Atoms	Coordination	R
Modify an Element Modify a Position		
Relative Size		
<input checked="" type="checkbox"/> No Label Atom Symbol Label Atom Number Label Atom Position Label		
Expand Coordination Hide Selected Atom		
Show All		

Figure 4.4 **Atoms** menu

Modify an Element

This command opens a dialog box that lets you change the colour and appearance of a specific element. The elements can be edited by selecting the element from the **Current Element** popup menu, which contains all the elements in the drawing. Figure 4.5 shows you the Modify Element dialog box.

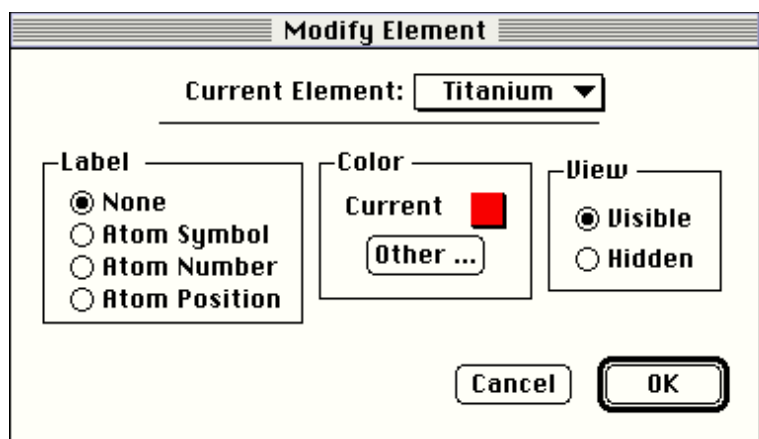


Figure 4.5. A dialog box that allows you to change the formatting of the elements.

You can label the elements with atom symbol, atom number or atom position. If your displayed atoms are too small to incorporate the label within the atom, the label will not be drawn. If some labels are hidden, you can make them visible by increasing the relative size of atoms or by making the graph window larger.

Click **OK** when you are finished with the formatting of the elements.

Modify a Position

This command opens a dialog box that lets you change the colour of a specific position in your active crystal structure. Figure 4.6 shows you the Modify Atom Position dialog box.

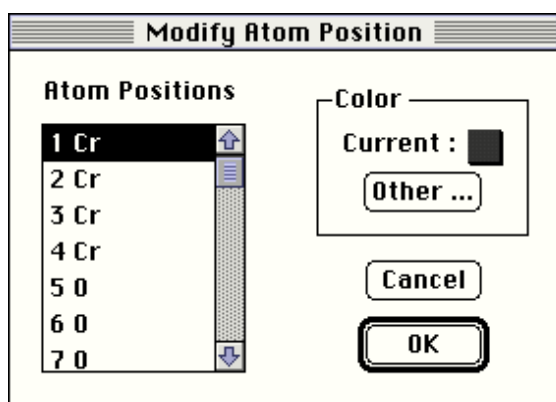


Figure 4.6 The Modify Atom Position dialog box.

You will typically use this dialog if one of your elements in the drawing consists of more than one atom position. You can set a unique colour for each atom position. If you change the colour of an element in the Modify Element dialog, only the atom positions with the same defined colour as the defined element colour will be changed.

Relative Size

This command opens a dialog box that lets you change the relative size of the atoms in the drawing. You can enter integer values from 1 to 100. When the relative size is set to 100, the displayed radius of the atoms correspond to the radius given by the atom positions.

No label

Atom Symbol Label

Atom Number Label

Atom Symbol Label

With these commands you are able to label the atoms in different ways. Please note that if your displayed atoms are too small to incorporate the label, the label will not be drawn. If some labels are hidden, you can make them visible by increasing the relative size of atoms or by making the graph window larger. Please note that these command entries override the element labelling done in the Modify Element dialog.

Expand Coordination

This command is enabled if a single atom is selected. By choosing this command a new graph window will appear displaying the coordination around the selected atom.

Hide Atom

This command is enabled if a single atom is selected. By choosing the **Hide Atom** command the atom and all the bonds connected to the atom will be hidden. If the hidden atom is a core atom of a polyhedron, the polyhedron will not be shown in the **Atom and Polyhedra Mode**. To display the hidden objects, choose **Show All** from the **Atoms** menu.

Show All

This command makes all the hidden atoms and the bonds connected to the hidden atoms visible again.

The Coordination Menu

The **Coordination** menu contains commands for creating bonds and polyhedra around atoms.

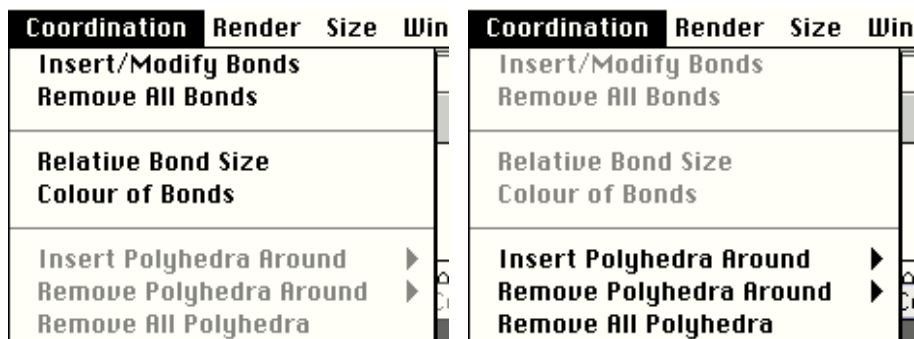


Figure 4.7 The **Coordination** menu.

When your active graph window is in **Atoms and Bonds Mode**, the upper part of the **Coordination** menu is enabled, shown to the left in figure 4.7. When your active graph window is in **Atoms and Polyhedra Mode**, the lower part of the menu is active, shown to the right in figure 4.7. When the active graph window is in **Atoms Only Mode** all the **Coordination** menu commands are dimmed. The different modes are explained in the section describing the Tool Window on page 40.

Insert/ Modify bonds

This command opens a dialog box that allows you to insert new bonds between elements or to modify already defined bonds. Figure 4.8 shows this dialog box.

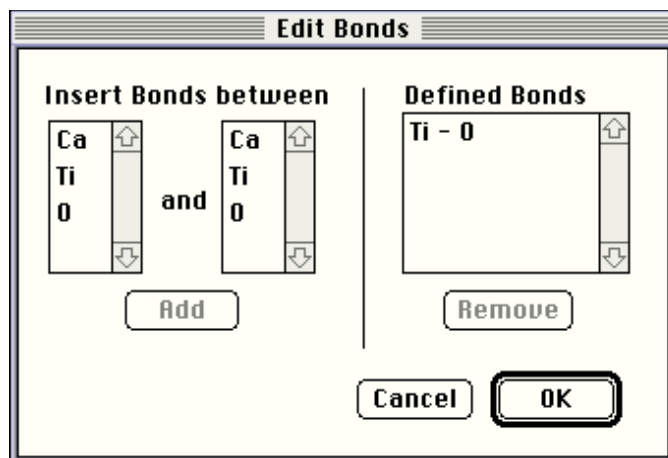


Figure 4.8 A dialog box for inserting and modifying bonds between elements. Here, bonds between titanium and oxygen have been defined.

Remove All bonds

This command removes all defined bonds in the active graph window.

Relative Bond Size

This command opens a dialog box that lets you change the relative bond size of all the bonds in the active graph window. The relative bond size is defined as the radius of the smallest atom in the bond times the relative size / by hundred.

Colour of Bonds

This command lets you open a dialog to change the current bond colour.

Insert polyhedra Around

When you choose this command, you see a hierarchical menu with the elements that you can define polyhedra around. If an element is a part of corner of a already defined polyhedron or is a core atom of a polyhedron, the element will not be visible in the hierarchical menu.

CrystalDesigner DR4 supports square, tetrahedron and octahedron. CrystalDesigner DR5 will expand the support by several new polyhedra. Our goal is to support polyhedra around elements that have coordination twelve or less by the introduction of CrystalDesigner DR5.

Remove polyhedra around

Remove all Polyhedra

Removes polyhedra around a specific element or removes all the polyhedra in the active graph window. These commands are not undoable.

The Render Menu

The **Render** menu contains commands that lets you control how the crystal structure should be converted into an image on the screen. You have the possibility to choose the projection method and how the atoms, bonds and polyhedra will be displayed. In addition you can also add a reference framework and a colour background to your displayed drawing. Figure 4.9 shows you the **Render** menu.

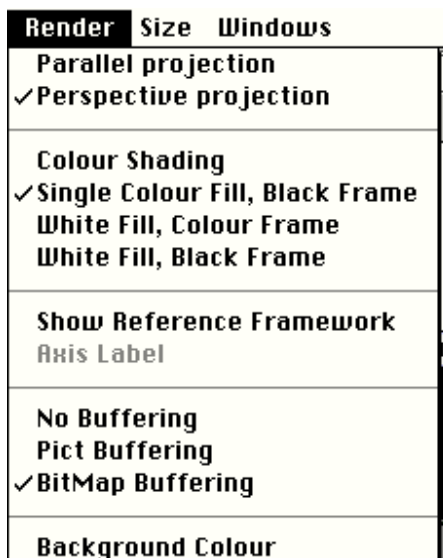


Figure 4.9 The **Render** menu.

Parallel projection

In parallel projection mode equal objects are displayed with same size independent of the distance from the viewer.

Perspective projection

In perspective projection mode equal objects are displayed with different size independent of the distance to the viewer. The nearest objects are largest.

Colour Shading

When this command is selected, atoms are drawn as spheres and bonds are drawn as cylinders. The colour of surface of the objects is determined by the angle between surface normal and the vector from the surface to the viewer.

Building up a drawing in this mode increases the update time by a factor 100. We recommend that you use this mode only when you are satisfied with all the other view parameters.

Single colour Fill, Black Frame

When this command is selected, atoms are drawn as circles and bonds are drawn as planar polygons. The objects are filled with the default or user defined colour with a black frame around. In the case where the atoms are smaller or equal to a dot on the screen, the atoms are displayed as a point. Equally, the bonds are displayed as lines.

White Fill, Colour Frame

When this command is selected, atoms are drawn as circles and bonds are drawn as planar polygons. The objects are filled with white colour and as a user default or user defined colour around.

White Fill, Black Frame

When this command is selected, atoms are drawn as circles and bonds are drawn as planar polygons. The objects are filled with white colour and the frame around the object is drawn in black.

Show/ Hide Reference Framework

With is menu command you can toggle off and on the reference framework in your drawing. The reference framework is dependent on which kind of graph you are displaying. When it is a unit cell view a framework showing the unit cell bonds is drawn. If you are displaying a plane of your crystal structure the unit cell axis and the boundary of the plane is displayed. If you are displaying a coordination around an atom the reference framework shows the crystal system axes though the centre.

Show/ Hide Axis Label

This command is only enabled when the reference framework is drawn. By using this command you can toggle between showing or hiding the axis labels.

No Buffering

When this menu entry is selected CrystalDesigner draws directly in the window. If an update event occur CrystalDesigner redraws the whole crystal structure. This will slow down your the speed of the program. An advantage using this mode is that you see the progress in drawing and you do not need memory available for making a off screen image.

PICT Buffering

This option is likely to be removed in the next update.

BitMap Buffering

When this menu entry is selected CrystalDesigner makes an off screen image before the program copies the image into the graph window. If an update event occur the stored image will be copied into the window. CrystalDesigner stores the off screen image in the system memory. If you have problems with activating this command, you should try to close other open program in order to release more memory to the system.

Background Colour

By choosing this command a dialog box is opened. The dialog lets you change the background colour of the active graph window.

The Size Menu

The **Size** menu contains commands that lets you change the size of your drawing. When a unit cell view is active the upper part of the menu is enabled as shown to the left in figure 4.10. When a plane view is active the part in the middle of the menu is enabled and finally when a coordination view is active the lower part of the menu is active, shown to the left in figure 4.10.

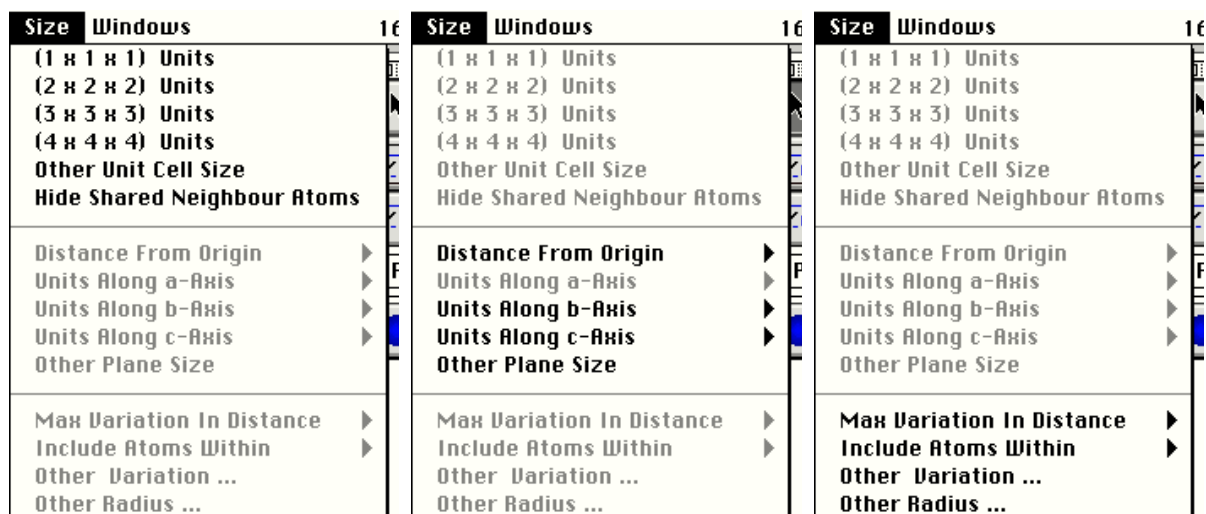


Figure 4.10 The **Size** menu

(1 x 1 x 1) Units
(2 x 2 x 2) Units
(3 x 3 x 3) Units
(4 x 4 x 4) Units

These commands let you control how many unit cells should be displayed in each crystal system direction. For example the command **(2 x 2 x 2) Units** changes the drawing to include two unit cells in each direction with the result that eight unit cells are displayed.

Other Unit Cell Size

This command opens a dialog box that lets you set the number of unit cells that should be displayed in each crystal system direction. You can enter integer values 1 to 1000 in the input fields. The initial values displayed are the current size of the drawing. Figure 4.11 shows you the dialog.

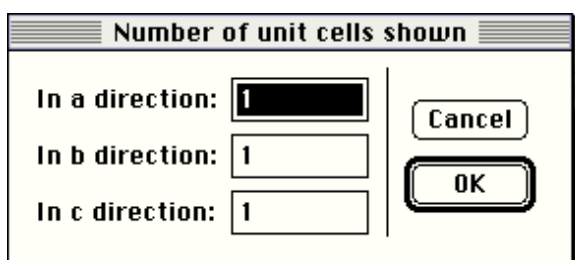


Figure 4.11 A dialog box for setting the number of unit cells that should be displayed in each crystal system direction.

Hide/ Show shared Neighbour Atoms

This command lets you include or exclude atoms from neighbouring unit cells that share corner, axes or surfaces with the unit cell(s) you are displaying. If the menu entry text is **Hide shared Neighbour Atoms**, the shared neighbouring atoms will be removed from the drawing. When the menu entry text is **Show shared Neighbour Atoms**, the shared neighbouring atoms will be added to the drawing.

For instance, suppose that you have a crystal structure containing only atoms located in origin (0,0,0) of the unit cell. When you display it as a unit cell with shared neighbouring atoms, you will see 8 atoms. By hiding the shared neighbouring atoms, only one atom will be displayed.

Distance from Origin

When you choose this command, you see a hierarchical menu with different choices of distances from origin. The boundary of the plane displayed is defined by the first octant. You can therefore incorporate more atoms in the drawing by transferring the defined plane away from origin.

Units Along a-Axis
Units Along b-Axis
Units Along c-Axis

With these commands you can define how many unit cells that should be included in the specific direction in the case where one of the crystallographic axes is parallel to the plane. If the plane is not parallel to a specific direction, the specific menu entry is disabled. Please note that the boundary of the plane displayed is defined by the first octant.

Other Plane Size

This command opens a dialog box that lets you set all the boundary conditions for the active plane view, shown in figure 4.12.

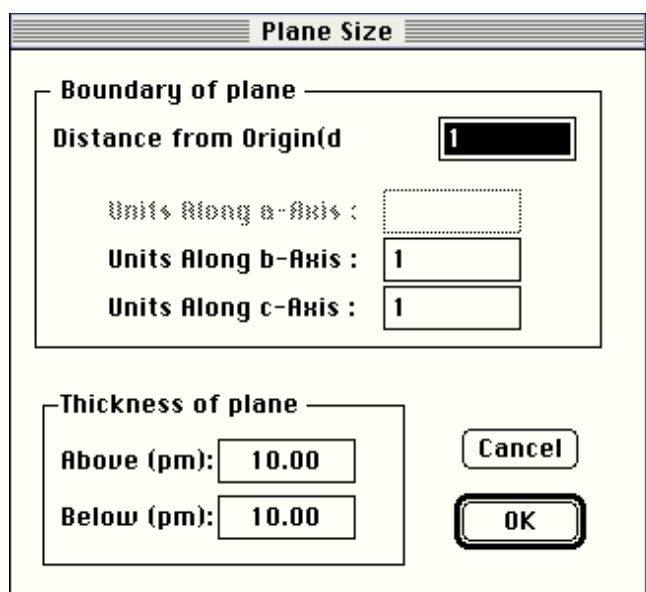


Figure 4.12 The plane size dialog.

In the upper part of the dialog you can set the boundary of the plane. Please note that in the cases where the plane is not parallel with the crystal system axes, the boundary of the plane is defined by the first octant. The effect of this definition is that when you transfer the plane away from origin the plane size is increasing. If the plane is parallel with any of the crystal system axes you can define how many unit cells that should be included in the specific direction.

In the lower part of dialog you can specify the thickness of the plane.

Max Variation in Distance

When you choose this command, you see a hierarchical menu with different choices of the maximum allowed variation in distance between the core atom and the surrounding nearest neighbours. Atoms within a given radius will be included in drawing dependent on which value you choose. The given radius (R) is calculated by the equation

$$R = r_0 + \delta$$

where r_0 is the distance to the nearest neighbour and δ is the maximum allowed variation in distance from the core atom between the nearest neighbouring atoms.

Include Atoms Within

When you choose this command, you see a hierarchical menu with different choices of the radius to include atoms within from the core atom. All atoms within the radius you have chosen will be included in the drawing.

Other Variation ...

This command opens a dialog box that lets you manually change the maximum variation in distance from the core atom to the surrounding nearest neighbours, figure 4.13. Atoms within a given radius will be included in drawing. The radius (R) is calculated by the equation

$$R = r_0 + \delta$$

where r_0 is the distance to the nearest neighbour and δ is the max variation in distance from the core atom between the nearest neighbouring atoms.

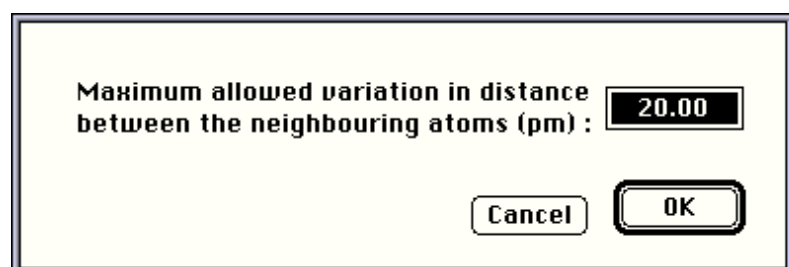


Figure 4.13 A dialog box for changing the maximum variation in distance from the core atom to the surrounding nearest neighbours

Other Radius ...

This command opens a dialog box that lets you manually change the radius you want to include atoms within.

The Windows Menu

The **Windows** menu contains commands creating new graph views. In addition this menu displays a list containing all the currently open windows. The list is located in the bottom of the menu. Figure 4.14 shows the menu.

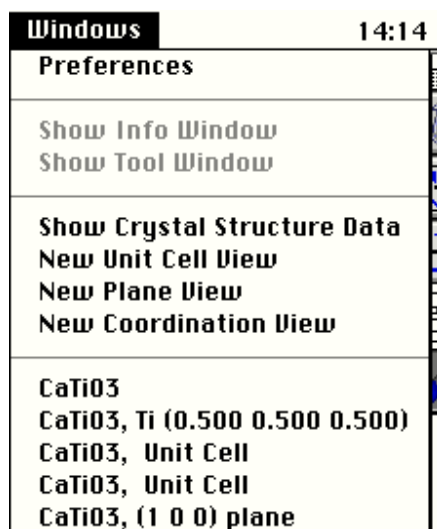


Figure 4.14 The **Windows** menu

Preferences

The **Preferences** command opens a dialog box that ables you to change the default settings in the program. You can change the default settings of: the graph windows, rendering options, rotation steps, element colours, element ratios, atom design, bond design, unit cell view parameters, plane view parameters and the coordination view parameters.

Show Info Window

If a graph view is active and the info window has been closed, this command will make the info window visible again

Show Tool Window

If a graph view is active and the tool window has been closed, this command will make the tool window visible again.

Show Crystal Structure Data

This command opens a window that displays the general positions of the chosen space group and the atom position in the unit cell generated from the general position and the atom position list. If the window is already open this command is disabled. You can then instead access the window by choosing its menu entry in the lower part of the **Windows** menu.

New Unit Cell View

This command creates a new unit cell view window based on the default settings. You can view the different default settings by choosing the command **Preferences** in the **Windows** menu.

New Plane View

This command opens a dialog that lets you specify which plane you want to view, see figure 4.15. You are only allowed to enter integer values. Inside the dialog box there is a popup menu that lets you choose the most common planes. The graph on the left side in the dialog display the current selected plane in a distance d from origin.

The parameters for the initial plane view is defined in the default settings. You can view the different default settings by choosing the command **Preferences** in the **Windows** menu.

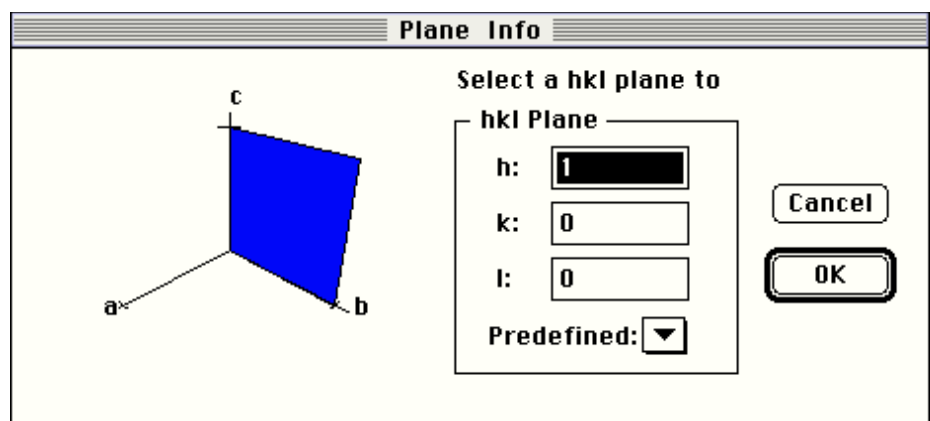


Figure 4.15 A dialog box for choosing a plane to view.

New Coordination View

This command opens a dialog that lets you specify which position in the unit cell you want to view coordination around, shown in figure 4.16. Select a atom and click OK to view the specific coordination.

The parameters for the initial coordination view is defined in the default settings. You can view the different default settings by choosing the command **Preferences** in the **Windows** menu.

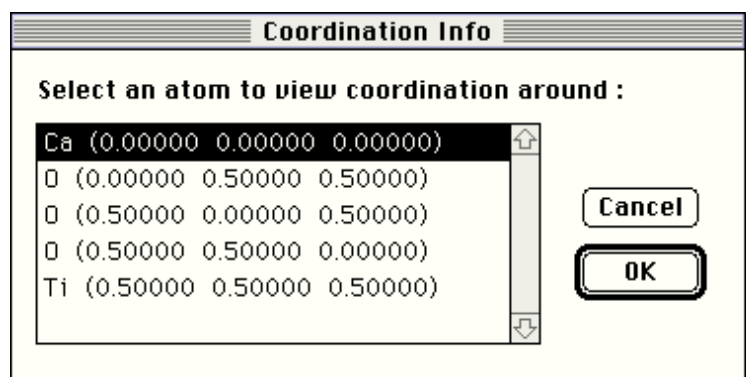


Figure 4.16. A dialog box for choosing an atom to view coordination around.

The Info Window

The info window is a floating window that is only visible when a graph window is active. The info window gives you information about the position of the selected atoms in the active graph window. If two atoms are selected the distance between them is also shown, see Figure 4.17. If three atoms are selected both the distance and the angle between the different atoms are shown. You can copy the contents of the info window to clipboard by choosing **Copy Info Window** in the **Edit** menu. Shift-click to selected one atom simultaneously.

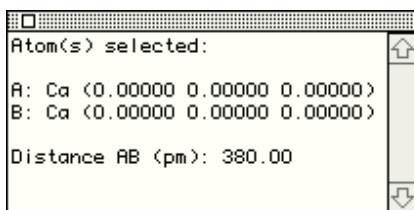


Figure 4.17 The Info Window shows the positions and distance between two selected atoms.

The Tool Window

The tool window in figure 4.18 is a floating window that is only visible when a graph window is active. By activating the document window containing the crystal structure data the tool window will disappear. By using the different tools in this window you can control the view direction and graph mode of your drawing.

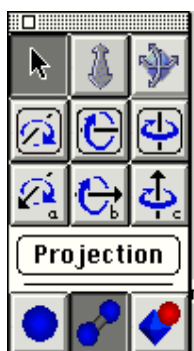


Figure 4.18 The Tool Window

The tool window consist of three main regions. The upper part of the window consist of a region containing of nine icons. Only one icon can be selected. Their properties are as described below:



The **Selection Tool**. With this tool selected you can select different atoms in the drawing. By shift clicking you can select up to three atoms simultaneously.



The **Magnification Tool**. With this tool selected you can change the magnification by dragging the mouse up or down inside your drawing.



The **Free Rotation Tool**. With this tool selected you can rotate your crystal structure in any direction. You are rotating around the centre of your crystal structure.



The **Screen Normal Rotation Tool**. This tool lets you rotate the crystal structure around an axis that goes through the centre of your model in a direction normal to the screen.



The **Screen Horizontal Rotation Tool**. This tool lets you rotate the crystal structure around an axis that goes through the centre of your model in horizontal direction.



The **Screen Vertical Rotation Tool**. This tool lets you rotate the crystal structure around an axis that goes through the centre of your model in vertical direction.



The **a-Axis Rotation Tool** lets you rotate around an axis that is parallel to the a-axis of your crystal structure. The axis goes through the centre of your model.



The **b-Axis Rotation Tool** lets you rotate around an axis that is parallel to the b-axis of your crystal structure. The axis goes through the centre of your model.



The **c-Axis Rotation Tool** lets you rotate around an axis that is parallel to the c-axis of your crystal structure. The axis goes through the centre of your model.

In the centre of the tool window there is a button named **Projection**. By choosing this button a dialog box will be opened as shown in figure 4.19.

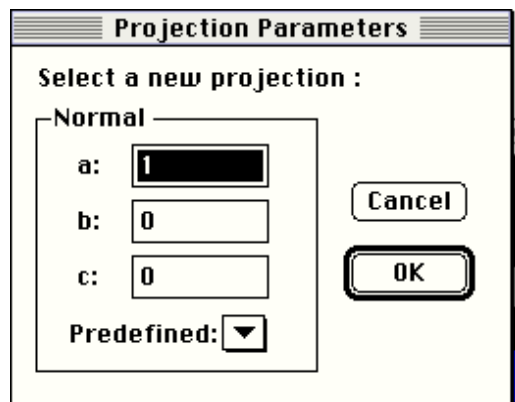


Figure 4.19. The projection dialog box.

Inside this dialog box you can set which crystallographic direction that should be parallel with the screen normal. You are only allowed to enter integer values in the input fields. Click OK to update your graph to the new view direction.

In the lower part of the tool window three icons are located. With these three icons you can control the graph mode of your drawing. The different graph modes are:



Atoms Only Mode. Only atoms are drawn.



Atoms and Bonds Mode. In this mode bonds and atoms are drawn and it is possible to create or modify coordination bonds between elements.



Atoms and Polyhedra Mode. Polyhedra and atoms are drawn and it is possible to create new coordination polyhedra around an element.