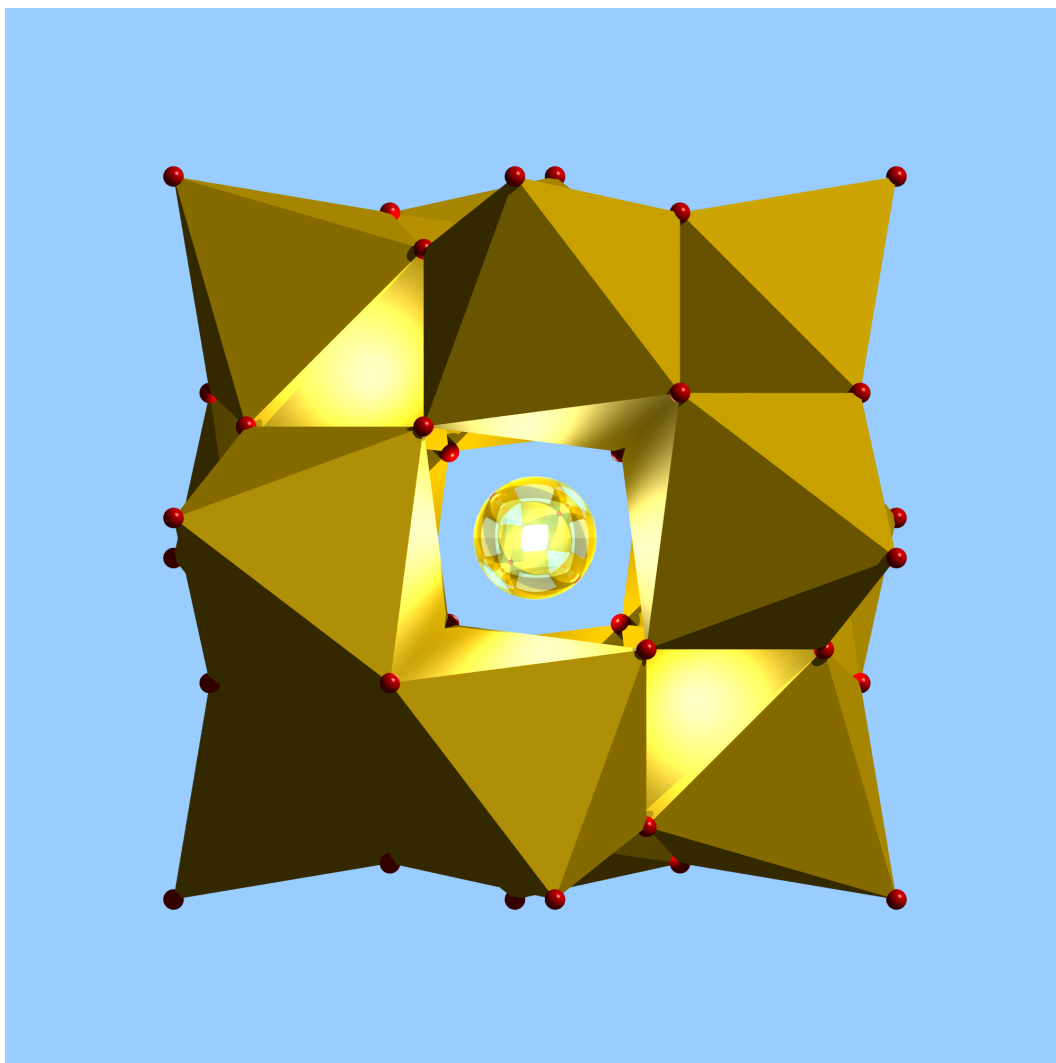




# DIAMOND

Crystal and Molecular Structure Visualization



User Manual





# DIAMOND

User Manual

Version 4.4





## User Manual



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## Introduction

You have crystal structure data (either space group/unit cell/atomic parameters or a file (e.g. CIF)) and would like to...

- create high-quality pictures for a presentation or publication?
- understand the construction principles of the structure?
- visualize the construction principles in various ways for your students?

Excellent. That's exactly what you can do with DIAMOND, a modern software package for visualizing crystal structures at the atomic level. The new version 4 has been improved again over the previous versions to make the initial steps as simple as possible<sup>1</sup>. As a result, you can create beautiful pictures of your crystal structure without ever reading this manual.

Nevertheless, Diamond is a really powerful package offering a large variety of options far beyond these initial steps. In order to be able to use the full power of Diamond, we strongly recommend to read this manual, following our recommendations:

1. First of all, you are certainly eager to get your new DIAMOND software package running on your computer straight away and create some pictures for testing. Hence, please install the software as described on p. 59 (if you have not already done so), and work through the tutorial session A (p. 2), following the instructions given in the text.
2. Once you have created your first pictures, we recommend to reserve a little bit of time for reflection, preferably not during a busy day between several phone calls, meetings and frequently interrupting colleagues.
3. Have a seat in an armchair with the manual and a nice cup of coffee or tea, and read the chapter "Reflection" on p. 17. Think about your first steps in tutorial A, and consider what you would like to do with the software concerning your own research.
4. You might even want to have a first look at the chapter "Tutorial B: Advanced Examples" (p. 20) while sitting in your chair, in order to get an impression of what will happen next.
5. Afterwards, return to your computer and perform Tutorial B. In doing so, you will learn a lot about DIAMOND's most prominent features.
6. Now that you been introduced into the way of working in DIAMOND, you should read the "What's New in Diamond Version 4" article which serves as a starting point through a tour of the new features of version 4. This article and the feature tour are available through the command "What's New" in the "Help" menu.
7. Finally, you should try to "play around" with the software as you like, probably trying some examples from your own research activities.
8. If you need help, please refer to the corresponding chapter on p. 57 in this manual in order to get an overview over the various ways DIAMOND can support you.

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<sup>1</sup>If you have already used the previous DIAMOND version 3, you should read the chapter "What's New for Diamond 3 Users" (p. 61) in the appendix. This chapter may also be interesting for new users who would like to get an overview over the highlighting new features in DIAMOND version 4.



## Tutorial A: Introductory Examples

### First Steps

In this very first tutorial session you will learn:

- How to **import crystal structure data files**, e.g. CIF-files.
- How to let DIAMOND **create a structure picture automatically**
- How the **user interface is organized**
- How to **display crystal structure data, table of distances and angles, and powder diffraction pattern**

We will start the tutorial with a rather typical situation: The crystal structure data of a certain compound are present in a CIF-file<sup>2</sup>, based on which a picture of the crystal structure shall be created. In our case, the CIF-file of Fullerene (C<sub>60</sub>) has been exported from the Pauling File Binaries Edition<sup>3</sup>.

If you have not already done so, please start the DIAMOND software now<sup>4</sup>. It will display the so-called "Start Screen", using which you can perform the most common operations (like importing a crystal structure file or opening a recently used document) by just a single mouse click (fig. 1).

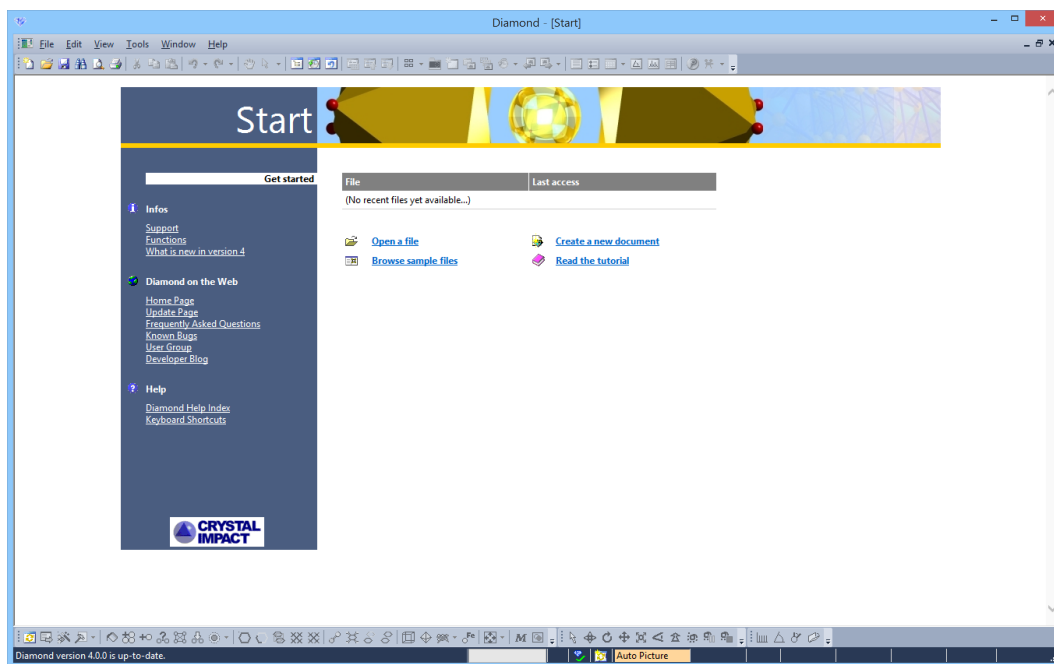


Fig. 1: The so-called "start screen" offering a variety of typical file operations, e.g. import or opening of recently used documents.

Please click on "Open a file" in order to import the structure data; the "Open" dialog will be displayed. Make sure that the file type at the bottom of the dialog is set to "CIF (\*.cif)", then select the file "c60.cif" in the "Tutorial" subdirectory of the DIAMOND program directory (e.g. "C:\Program Files\Diamond 3 \Tutorial"). Finally, please press "Open".


<sup>2</sup>CIF (= Crystallographic Information File) is one of the most common file formats for storing and exchanging crystal structure data. For example, IUCr-journals like "Acta Crystallographica" offer downloads of CIF-files for published crystal structures. More information about CIF can be found at <http://www.iucr.org/iucr-top/cif/index.html>

<sup>3</sup>Pauling File Binaries Edition, published by ASM International, Materials Park, Ohio, U.S.A.

<sup>4</sup>If your colleagues have used DIAMOND on your PC before, we strongly recommend to restore the default (factory) settings as described in the appendix (p. 60) before you follow the tutorial sessions in this manual.



A lot of frequently used commands can also be executed by pressing the corresponding button in the toolbar or by pressing a certain combination of keyboard buttons. Once you know these buttons and key combinations by heart, your work will become more quick and fluently. If a menu command can also be executed using a toolbar button or key combination, this is indicated by a small pictogram to its left and/or the key combination to its right.

In our case, you could e.g. have selected the "Open" command from the "File" menu, pressed the toolbar button  or pressed the key combination "Ctrl+O". ("Ctrl+O" means that you keep the Ctrl-button on your keyboard pressed and press the "O").

If you have just installed DIAMOND (i.e. if the option settings are still equivalent to the factory settings), the "File Import Assistant" will be displayed (fig. 2), using which you can control the individual steps of the import procedure (e.g. recognition of file type etc.).

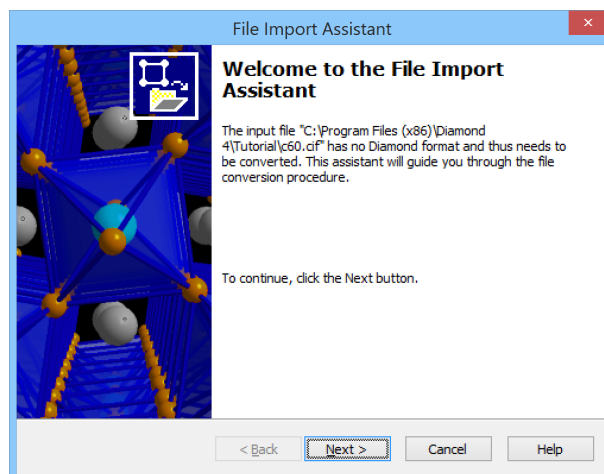


Fig. 2: The "File Import Assistant" guides you through the options which apply to the import of crystal structure data files.

Please click on the "Next" button at the bottom of the assistant, and check if the file format which has been determined automatically from the contents of the selected file is correct. Below, the number of data sets which can be imported from the file (1 in our case) is displayed (fig. 3).

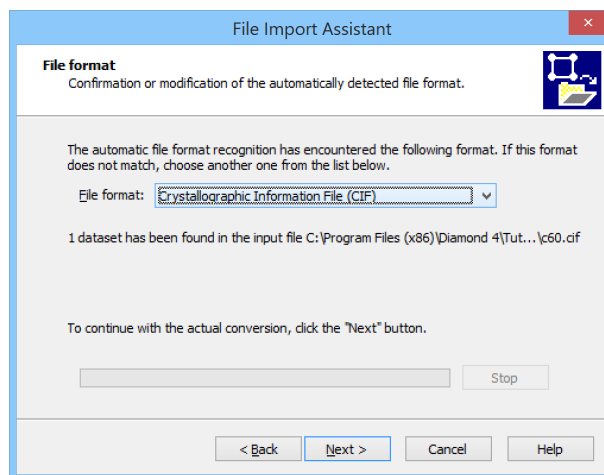


Fig. 3: On the second page of the "File Import Assistant" you should check if the file format which has been determined automatically is correct. If not, please select the correct format using the "drop-down" box in the center of the dialog.

Please press "Next" to advance to page 3 of the assistant. Here, you can select if you would like to let DIAMOND create a structure picture automatically, use the "Structure Picture Creation Assistant" or the new "Auto Picture Creator", or start with a blank picture. In our case, we would like to keep this first tutorial as simple as possible, so please select "Create picture automatically (proposal based upon structural parameters)" from the "Select if and what to do with the structure picture(s)" combobox (fig. 4).

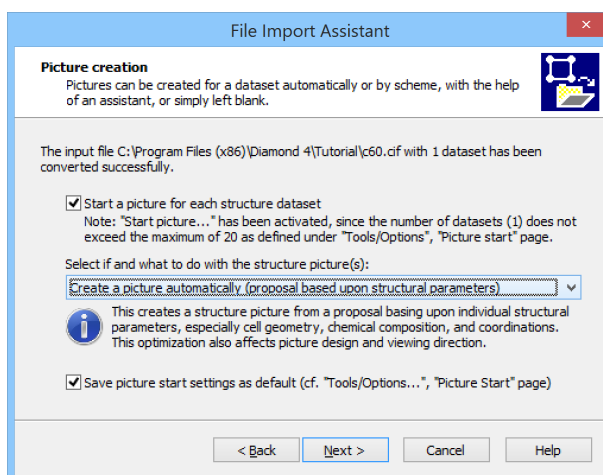


Fig. 4: On the third page of the "File Import Assistant" you can select if (and how) you would like to create a first picture for the imported crystal structure data.

Please click on the "Next" button to advance to the fourth (and final) page of the file import assistant (fig. 5). If you mark the "Do not show this assistant again" checkbox (don't do this now), the complete "file import" operation will be performed automatically next time you import a structure file. Press the "Finish" at the bottom of the assistant. DIAMOND will import the crystal structure data and display a picture which has been created automatically (fig. 6).

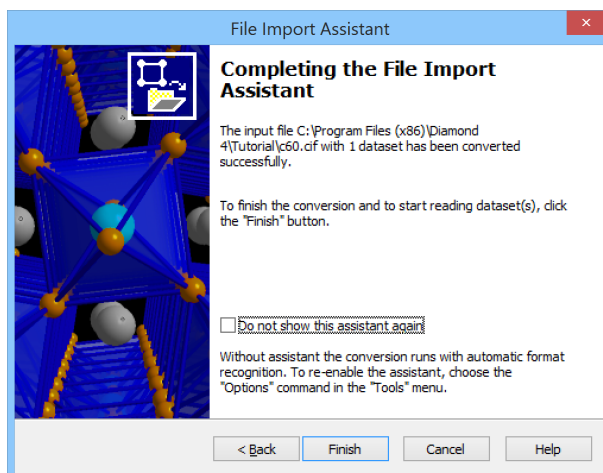


Fig. 5: On the final page of the "File Import Assistant" you can select if the assistant shall be displayed again on your next file import, or if the import procedure shall be performed "in silence" (i.e. automatically).

Now that both crystal structure data have been imported as well as a structure picture has been created, we will explore the DIAMOND user interface in order to learn about the various displaying options. Please have a look at the screen (or fig. 6):

The dominating view in the working area<sup>5</sup> is the **structure picture**, currently displaying the cubic arrangement of C<sub>60</sub> "balls". To the right of the structure picture, two so-called "panes" are displayed: On the upper right-hand side, the **Tables pane** by default displays a short overview of the most important crystal structure data (**Data sheet**). In this pane, you can also display various other tables (e.g. atomic parameters, created atoms, molecules, or planes, distances and angles measured by the user etc.). These tables are accessible by clicking on the phrase with the small "arrow down" to its right (currently "Data sheet") at the top of the tables pane.

Please go ahead and try to display the "Table of created atoms": Click on "Data sheet", then select "Table of Created Atoms" from the drop-down list. Afterwards, please display the "Data sheet"

<sup>5</sup>The working area in DIAMOND is the space between the toolbar at the top and toolbar and status bar at the bottom.

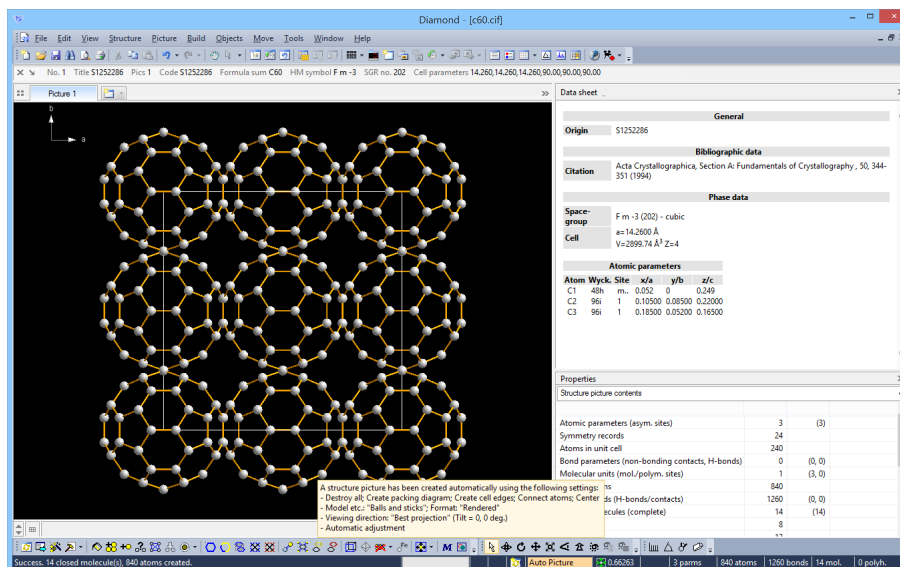


Fig. 6: The crystal structure data have been imported from the file "c60.cif". DIAMOND has created a picture automatically; besides this, a short overview of the most important crystal structure data ("data brief") as well as a summary of the contents of the picture are displayed.

again by selecting it from the drop-down list, and click on the black background in the structure picture (left mouse button) to make it the active pane again.

On the lower right-hand side, the so-called **Properties pane** displays various kinds of information about the structure picture and the currently selected objects, e.g.

- Structure picture contents
- Created atoms in structure picture
- Selected objects
- Distances between/around selected atoms
- Linearity/planarity of selected atoms
- etc.

The Properties pane can be set to "Automatic" mode (by selecting the corresponding first line in the dropdown box at its top) so that it always displays information depending on the currently selected objects. This "Automatic mode" is also the default setting, so there is no need to change it now.

There are several bars and windows that enable quick and easy navigation through the structures and pictures of a DIAMOND document (fig. 7). Unlike in this tutorial sample, DIAMOND **document files (\*.diamdoc) can contain more than a single crystal structure as well as more than one picture for each crystal structure!**

**Picture Tab Bar** The "Picture Tab Bar", located above the actual structure picture, allows to switch between multiple pictures, provided there are multiple pictures in a document.

**Navigation Tree** The so-called "Navigation Tree" provides a hierarchic overview over all crystal structures and pictures in all open documents. It can be displayed by selecting the "Navigation" command from the "View" menu. If you click on a "leaf" in this tree, the corresponding picture will be displayed in the main window area. By clicking on a "branch" you will obtain an overview of all pictures associated to the clicked structure or of the entire (clicked) document node as small so-called "thumbnails".



**Structure Info Bar** The "Structure Info Bar", located above the Picture Tab Bar, gives a brief summary of some structural parameters, like title/code, formula sum, space group, and cell parameters. If the document contains multiple structure parameter sets, this info bar can be expanded to the "Structure Table", a report-like representation of all structures of the current document.

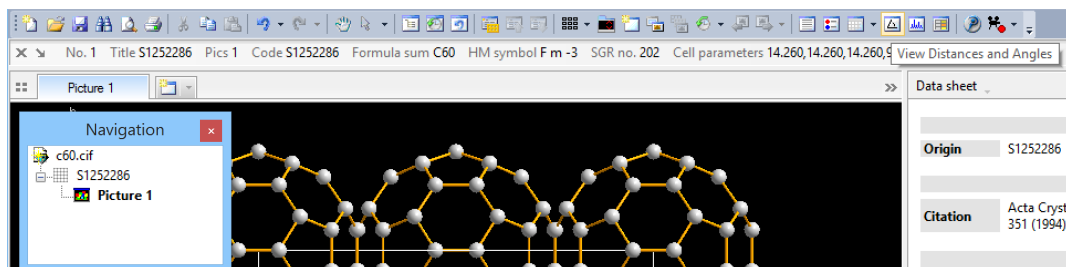


Fig. 7: The **Navigation window** provides quick access to all pictures of all structures of all open documents as well as "nodes" to the "structure level" and the "document level". (Here: Only one document "c60.cif" with one structure data set "S1252286" and one picture with default title "Picture 1".) The **Picture Tab Bar** above the actual structure picture allows to switch between multiple pictures (here: only one tab for "Picture 1"). The **Structure Info Bar** above the Picture Tab Bar gives a brief summary of the current structure data set. The icons to view data sheet, distances and angles analysis, powder diffraction pattern, etc. of the current structure picture are located in the right part of the main toolbar

In addition to the structure picture(s) view, there are several different views available for the current structure. These views are located in the so-called "data pane", which is located right of the actual structure picture(s) view:



**Data sheet** The data sheet contains all information that is currently known about the structure and is available in brief and in comprehensive form.



**Atom list** The default setting of the atom list uses the hierarchy of atom groups and their associated atom sites as well as the associated created (symmetry-equivalent) atoms present in the current structure picture. This hierarchical list gives you enhanced access to single or some atoms or some or all atoms of a site or group, e.g. to edit properties and designs or to select them. Another setting shows all molecular units and their constituent atoms.



**Various data tables** Several tables are available to list the atoms of the parameter list, to list all atoms, bonds, molecules, or polyhedra in the structure picture, etc.



**Distances and angles** This displays a table as well as a histogram representation of the distances and angles between the various atoms in the structure.



**Powder pattern** The powder diffraction pattern is calculated from the crystal structure data. Both a list of individual reflections as well as a diffraction diagram are presented. Various parameters of the diffraction pattern calculation (radiation, wavelength, LP-correction, profile function etc.) as well as the diagram (scaling, colors etc.) can be adjusted.

Please walk through these views by clicking on the corresponding symbols in the main toolbar, and try to change the settings e.g. for the diffraction pattern or the distances and angles calculation.

If you click on the structure name (node) in the navigation tree (in our case "S1252286"), you will obtain a thumbnail overview of all pictures which have been created for the current crystal structure ("structure level"), as well as the "Data sheet" providing a quick overview over the most important crystal structure data. This is also available as "Structure Overview" from the "View" menu.

The first tutorial session is finished at this point; you have got an overview over the user interface and some important dialog elements. We will now start working with DIAMOND in the next chapter, by manually entering the crystal structure data and creating a picture "on your own".



## Creating a Picture

In this tutorial session you will learn:

- How to **manually enter the crystal structure data**
- How to **create a picture using the Structure Picture Creation Assistant**

You will now learn how to enter crystal structure data manually which may be necessary if no structure data file is available (e.g. if the crystal structure data are given in some printed publication): Please execute DIAMOND if it is not already running. Afterwards, you will have to create a new DIAMOND document (in the previous session, this has been done automatically during the file import procedure): Please select the "New" command from the "File" menu (or press the corresponding toolbar button). A completely empty document will be displayed.



Now you have to enter the crystal structure data; we will use the data of quartz ( $\text{SiO}_2$ ) taken from the entry "S541934" of the Pauling File Binaries Edition: Please select the "New Structure..." command from the "Structure" menu; this will open the **New structure assistant** guiding you through the input of the required data (like space group, unit cell or atomic parameters). The assistant will display an opening screen with some hints about its purpose; please press "Next" to advance to the second page (fig. 8) on which you will start entering your data.

Fig. 8: On this page of the New structure assistant, you can select if you would like to enter crystal structure or molecule structure data. For crystal structure data, you have to provide space group and unit cell parameters.

Please make sure that "Crystal structure with cell and space group" is selected, then click on the "Browse" button to the right of the "space group" input line. In the dialog which opens, please select the space group "P 31 2 1 (152)" (fig. 9) and click "OK". The space group will be copied to the New structure assistant page.

Fig. 9: Using this dialog you can select the appropriate space group, supported by additional information about the currently selected space group on the right hand side.





Afterwards, please enter the unit cell parameters  $a = 4.535\text{\AA}$  and  $c = 5.17\text{\AA}$  (all input fields which are fixed by the space group are automatically disabled). Finally, change the "Title of the new structure" at the bottom of the page to "Quartz low", since the data correspond to the low temperature modification of quartz. Your window should now look similar to fig. 10.

**New Structure**

**Cell parameters, space-group, and title**  
The new structure may be a crystal structure (with cell and space-group) or just a "molecular structure" with atoms only.

Choose if the new structure is a crystal structure (translational symmetry and fractional atom coordinates), or a "molecular structure" (just atoms in orthogonal coordinates).

☒ Crystal structure with cell and space-group

Space-group:

Cell length  $a$  [ $\text{\AA}$ ]:   $b$ :   $c$ :

Cell angle  $\alpha$  [ $^\circ$ ]:   $\beta$ :   $\gamma$ :

☐ "Molecular structure", no cell, no space-group

Title of the new structure:

Fig. 10: Space group, unit cell parameters and title of the structure have been entered.

Please press "Next" to advance to the next page of the assistant where you have to enter the atomic parameters (elements, oxidation states and coordinates). The element of the first atom you would like to enter is Si; its oxidation state in this compound is +4. The oxidation state of an element must be given right after the element symbol, so please enter "si+4" as element symbol in the "Atom" input field. Afterwards, press the <Tab> button on your keyboard to advance to the input field "x/a". Please enter 0.4487 in this field and press <Tab> to advance to "y/b". Enter 0, advance to "z/c" (<Tab>) and enter 0.3333. Now that you have entered all data for the atom, press the "Add" button to the right (or simply <Return>) to add the data to the table below (fig. 11).

**New Structure**

**Atomic parameters**  
The atomic parameters use fractional coordinates for a crystal structure but orthogonal coordinates (in Angstrom units) for a "molecular structure".

Here you can define element (with oxidation number) as well as x, y, and z for every atom. For mixed or defect sites, standard uncertainties, and displacement parameters, use the "Atomic Parameters" dialog ("Structure" menu) instead.

Atom:   $x/a$ :   $y/b$ :   $z/c$ :

Atoms in the asymmetric unit:

Atom	x	y	z
si	0.4487	0	0.3333

Fig. 11: The atomic parameters for the first atom (Si+4 (0.4487,0.0,0.3333)) have been entered.

Now, you have to enter the parameters for the second atom (O-2) which are "O-2 (0.367,0.2952,0.2427)". Simply follow the procedure described above for Si+4. Once you have pressed the "Add" button, please compare your window to fig. 12.

Afterwards, press "Next" to advance to the final page of the assistant. Here you can select if (and how) you would like to create a structure picture for the data you have just entered. While in the previous session the picture has been created automatically, you will now learn how this can be achieved "semi-manually" using the so-called **Structure picture creation assistant** (which provides the most common options for creating crystal structure pictures). We recommend to use it until you have gained some experience and can perform the individual steps using the menu or toolbar buttons.





**New Structure**

**Atomic parameters**  
The atomic parameters use fractional coordinates for a crystal structure but orthogonal coordinates (in Angstrom units) for a "molecular structure".

Here you can define element (with oxidation number) as well as x, y, and z for every atom. For mixed or defect sites, standard uncertainties, and displacement parameters, use the "Atomic Parameters" dialog ("Structure" menu) instead.


Atom:  x/a:  y/b:  z/c:

Atoms in the asymmetric unit:

Atom	x	y	z
Si	0.4487	0	0.3333
O	0.367	0.2952	0.2427

Fig. 12: The atomic parameters for both atoms in the asymmetric unit of the quartz structure have been entered.

Please make sure that the box to the left of "Start structure picture" is checked and "Launch the Picture Creation Assistant" is selected in the combobox right beneath the "Create picture" label. Then click "Finish".

 Note that the structure picture in the background is still empty; you now have to build a structural model based on the crystal structure data you have just entered. This is central aspect of the DIAMOND concept which is described in more detail in the next chapter on p. 17.

Right after the New Structure Assistant has closed, a new (empty) picture will be created, and the Structure Picture Creation Assistant will open. The first page of the assistant offers the option to destroy all objects currently present in the structure picture as well as to initialize the input fields on the following pages of the assistant from a proposal that DIAMOND has derived from the structure parameters. Since the structure picture is still empty and we do not want to follow the proposal, leave the two checkboxes left beneath "Destroy all atoms, bonds, etc." as well as "Get a proposal from structure parameters" blank, and press "Next" to advance to the second page of the assistant (fig. 13).

**Create Structure Picture**

**Picture building basics**  
This defines the basic set of atoms and bonds in the structure picture.

Select if and what part of the structure is to be built up.

☐ Add all atoms (and connections) from parameter list(s)  
☒ Add all bonds ☐ Add all H-bonds ☐ Add all non-bonding contacts


☐ Get molecule(s) (or polymeric fragment)  
☒ Fill cell range with atoms ☐ Create packing diagram

Range:

x/a-min:  y/b-min:  z/c-min:   
x/a-max:  y/b-max:  z/c-max:

☐ None of the above mentioned

Fig. 13: The first step when building up a structural model is to select the atoms which shall be displayed. The second page of the Structure picture creation assistant offers a variety of options for this task.

 The Structure picture creation assistant cannot only be used to build new structure pictures but also to modify existing ones. You can generally call this assistant by selecting the "Picture Creation Assistant..." command from the "Picture" menu.

The first thing you generally have to do when creating a structure picture is to define the atoms which shall be displayed. The second page of the Structure Picture Creation Assistant offers the



most common methods to do this. You should select the method depending on your compound. In our case, we would like to fill two unit cells in each direction, so please mark "Fill cell range with atoms", and select "2 x 2 x 2 cells" from the "Range" combobox (fig. 14). Afterwards, press "Next" to advance to the third page of the assistant.

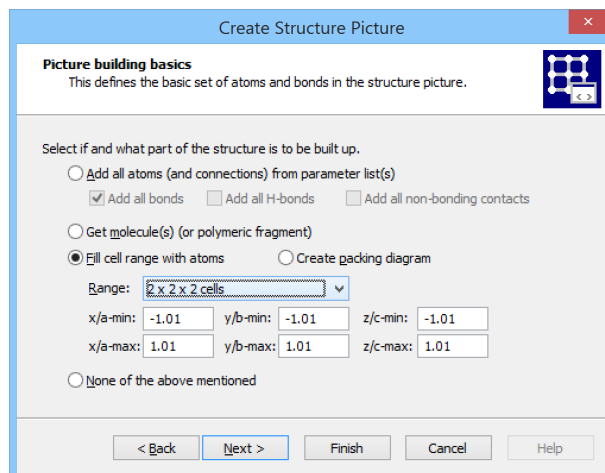


Fig. 14: DIAMOND will fill eight unit cells (two in each direction) with atoms.

This page is dedicated to the completion of structural fragments to which the atoms created on the previous page belong. In our case, we would like to draw polyhedra around the Si-atoms: Please deselect "Fill coordination spheres", and mark the checkbox "Create polyhedra around" instead. Afterwards, enter "Si" in the input line to the right of "Central atom elements". Besides this, make sure that the "Create cell edges" as well as the "Connect atoms" checkbox at the top of the page are checked. All other options should be unchecked (fig. 15). Finally, press "Next".

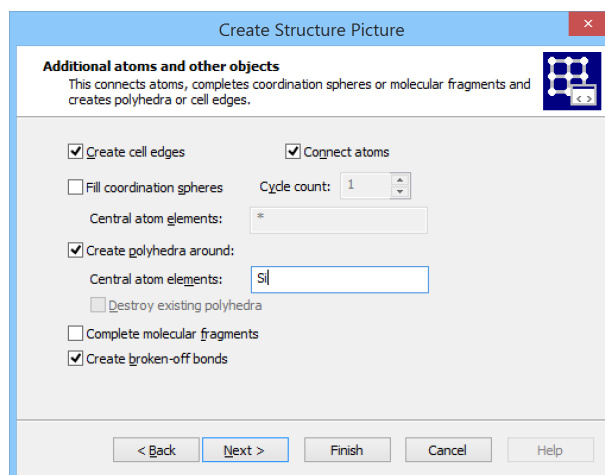


Fig. 15: The atoms will be connected by bonds (based on the current connectivity settings), and the unit cell edges will be displayed as well. We would also like DIAMOND to create polyhedra around the Si-atoms which are created by the options selected on the previous page.



The method described here to create polyhedra is only one of several ways to perform this task in DIAMOND. Other possibilities are e.g. to select a center atom as well as the ligand atoms in the structure picture and execute the "Construct polyhedron" command from the "Build"/"Polyhedra" submenu afterwards, or to use the "Build"/"Polyhedra"/"Add polyhedra" dialog in which you can define the atom groups for center as well as ligand atoms separately.

While the previous two pages of the assistant were basically dedicated to **building up the structural model** (sometimes also called the "creation of the primary atoms"), the fourth page provides some options to define the **design** of the picture. You can e.g. change the model from the default "Balls and Sticks" to "Wires" or "Space filling", select the layout of the screen (e.g. screen or A4-page), and define the quality of the display (rendered etc.). An important option on this page is "Avoid duplicate atom main colors" which should generally be checked if a new picture is created. We will



use the default settings on this page, so simply press "Next" to advance to the following page.

Here, you can select the way you would like to look at the structural model. For example, you could choose viewing along a certain unit cell axis: Please select "[001] projection (view along c axis)" which is generally quite appropriate for monoclinic axis b settings. Please select "(No change)" from the "Projection" combobox.

The final option on this page is also important; you should normally check the "Adjust enlargement factor and position to fit picture in drawing area" so that the complete structural model is displayed as large as possible automatically. Afterwards, please click on "Finish". The structure picture will be created according to the options you selected (fig. 16).

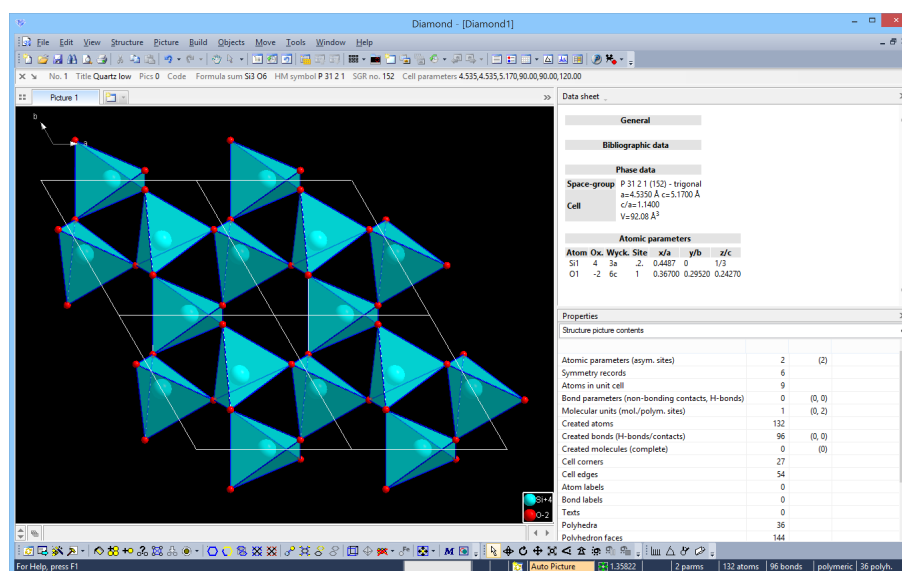


Fig. 16: Using the Structure picture creation assistant, you have created your first structural model.

Congratulations! You have just finished creating your first picture of a crystal structure on your own! However, please do not close this picture yet: The next important thing to do is to adapt the design of the picture to your requirements. This will be described in the next chapter.



## Adapting the Design of the Picture

In this tutorial session you will learn:

- How to **change designs** (e.g. **atom colors**) in order to best match your requirements
- How the **unlimited undo/redo functionality** can help you to find the best solution
- How to change the **orientation** of the structure model.

In the previous chapter, you have created a structural model of quartz. Now, we will see how the design of the model can be changed to emphasize certain aspects you would like to present to your audience. We will continue working on the structure picture right at the point where we stopped in the previous chapter.



Please note that from now on we will no longer include the complete contents of the DIAMOND window in structure pictures. Besides this, we will display the contents of the actual structure picture with a white background in the manual which is more appropriate for printing and reading. Of course, the background of your structure picture on the screen will be black like in the previous tutorial sessions.

Your aim concerning this structure picture is to present different aspects of the crystal structure of quartz to your audience. In this context, it would be nice to have parts of the structure being displayed in different models, each focusing on different aspects (like packing of atoms, 3d-network, local atomic environments).

We will start by displaying some atoms in the corner on the lower right hand side of the picture in the space-filling model (and not in the "Balls and Sticks" model which is the default representation). The first thing you have to do is to select the atoms for which the "displaying model" shall be changed. Please press the left mouse button somewhere in the lower right hand corner inside the structure picture, and move the mouse up and to the left, thus spanning a selection rectangle on the screen. When the mouse cursor is close to the center of the structure picture, release the mouse button; all atoms within this rectangle will be selected (which can be seen by a yellow/blue frame around them) (fig. 17).

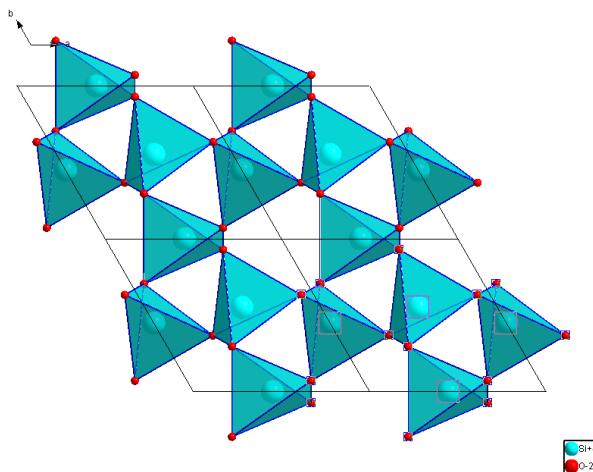


Fig. 17: The atoms in the corner on the lower right hand side have been selected, as indicated by the blue frames around them. Note: On a black background the selection frames are yellow instead, cf. the remark above concerning the background color of the structure picture!

Now that the atoms for which the displaying model shall be changed have been selected, please choose the "Model and Radii..." command from the "Picture" menu.



You will find commands to **build** a structural model (e.g. add atoms or bonds) in the "Build" menu, while commands which change the design of individual atoms or even the whole structure picture are present in the "Picture" menu. If you would like to add abstract objects (like planes, atom vectors or labels), you will find appropriate commands in the "Objects" menu.

From the "Model" combobox at the top, please select "Space-filling", then press "OK". The atoms



you have selected in the structure picture will be displayed with their "space-filling" radii. The selection frames are still present around them, so please click into a blank part of the structure picture to release the selection and remove the frames (fig. 18).

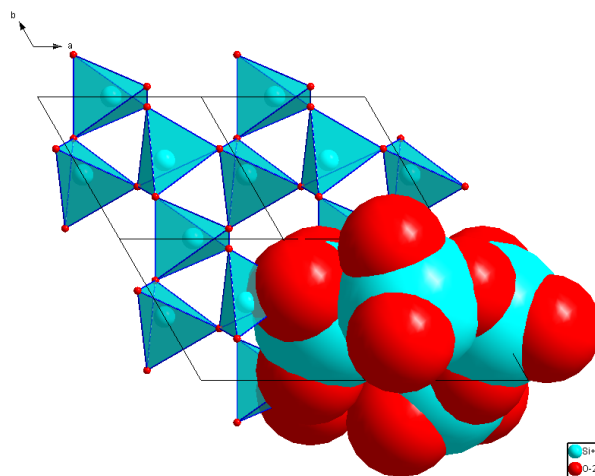


Fig. 18: The atoms which have been selected in the previous step are now drawn with their "space-filling" radii.

Let's summarize what we have up to now: One part of the structure picture presents the crystal structure of quartz as corner-connected  $\text{SiO}_4$ -tetrahedra, another part shows the space filling character of the atomic arrangement. A third way to look at the crystal structure of quartz is to describe it as a three-dimensional network of covalent bonded atoms. Hence, we will change the model for a part of the structure picture to "wires/sticks" to emphasize this important point of view.

Please draw a selection rectangle somewhere in the center of the picture similar to the one used for the space-filling model (press the left mouse button, move the mouse until the selection rectangle which is displayed contains the objects you would like to select, and finally release the mouse button).

Before we can actually change the model to "wires/sticks", we have to remove all polyhedra within the selection rectangle in order to make the actual bonds visible: Please select the "Polyhedra" command from the "Destroy" submenu of the "Build" menu (in short: select "Build/Destroy/Polyhedra" in the menu). The atoms and bonds previously hidden by the polyhedra surfaces will become visible. Note that the atoms are still selected (fig. 19)!

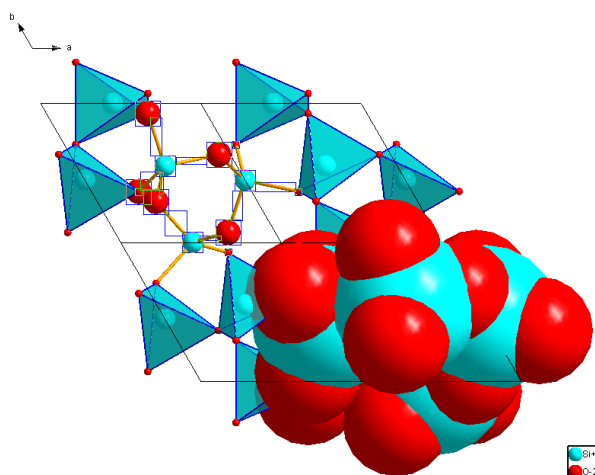


Fig. 19: In the center of the structure, some polyhedra have been removed in order to make the bonds visible.

Now, you can change the model for the selected atoms: Please open the "Model and Radii..." dialog from the "Picture" menu, then select the model "Wires/Sticks" in the combobox at the top of the dialog. Afterwards, click "OK" (the dialog will close) and click into a blank part of the picture in



order to release the current selection. As you see, the network consisting of four-bonded (Si) and two-bonded (O) atoms clearly becomes visible (fig. 20).

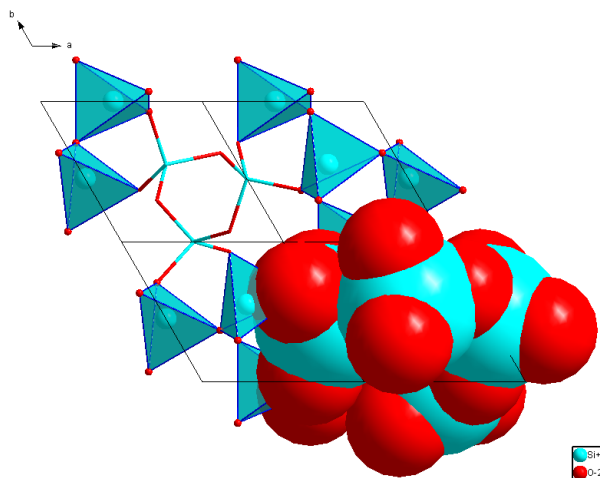


Fig. 20: Three models in the same structure picture reveal different aspects of the crystal structure of quartz.

Let's assume that you are still not really satisfied with the picture...the cyan color of the Si atoms is a little bit too dominating; perhaps a different color would be better. In order to change the design (here: the color) of objects (here: atoms), you first have to select them. You have already selected atoms using the mouse in the structure picture; however, this method is a little bit too complicated for our current purpose. We would like to change the color of **all Si+4 atoms**, or, in other words, the design (color) of the **atom group** "Si+4" shall be changed.



DIAMOND creates groups of atoms from the list of atomic parameters: All atoms which have the same element (here: Si) and the same oxidation state (here: +4) are (at least by default) assigned to the same group. You can change the design for an atom group, with the result that the individual designs of all atoms belonging to this group will be changed. Of course, you can also change the design of individual atoms, e.g. by right-clicking on an atom in the structure picture and selecting the "Edit.../Atom design" command from the context menu.

Please select the "Atom designs..." command from the "Picture" menu. The "Atom Group and Site Designs" dialog will open (fig. 21).

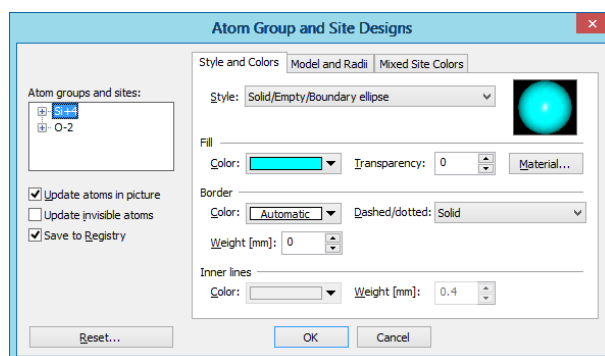


Fig. 21: In the Atom Group and Site Designs dialog, you can change the design (color, radii etc.) for all atoms belonging to the group selected on the upper left hand side.

Make sure that the atom group for which you would like to change the color (Si+4) is selected on the left hand side, and that the "Update atoms in picture" box (also to the left) is checked, then click on the "Color" button under "Fill". The color selection panel will open; please select (click on) the brown color close to the upper left corner of the color table. Afterwards, simply close the "Atom Group and Site Designs" dialog by clicking "OK". All Si+4 atoms will now be displayed in brown color.



In the "Atom Group and Site Designs" or "Atom Design" dialog, it is not only possible to change the color of atoms, but also of a large variety of other settings, among which are atom styles, radii for the different models, "material" properties (which are especially useful when creating POV-Ray images, see p. 44), etc.

However, when you look at the picture, you most probably will realize that brown was not an overly good select...the contrast to the red oxygen atoms is too small now. It would be nice if one could undo the coloring of the Si+4 atoms. This can easily be achieved by selecting the "Undo" command from the "Edit" menu, by pressing the corresponding toolbar button, or simply by pressing the combination <Ctrl+Z> on your keyboard. Please do so now to return to the picture with Si+4 atoms in cyan color.



Though the "undo" functionality does not seem to be that much important at the first glance, it is indeed one of the most frequently used features in DIAMOND! You should always keep in mind that you cannot just undo the last operation, but can go back step by step right to the beginning of your work. There is no limitation to the number of undo steps except the memory capacity of your computer.

You can see a list of the last operations as well as a thumbnail picture of the picture state before the operation each, when you click on the dropdown arrow right beneath the actual "undo" symbol in the toolbar.

In addition to the "undo" function, the opposite is also possible: You can "redo" an unlimited number of steps, i.e. return to the point at which you performed the last undo operation. Using undo and redo, you can go back and forth your modifications to the structure picture, so it is extremely simple to try modifications and test alternatives.

Let's now use a different color for Si+4 atoms...gray for example. Please select the "Atom Designs..." command from the "Picture" menu again, make sure that Si+4 is selected to the left, and open the color selection panel by clicking on the corresponding button in the center of the dialog. Afterwards, select the color "Gray-25" in the right part of the panel, guided by the tooltips when moving the mouse pointer over the selection panel. Finally, close the "Atom Group Designs" dialog by pressing "OK". The contrast between Si and O atoms is better now and the coordination polyhedra look less intrusive.

While you look at the structural model, you somehow feel that you are still not fully satisfied. The unit cell edges in the picture do not seem to be favourable for your presentation. In order to delete them, please select "Destroy/All cell edges" in the "Build" menu. The result is shown in fig. 22.

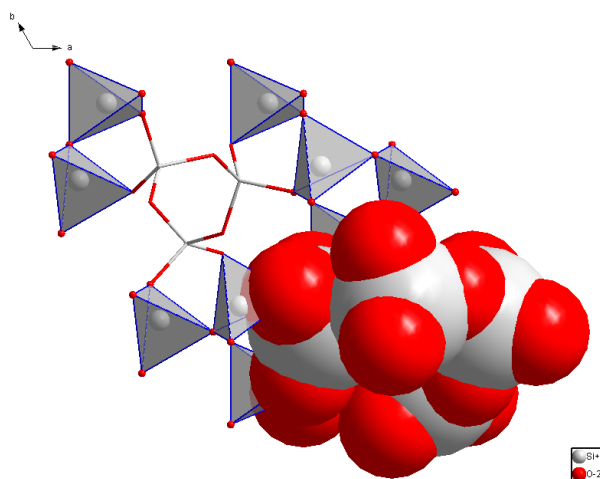


Fig. 22: The color of all atoms belonging to the "Si+4" atom group has been changed to gray. Besides this, the unit cell edges have been removed ("destroyed") to provide a better view of the different aspects of the structure.

The structure picture has now been finished. However, in order to present it to your audience, you would like to rotate the model in order to find the most suitable representation. Please select the "Rotate along x-/y-axis" command from the "Move" menu (or press the corresponding button in the toolbar at the bottom) in order to switch to the so-called "tracking mode", indicated by the different mouse cursor. Afterwards, press the left mouse button inside the structure picture and move the mouse around while keeping the button pressed; the structure picture will rotate following your mouse movements. Once you have found a suitable orientation, you should release the mouse button. Afterwards, you should select the "(no tracking)" command from the "Move" menu (or press







the corresponding toolbar button) in order to return to the normal "selection" mode.



It is also possible to let the model rotate continuously around one or more axes. For example, you can simply "push" the model into rotation using your mouse<sup>6</sup>: Please activate the so-called "Spin mode" by pressing the corresponding button in the toolbar at the bottom, and switch to the "Rotate along x/y-axis" tracking mode afterwards by pressing the appropriate button which is located in the bottom toolbar as well. Now you can push your model into rotation: Simply move the mouse into the structure picture, press the left mouse button and keep it pressed while you rapidly move the mouse in some direction. Finally, release the mouse button. The model in the structure picture will start rotating around the x- and y-axis according to the direction in which you moved the mouse.



The x-axis of the so-called "view coordinate system" is the horizontal axis in the plane of the screen, the y-axis is the vertical axis in this plane. The z-axis "comes out of the screen", pointing towards you.



You can change the rotation simply by repeating the "mouse pushing" procedure described above. The closer the mouse pointer to the rotation center, the slower will be the rotation, and vice versa. If you would like to stop the rotation, simple select the "Stop motion" command from the "Move" menu, or press the corresponding button in the toolbar below. Afterwards, you should also disable the "Spin" mode (push the corresponding button again) in order to prevent yourself from surprising results during tracking operations later on. Please return also to the default viewing of the structure by executing the "Viewing Direction..." command from the picture menu, pressing the "c" button in the "View along axis" rectangle at the top of the dialog, and finally pressing "Close".



The final step in this tutorial session will be to prepare the structure picture you have created for a printed publication: Even nowadays, it may be quite difficult to include a "normal" structure picture created with DIAMOND in a printed publication with sufficient quality. In these cases, it is generally recommended to use DIAMOND's so-called "flat mode" without any rendering. In this mode, the structure picture looks more like a drawing than like an arrangement of shaded spheres and tubes. Please select (disable) the "Rendering" option in the "Representation Settings" popup menu in the toolbar at the bottom<sup>7</sup>. Alternatively, you could also select the "Picture Settings..." command from the "Picture" menu, disable the "Rendering" checkbox on the "Representaton" tabsheet, and press "OK". The shaded (OpenGL) representation of the structure will be replaced by one which looks much more "flat" (fig. 23).

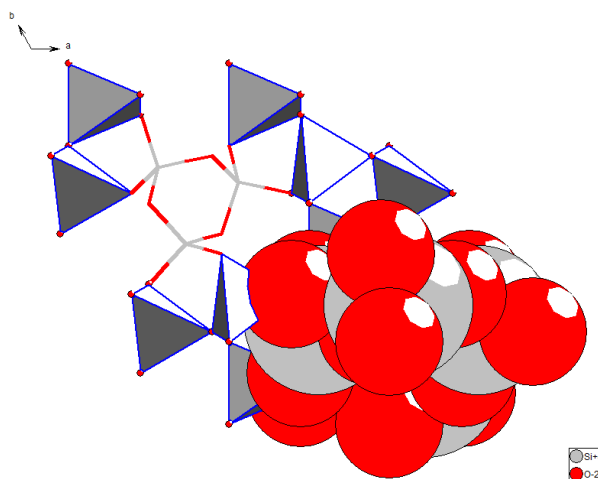


Fig. 23: The so-called "flat mode" is often more appropriate for printed publications than the normal "rendered" or "OpenGL" mode.

It should be noted that you can use the flat mode equivalent to the rendered mode, i.e. you can perform all operations in both modes, depending on your personal preferences, the only exception being planes which can only be displayed in the rendered mode.

<sup>6</sup>You could also use the "Rock'n Roll" command in the "Move" menu where you define the rotation axes and angles in a dialog.

<sup>7</sup>You can open a so-called "popup menu" in the toolbar by clicking on the "arrow down" button to the right of the corresponding button/icon.





## Reflection: The DIAMOND Concept

Now that you have created your first pictures with DIAMOND, we would like to insert a short reflection explaining the concept of this software in somewhat more detail. Wait a minute...don't be afraid! This will not become a long and exhausting introduction to every single idea behind DIAMOND; however, the knowledge of a few basic concepts will help you to not only successfully operate the software but really get the most out of its elaborate features.

### Task

In fact, the basic task when using DIAMOND is rather straight forward:

What you *have* is an abstract numerical description of a crystal structure, typically consisting of unit cell parameters, space group and atomic parameters (elements, fractional coordinates etc.), either in print or as a file (e.g. CIF-file).

What you *would like to have* is one or more pictures visualizing both the overall crystal structure as well as the basic construction principles, e.g. the packing of atoms or molecules, the atomic environments, the building blocks and their connections among each other etc. If the crystal structure is new or unknown, it may even be necessary to *explore* its construction principles before you can actually create pictures. The pictures can then be used to present your results to a scientific audience or to your students.

### Step-by-Step

As you have seen in the previous tutorial sessions, the first step when working with DIAMOND is to either import (from a file) or manually enter the abstract crystal structure data. Immediately after entering/importing the crystal structure data, the graphics pane is still empty, i.e. there is no structure picture yet (at least if you did not apply the "automatic picture creation" function!).



Especially unexperienced users of previous versions of DIAMOND sometimes were a little bit confused at this point because there was no obvious way how to proceed.

At this point, DIAMOND "knows" about the infinite three-dimensional arrangement of atoms described by the crystal structure data, however, it does not know what you would like to visualize. Hence, the next step is to create a picture **based on the data which have been entered/imported**, or, in other words, to **build up a structural model**.

This is straight forward: All you have to do is to tell DIAMOND which atoms or parts of the crystal structure described by your data shall be displayed. Once the model has been built (all atoms, molecules, polyhedra etc. are visible on the screen), you can **modify the design** of the picture (e.g. the colors of the atoms or bonds) in order to best express your understanding of the structure.

In summary, the following steps generally have to be performed to obtain a picture:

1. Open the file containing the crystal structure data (e.g. CIF-file) (menu "File/Open"), or enter the crystal structure data manually (menu "File/New..." or menu "Structure/New Structure...").
2. Build the structural model (i.e. atoms, unit cell edges etc.) you would like to display (menu "Build"). You might want to use the "Picture Creation Assistant" or the "Create automatically" function (menu "Picture").
3. Modify the design of the picture or of individual objects (e.g. atom colors) (menu "Picture").



Of course, this description is very schematic...DIAMOND is not a one-way street as may be suggested by this scheme! For example, you certainly can add new atoms or molecules to the current structural model also when you have already worked on the design. However, this simplified description shall help you to really understand what you are doing.



## Connectivity and Filter

While creating a picture using DIAMOND, it is generally helpful to imagine that you are somehow building a structural model: A lot of functions and settings do not affect the current model but only apply to future building operations. Hence, they should be regarded as "tools" that are temporarily applied during the model building process.



A typical example is the so-called **"Connectivity"** (which can be set using the corresponding command in the "Build" menu or the toolbar button): On the "Bonds" page (tab)<sup>8</sup> of this dialog, you can define interatomic distance interval(s) based on which DIAMOND decides if some atom belongs to the coordination sphere of some other atom, or, in other words, which atoms are chemically bonded. These distance intervals can be adjusted individually for each pair of atom groups (the so-called "bond groups"). Once you have defined appropriate distance intervals for each bond group, you can easily use building operations like the creation of polyhedra, the automatic search for molecules in the atomic parameter list, or the filling of coordination spheres. After the building operation(s) has/have been carried out, you can change the "Connectivity" settings for the next building operation without affecting the current structural model.

Another example is the **"Filter"** ("Build" menu): This command enables you to exclude selected atoms of the parameter list or selected symmetry operators temporarily from manual building operations. Once you have defined filter settings, the excluded atoms and symmetry operations won't be taken into account during the next building operations (e.g. filling the unit cell). However, when the building operation(s) have been carried out, you can perfectly change or even disable the filter settings without any harm to the current structure picture.



Do not mix up the "Filter" settings (menu "Build") with the "Hide" option (menu "Picture"): Using "Filter" you can define which atoms, symmetry operations etc. shall be involved in the future building operations (e.g. the filling of coordination spheres), while "Hide" affects only objects that are already present in the structure picture.

Nevertheless, both commands have in common that they are only temporary, in the sense that they are not saved in the DIAMOND document files: If you save a DIAMOND document and restore it later on to continue working on your structure picture, both options ("Filter" and "Hide") will be disabled again, independent on their status when the document was saved.

## Exploring Crystal Structures

If your data describe a new or even unknown crystal structure, it is quite difficult to create pictures revealing the underlying principles right away. Instead, you should first use DIAMOND's various options to explore the structure. For example, you might want to start exploring the individual atomic environments, and study the three-dimensional arrangement of these building blocks afterwards.

Typically, the first step when exploring a new crystal structure is to have a look at the distances between the various atoms. By comparing interatomic distances with typical distances, the intervals for chemical bonding and coordination spheres can be defined (the so-called "connectivity", see above). Once these distance intervals have been fixed, you can e.g. start from some individual atom, add its coordinating atoms, use the created atoms as new starting points, etc. By doing so, you can build a complete crystal structure or molecule starting with one single atom. Step-by-step you learn about the atomic environments as well as about their connection, helping you to fully understand the fundamental building principles of the structure.

In summary, you should use the following steps when creating pictures for unknown crystal structures:

1. Import or enter crystal structure data.
2. Check the connectivity based on interatomic distances, supported by distance statistics.
3. Build fragments for the structure by creating individual atoms and filling their coordination spheres stepwise until you understand the structural principles.

<sup>8</sup>The "Connectivity" dialog consists of three pages, where the first deals with the "actual" bonds, i.e. strong interactions, whereas the two other pages deal with H-bonds and non-bonding contacts.



4. Create one or more new picture(s) clearly showing these principles for publication and/or your students.

The exploration of an "unknown" crystal structure will be demonstrated on p. 25.

## Using Crystal Structure Pictures

Once you have created one or more pictures, you can use or export it in various ways:

- Copy to the clipboard (menu "Edit/Copy") and paste to another application (e.g. Microsoft Word or PowerPoint)
- Save (export) to a graphics file (e.g. JPEG, BMP) (menu "File/Save As"). You can adjust the format and resolution of the picture in the "Layout" dialog which can be opened from the "Picture" menu.
- Print it (menu File/Print)
- Create a photorealistic picture using POV-Ray (menu "Tools/POV-Ray")

In addition to single pictures, you can also create video sequences (menu "Tools/Video Sequence"): In this mode, DIAMOND takes snapshots (similar to the creation of an animated cartoon) while you e.g. move and rotate your model. The results is a so-called "AVI-file" which can e.g. be imported in Microsoft PowerPoint to visualize certain dynamic effects during your talk. Of course, the AVI-files can also be viewed directly on nearly any PC using e.g. the Windows Media Player. You can also use the Windows Movie Maker to rework your video sequence, add titles and fading effects etc.



## Tutorial B: Advanced Examples

### Molecular Structures

In this session you will learn:

- How **molecular structures** can be displayed by DIAMOND.
- How to easily create a **packing diagram**.
- How to **perform geometric investigations**, e.g. measure distances and angles.



In this tutorial session you will learn how molecular structures can be visualized using DIAMOND. The first thing you have to do is to import the crystal structure from the CIF-file in which it is described: If you have not already done so, please start the DIAMOND software now. Afterwards, select the "Open" command from the "File" menu, make sure that the file type at the bottom of the "Open" dialog is set to "CIF (\*.cif)", and select the file "pyrene.cif" from the "Tutorial" subdirectory of the DIAMOND program directory (e.g. "C:\Program Files\Diamond 4\Tutorial"). Finally, please press "Open", and walk through the individual steps of the "File Import Assistant". On the "Picture creation" page of the assistant, please make sure that "Launch the Picture Creation Assistant" is selected for "Select if and what to do with the structure picture(s)", press "Next" (to advance to the final page) and "Finish" afterwards.

The "Structure Picture Creation Assistant" which is displayed now has already been used earlier to create a picture for quartz. This time, we will only use a single option: On the second page of the assistant, please select "Get molecule(s) (or polymeric fragment)", adjust all remaining settings according to fig. 24, and press "Next" to advance to page 3. Here, you should clear the checkmark at "Create cell edges", then press "Finish" at the bottom of the assistant<sup>9</sup>.

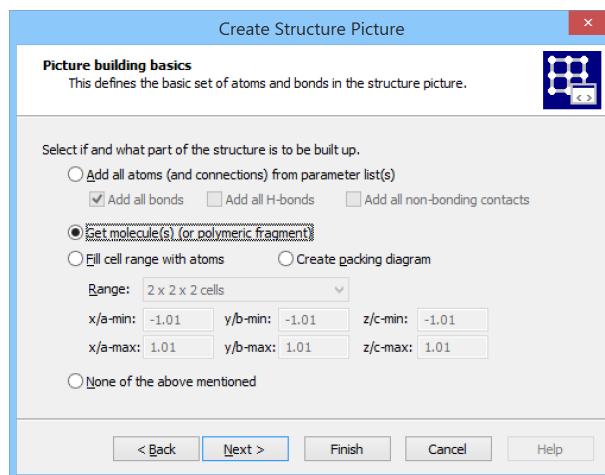


Fig. 24: The only thing you would like the assistant to do is to display the molecule.

Once you have pressed "Finish", the molecule will be displayed in the structure picture (fig. 25).



You should rotate the molecule using your mouse in order to get a three-dimensional impression: Please press the "Rotate x/y" button in the bottom toolbar, thus enabling the so-called "tracking mode". Afterwards, press the left mouse button somewhere inside the structure picture and move the mouse around. As you see, the molecule consists of four condensed benzene rings and is completely flat.

Now that you know about the structure of the molecule itself, it should be worth while to create a so-called "packing diagram" in order to understand the three-dimensional arrangement of the molecules in the crystal structure. This can be done rather quickly with two different methods:

<sup>9</sup>In this case, it is not necessary to walk through all remaining steps of the assistant.

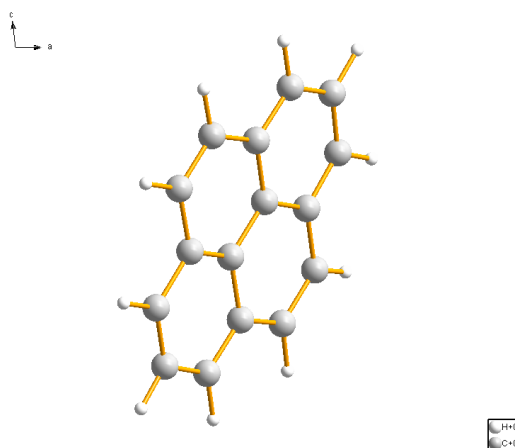


Fig. 25: A single molecule is present in the asymmetric unit of the crystal structure of Pyrene.

**Fill unit cell and complete fragments** Please "fill the unit cell" (i.e. create all atoms in the unit cell) by clicking on the corresponding button in the bottom toolbar.

As you see, the individual atoms are displayed within the unit cell, however, they are not connected (i.e. there are no bonds displayed between them). In addition, there are only fragments of molecules in the unit cell. In order to account for this, please click the "Complete fragments" button in the bottom toolbar. The atoms will now be connected by bonds, and all molecular fragments in the unit cell will be completed.

**Packing diagram function** First destroy the contents of the structure picture by running the command "All" from the "Build/Destroy" submenu (or the corresponding toolbar button or the key combination <Shift+Ctrl+D>).

Then open the "Packing" dialog with the "Packing..." command in the "Build" menu. The default range is the unit cell, and the default option to handle molecules is to include the whole molecule each, if its reference position fits. The reference position is the centroid of the molecule. In our tutorial sample, this would lead to a packing diagram containing four molecules. But we want to catch every molecule where at least one of its atoms is inside the unit cell range. So please activate the radio button "Include whole molecule, if any of its atoms fit" in the group "How to include molecules" on the "Choose Atoms" page (tab) of the dialog (fig. 26) and press "OK".

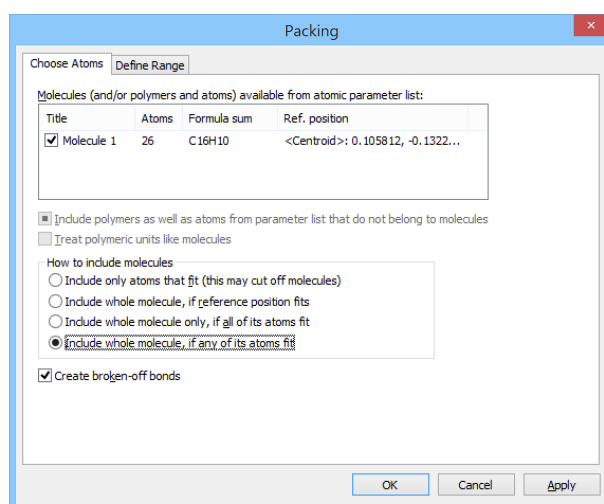


Fig. 26: On the "Choose Atoms" page of the "Packing" dialog you define, which of the molecular units, generated from the atoms of the parameter list, to include in the cell range of the packing diagram.

Both methods lead to the same packing diagram with a total of 16 molecules. However, it looks a little bit confusing, due to the large number of molecules and their orientation. In similar cases, it is



always worth while to try to look along the unit cell axes in order to find an orientation in which the molecular arrangement is more clear. Please select the "Viewing Direction..." command from the "Picture" menu. This will bring up a dialog in which you can exactly define your viewing direction along certain axes or towards certain planes (fig. 27).

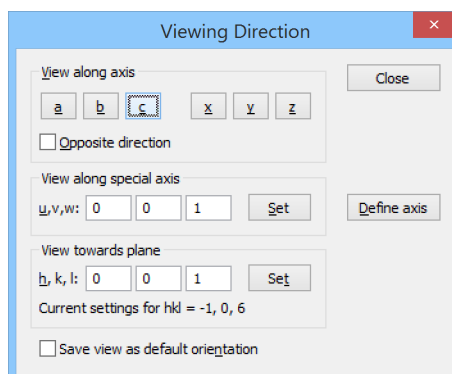


Fig. 27: You can precisely define your viewing direction using this dialog.

You should at least try to view along the three axes of the unit cell (a,b,c), by subsequently pressing the corresponding buttons at the top of the dialog. The best projection will be along axis c, so please press button "c" and close the dialog. The arrangement of the molecules in the packing diagram now looks rather clear (fig. 28).

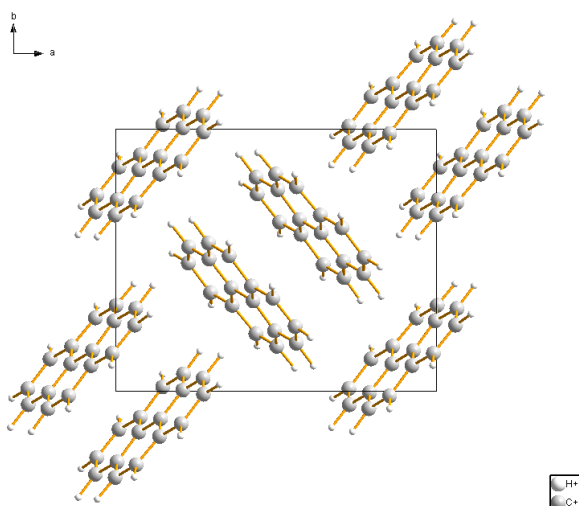


Fig. 28: Viewing along the c-axis of the unit cell is the best perspective for the investigation of the packing of the molecules.

It may be interesting to investigate the inter-planar distance between two molecules staggered more or less on top of each other. In order to do this, we will first create so-called "least-squares" planes through two adjacent parallel molecules and measure the distances between the planes afterwards.

The first plane will be created through the molecule in the top right corner: Please right-click on one of its atoms, then select "Select Molecule(s)" from the context menu. All atoms and bonds of the molecule will be selected, as indicated by the yellow frames. Afterwards, select the command "Create Plane Through Atoms..." in the "Objects/Planes..." submenu. In the "Plane through Atoms" dialog, you can select which atoms shall be included or excluded in the least-squares calculation of the plane. By default, all atoms you had selected in the structure picture will be included, as indicated by the checkboxes on the left hand side (fig. 29).

Simply accept the default settings for the first plane, close the dialog by pressing "OK", and release the selections by clicking into a blank part of the structure picture. The plane will be displayed in the structure picture (fig. 30),

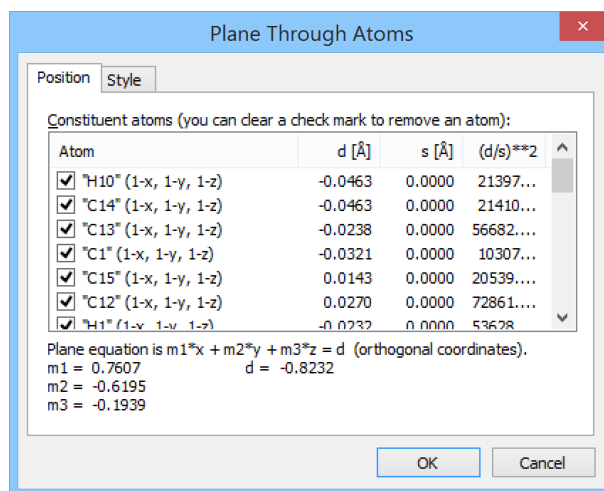


Fig. 29: This dialog provides a list of all atoms you had selected in the structure picture when calling the "Create Plane Through Atoms" command. Individual atoms can be included/excluded from the least-squares calculation of the plane by marking the corresponding checkboxes. Besides this, the equation of the current plane is displayed at the bottom of the dialog.

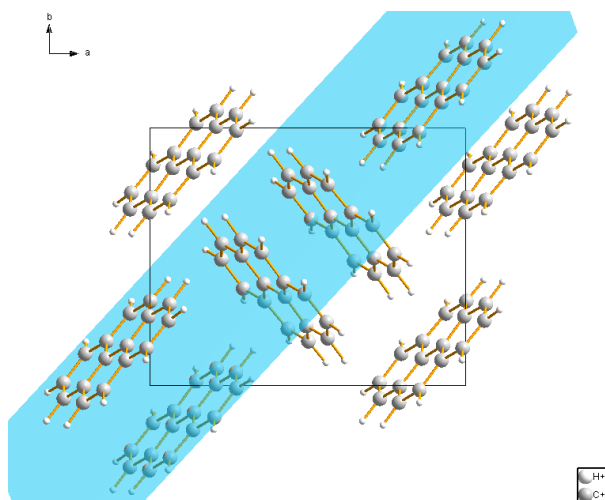


Fig. 30: The first plane defined by the atoms of the molecule on the upper right hand side has been created.



With the current version of DIAMOND, it is not possible to select a plane directly in the structure picture. If you would like to change settings (e.g. color or title) of an existing plane, please display the "Table of Planes" in the tables pane on the upper right hand side of the screen, and mark the plane for which you would like to change the design. Afterwards, select the "Edit Plane" command from the "Objects/Planes..." submenu.

Besides this, it is not possible to change the atoms which contribute to the plane once it has been created. If you would like to change them, you have to delete the plane and create a new one. In order to delete a plane, please mark the corresponding line in the "Table of Planes" in the tables pane, then select the "Delete Plane(s)" command from the "Objects/Planes..." submenu.

Once the first plane has been created, you should create the second one: Please right-click on an atom of the molecule "below" the previously selected molecule on the far right of the structure picture, then select "Select Molecule(s)" from the context menu. Afterwards, select the "Create Plane through Atoms" command from the "Objects/Planes..." submenu which will again open the "Plane Through Atoms" dialog.

This time, we would like to use a different color for the plane: Please click on the "Style" tabsheet in the dialog to bring it into front, open the color selection box, and select the light yellow color in the bottom row. Afterwards, close the dialog by clicking on the "OK" button, and remove the selection frames from the atoms by clicking in a blank part of the picture. The second plane will be displayed below the first one (fig. 31).

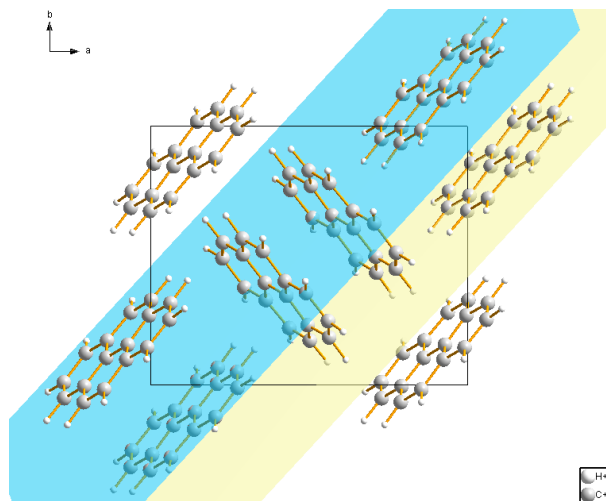


Fig. 31: The second plane has been created; this time in yellow color.

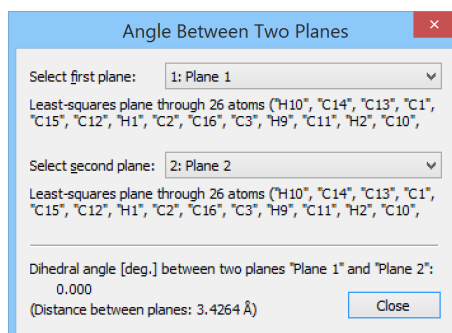


Fig. 32: The dihedral angle between the two planes is  $0.0^\circ$ .



If you rotate the structure picture (e.g. by selecting the "Rotate along x/y-axis" tracking mode), you will see that the two planes seem to be parallel to each other. You can check this by selecting the "Angle Between Planes" command from the "Tools/Calculate" submenu: At the bottom of the dialog the dihedral angle between the two planes is given as  $0.0^\circ$  (fig. 32).

As you may remember, our original intention for the creation of the planes was to measure the distance between them. Due to the fact that the planes are parallel, this has already been done automatically: At the bottom of the "Angle between Planes or Lines" dialog, you can see that the distance between the two planes is given as 3.4264 Å.





## Exploring an Unknown Structure

In this tutorial session you will learn:

- How to **explore an unknown crystal structure step-by-step** in order to understand its basic construction principles
- How to **use some of DIAMOND's many functions to visualize your increased knowledge about the structure**

From time to time, you certainly will obtain data describing a new or unknown crystal structure. In these cases, you can use DIAMOND's comfortable features to explore the new structure step-by-step until you fully understand the underlying principles. This chapter will demonstrate how to tackle these kind of problems.

In our case, the unknown crystal structure is described in a CIF-file called "unknown.cif". The first thing you have to do is to import the crystal structure data from this file: If you have not already done so, please start the DIAMOND software now. Afterwards, select the "Open" command from the "File" menu, make sure that the file type at the bottom of the "Open" dialog is set to "CIF (\*.cif)", and select the file "unknown.cif" from the "Tutorial" subdirectory of the DIAMOND program directory (e.g. "C:\Program Files\Diamond 4\Tutorial"). Finally, please press "Open", and walk through the individual steps of the "File Import Assistant" similar to the first tutorial. On the "Picture creation" page of the assistant, please set the action belonging to "Select if and what to do with the structure picture(s)" to "Create a blank picture", press "Next" (to advance to the final page) and "Finish" afterwards. The crystal structure data are now displayed in the data sheet on the upper right hand side, however, the structure picture itself is completely empty.

After having imported new crystal structure data into DIAMOND, it is generally appropriate to let DIAMOND create a picture automatically in order to get a very first impression of the structure. This can also be achieved very easily if you have missed the corresponding selection in the "File import" assistant (as in this case): Simply click on the corresponding button in the bottom toolbar, or alternatively select the corresponding command from the "Picture" menu. Please click on this button now; DIAMOND will display the crystal structure (fig. 33).

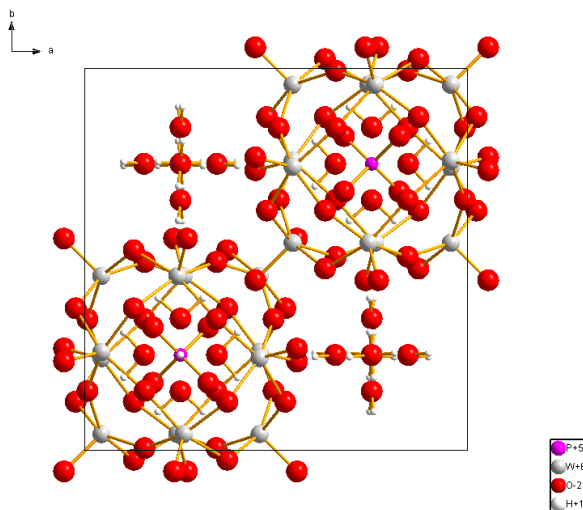


Fig. 33: This picture of the unknown structure has been created by DIAMOND automatically, revealing that the crystal structure is rather complex.

There are quite a lot of atoms and bonds in the unit cell; at first glance, their arrangement looks rather complex. Hence, it is certainly a good idea to restart from scratch with a single atom and build the structure step-by-step from there, e.g. by adding the coordinating atoms to this initial atom, then the coordinating atoms of the initial atom's neighbours, etc. Before we can actually do this, the current contents of the structure picture has to be deleted. Please click on the "Destroy all" button in the bottom toolbar, or select the command "All" from the "Build/Destroy" submenu. The structure



picture will now be empty again, so we can start to build up the structure.

The first step required is to check the interatomic distance intervals based on which DIAMOND decides if some atom belongs to the coordination sphere of some other atom or not, the so-called "connectivity". Please open the "Connectivity" dialog (fig. 34), either by selecting the corresponding command from the "Build" menu, or by pressing the corresponding toolbar button. If not already visible, switch to the "Bonds" page by clicking on the "Bonds" tab in the top left of the dialog.

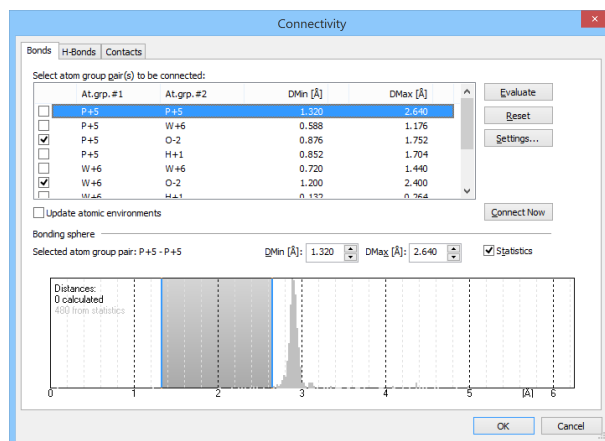


Fig. 34: The so-called "Connectivity" dialog is one of the fundamental tools of DIAMOND. On the "Bonds" page, the user can fix distance intervals for all possible pairs of atom groups. DIAMOND will create bonds, polyhedra etc. based on these intervals.

In the table in the upper half, all atom group pairs of the current data set are listed, along with minimum and maximum values for the distance intervals. If an interatomic distance between two atoms lies inside the corresponding interval, DIAMOND considers them as being chemically bonded. This information is used e.g. for the creation of bonds, polyhedra etc.



An **atom group** is by default defined by all atoms of a certain element which have the same oxidation state. You can change the assignment of individual atoms of the parameter list to certain atom groups in the "Atom groups" dialog which can be opened from the "Build" menu.

Please do not mix up *atom groups* and *atom types*! Atom types are **always** defined by the element and oxidation state; the assignment of atoms to atom types cannot be changed, in contrast to atom groups. Atom types are e.g. used in the "Distances and angles" view.

DIAMOND already contains upper and lower distance limits for most pairs of elements, which are based on effective radii defined for each atom group. However, due to the fundamental character of the distance intervals, **we strongly recommend to check them for all atom group pairs before starting to create a picture for a compound.** In order to help you to find reasonable values for "DMin" and "DMax", DIAMOND can display a distance statistics histogram over all corresponding distances found in the ICSD database<sup>10</sup>. Please make sure that the box "Statistics" on the right hand side of the dialog is checked!

Afterwards, click on the first line in the atom group pairs table, which belongs to "P+5 - P+5". Watch the distance histogram at the bottom of the dialog: There are no interatomic distances (black bars) between the two red lines which mark the upper and the lower boundary of the coordination interval. This is reasonable, since we do not expect any bonds between two P atoms in a compound containing excess oxygen. The same holds also for "P+5 - W+6", so please advance to the third line ("P+5 - O-2"). Here, there are clearly some interatomic distances (black bars) inside the interval. Any two atoms contributing to these distances will be regarded as being bonded. Please note that there is a large gap between the upper distance limit (DMax = 1.752 Å) and the next P-O distance at about 3.4 Å, a clear evidence that all relevant interatomic distances have been taken into account (maximum gap criterion; fig. 35).

Continue to walk through the list and watch the histogram, until you reach the atom group pair "W+6 - O-2". Here, you will find an interatomic distance below the maximum gap but above the current "Dmax" limit which is 2.4 Å. This interaction certainly must also be taken into account concerning

<sup>10</sup>The ICSD (Inorganic Crystal Structure Database) is created distributed by Fachinformationszentrum Karlsruhe, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany.

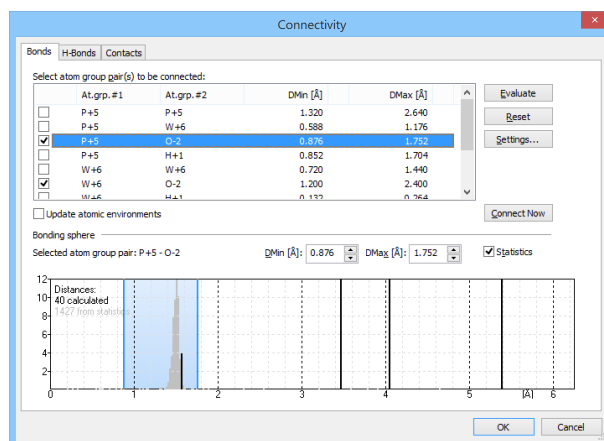


Fig. 35: For the atom group pair P-O, there is a large gap between the maximum distance value for bonding and the next interatomic distance.

the bonding situation, so please adjust the right vertical bar to the right to a value of about 2.6 Å in order to also include this distance: Move the mouse cursor over the right one of the two blue vertical bars, then press the left mouse button and move the mouse to the right. When the relevant interatomic distance lies between the two blue bars, i.e. inside the bonding range, simply release the mouse button<sup>11</sup>.

Afterwards, please advance to the atom group pair "O-2 - O-2". Here, a remarkably short interatomic distance of 1.685 Å has been found, a rather strange value with regard to the composition which is (H<sub>5</sub>O<sub>2</sub>)<sub>3</sub> P W<sub>12</sub> O<sub>40</sub>, for which no O-O-bonds are expected. Typically, extremely short interatomic distances can be present due to at least two different reasons:

1. Some atomic positions are not fully occupied; the corresponding atoms have site occupation factors below 1.0. Generally, this has been introduced during the crystal structure solution or refinement phase to account for some sort of disorder.
2. There is an error in the crystal structure data. Quite frequently, the space group setting is not correct.

In our case, there is one O-atom in the parameter list with a site occupation factor of 0.5, so the extremely short distances is nothing to worry about<sup>12</sup>. However, you should **generally always check short interatomic distances until you fully understand their origin!** Please advance to the next atom group pair "O-H" (fig. 36).

This histogram is rather interesting: There are two bonding spheres of O-H-bonds, one between appr. 0.995 and 1.19Å, and the second one between appr. 1.81 and 1.91Å. This second bonding sphere is a clear hint for the existence of so-called "H-bonds" (O-H-O) in addition to the normal covalent bonds (O-H). We will focus here only on the covalent bonds; the creation of H-bonds using DIAMOND is described later on p. 33.

Please note also that the upper boundary for the covalent O-H-bonds is a little bit too low (similar to "W+6 - O2-"); there are some reasonable distances at appr. 1.19Å which are currently not taken into account. Please adjust the upper boundary in order to also include these interatomic distances (DMax should be around 1.3 Å) (fig. 37).

You may finally have a look at the H-H-distances; afterwards, close the "Connectivity" dialog by pressing "OK". At this point, we have clearly defined the bonding spheres for the atoms required by many DIAMOND functions. We can now start to actually create the structure picture.

As has already been mentioned, we would like to start with a single atom. In order to add a single atom to the structure picture, please select the "Add Atoms..." command from the "Build" menu,

<sup>11</sup>You also could have entered the value 2.6 numerically in the "DMax" field at the top of the histogram.

<sup>12</sup>Normally, you should of course check if the atoms which correspond to the short distance (in our case O5) also have the reduced site occupation factor!

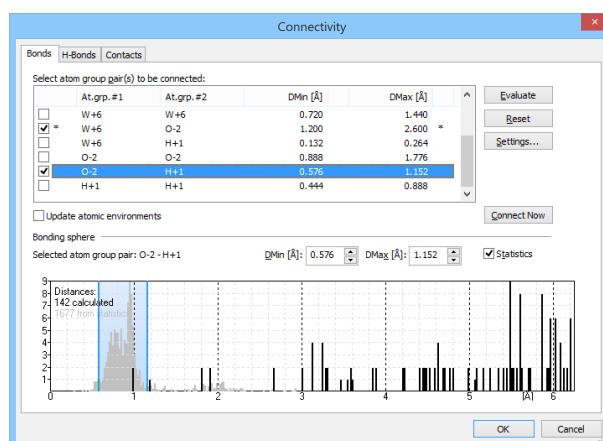


Fig. 36: The O-H-distance histogram reveals two bonding spheres between atoms of these two atom groups.

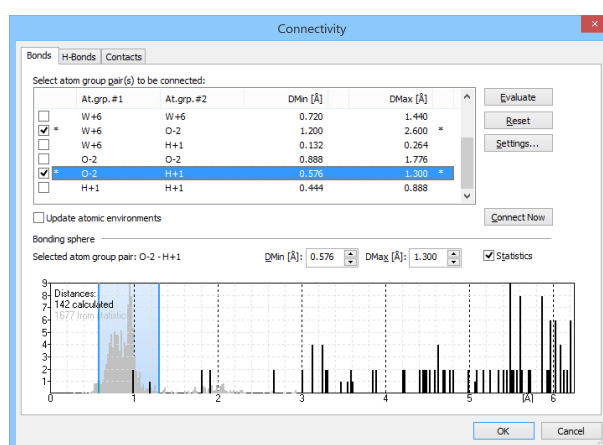


Fig. 37: The upper boundary for the O-H-bonding interval has been adjusted. The asterisks in the atom group pair table indicate which bonding spheres have been adjusted during the current dialog session.



or use the corresponding toolbar button. The "Add Atoms" dialog will be displayed (fig. 38) using which you can precisely define which atoms of the infinite atomic arrangement described by the crystal structure data shall be displayed in the structure picture.

In the table at the top, you select the atom(s) of the atomic parameter list based on which the atom(s) in the structure picture shall be created. Below, you can define the symmetry operation(s) as well as Bravais translation(s) which shall be applied to the selected atom. Finally, you can select if a cell translation shall be applied to the coordinates resulting from the application of the symmetry operation(s) and Bravais translation(s). For example, you could define that the atom shall be created in the next but one cell in X direction.

In our case, we will start rather simple: We would like to create only the phosphorus atom in the asymmetric unit: Please select the atom "P1" in the table at the top and make sure that only the symmetry operation "identity" (x,y,z) is marked. If your dialog window corresponds to fig. 38, please click "OK". A single purple P-atom will be displayed in the center of the structure picture.



Due to the connectivity which has already been fixed, the next building steps are rather straightforward: Simply click on the "Fill Coordination Spheres" button in the bottom toolbar (or press the combination <Shift+Ctrl+S> on your keyboard) in order to add the neighbouring atoms of the phosphorus atom. The typical P-O-tetrahedron is clearly visible.



Please add the next coordination spheres (the ones of the O atoms), simply by clicking on the "Fill Coordination Spheres" button again. As you see, there are three W-atoms connected to each O-atom coordinating the central P-atom (fig. 39).

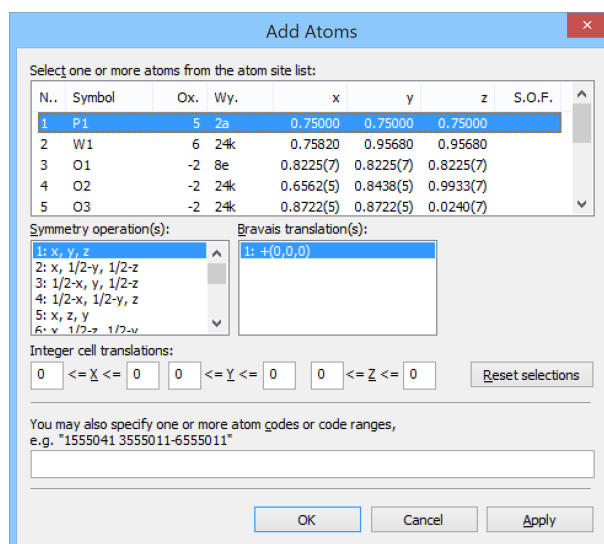


Fig. 38: Using the "Add Atoms" dialog, you can precisely define which atoms shall be added to the structural picture.

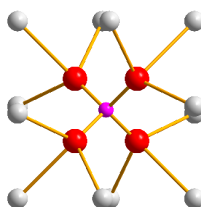


Fig. 39: The P-atoms in the structure are tetrahedrally coordinated by O-atoms, which themselves are connected to three W-atoms each.

Of course, the coordination spheres of the W-atoms are still incomplete. Please press on the "Fill Coordination Spheres" button again in order to complete them. A rather large number of O-atoms will be added. If you click on the "Fill Coordination Spheres" button again, nothing will happen. Obviously, you have found some isolated building block which is not directly bonded to the rest of the structure. It should be worth while to further investigate this building block.



The typical "ball-and-stick" representation is not really appropriate in this case, since the large number of bonds per atom is a little bit confusing. Due to the fact that this is a typical inorganic oxide building block, a polyhedra representation (metal/non-metal atoms coordinated by oxygen) should be better. Please select the "Add Polyhedra..." command from the "Build/Polyhedra" submenu in order to open the "Add Polyhedra" dialog (fig. 40).

At the top of the dialog, you can select the type of sphere to include the coordinating atoms for the new coordination polyhedra:

- **Atomic environments**, which can be defined individually for an atom site each using the "Atomic Environments..." command in the "Build" menu.
- **"Generic"**, which means the bonding spheres from the connectivity list.
- A sphere with **fixed boundaries** *RMin* and *RMax* that is independent from the atom sites' environments or from the atom group pairs' bonding spheres.
- **"As is"**, which means "do not change the current coordination spheres present in the picture", i.e. do not add atoms, if a coordination sphere should be incomplete.

We will use the second option ("Generic"). In the center of the dialog, you have to select the atom group(s) (or even certain atom sites) that shall represent the centers of the polyhedra and the ones which shall be ligands. We would like to create polyhedra around P and W, so please clear the

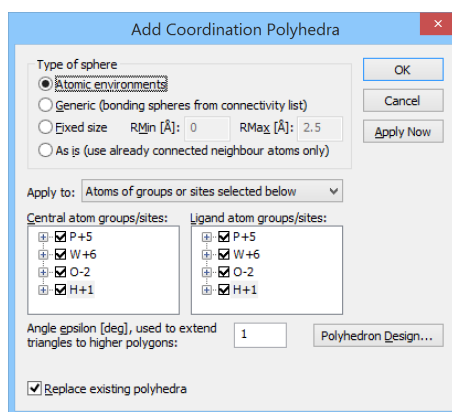


Fig. 40: In this dialog, you can e.g. select central and ligand atoms for the polyhedra which shall be created.

checkmarks at O and H in the "Central atom groups" list to the left. On the other hand, we would like to have O atoms at the corners of the polyhedra, so clear the checkmarks for P, W, and H in the "Ligand atom groups" list to the right. Your dialog should now look similar to fig. 41.

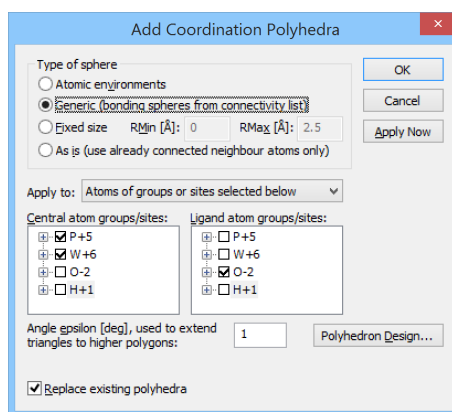


Fig. 41: According to these settings, DIAMOND will create polyhedra around the W and P atoms with O at the corners of the polyhedra. The coordinating atoms are selected according to the settings in the "Connectivity" dialog.

Though it could also be accomplished later on, we will modify the design of the polyhedra now. Please click on the "Polyhedron Design..." button on the right hand side of the "Add Coordination Polyhedra" dialog which will open the "Polyhedron Design" dialog. We would like to change the transparency setting of the polyhedron faces to opaque, i.e. non-transparent, as well as to change the thick blue edges to thin lines. Change the value in the input box "Transparency" to zero. Click on the "Color" button below "Border" and choose "Automatic" from the color selection panel (fig. 42). Set "Weight" to zero, which means Diamond will use only one pixel thin lines for the polyhedron edges. (An "automatic" line color means white lines on dark background but black lines on white background.) Afterwards, close the "Polyhedron Design" dialog by pressing "OK".

Now all settings for the creation of the polyhedra have been adjusted; please press "OK" in the "Add Coordination Polyhedra" dialog which will close it and create the polyhedra (fig. 43).



We would like to use the current structure picture later on in the demonstration of DIAMOND's POV-Ray interface (p. 44), so please save it as a DIAMOND document file<sup>13</sup>: Please press the "Save" button in the toolbar. Afterwards, a message will be displayed that you have to use the DIAMOND document file format in order to save the complete information and picture you have created up to now. Please accept by clicking "Yes" which will open the "Save Document As" dialog. Select the Tutorial subdirectory of your DIAMOND program directory (e.g. "C:\Program Files\Diamond

<sup>13</sup>If you are using the demonstration version, saving is disabled. In this case, you can use the corresponding file "unknown.diamdoc" later on which is already present in the "Tutorial" directory, so you can simply skip this step.

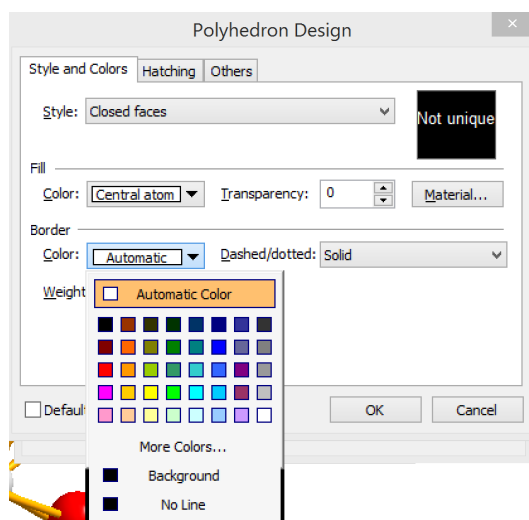


Fig. 42: We would like the colors of the faces of the polyhedra to correspond to the colors of their central atoms and opaque faces with thin edges in "automatic" color, which means black on white or white on black background, resp.

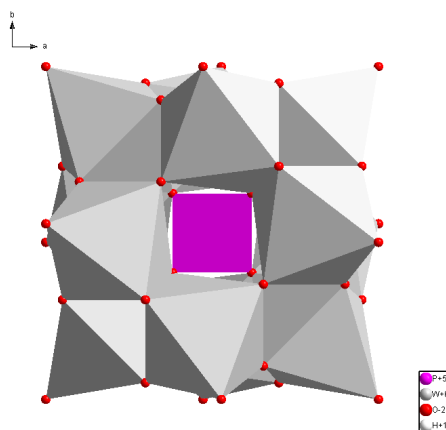


Fig. 43: The building block you have found in the unknown structure is now displayed using polyhedra around P and W.

4\Tutorial"), accept the proposed filename "unknown.diamdoc" and press "Save".



Remember that you have opened a CIF-file at the beginning of the session. It is not possible to store all information of a DIAMOND session (e.g. the contents of the structure picture or the design of the polyhedra) in a CIF-file, so you have to use DIAMOND's proprietary file format "\*.diamdoc" in order to be able to restore the current contents of the DIAMOND window later on. Please note also that the name of the current session document which is displayed in the title bar of the DIAMOND window will have changed afterwards.

In order to fully understand the construction principles of the building block, you should rotate it using your mouse. This will provide you with a much better three-dimensional impression of the structure. Please select the "Rotate along x/y-axis" from the "Move" menu, or simply press the corresponding button in the bottom toolbar, thus enabling the so-called "tracking mode". Afterwards, press the left mouse button somewhere inside the structure picture and move the mouse around. You will clearly see the  $\text{PO}_4$ -tetrahedron at the center of the building block. Each corner of this tetrahedron is capped by a group of three edge-connected  $\text{WO}_6$ -octahedra. These  $\text{W}_3\text{O}_{13}$  units are connected by corners. This is the so-called "Keggin structure" or "Keggin ion".



The next step is to investigate how these Keggin ions are arranged in the overall crystal structure. Leave the tracking mode by clicking the "No tracking" button in the bottom toolbar. Afterwards, please return to the previous viewing direction along the c-axis in order to have a better overview: Select the "Viewing direction..." command from the "Picture" menu in order to open the corresponding dialog (fig. 44). As has already been mentioned, we would like to view along the c-axis, so please







click on the corresponding button at the top of the dialog and close it by pressing "OK".

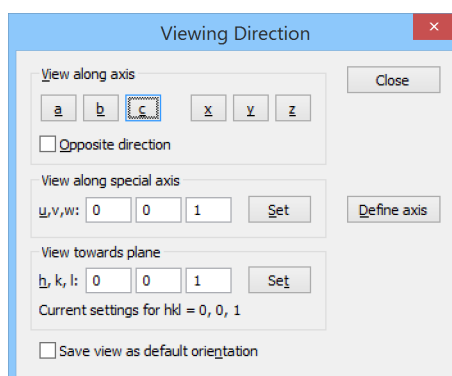


Fig. 44: You can select the viewing direction in various different ways using this dialog.



We now have to add the rest of the unit cell. This can easily be achieved by pressing the "Fill Unit Cell" button in the toolbar in the lower corner on the left hand side. As you see, the Keggin ion is placed in one octant of the unit cell. Obviously, there is a second Keggin ion in the opposite octant of the cell for which we should also create polyhedra similar to the first one. Select "Build/Polyhedra/Add Polyhedra...", then click on the "Polyhedron Design..." button in the "Add Coordination Polyhedra" dialog which opens. Change to the same design settings as described above, and press "OK". The atom groups for the central atoms and ligands are still present from the previous usage of this dialog, so simply close the dialog by pressing "OK". The second Keggin unit in the cell will now become clearly visible (fig. 45).

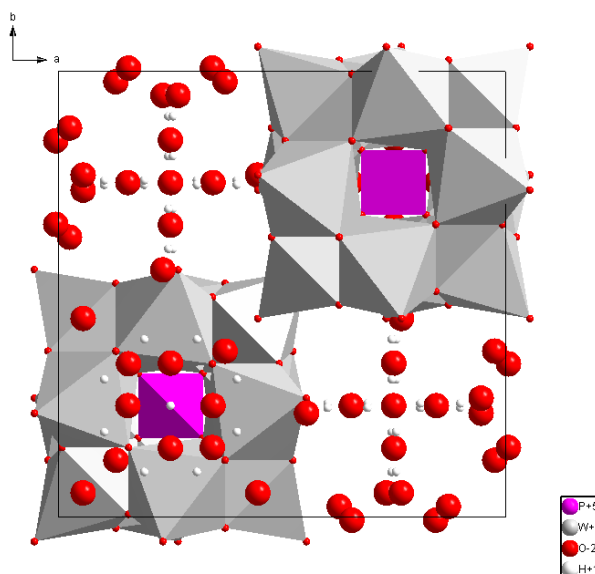



Fig. 45: There are two Keggin ion building blocks present in the unit cell.



You can now see that the space between the Keggin ions is filled by O and H atoms, most probably water molecules. In order to check this, you should connect the atoms (i.e. create bonds between them, based on the settings in the "Connectivity" dialog). You can achieve this rather quickly, either by clicking on the "Connect Atoms" button in the bottom toolbar or simply by pressing the combination <Shift+Ctrl+N> on your keyboard. The water molecules will now become clearly visible.

Finally, we recommend to remove the remaining non-bonded O-atoms which belong to  $\text{WO}_6$ -octahedra in the neighbouring unit cells. This can easily be achieved by selecting the command "Non-bonded atoms" in the "Build/Destroy" submenu, or (more quickly) by clicking on the small arrow ▼ to the right of the  button in the bottom toolbar and selecting "Destroy non-bonded atoms". At this stage, the construction principles of the structure are clearly visible (fig. 46).



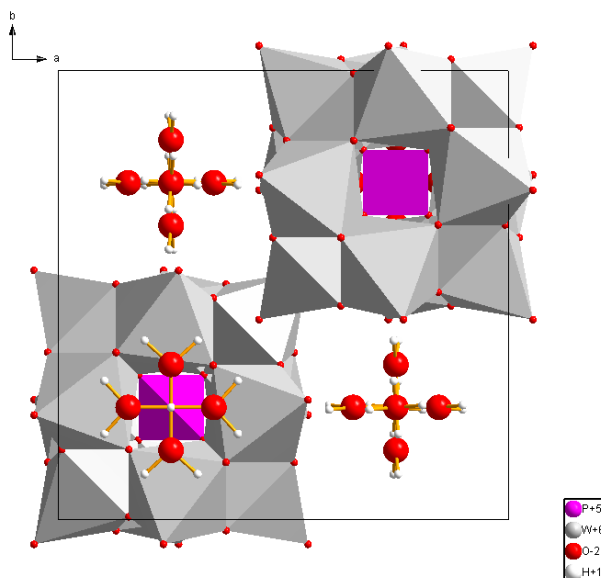


Fig. 46: Now that the "non-bonded" O-atoms (which are in fact bonded to W-atoms in the neighbouring unit cells) have been removed, the structure becomes even more transparent.

There is just one remaining question arising while you look at the structure: There must be some kind of bonding between the Keggin-ions and the water molecules...but what is it? With a little bit of experience, you certainly will suspect that there must be so-called "H bonds" between the two parts of the structure. In order to see this more clearly, you should add these bonds to the structure picture: Please select the "Create H-bonds..." command from the "Build" menu; this will bring up the "Create H-Bonds" dialog. In this dialog, you can enter criteria which must be fulfilled by the contributing atoms in order to create an H-bond. You can enter minimum and maximum interatomic distances, minimum and maximum angle between donor (D), H-atom and acceptor (A), atom groups which are applicable as donor or acceptor etc. Please change the settings in your dialog according to fig. 47, then press "OK". The H bonds are introduced in the structure picture as dashed lines; now you can clearly see how they connect both parts of the structure as well as the water molecules among each other.

Fig. 47: These are the criteria defined for the creation of H bonds in the structure picture: "Direct definition" of H-bonds, distance range 1.5 to 2.5 Å, and atoms of group "O-2" as both donors and acceptors.

That's it! As you see, DIAMOND provides a large amount of features which can help you to understand construction principles of crystal structures. Once you have explored these principles, you can use similar functions to present your understanding of the structure to an audience.



## Zeolite Framework

In this session you will learn:

- How to present even complex structures in a few steps.
- How to apply **filter**, **dummy atoms** and **selections** effectively.

Faujasite is a famous representative of the zeolites. One of the components in the linking pattern of this aluminosilicate is the so-called " $\beta$ -cage". Each corner of this polyhedron contains one silicon or aluminium atom; each edge contains an oxygen atom which links two atoms in the corners. The  $\beta$ -cages are connected with each other via hexagonal prisms.

In this tutorial session we will create a structure picture in which the  $\beta$ -cages in the Faujasite structure as well as their connection among each other by hexagonal prisms will be clearly visible.



Please start the DIAMOND software now if it is not already running. Select the "Open" command from the "File" menu, make sure that the file type at the bottom of the "Open" dialog is set to "CIF (\*.cif)", and select the file "faujasite.cif" from the "Tutorial" subdirectory of the DIAMOND program directory (e.g. "C:\Program Files\Diamond 4 \Tutorial"). Afterwards, press "Open", and walk through the individual steps of the "File Import Assistant". On the "Picture creation" page of the assistant, please make sure that "Create a blank picture" is selected for "Select if and what to do with the structure picture(s)", then press "Next" and "Finish" afterwards. The crystal structure data will now be displayed in the data sheet on the upper right hand side; the structure picture will be completely empty.

Unfortunately, there is a little problem with the space group setting in context with this CIF-file: There are two origin choice options available for this space group (choice one (non-centrosymmetric) and choice two (centrosymmetric)). From the contents of the CIF-file, DIAMOND is not able to determine the correct origin choice, so it will use origin choice one which is not correct in this case. Fortunately, the author of the CIF-file added a personal note that he used the standard setting which is origin choice two. This information must be applied to the space group setting in DIAMOND: Please execute the "Symmetry" command from the "Structure" menu, which opens the "Symmetry" dialog with the data of the wrong space group setting. In the uppermost input field "Space group" enter the space group number "227". DIAMOND then lists both origin choices (but also some special settings available from ICSD). Select the centrosymmetric setting for space-group 227 (internal no. 22701) in the "Results matching current space group symbol" list, according to fig. 48. Afterwards, press "OK".

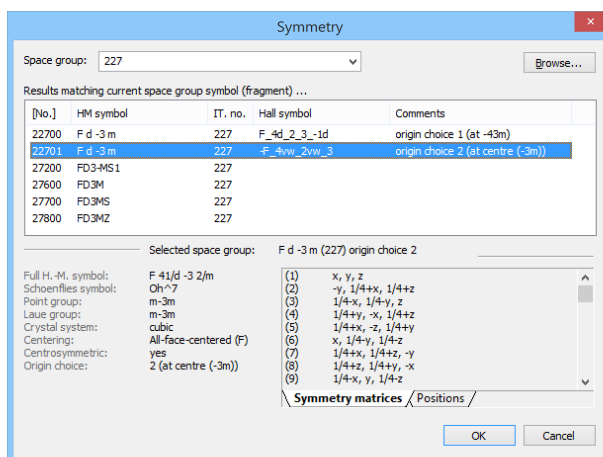


Fig. 48: We have to select the correct setting (origin choice 2, centrosymmetric) of the space group manually, since DIAMOND was not able to determine it from the contents of the CIF-file.



We strongly recommend to check the space group setting each time you have imported a crystal structure file! This can e.g. be done by checking the interatomic distances in the "Connectivity" dialog. Quite frequently, a wrong space group setting will lead to extremely short interatomic distances. However, short interatomic distances may also be present due to other reasons (p. 27).



We will now create a single atom based on which we will build the complete structure picture afterwards: Click on the "Add atom(s)" button to open the "Add atoms" dialog. Select the atom "Si1—Al1" from the parameter list<sup>14</sup> and leave the other settings as before (fig. 49). Confirmation with "OK" will create a single atom in the center of the structure picture.



If you do not see the atom in the center of the picture, the so-called "Automatic adjustment" has been disabled most probably. In order to center and adjust the picture (i.e. place the center of rotation in the center of the screen and adjust the enlargement factor so that the complete structure fits into the current size of the screen), please press the F9 key on your keyboard. In order to activate the automatic adjustment for the future, please select the "Adjust..." command in the "Picture" menu, mark the checkbox "Automatic adjustment", and press "Adjust" (which will also close the dialog).

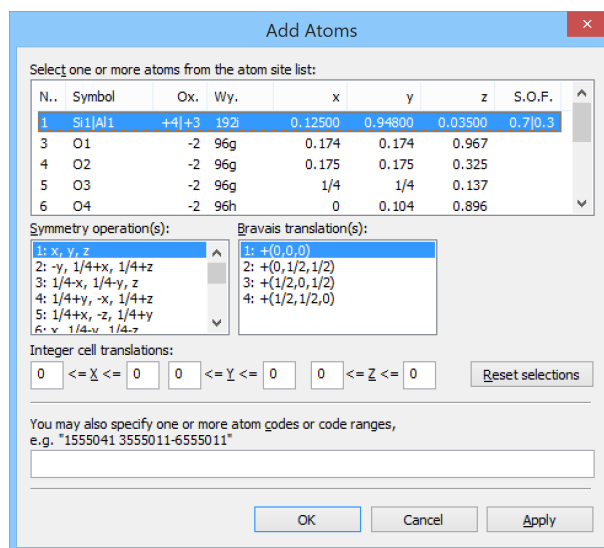


Fig. 49: A single Si/Al atom shall be created in the structure picture. It will be placed at the original coordinates from the parameter list: Only the symmetry operation "identity" (x,y,z) and the Bravais translation (0,0,0) will be applied.

As has already been mentioned in the introduction to this chapter, we would like to create a structure picture of the  $\beta$ -cages. Hence, only the Si/Al atoms and their connections are of interest; all other atom types shall be excluded from the construction. This can be achieved using DIAMOND's so-called "filter" functionality:

Please select the "Filter..." command from the "Build" menu in order to open the "Filter" dialog. In the "Atom groups" list at the top, clear all checkboxes but the one for "SiAl". Additionally, clear all checkboxes but "+(0,0,0)" from the "Bravais translations" list (not the ones from the "Symmetry operations list" !) (fig. 50). If you now confirm with "OK", only atoms of the mixed site Si/Al can be created, and no Bravais translations will be applied. To remind you of the active filter, Diamond displays a warning symbol in the lower left corner of the structure window.



If you would like to disable the filter later on, all you have to do is to double-click on the filter warning symbol in the structure picture. Please don't do this now!

Since we would like our structure model to have direct connections between Si/Al atoms (which makes no sense in a compound containing excess oxygen from the chemical bonding point of view, of course), the connectivity needs to be adjusted. Remember that the bonds created in the structure picture depend on the connectivity settings!

Please open the "Connectivity" dialog by clicking on the corresponding button in the bottom toolbar (or alternatively by selecting the corresponding command from the "Build" menu). For the atom type pair "SiAl - SiAl", please define a bonding sphere of approximately 3.0 to 3.5 Å in the lower half of the dialog box (fig. 51) and press OK.



Now that we have adjusted the filter and connectivity settings, we can use DIAMOND's comfortable building functions: Click on the "Complete fragments" button. DIAMOND will complete the frag-



<sup>14</sup>Si and Al share the same position in the parameter list, since in many zeolites they are randomly distributed to these

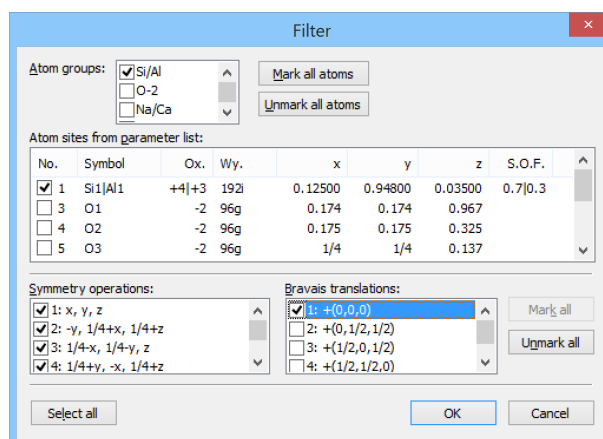


Fig. 50: Only atoms of the mixed site Si/Al will be taken into account during construction operations in the structure picture.

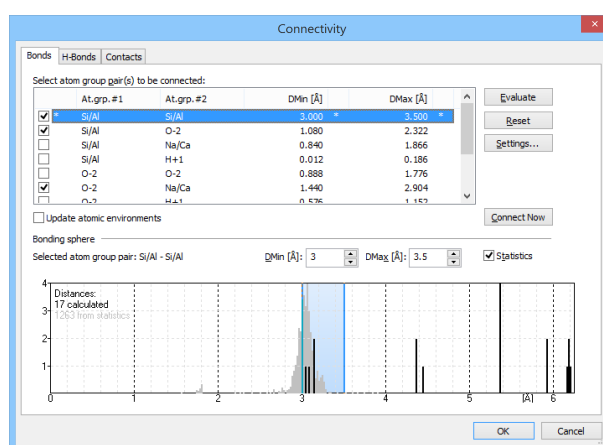


Fig. 51: The coordination sphere of the Si/Al atoms has to be adjusted manually to 3.0-3.5 Å since we would like to introduce "unphysical" bonds between Si/Al-atoms in the structure picture.

ment and generate a  $\beta$ -cage as well as four attached hexagonal prisms. By means of the active filter, only Si/Al atoms will be created, and the recursive search for neighbouring atoms will be cancelled because of the excluded Bravais translations (fig. 52).

In the second step, the  $\beta$ -cage will be displayed as a closed polyhedron. In DIAMOND, all polyhedra require a central atom. Unfortunately, the  $\beta$ -cage does not contain a central atom, so this atom must be inserted first before the actual polyhedra can be created. If the structure in use does not have any appropriate atom that can be used as central atom (as in this case), we can add a so-called "dummy atom".

The first thing you should do is to change the orientation leading to a view along the cubic diagonal of the unit cell (1,1,1). This can be done by choosing the "Viewing Direction..." command from the "Picture" menu which will open the "Viewing Direction" dialog. In the three input fields next to "h, k, l" enter "1" (fig. 53). Afterwards, push the "Set" button; DIAMOND will change the viewing direction (fig. 54). Afterwards, close the dialog by pressing "OK". You may have to press <F9> afterwards in order to readjust the enlargement factor.

We would like to create a dummy atom right in the center of the  $\beta$ -cage. This can easily be achieved: First, please select all objects of the picture by pressing the key combination <Ctrl+A>. Afterwards, select the "Insert Atom..." command from the "Structure" menu in order to open the "Insert Atom" dialog. DIAMOND has calculated the center of all selected atoms and proposes this center as position for a dummy atom (fig. 55). Confirm with "OK", then click into a blank area of the picture to remove all selection frames from the structure picture.

positions.

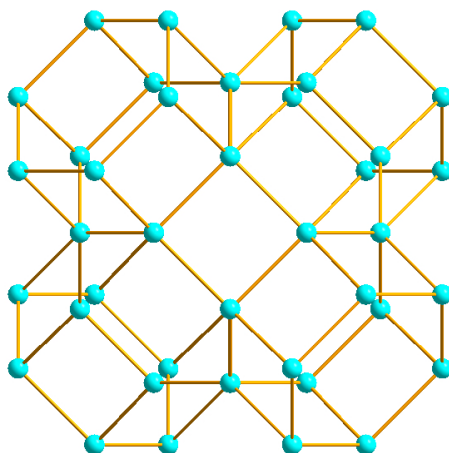


Fig. 52: View of the Si-Al-substructure in Faujasite

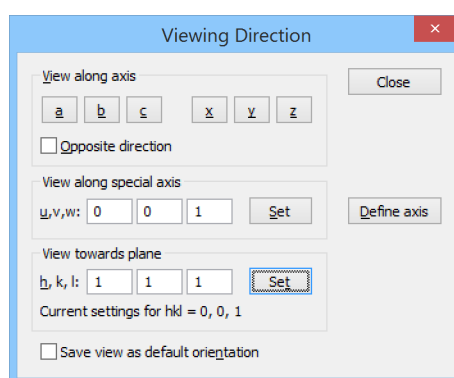


Fig. 53: In the "Viewing Direction" dialog, you can adjust the direction in which you look at the structure picture. Here, we would like to look in the direction perpendicular to the hkl-plane (111).

You will now see that there is a dummy atom in the center of the structure, which can be used as central atom for a polyhedron. In the data sheet to the right of the structure picture you will see a new entry for the dummy atom at the bottom of the atomic parameter list.

Now choose the "Add Coordination Polyhedra" command from the "Polyhedra" submenu of the "Build" menu. In the "Add Coordination Polyhedra" dialog, please select "?" (which represents the dummy atom) as central atom type and "SiAl" as ligand atom type. Set the type of sphere to "Fixed" and "RMin" to 1 and "RMax" to 5. Your dialog should now look similar to fig. 56.

We will define the design of the polyhedra to be created right away, so please click on the "Design..." button on the right hand side of the dialog. In the "Polyhedron Design" dialog, please adjust the settings according to fig. 57.

Afterwards, bring the "Others" tabsheet into front by clicking on its header, and change the "Ligand atoms reducing factor" to 0.01. This factor results in a size reduction of all atoms at the corners of the polyhedra so that they are rather indiscernible but can still be selected. Finally, mark the checkbox "Default for new polyhedra" at the bottom of the dialog and press "OK". Once you have returned to the "Add Polyhedra" dialog, push the "OK" button here, too. DIAMOND will create the polyhedron (fig. 58).

In the third step, the hexagonal prisms connecting the  $\beta$ -cages will be displayed as polyhedra, too. For this, we will use a similar strategy like for the  $\beta$ -cage itself.

Again, we will change the orientation in a suitable way before we will add the dummy atoms in the center of the polyhedra which shall be created. Please select the "Rotate Incrementally..." command from the "Move" menu to open the "Rotate Structure Picture" dialog. Enter a value of 30 degrees for the z-axis and assert zero for both x- and y-axis. Then click on the "Apply Now" button. This will cause the desired rotation without closing the dialog. Now set the value for the z-axis to zero,

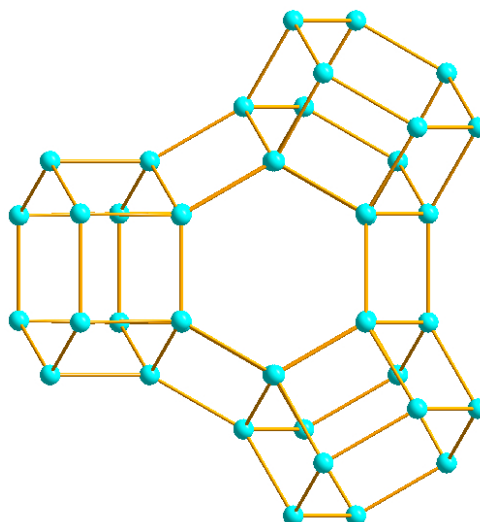


Fig. 54: View towards the (1,1,1)-plane of the Faujasite Si-Al-substructure

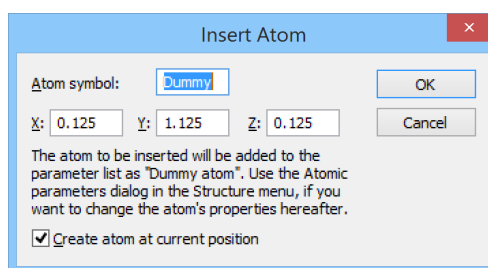


Fig. 55: Using this dialog, you can add new atoms to the atomic parameter list. In our case, the coordinates for the new atom have been calculated by DIAMOND automatically in the center of the selected atoms.

but that for the x-axis to -20 degrees. Then confirm with "OK" (Fig. 59).

Select all atoms of the hexagonal prism at the bottom by pulling up a frame around the atoms concerned using the mouse. Afterwards, select the "Insert Atom..." command again. DIAMOND will calculate the center of all selected atoms and will now propose the position (1/4, 1, 1/4) for a dummy atom. Confirm with "OK", then click into a blank area of the picture in order to remove all selection frames from the structure window. The new dummy atom can now clearly be seen inside the prism (fig. 60). The data sheet to the right of the structure picture displays the new dummy atom in its atomic parameter list, too.

The central atoms of the other prisms need no further dummy atom in the list of atomic parameters; they can be generated from the previously inserted dummy atoms using suitable symmetry operations. For this procedure, the filter needs to be adjusted first (remember that we locked out all Bravais translations except (0,0,0) at the beginning!).

Please select the "Filter..." command from the "Build" menu to open the "Filter" dialog. At the top, exclude all atom groups except "?", which represents the two dummy atoms. Note that you have to reactivate the atom group "?", since new atoms have been created in the meantime. Click the "Mark all" button to the right of the list of Bravais translations and compare your screen to fig. 61. Afterwards, please press "OK".

With the filter having been changed, the missing dummy atoms in the hexagonal prisms are now accessible for build operations: Please select the "Coordination Spheres" command from the "Build" menu to open the corresponding dialog. Set the type of sphere to "Fixed size" and "RMin" to 0 and "RMax" to 4 Å, clear the checkmark at "Connect atoms", and set "Apply to" to "All atoms in structure picture" (fig. 62). Once you have confirmed by clicking "OK", DIAMOND will start to search all missing dummy atoms, which have a maximum distance of 4 Å from all atoms currently present in the structure picture. This will generate one dummy atom in the center of each hexagonal

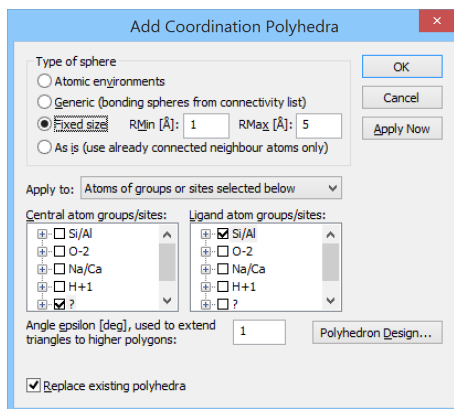


Fig. 56: We would like to build polyhedra around the '?' (dummy) atoms. The ligand atoms should be Si/Al and must be placed at a distance between 1 and 5 Å from the central dummy atom.

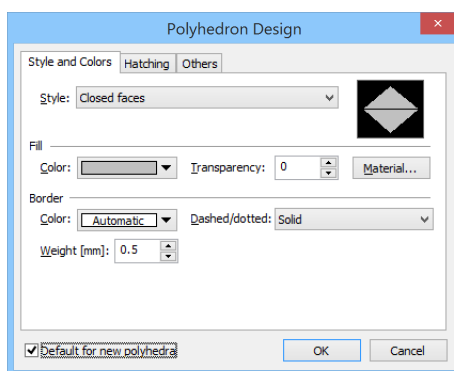


Fig. 57: Please use these settings for the design of the polyhedron.



prism.

Before the polyhedra around the dummy atoms in the hexagonal prisms can be created, the Si/Al atoms must be unlocked from the filter. The reason is that these atoms will be newly created during the polyeder creation process, which is only possible if they are not blocked by the filter function. Please select the "Filter..." command from the "Build" menu to open the "Filter" dialog. In the list "Atom groups" select "SiAl" additionally to "?". Afterwards, press "OK".

Now we are ready to create the polyhedra: Please select the "Add Coordination Polyhedra" command from the "Build/Polyhedra" submenu to open the "Add Coordination Polyhedra" dialog. Select the atom type "?" for the central atoms and "SiAl" for the ligand atoms. Set the type of sphere to "Fixed" and "RMin" to 1 and "RMax" to 5. Finally, close the "Add Coordination Polyhedra" dialog by clicking "OK" (fig. 63).

In the fourth and final step, the connection of the  $\beta$ -cages with each other will be visualized. For that, we have to change the orientation again in order to view along the (1,1,1)-axis: Choose the "Viewing Direction" command from the "Picture" menu, set the input fields next to "h,k,l" to 1, then confirm with "Set", then close the dialog box. You will now look at the structure picture in the direction perpendicular to the (111) plane (fig. 64). Again, you may have to press <F9> afterwards in order to readjust the enlargement factor.

Afterwards, please select the "Coordination Spheres..." command from the "Build" menu again in order to open the corresponding dialog. Please define a "fixed size" sphere of 0 to 5 Å this time (fig. 65), then confirm by pressing "OK". New Si/Al and dummy (?) atoms will be created close to the hexagonal prisms (fig. 66).

Please click on the small arrow  to the right of the  button in the toolbar at the bottom of the DIAMOND window, then select "Fill Fixed Spheres Directly". This will perform the search for neighbouring atoms with the previously set search radius again. Repeat this step; your structure



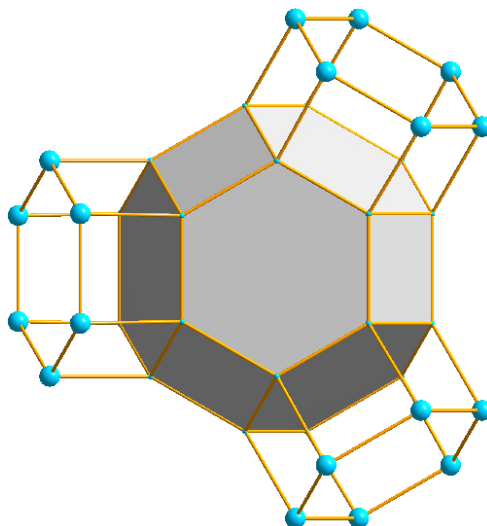


Fig. 58: Polyhedron view of the  $\beta$ -cage in Faujasite

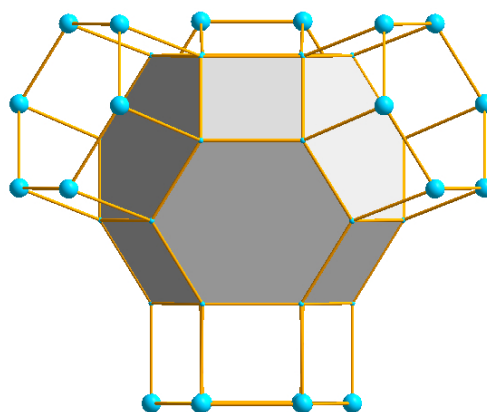


Fig. 59: The picture has been rotated so that the atoms of the prism at the bottom can be selected more easily.

picture should now look similar to fig. 67.

Finally, you have to create polyhedra for the newly created atoms: Select the "Add Coordination Polyhedra" command from the "Build/Polyhedra" submenu to open the "Add Coordination Polyhedra" dialog. We use the previously defined sphere size but have to update the selections in the "Central atom groups/sites" and "Ligand atom groups/sites" trees: "?" must be selected for central atoms and "Si/Al" for ligand atoms. Then confirm by pressing "OK". The structural part being displayed (fig. 68) gives a quite good impression how the structure of faujasite is built up.

You may extend the given structural part using the previously described operations (first complete spheres, then create polyhedra) as much as you like. We will do so when we will demonstrate the "walk in" and "video sequence" features of DIAMOND later on on p. 51. For the moment, please save the current document<sup>15</sup>: Select the "Save Document As..." command from the "File/Save As" submenu. In the "Save Document As" dialog which opens, select the "Tutorial" directory of the DIAMOND program directory (e.g. "C:\Program Files\Diamond 4\Tutorial"). Afterwards, change the file type at the bottom of the dialog to "Diamond 3 Document (\*.diamdoc)", and use the filename "faujasite.diamdoc". Finally, please press "Save". That's it!

<sup>15</sup>If you are using the demonstration version, saving is disabled. In this case, you can use the corresponding file "faujasite.diamdoc" later on which is already present in the "Tutorial" directory, so you can simply skip this step.



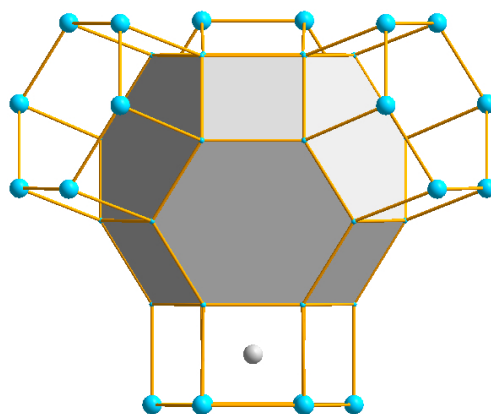


Fig. 60: A dummy atom has been created in the center of the prism at the bottom.

No.	Symbol	Ox.	Wy.	x	y	z	S.O.F.
<input type="checkbox"/> 11	O5	-2	?				1.37
<input type="checkbox"/> 12	H1	1	?				2.74
<input checked="" type="checkbox"/> 13	Dummy	8a		1/8	9/8	1/8	
<input checked="" type="checkbox"/> 14	Dummy1	16c		1/4	1	1/4	

Fig. 61: We would like to add some dummy ('?') atoms by application of the space group symmetry; all other atom groups should be excluded from these build operations.

Type of sphere:  
☐ Atomic environments  
☐ Generic (bonding spheres from connectivity list)  
☒ Fixed size RMin [Å]: 0 RMax [Å]: 4

Number of cycles: 1

☐ Connect atoms ☐ Create broken-off bonds

Apply to: All atoms in structure picture

Central atom groups/sites: (Not applicable, cf. "Apply to")

Ligand atom groups/sites:  
☒ Si/Al  
☒ O-2  
☒ Na/Ca  
☒ H+1  
☒ ?

Fig. 62: We use a sphere with a radius of 4 Å to add dummy atoms into the centers of the hexagonal prisms, without having the central atoms connected with the coordinating atoms.

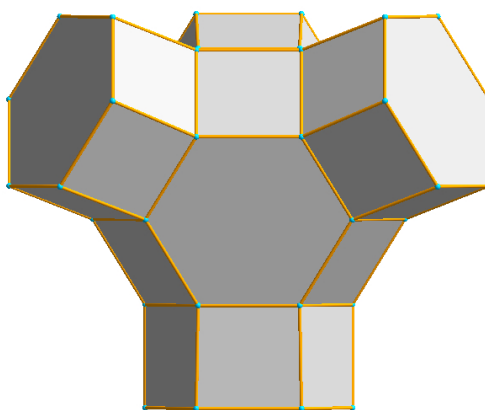


Fig. 63: The prisms are now visualized as polyhedra, too.

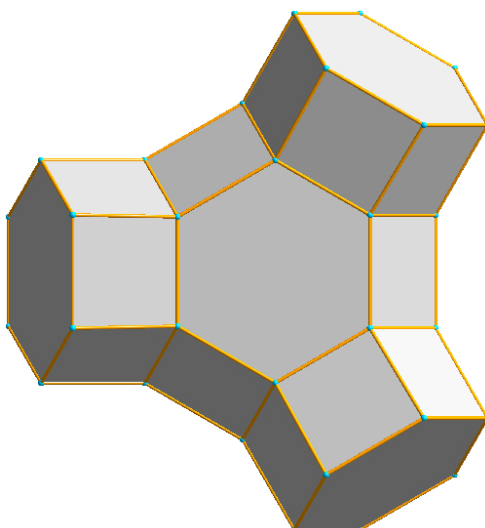


Fig. 64: The structure is again viewed towards the (1,1,1)-plane.

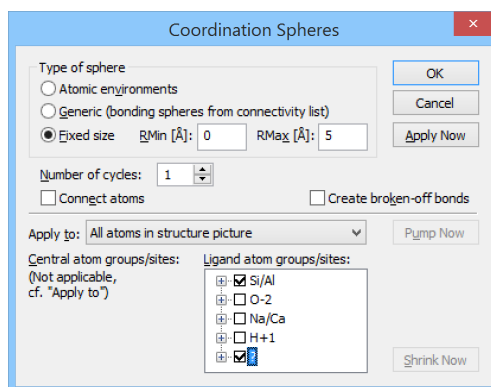
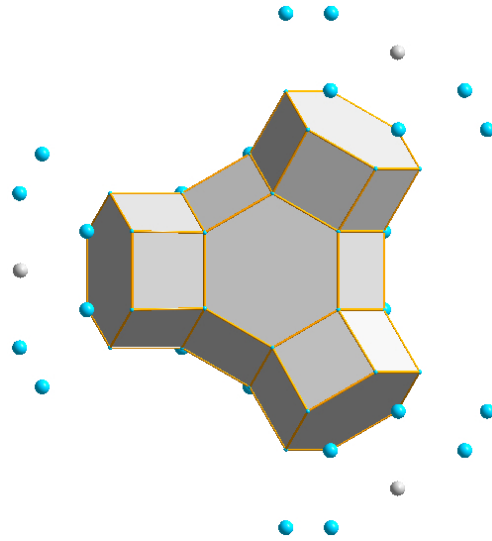
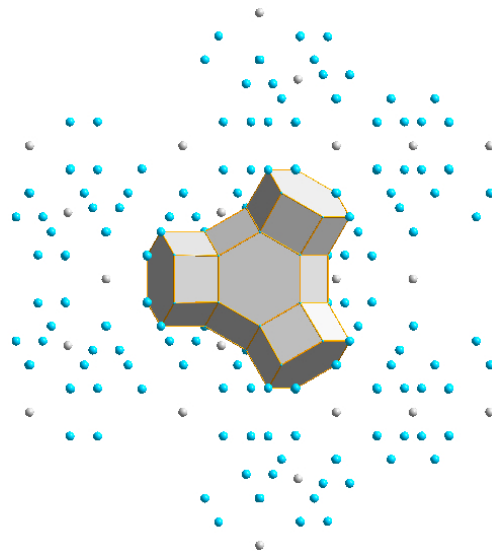


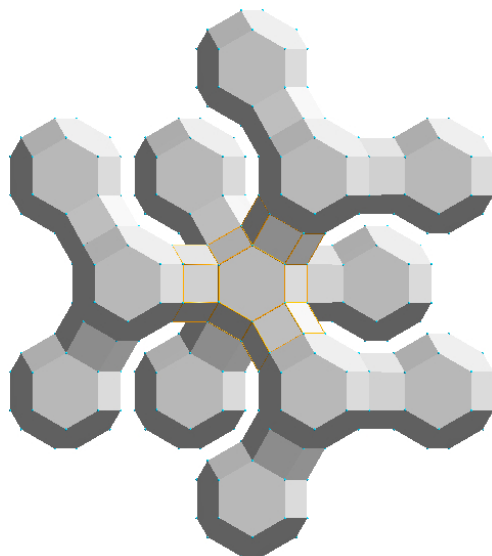
Fig. 65: New Si/Al and dummy (?) atoms will be created close to the hexagonal prisms.



*Fig. 66: Another coordination sphere has been added to the structure.*



*Fig. 67: Two more coordination spheres have been added.*



*Fig. 68: Final view of the Faujasite structure using polyhedra*



## Creating High Quality Pictures Using POV-Ray<sup>TM</sup>

In this session you will learn:

- How to **use POV-Ray<sup>TM</sup>** to create photorealistic pictures of your structure
- How to **design POV-Ray<sup>TM</sup> scenes**

POV-Ray<sup>TM</sup> is the current standard software to create photorealistic pictures by rendering a so-called "scene", i.e. a description which objects are present at which position in the structure picture and how they are illuminated. DIAMOND is able to create these descriptions (the so-called "scene files") for crystal structure pictures. In this tutorial session, you will learn how to create a photorealistic picture of the Keggin-ion structure which has been created earlier in this manual (p. 25).

The first thing you should do before following this tutorial session is to check if POV-Ray<sup>TM</sup> is already installed on your PC. If this is not the case, please follow the instructions given in the chapter "Installation" on p. 59 in the appendix before you continue.



Afterwards, please start DIAMOND if it is not already running. Load the file "unknown.diamdoc" you have saved in the "Exploring an Unknown Structure" tutorial session<sup>16</sup>: Select the "Open" command from the "File" menu, make sure that the file type at the bottom of the "Open" dialog is set to "Diamond 3 Document (\*.diamdoc)" or "All files (\*.\*)", and select the file "unknown.diamdoc" from the "Tutorial" subdirectory of the DIAMOND program directory (e.g. "C:\Program Files\Diamond 4\Tutorial"). Finally, please press "Open". The so-called "Keggin ion" will be displayed as an arrangement of polyhedra (fig. 69).

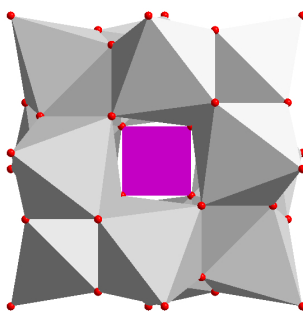


Fig. 69: This picture of the Keggin ion has been created in the "Exploring an Unknown Structure" tutorial.

For a photorealistic representation, we would prefer a space-filling representation of the ion rather than the polyhedra. However, we do not want to destroy the polyhedron picture, so we will add a new picture for the current structure, copy the contents of the existing one (the polyhedron model), and finally change the model to space filling:

Please select the "New Picture..." command from the "Picture" menu which will display the "New Structure Picture" assistant. On the second page of the assistant, please mark "Create a copy of an existing picture", and make sure that "Picture 1" is given as source picture. At the bottom of the assistant, please change the name of the new picture from "Picture 2" to "Space filling" (fig. 70). Afterwards, press "Next".

On the third page of the assistant, you can select if you would like to use some tool to create or modify the contents of the structure picture. In our case, this would not be appropriate, since the only thing we would like to change is the model. Hence, please select "No, I want to build up or change the structure picture manually" at the top (fig. 71), then press "Finish". Once the assistant has been closed, nothing seems to have changed on first glance. However, please note the second tab labelled "Space filling" in the "Picture Tab Bar" at the top of the structure picture (fig. 72). As you see, there are now two structure pictures available ("Picture 1" and "Space filling") for the current structure.

<sup>16</sup>If you are using the demonstration version, you can use the corresponding file shipped with DIAMOND instead.

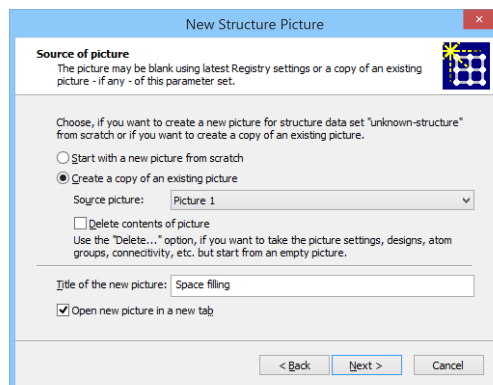


Fig. 70: We would like the newly created picture to contain a copy of the existing picture "Picture 1". Besides this, we would like to change the title of the new picture to "Space filling".

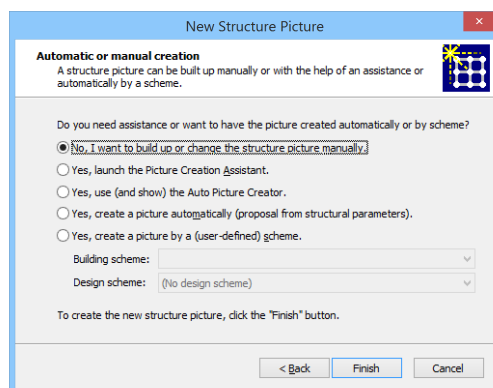


Fig. 71: We do neither want changes nor assistance for the copy of the picture the "New Structure Picture" assistant will create for us.

In order to select the model for the current (new) picture "Space filling", please select the "Model and Radii..." command from the "Picture" menu. In the corresponding dialog, select "Space-filling" from the "Model" combobox at the top, then press "OK". Now the ion is displayed using the space filling radii of the atoms; unfortunately, it does not yet really fit into the structure picture. Please press the F9 key on your keyboard (or select the "Center and Adjust now" from the "Center and Adjust" popup menu in the bottom toolbar. Now the structure picture will be properly scaled (fig. 73).



Though we have just re-adjusted the picture, we do not want the Keggin ion to cover the complete picture in the picture created by POV-Ray<sup>TM</sup> later on. Hence, you have to disable the "Automatic Adjustment" option which is active by default. This can either be achieved by selecting the "Adjust..." command from the "Picture" menu and removing the hook from the checkbox "Automatic adjustment" in the dialog which is opened, or alternatively by selecting the corresponding option from the "Center and Adjust" popup menu in the bottom toolbar (check that the hook in front of "Automatic adjustment" has been removed!).



Another important setting should also be checked in context with POV-Ray<sup>TM</sup>: While most users display their crystal structure in the so-called "parallel projection" (i.e. without perspective impression), this mode is not really appropriate for POV-Ray<sup>TM</sup>. Instead, you should use the so-called "central projection": Please select the "Picture Settings..." command from the "Picture" menu. In the "Picture Settings" dialog, please select (click on) the tabsheet "Projection". Change the "Projection" to "Central", and enter an enlargement factor of 0.8. Finally, compare your window to fig. 74 and press "OK".

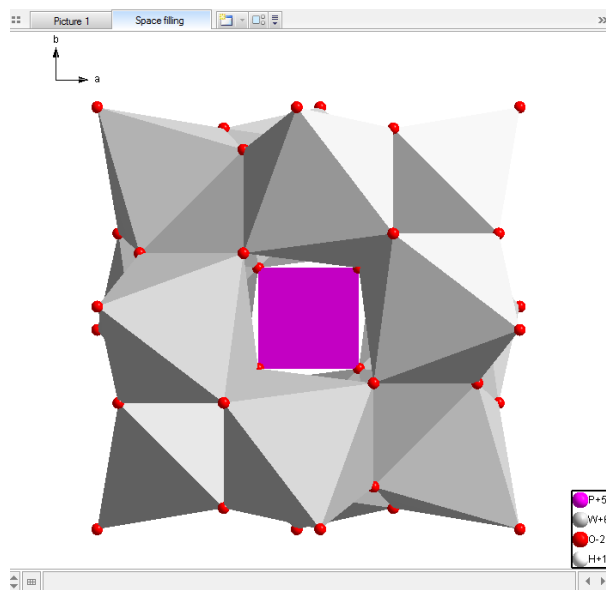


Fig. 72: The two pictures "Picture 1" and "Space filling" are now available from the "Picture Tab Bar". If there are multiple pictures for a structure, these may appear in the "Picture Link Bar" below the structure picture - either as buttons with titles or as small thumbnails. In our example, we only have the two mentioned pictures, so the link bar is empty.

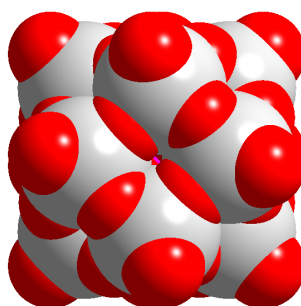


Fig. 73: The display of the Keggin ion has been changed to space-filling model.



By adjusting the parameter "enlargement factor", you can resize your model in the crystal structure picture. The enlargement factor is given as  $\text{cm}/\text{\AA}$ : A value of 1.0 means that 1 cm on the screen corresponds to 1  $\text{\AA}$  in the structure; a value of 0.5 means that 1 cm on the screen corresponds to 2  $\text{\AA}$  in the structure. As a result, the model will be smaller in the second case. On the other hand, there is little sense in changing the parameter "Camera distance (cm)" in this context. The background is that DIAMOND will internally adjust the camera aperture if you change the camera distance in such a way that the same part of the structure picture is displayed. If you increase the camera distance, the aperture will be reduced. This can be compared to your reflex camera: If you would like to take a picture of some object but the object has moved off from you in the meantime, you have to increase the zoom (enlarge the focal length) in order to get "the same picture". As a result, the size of the structural model in the picture is hardly affected by changing the camera distance; the only effect is the degree of perspective distortion which increases with decreasing camera distance.

Since POV-Ray<sup>TM</sup> is a raytracing software, it calculates the reflection of the light on the surfaces of the objects. As a result, it is perfectly possible to let the atoms look as if they were made of stone, metal, glass etc. In our case, we would like to display the W atoms in the ion as shining balls made of solid chrome. In order to achieve this, you have to change the "Material" property for the atom group "W+6":

Please select the "Atom Designs..." command from the picture in order to open the "Atom Group Designs" dialog<sup>17</sup>. On the left hand side, select (mark) the atom group "W+6", then click on the "Material..." button on the right hand side of the dialog. Once the "Material Settings" dialog has

<sup>17</sup>If you had selected an atom before selecting the command, you would be prompted to open the "Atom Design" dialog for this individual atom would be displayed instead.

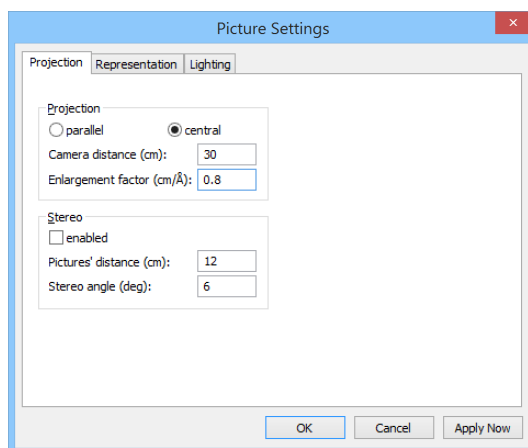


Fig. 74: You should use the central projection for the  $\text{POV-Ray}^{\text{TM}}$  picture.

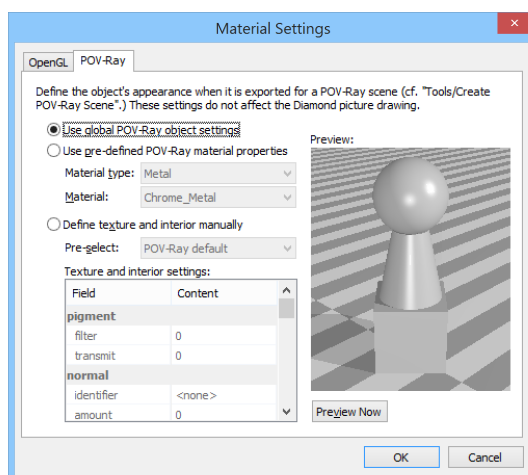


Fig. 75: In this dialog, you can select if you would like to use the global  $\text{POV-Ray}^{\text{TM}}$  settings for the current atom group, or if you would like to use an individual design.

been opened, select (click on) the "POV-Ray" tabsheet ( $\text{POV-Ray}^{\text{TM}}$  might display its so-called "splash screen"). Here, you can select if you would like to use the global  $\text{POV-Ray}^{\text{TM}}$  settings or select an individual design for the current atom group (fig. 75).

There are two options for individual designs: For one, you can use predefined material properties (textures). Besides this, you could also define a new texture on your own. We will use a predefined texture in this case: Please select "Use pre-defined POV-Ray material properties". Afterwards, select "Metal" for "Material type" and "Chrome\_Metal" for "Material" (fig. 76). Finally, press "OK", and close the "Atom Group Designs" afterwards also by pressing "OK".

We will now adjust some global  $\text{POV-Ray}^{\text{TM}}$  settings, i.e. define the background of the picture as well as the floor: We would like the model to float above the surface of the ocean, with a bright blue summer sky in the background. In order to adjust these options, please select the "Global Settings..." command from the "POV-Ray" submenu of the "Tools" menu.

The "Global POV-Ray Settings" dialog which is opened contains four tabsheets (Objects, Background, Bottom, Lights). On the first tabsheet (Objects), you can define the default material property which is applicated to all objects (e.g. atoms, bonds etc.) for which no individual design has been selected. The default selection "Plastic" is a not shiny enough for our purpose, so we will use "Shiny" instead (fig. 77). Please mark the corresponding line, then advance to the tabsheet "Background".

As has already been mentioned, a bright blue summer sky would be nice. Fortunately, a corresponding predefined texture is available: Please mark "Pre-defined texture", then select "Summer sky" from the list. You will see a preview of this background on the right hand side (fig. 78).

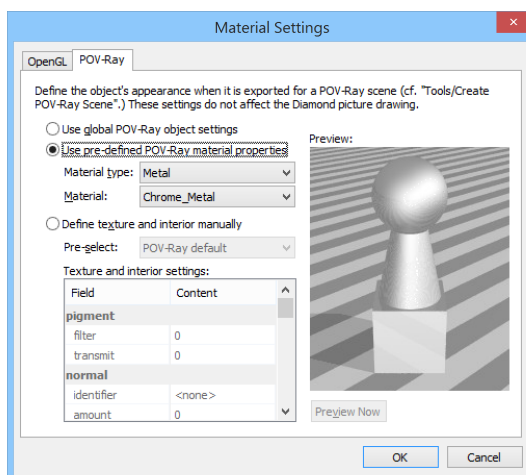


Fig. 76: We would like the W-atoms to look like metallic balls being made of chrome.

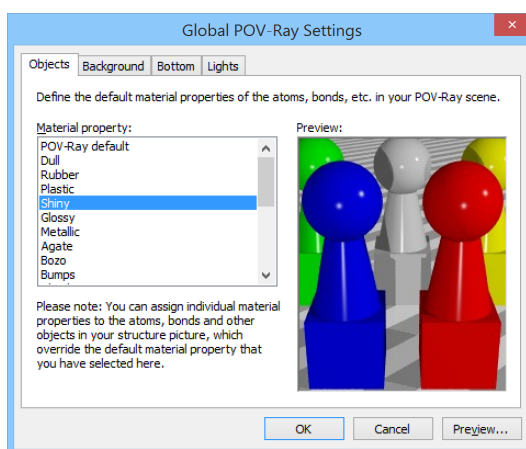


Fig. 77: We prefer a more shiny material for the atoms than the default "Plastic".

Afterwards, open (click on) the tabsheet "Bottom", on which you can define the texture of the floor below the model. Please mark "Ocean" near the bottom of the list (fig. 79), then close the "Settings" dialog by pressing "OK".

At this point, everything has been prepared for POV-Ray<sup>TM</sup>, so we can get things running now: Please select the "Render Into Bitmap..." command from the "Tools/POV-Ray" submenu. At the top of the dialog which opens, you have to define the size of the bitmap which will be created. If you are in doubt, you should use the size of your structure picture window which is given below the corresponding input fields. In our case, we will use a width of 703 and a height of 626 pixels.

The only other thing you have to define is the name and directory of the file to which you would like to save the result of the rendering operation: We choose the (current user's) "Pictures" (or "My Pictures") folder as destination. Please press the "File..." button, then select the path as shown in fig. 81. Afterwards, select the file type (Windows Bitmap (bmp) or Portable Network Graphics (png)), and enter the filename. In our case, we will use the bmp file format and the filename "keggin.bmp". Finally, please press "Save" to return to the "Render POV-Ray Scene" dialog.

All remaining options will be left at their current (default) setting, so your window should look similar to fig. 80.

You are now ready to let POV-Ray<sup>TM</sup> begin its work: Please press the "Render" button at the bottom of the dialog. POV-Ray<sup>TM</sup> may (depending on the version) first display its so-called "splash screen"; afterwards, the picture will be calculated starting from its top. You can watch the progress of the rendering in a window which is opened. Once the rendering has been completed, this window will be closed, and the newly created picture (fig. 82) will be displayed using the application which is associated on your PC to the file type you selected (e.g. image viewer).



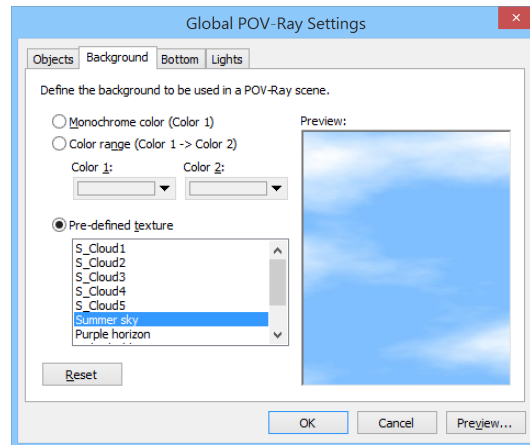


Fig. 78: In the background of our scene, a bright blue summer sky shall be displayed.

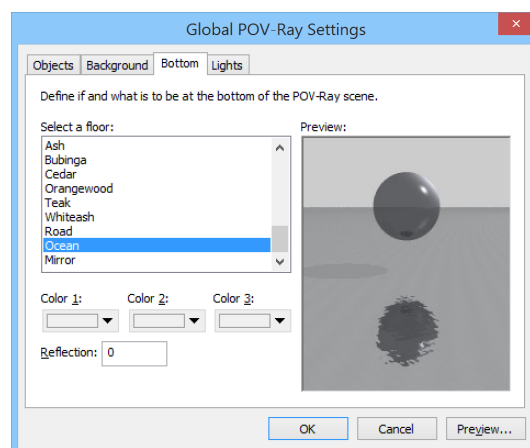


Fig. 79: We would like the structural model to float above the ocean.

Congratulations! You have created your first picture with POV-Ray<sup>TM</sup>! As you already may have noticed while working through this tutorial, there are a lot of design options which may be changed. We recommend to try at least some of these settings, using e.g. different settings for the atom materials or background. **Warning:** According to our own experiences, it may take some time before you will remember that you also have other things to do than just to play around with POV-Ray<sup>TM</sup>...



If you are no longer satisfied with the few POV-Ray<sup>TM</sup> options which can be accessed using DIAMOND, you can directly view and edit the so-called "scene file" created by DIAMOND in the POV-Ray<sup>TM</sup> environment. In order to do so, simply select the "Launch Environment..." command from the "Tools/POV-Ray" submenu. This will open the scene file directly in the POV-Ray<sup>TM</sup> editor where you now can really start working....

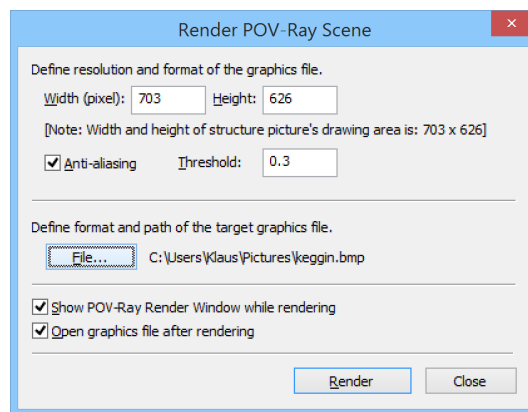


Fig. 80: We will use these settings for our example.

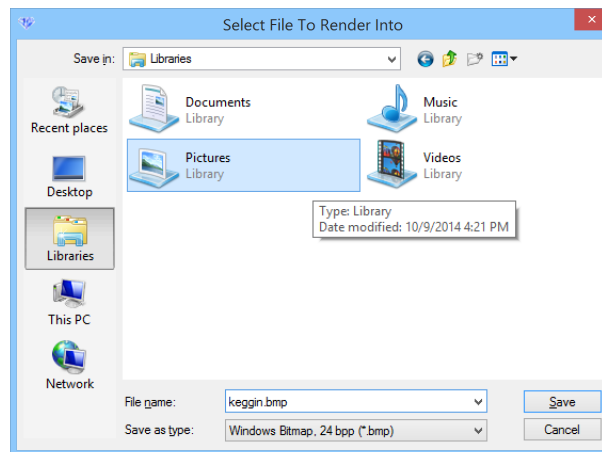


Fig. 81: The file destination dialog for the POV-Ray scene bitmap. We choose the "Pictures" folder via the "Libraries" link in the navigation bar on the left. Note: This dialog, here taken on MS Windows 8.1, may look different on other operating system versions.

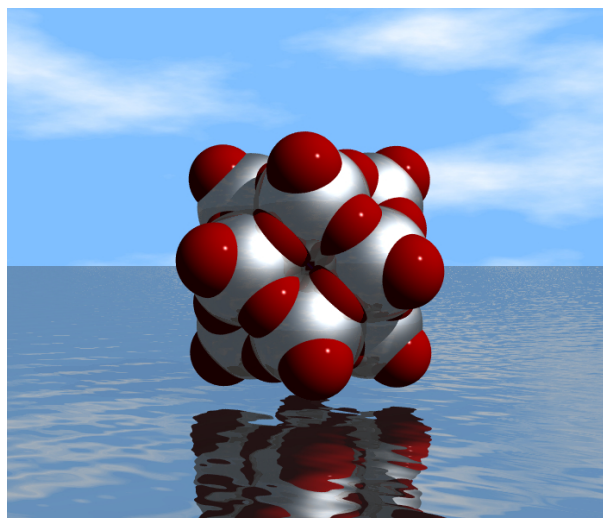


Fig. 82: This is the result of the rendering operation. Note that both the coordinate system as well as the legend are not displayed in the rendered picture.



## Creating Video Sequences

In this session you will learn:

- How to **create video sequences** for presentations and web publications
- How to **walk right into the structure** and not just watch from outside

The basic aim of this tutorial session is to demonstrate how you can create a video sequence using DIAMOND. The procedure is rather similar to recording some radio program on your tape deck or to creating a cartoon. In general, it works as follows:

1. The first thing you have to do is of course to decide what you would like to show in your video sequence. You should precisely define which pictures shall be included in the video sequence, and in which order.
2. When you are ready to go, create the first picture.
3. Afterwards, start the recording. DIAMOND will now **add a picture to the video sequence each time it redraws the structure picture**.
4. Modify your picture step by step while DIAMOND is recording.
5. If you would like to perform some intermediate drawing steps without recording, please press the "Pause" button, and "Continue" when you would like DIAMOND to continue recording.
6. Once your final picture has been created, stop the recording by pressing the "Stop" button. This will bring up a dialog in which you can define things like speed (frames per second), quality, and especially the filename to which you would like to save your video sequence to.
7. The video sequence file will be a so-called "AVI-file" which can easily be viewed using e.g. the Windows Media Player or imported as a "film" into Microsoft PowerPoint presentations.

Let's see how to do this step by step: We would like to use an enlarged version of the Faujasite structure picture which has been created in the tutorial session on p. 34. The first thing to do is to load the corresponding DIAMOND document which has been saved during this session<sup>18</sup>.

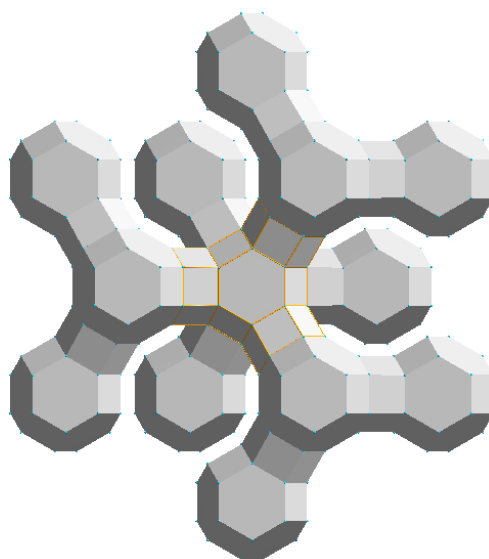


Fig. 83: You have created this view of the Faujasite structure earlier in this manual.

Select the "Open" command from the "File" menu, make sure that the file type at the bottom of



<sup>18</sup>If you are using the demonstration version, you can use the corresponding file shipped with DIAMOND instead.



the "Open" dialog is set to "Diamond 3 Document (\*.diamdoc)" or "All files (\*.\*)", and select the file "faujasite.diamdoc" from the "Tutorial" subdirectory of the DIAMOND program directory (e.g. "C:\Program Files\Diamond 4\Tutorial"). Finally, please press "Open". The picture of the Faujasite structure you have created earlier in this manual will be displayed (fig. 83).

Now we would like to extend the polyhedron structure a little bit. In principle, this will be done using the same building steps that have been used earlier, i.e. by adding fixed spheres to existing atoms and creating polyhedra afterwards. However, there is one important thing you should know: **The setting of the "Filter" which has been used to build the structure picture of Faujasite is not saved in the document file**, since it is not really a property of your structure picture but rather only a helper tool for the selection/exclusion of certain atoms during the building steps. Hence, you have to restore the "Filter" settings corresponding to the ones you have used earlier before you can continue to add spheres to the structural model.

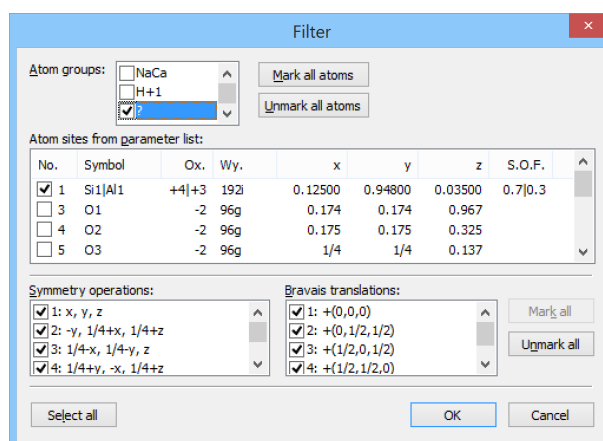


Fig. 84: Only atoms of the mixed site Si/Al and dummy atoms (" ? ") will be taken into account during construction operations in the structure picture.

Please select the "Filter..." command from the "Build" menu in order to open the "Filter" dialog. In the "Atom groups" list at the top, clear all checkboxes but the ones for "SiAl" and "?" (dummy atoms in the centers of the polyhedra) (fig. 84). If you now confirm with "OK", only atoms of the mixed site Si/Al and dummy atoms can be created. To remind you of the active filter, DIAMOND displays a warning symbol in the lower left corner of the structure window.



We can now continue to build the structure (i.e. add hexagonal prisms and  $\beta$ -cages) similar to the earlier session: First, the RMin and RMax settings for the creation of fixed spheres have to be checked: Please select the "Coordination Spheres" command from the "Build" menu to open the corresponding dialog. Set the sphere type to "Fixed size" and "RMin" to 0 and "RMax" to 5 Å. Ensure that the checkmark at "Connect atoms" is clear and "Apply to" reads "All atoms in structure picture", see fig. 85. In order to add three more spheres, press the "Apply Now" button three times, then close the dialog with "Close". Afterwards, confirm by clicking "OK". The next sphere of atoms will be added. Your structure picture should now look similar to fig. 86.

Afterwards, you have to create polyhedra for the newly created atoms: Please select the "Add Coordination Polyhedra" command from the "Polyhedra" submenu of the "Build" menu. In the "Add Coordination Polyhedra" dialog, please select "?" (which represents the dummy atom) as central atom group and "SiAl" as ligand atom group. Set the type of sphere to "Fixed" and "RMin" to 1 and "RMax" to 5. Your dialog should now look similar to fig. 87.

We also would like to define the design of the polyhedra, so please click on the "Polyhedron Design..." button on the right hand side of the dialog. In the "Polyhedron Design" dialog, please adjust the settings according to fig. 88.

Afterwards, bring the "Others" tabsheet into front by clicking on its header, and change the "Ligand atoms reducing factor" to 0.01. This factor results in a size reduction of all atoms at the corners of the polyhedra so that they are rather indiscernible but can still be selected. Finally, please press "OK" to return to the "Add Coordination Polyhedra dialog", and push the "OK" button here, too. DIAMOND will now create polyhedra around the atoms you have added using the "Coordination

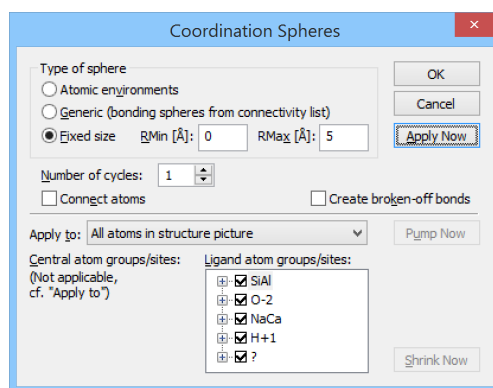


Fig. 85: We use the "Coordination Spheres" dialog to add three more spheres of Si/Al and the dummy atoms.

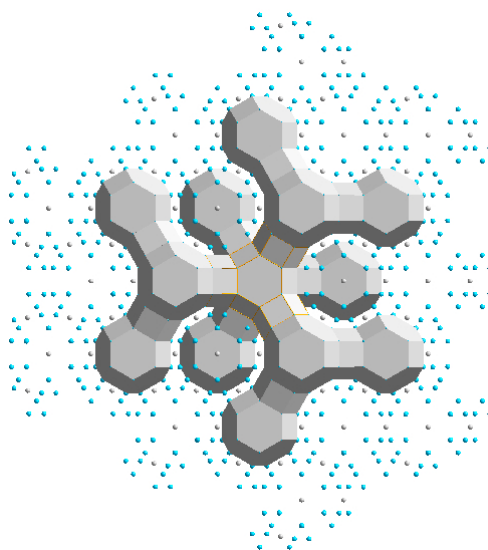


Fig. 86: Three more coordination spheres have been added.

Spheres" command (fig. 89).

At this point, the structural model has been prepared; it is now time to think about how this model shall be presented: We would like to start viewing the model from the distance and fly through the front "pore" right into the structure until we reach the central atom. In order to do so, several settings concerning the perspective have to be changed: Please select the "Picture Settings..." command from the "Picture" menu. In the dialog which opens, please click on the tabsheet "Projection".

You should switch from the normal parallel to the central projection. Besides this, please check that the camera distance is set to 30 cm (fig. 90). Afterwards, close the dialog by pressing "OK".

Now you can start the actual recording of the video sequence: Please select the "Start Recording" command in the "Tools/Video Sequence" submenu, or press the "Record" button in the toolbar at the top. You should now be extremely careful: From now on, each time DIAMOND updates the structure picture, it will also be added to the video sequence. The "Start Recording" toolbar button changes to "Pause Recording" while a video sequence recording is running.



It is not possible to remove individual pictures from a video sequence using DIAMOND. If you would like to do so (or perform similar editing operations), we recommend to use video editing software like Windows Movie Maker or similar.

We will now step-by-step fly into the structure. Normally (i.e. without recording), you could use the mouse by activating the corresponding tracking mode in the toolbar at the bottom. However, this is not really appropriate for recording, since it is rather difficult to achieve a constant mouse moving speed. In context of recording, we strongly recommend to use the keyboard, since a constant stepsize is associated with each button press event.



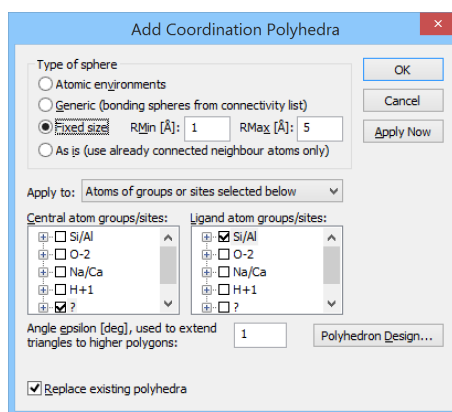


Fig. 87: We would like to build polyhedra around the '?' (dummy) atoms. The ligand atoms should be Si/Al and must be placed at a distance between 1 and 5 Å from the central dummy atom.

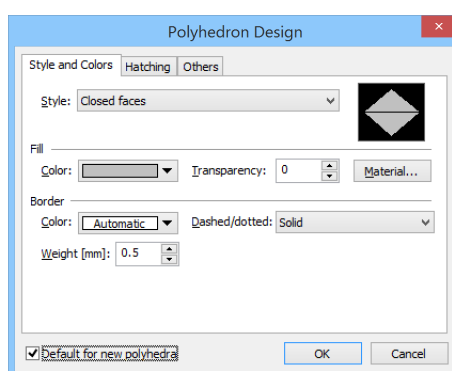


Fig. 88: Please use these settings for the design of the polyhedron.

The button for "walk in" is the "7" on the numerical button block to the right on your keyboard. **Please make sure that the "Numlock" function is active before you proceed!**

Please press the "7" on the numerical button block now; the structural model will get closer to you a little bit. Please repeat this step 28 times until you see the central (dummy) atom of the central  $\beta$ -cage. **Please wait with each new keystroke until DIAMOND has updated the structure picture** (which can be seen in the progress indicator in the status bar at the bottom).



There are two stepsizes available: Normally, the walk-in stepsize is 1cm. If you prefer a more smooth movement, you should use a smaller stepsize of 0.2cm per keystroke. This smaller stepsize can be accessed by pressing the "Ctrl"-button on your keyboard in combination with the "7" on your numerical block (<Ctrl+7>).

We will stop our walk-in here; however, it is worth while to add some more pictures of the central atom so that this picture is displayed for a few moments at the end of the video sequence. All you have to do is to let DIAMOND update the structure picture. This is achieved by pressing the F5 button on your keyboard. Please press this button now approximately 10 times.



Now that all pictures have been recorded, you can stop the recording mode, either by selecting the "Stop..." command in the "Tools/Video Sequence" submenu, or by **double-clicking**<sup>19</sup> the "Pause Recording" toolbar button. A dialog will be displayed where you have to select what to do with the sequence of structure pictures you have recorded (fig. 91). You can either create an AVI-file which can directly be imported e.g. into PowerPoint, or create a series of individual graphic files in some directory which can be imported in typical video creation software like Ulead GIF animator or similar products.

We would like to create an AVI-file directly, so please mark the first option. We recommend to use the "Preview" option in order to check if the so-called "Compression handler" which can be selected in the corresponding combobox is able to handle your pictures. Please press the "Preview..." button

<sup>19</sup>A single click pauses or continues the recording. You can also choose a command from the dropdown menu that opens when clicking on the arrow-down symbol right beneath the toolbar button.

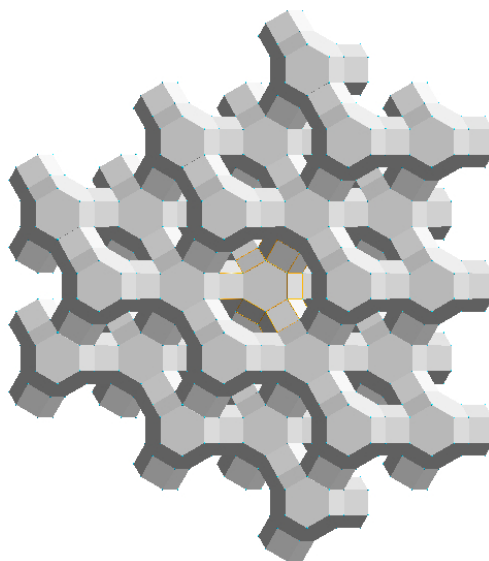


Fig. 89: The Faujasite structure from the earlier tutorial session has been extended.

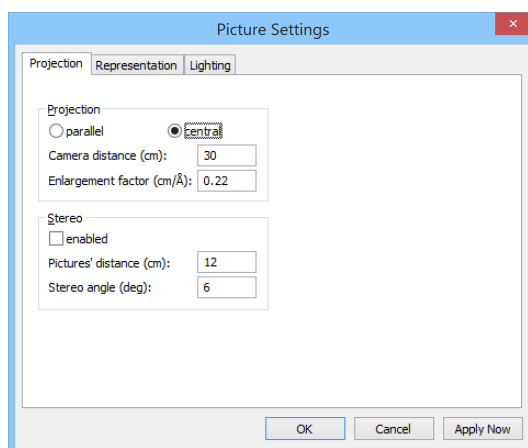


Fig. 90: The projection has been switched to central projection in order to obtain a perspective impression of the structure when flying into it.

now. If you get an error message (e.g. indicating that the "Video Stream Compressor rejected the bitmap format"), you should select a different compression handler or even "<no compression>". Of course, the latter option is only recommended if no compression handler seems to work at all, since the files created by this method are extremely large.

Once you have found a suitable compression handler and the preview was satisfactory, you should press "File name..." in order to define the filename and directory to which you AVI-file shall be written to. Once this has been done, please press "OK" at the bottom of the dialog. Your AVI-file will now be created; afterwards, the dialog will be closed.

That's it! You can now view your AVI-file simply by double-clicking on it in the Explorer (provided that a suitable software is installed on your PC which is associated with the file extension ".avi").

Of course, you can create much more elaborate video sequences than this one. Quite frequently, it is necessary to interrupt the recording if you would like to perform more than a single step between two recorded pictures. This can be achieved using the "Pause/Continue" command/button in the toolbar at the top. Here is just one example which you might want to try by yourself: We will simultaneously rotate the structure around the z-axis (i.e. the axis pointing out of the screen) while flying into it.



Open the "Picture/Picture Settings..." dialog and reset the "Camera distance" on the second tabsheet back to 30 cm in order to return to the starting point of the flight into the structure. Afterwards, start recording by pressing the corresponding toolbar button.



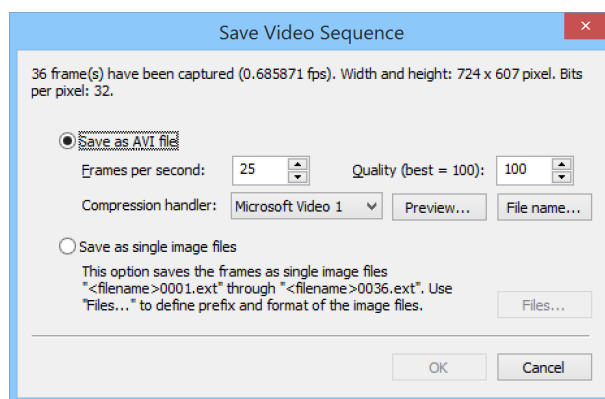


Fig. 91: In this dialog, you define what to do with the sequence of structure pictures you have recorded.

Now that the "camera is running", please repeat the following steps until you can see the central atom:

1. Fly a single step by pressing the 7 on the numerical block (NumLock!)
2. Pause the recording by pressing the corresponding "Pause/Continue" button in the toolbar
3. Rotate a single step around the z-axis by pressing the <PgUp> button on your keyboard
4. Continue the recording by pressing the corresponding "Pause/Continue" button in the toolbar

Again, please wait until DIAMOND has really updated the structure picture before you press the next key. When you see the central atom, you should update the final picture about 10 times (by pressing F5) afterwards. Finally, double-click the "Pause Recording" button in order to stop recording, and create the AVI-file as described above.

When you have finished creating video sequences, you should perhaps switch the projection back to "parallel projection" (menu "Picture/Picture Settings...") which is more suitable for normal structure investigations.





## Where to get Help

In addition to the tutorial sessions present in this manual, we strongly recommend to use DIAMOND's very detailed **online help**<sup>20</sup> for **reference** purposes. The online help system can be used in a variety of different ways:

- continuous "in-depth" reading guided by the links
- context sensitive
- index based
- searching for arbitrary keywords (free-text searching)

If you would like to obtain a context-sensitive help, please press the **F1** key on your keyboard. DIAMOND will display a helping text depending on your current situation (e.g. which dialog is currently open or which menu item is highlighted). If neither a dialog box is open nor a menu item is highlighted, pressing of the F1 key generally opens the help page for the part of the program window over which the mouse cursor is currently placed (e.g. toolbar).

A special mode, the "Help mode", is activated by pressing the key combination **Shift+F1**. This is an alternative method of getting context-sensitive help: When this mode has been activated, the mouse cursor changes to a symbol consisting of standard arrow and question mark. In this mode, you will get context-sensitive help if you click on a certain item of the DIAMOND window, e.g. the diffraction pattern or a toolbar. The Help mode ends automatically when you get help for a clicked item.

DIAMOND also offers several so-called "assistants" which can e.g. guide you through the steps of picture creation ("Structure Picture Creation Assistant", available in the "Picture" menu).

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<sup>20</sup>The online help can generally be opened by pressing the F1 button on your keyboard.



## Support

In case of trouble when using DIAMOND, please pay attention to the following hints:

- If you do not know how to operate in a dialog window, carefully read all information in the window. Make sure that you understand the meaning of the buttons, input fields, lists, etc. Look at the way several functions are grouped into frames and read the frame titles, too.
- Press the F1 key and examine the help text. Especially read the items mentioned under **Note:**, and check the help jumps, too.
- Look for appropriate keywords in the **Help Index**, and look for any related text on the **Help Find** tab.
- If you do not know how a command in a pulldown menu operates, press the **F1** key when the corresponding command is highlighted. This will open the help page for this command, where you can continue as mentioned above.
- If you do not find a command, use the **Help Index (Index** tab on the **Diamond Application Help** window) to get an alphabetic list of search items.
- Visit the DIAMOND update page at:

**<http://www.crystalimpact.com/diamond/update.htm>**

This page offers the latest versions of online help files, sample files, and software patches for the executables and DLL's.

- If this page does not give you an answer, or if the trouble is caused by an error in the software (a "bug"), check if the bug has already been listed on the "Known Bugs" web page (**[www.crystalimpact.com/diamond/bugs.htm](http://www.crystalimpact.com/diamond/bugs.htm)**) and what you may do as a workaround until a software "patch" (update) is available.
- If the bug you encountered is not listed, send an **e-mail** to **[support@crystalimpact.com](mailto:support@crystalimpact.com)**

Or - if you are not connected to the Internet - send a **fax** to: **++49 - 2 28 - 9 81 36 44**

or **write** to:

Crystal Impact  
Dr. H. Putz & Dr. K. Brandenburg GbR  
Kreuzherrenstr. 102  
D-53227 Bonn  
Germany



## Appendix

### Installation

Before you install and run DIAMOND, you should check the following

#### Minimum system requirements:

- Personal Computer with Microsoft Windows XP, Windows Vista, Windows 7, Windows 8/8.1, or Windows 10 operating system  
(note: does not run with Windows RT)
- Microsoft Internet Explorer 8 or higher
- Intel or AMD (or compatible) processor with "x86" instruction set
- 512 MB of RAM
- 3.8 GB of free disk space (6 GB during installation procedure, for unpacking of Crystallography Open Database)
- Graphics resolution of 1024 x 768 pixels with 32,768 colors ("High Color") or higher (1280 x 800 pixels or more recommended)
- DVD-ROM drive (for installation from DVD)
- Microsoft-compatible mouse

#### Installing from DVD-ROM:

Please insert the DIAMOND DVD into your DVD-ROM drive and wait a few seconds; an installation selection program will start automatically. Afterwards, please click on the big Diamond logo next to "Install Diamond". The actual DIAMOND installation program will start and lead you through the setup process. Please follow the instructions on the screen.



If nothing happens for a reasonable amount of time after you inserted the DVD-ROM into your drive, start the Windows-explorer, right-click on your DVD-ROM icon, and select "Autoplay".

#### Installing from Download Package:

If you have not already done so, download the installer from:

<http://www.crystalimpact.de/diamond/download.htm>

Then run the downloaded setup executable to launch the installation procedure and follow the instructions on the screen.

#### License Installation:

If you have installed DIAMOND from a download package or from a Crystal Impact software demonstration DVD (or other media), the program runs in demonstration mode. In order to turn DIAMOND into a full-featured version, you need a personal license file, which you most likely have received by e-mail when purchasing the software. Copy your personal license file ("yourlicense.lic") (and replace the demo license file) into the Diamond program directory (which is by default located at: "C:\Program Files\Diamond 4\"). You may need administrator rights to copy the license file into the Diamond program directory!

Note that you need to run the installer using administrator rights explicitly. If you are not running the PC as administrator, you can right-click on the installer file, then select "Run as administrator" from the context menu.

Please read the terms of the "End User License Agreement", which will appear in one of the dialog windows of the setup program!

#### POV-Ray installation:



Once you have installed DIAMOND, you should also install POV-Ray<sup>TM</sup> (if it is not already present on your computer) in order to be able to produce photorealistic pictures. Please follow the instructions below:



### Install POV-Ray<sup>TM</sup>

You can install POV-Ray<sup>TM</sup> ([www.povray.org](http://www.povray.org)) either by clicking on the corresponding button in the installation selection program, or by double-clicking on the file "povwin-3.7-agpl3-setup.exe" in the "POV-Ray" directory on the DIAMOND DVD-ROM. If you install from separately downloaded files, simply double-click on this file in the directory where you have stored it on your hard disk. The POV-Ray<sup>TM</sup> installation program will start and lead you through the setup process. Please follow the instructions on the screen.

If POV-Ray<sup>TM</sup> is already installed on your PC, it might be necessary to inform DIAMOND about the directory in which it is present. DIAMOND will ask for it if necessary.

### Online Update

Diamond is able to automatically download and install a new version once it has become available. It connects to the Crystal Impact webserver and compares the version of the most recent update available there to the version which is currently installed on your PC. In order to achieve this, a working connection to the internet is required, of course. If you are not connected to the internet, Diamond will ask you to do so before continuing.

If a more recent version is found on the webserver, a list of changes and improved features in the new version will be displayed, and you will be asked if you would like to download the corresponding update. Once you have acknowledged and the corresponding files have been downloaded, you will be asked to close all open Diamond windows so that the update program can replace the program executable. After the update has been completed, Diamond will be restarted so that you can check if the update was successful. This can e.g. be achieved by selecting the "About Diamond..." command in the "Help" menu and checking the version number and date in the dialog which is displayed.

By default, Diamond checks the Crystal Impact webserver for a new version automatically each time it is executed. If you would like to disable this feature (e.g. if you are not permanently connected to the internet), you can do so on the "Desktop" page of the "Tools/Options" dialog, simply by removing the hook in front of "Check for available updates when starting" at the bottom of the dialog.

If you have disabled the "Check for available updates" option, you can update your software online manually by selecting the "Online Update" command from the "Help" menu. The procedure will be the same as the one described above for the automatic update.

### Restore Factory Settings

If your colleagues use DIAMOND on the same PC as you, you might want to restore the default settings from time to time. This is also appropriate if you are a beginner and would like to work through the individual tutorial sessions step-by-step.

In order to restore all options and settings to the original ones selected by Crystal Impact ("factory settings"), please start DIAMOND<sup>21,22</sup> if it is not already running. Afterwards, select the "Reset Settings..." command from the "Tools" menu. A dialog will open indicating that DIAMOND will have to be closed, so that you will have to restart it afterwards. Simply accept by clicking "OK", and accept the question "Close application now?" as well. Finally, restart DIAMOND; it will now operate exactly like it has just been installed.

<sup>21</sup>In order to start DIAMOND, press the Windows "Start" button, select the "Diamond 4" folder of the "Program Files" branch, and finally click on "Diamond".

<sup>22</sup>If DIAMOND has not been installed on your computer yet, you should read the chapter "Installation" on p. 59 and follow the instructions given. Of course, you don't need to restore the factory settings in this case.



## What's New for Diamond 3 Users

Although the basic principles as well as the most common operations have been retained, users of the previous DIAMOND version 3 will find a lot of new features and options:

### New arrangement of views

Since the average screen size (especially width) is higher than at the times of Diamond 3, version 4 has a closer correlation and thus better integration between the actual pictures view and the other views. So you can arrange structure picture and distances or powder pattern side-by-side rather than in separate main views.

A Diamond document window consists of a **Structure Pictures** view (which may contain one picture or multiple pictures) in the main (left) pane, assisted by several textual views in the right data pane:

- tables (e.g. of atomic parameters),
- data sheet (formerly called "data brief" at that position),
- the new "**Atom List**" (see description below),
- table of distances and/or angles,
- table of reflection parameters.

The separate views (as used in Diamond 3 and available from Navigation bar or Navigation window) "Data sheet", "Powder pattern", and "Distances/angles" have become obsolete.

You will find the **Structure Table** (for a document with more than only one structure parameter set) in a new pane above structure picture and data pane. (In Diamond there was a separate view for that table with just picture thumbnails previews and the "data brief" below available.) The structure table can collapse to save room to show only the row of the current structure, that is the **Structure Info Bar**.

While there was a separate "Distances and angles" view in Diamond 3, the **table of distances and/or angles** is now positioned right beneath the structure picture (i.e. in the data pane), and the distances histogram appears in the **Properties** view in the bottom right. Analogously, **powder diffraction** data can be displayed there: reflection parameter table and diffraction diagram in Properties pane below.

To activate data sheet, distances table etc., run the corresponding commands from the "View" menu.

### Integration of picture thumbnails

You can now edit a structure picture side-by-side with the other pictures' thumbnails in a multiple picture document:

- The **active picture** is now indicated by a **tab** showing the picture's title.
- The separate docking window "Picture thumbnails" has been replaced. Now you can view structure pictures (if a document contains multiple structure pictures) side-by-side: A preferred picture under a **tab**, whereas the residual N-1 pictures appear either as **link buttons** or as **thumbnails** below the picture in the edit view. (The "Navigation bar" of version 3 has become obsolete.)
- **Multiple tabs**: Edit another picture in the same tab by clicking on the link button (or link thumbnail), or edit the other picture in a new tab. So two or more tabs for these "preferred" pictures can appear in the **Picture Tab Bar** you can easily switch between.
- You can be in **Picture Edit** mode (i.e. have full access to building and designing functions) while the thumbnails of the residual preferred ("tabbed") pictures are arranged right beneath the edit view.



## Auto Picture Creator

The new "Auto Picture Creator" is a dialog-like window nested in a **docking window** and offers the most useful features in the categories picture building, picture design and picture viewing at a glance.

Like the "Navigation window" it can be docked, floating or completely hidden. Additionally it can reduce its size to nothing but the tab – enabling quick reappearance when the mouse hovers it. This is useful when your screen size is limited due to open data sheet or other windows or panes. The activity status of the Auto Picture Creator is signalled with a yellow-orange field in the middle of the **status bar**.

To show the Auto Picture Creator, run the corresponding command in the "View" menu.

For examples, read the article "Auto Picture Creator", available from "What's New in Diamond Version 4" ("Help/What's New").

## Building schemes

The "Building schemes" (formerly called "Auto-Build schemes") have been improved:

- Several commands to apply or manage building schemes are available through the "Build/Building Scheme" sub-menu.
- The command "Define Scheme" defines a new scheme or by modification of an existing scheme.
- The command "Run Proposal" runs the building scheme that Diamond suggests basing upon structure data.
- Apply Building schemes directly from a list in the sub-menu or in the bottom ("Picture") toolbar or from the "Run Building Scheme..." dialog.
- The option "Packing diagram" (with several choices how to include molecules) is new in "Basics".
- The option "Add all atoms" has been extended by H-bond and contact definitions. (Cf. "Build/Add All Atoms and Connections" command.)

## Design schemes

A "design scheme" is a kind of style sheet and contains some basic picture design settings plus optionally the whole current design and viewing settings of a structure picture. The basic picture design settings as well as the viewing settings are already known from the "Picture Creation Assistant" that is in use since Diamond version 3.

You find the design schemes in the corresponding submenu of the "Picture" menu. The first command "Create Design Scheme..." initializes a design scheme from the current picture settings – from layout, model, rendering or not, across the atom, bond etc. designs up to the viewing direction. Use the checkboxes to decide what the new design scheme may change when applied later. For instance, you can create a design scheme that only reflects the atom (type) designs. So you can easily change current atoms' designs to have different colors, ellipsoid styles, etc.:

- Apply a previously defined design scheme directly to the current structure picture.
- Run "Apply Design Scheme": Choose a design scheme from the dropdown combobox list and apply it – either directly or after some modifications.
- The "Design Scheme Manager" (Picture sub-menu or Tools menu) can be used to manage design schemes.



## Crystallography Open Database (COD)

The crystal structure database **COD** ("Crystallography Open Database")<sup>23</sup> including (amongst others) **AMCSD** ("American Mineralogist Crystal Structure Database") as well as **CIF files** from the **IUCr journals**, has been setup (and will be updated regularly) for direct access by Diamond. In 2010, this database of inorganic as well as organic crystal structures has crossed the 100,000 entry border. Now (May 2017) there are almost 378,000 datasets. (The COD version delivered with Diamond versions 4.0 through 4.4 is dated April 3, 2012, and contains approximately 156,000 entries.)

The database can be accessed via the "Search" command from the "File" menu, where you can also (like in earlier Diamond versions) search files and folders on your hard disk for structure data.

A subset of COD entries is also available through the command "From Structure Type Database" in the "Structure" menu, where you can browse through a list of the most common inorganic structure types and can load ready-to-use structure pictures.

## Connection parameters

The new "Connection Parameters" command ("Structure" menu) offers three new parameter tables that complement the atomic parameters:

- The **bond parameters** are usually derived from CIF "\_geom\_bond\_xxx" loops and define selected bonds (that may be important in a publication for instance) or even a whole (ensemble of) molecule(s).
- The **contact parameters**. Like the bond parameters, these usually come from "\_geom\_contact\_xxx" loops.
- The **H-bond parameters**. These describe relations between an H-atom, a donor atom and an acceptor atom each with bond lengths/atom distances and an angle each (usually from "\_geom\_hbond\_xxx").

Tables of bond, H-bond, and contact parameters are available from the "Tables" sub-menu of the "View" menu. These tables offer several commands in their context menus to create bonds, H-bonds or contacts, resp., directly or to expand to neighbouring molecules via selected contacts or H-bonds.

## Atomic environments

The "Atomic environment" ("Build"/"Atomic Environments") is an additional (optional) criterion when filling coordination spheres or adding coordination polyhedra.

- It enables more precise definition of neighbouring atoms connected with strong bonds than just the connectivity, which is defined between atom groups and by rather simple two sphere boundary values *rmin* and *rmax* each.
- The "Atomic Environments" dialog offers two presentations for an atom site's environment each: Distances table and histogram.
- Atomic environments are (optionally) updated when changing the bonding spheres (connectivity) or vice versa.
- Atomic environments can be derived from the **Dirichlet domain (Voronoi polyhedron)** of the central atom site each.

<sup>23</sup>www.crystallography.net. Crystal Impact would like to thank Pete Strickland (IUCr), Armel Le Bail (COD) and Bob Downs (AMCSD) for their kind permission to download and distribute their data free-of-charge.



## Handling of molecules

The generation of molecules and the completion of fragments has been enhanced:

- The new command "Build/Molecules/Define Molecules..." defines "**molecular units**" from the atomic parameter list basing upon connectivity or atomic environments.
- The new command "Build/Molecules/Add Molecules..." creates molecules at symmetry-equivalent positions (by applying symmetry operations, and/or Bravais translations and/or integer cell translations) to the molecular units.
- The **completion of fragments**, now under "Build/Molecules/Complete Fragments", has been improved. It can be applied to all atoms or the currently selected atoms - but also to atoms of selected atom groups or selected sites. (Tree view as in the Coordination Spheres dialog or the new Connect Atoms dialog.)

## Packing diagram

The new command "Build/Packing..." offers a comprehensive two-pages dialog with:

- Page "Choose Atoms" to choose the molecules to be considered, how to treat polymers and vagabonding atoms, and if and how to include, exclude or cut molecules at the packing boundaries.
- Page "Define Range" to define the boundaries of the parallel piped. You may also define a sphere instead of a parallel piped.
- Additional option to fill a slab or slice parallel to an hkl plane (compare command "Build/Fill/Slab"), with the cell range as delimiters.

A shortcut is available from the bottom toolbar or **Shift+Ctrl+G** to create a **packing of the unit cell** containing molecules whose centroid is inside the unit cell.

## Grow and cut, pump up and shrink

The coordination spheres and fragment completion functions have been enhanced and come closer to each other:

- Add another series of spheres to a polymer or a molecular fragment (or remove) with "Build/Grow or Cut": Apply to all or selected atoms (molecules or polymers), with the option to step over broken-off bonds.
- Shortcuts are also available from bottom ("Picture") toolbar: "Grow directly" and "Cut directly".
- New command "Shrink" to reduce (dismantle) a coordination sphere around a central atom or central atoms of selected atom groups or sites or currently marked in structure picture.
- Available as push buttons "Pump now" and "Shrink now" from within "Coordination Spheres" dialog or to perform directly from the dropdown menu of the "Fill coordination spheres directly" button in the "Build" toolbar.

## H-bonds and non-bonding contacts

The Connectivity dialog ("Build" menu) now has additional pages to define non-bonding contacts and for improved handling of H-bonds:





- Consideration of connection parameters for bonds as well as for H-bonds and contacts.
- Support for multiple sets of H-bond and contact definitions: Contact and H-bond definition groups – as there are "Standard contacts" and "Standard H-bonds", resp., defined between the atom group pairs (like bonds are) and using van der Waals radii sum plus an offset as default.
- User-defined, special contact definition groups and H-bond definition groups, resp. These may be defined on atom site level.
- Reported contacts/H-bonds (from connection parameters) are compiled in "Reported contacts" and "Reported H-bonds" definition groups, resp., each.

The new command "Build/Add contacts" creates contacts according to connectivity settings or with fixed boundary values. The command "Create H-Bonds" has been enhanced to regard the H-bond definitions from the connectivity dialog, too.

### Expansion and reduction of molecule clusters

Several new functions allow the building up ("Expand") of a **molecule cluster**, using contacts, H-bonds or shortest distances: "Reduce" is the reversal function.

- Dialog "Build/Expand" with several settings if to apply to all atoms or selected atoms or selected molecules, to enable intramolecular contacts, to regard H-bond definitions, too, and what to do with the contacted neighbouring atoms (broken-off bonds around or complete fragments).
- "Settings" page in that dialog, so you can choose the current connectivity settings or use different contact spheres, either relative to van der Waals radii or in absolute Angstrom boundaries.
- Push buttons to do expansion step-by-step: Add contacts now, Expand now. Push buttons to remove contacts or fragments, that means to step back.
- Dialog "Build/Reduce" to remove molecules step-by-step, either the farthest molecules or all neighbouring molecules. Several settings to apply to or to start from and if and how to consider H-bonds and contacts.
- Accelerator keys and toolbar icons to expand or to reduce: "Create atoms' neighbouring atoms", "Create molecules' neighbouring atoms", "Create neighbouring molecules", and "Reduce directly".

### Voronoi polyhedra

Diamond now supports Dirichlet domains and Voronoi polyhedra<sup>24</sup>:

- Voronoi polyhedra can be created for selected atoms or atoms of selected sites basing upon their Dirichlet domains ("Build/Polyhedra/Voronoi Polyhedra").
- There are several options for the style of the polyhedron as well as if and how to show and connect the neighbouring atoms.
- Infos about a selected Voronoi polyhedron (neighbouring atoms, distances, bond strengths, solid angles, etc.) are available from the Properties view.

<sup>24</sup>Diamond uses "Dirichlet domain" to define which neighbouring atoms of an atom site belong to the domain, whereas "Voronoi polyhedron" describes the polyhedron building with its central atom and its vertices, faces and edges.



## Grab mode

The "grab mode" ("Edit" menu) is an alternative to the several "tracking modes" ("Move" menu) with the advantage to be able to rotate, shift, or zoom in/out without the need to change between the several tracking modes. Features of grab mode are:

- **Rotation** with left mouse button with the possibility to grab an atom, i.e. turn the structure while the atom stays under the mouse cursor.
- **Shifting** with right mouse button.
- Changing **enlargement factor** or camera distance with mouse wheel.
- Several options available with mouse button double click.

## Neighbourhood preview

The new "Neighbourhood preview" ("Tools" menu) shows the environment of the atom (or molecule) under the mouse cursor:

- Move the mouse cursor over an atom and see its neighbouring atoms (and molecules, if molecular structure) as semi-transparent preview.
- Turn the mouse wheel forward/backward to increase/decrease the preview sphere size.
- The neighbourhood preview can also be applied to whole molecules.

## Changing properties with mouse wheel

Several new operational modes ("Tools/Mouse Wheeling" submenu) use the mouse wheel to change properties or to explore the environments of atoms or molecules:

- Change the **radii of atoms**, up to space-filling radii and down to wire/stick model.
- Change the **radii** of thick (stick) **bonds**.
- **Expand** the current **selection** to the next bonds and atoms, etc. with a mouse wheel tick each.
- Blow up a **coordination sphere** (i.e. increase the coordination number), also available to coordination polyhedra.
- Find non-bonding **contacts** by varying an offset to van der Waals radii sums.
- Expand molecules to **clusters**, i.e. find next neighbouring molecules with a mouse wheel tick each.

## Recent Pictures list

The "Recent pictures" list gives you comfortable access to the latest viewed or edited structure pictures:

- Applies to pictures from **current** as well as **earlier Diamond sessions**.
- The "Recent Pictures" **docking window** ("View" menu) contains the latest edited structure pictures of open document as well as of recently closed documents (files) as small thumbnails.
- The command "View/Last Pictures" offers access to the latest edited pictures of the current open document (also available from toolbar).
- A **toolbar button** enables direct access to the latest edited picture, so you can easily swap between two pictures of interest.



## Undo and Redo buffer

The "Undo buffer" enables to undo or redo multiple steps together.

- Undo/Redo can be done now with multiple steps together, assisted by **thumbnail pictures** of the previous conditions each.
- In the "Undo/Redo" **docking window** ("View" menu), you can click on a thumbnail to restore all undo steps through the clicked one. The same works for redo steps, if undo steps have been performed immediately before. (Slight differences in shape between the two kind of undo and redo thumbnails.)
- A **dropdown list** is available from the main **toolbar** with a thumbnail of the last undo and redo, resp., step each.

## Atom list

The new "Atom list" ("View" menu) in the data pane is a **hierarchical list** of atom groups, atom sites, and created atoms of a structure picture:

- Used for instance to edit properties and designs or to select from.
- Two kinds of arrangements: 1) For atom **groups, sites** and created atoms. 2) For **molecules** and their constituent atoms.
- Settings, if and how to **group items** (context menu of atom list).
- Plus/minus signs (and commands) to **collapse or expand** trees of items.
- **Preview** of atom design in first column each.

## Other Improvements

In addition to the topics mentioned above, the new DIAMOND version 4 contains a large number of more-or-less "minor" improvements which shall only be given as a list here. For more details, please read the "What's New in Diamond Version 4" document that is available through the command "What's New" in the "Help" menu. We also recommend to have a look at the online help for the corresponding command and/or dialog window, which can be opened by pressing F1.

**Enhanced search for structure data** (File/Search) Improved file, folder, and format selection for searching files on your hard disk for structure data. The sequential search in files use the enhanced restraints for chemical composition, crystallography, as well as bibliographic references, as described above for "Crystallography Open Database".

**Color coding of structure parameter sets** (View/Color Coding) Multiple structure data sets in a document can now be differentiated by different colors: Colored rows in structure table, colored group headers in data sheet, colored tabs of preferred structure pictures as well as link buttons, and colored frames around picture thumbnails.

**Symmetry dialog** (Structure/Symmetry) A new symmetry dialog where you enter a space group symbol (or fraction of) or one or more space group numbers or a range, and Diamond automatically updates a list of matching space group settings. The Diamond 3 space group dialog is also still available as "Space Group Browser".

**Atomic parameters dialog** (Structure/Atomic Parameters) The new atomic parameters dialog gives a tabular representation of the atoms. Editing of atom's properties is now easier, since it can be performed directly in the row rather than in separate edit fields as in Diamond versions 2 and 3. Multiple atomic parameters on one and the same site each, i.e. the mixed sites' components, are displayed under a tree branch. Symmetry equivalent positions (as come often from



CSD-imported CIF files, in order to describe complete molecules when the asymmetric unit only reflects a fraction of those molecules) are marked separately.

**Picture start options** In version 3, the options, if and how far to create a structure picture for every dataset in a non-Diamond input file were somewhat hidden in the "File Import Assistant" (page "Picture creation") and not reachable, if the File Import Assistant was disabled. The picture start options are now available from the "Options" command of the "Tools" menu, which opens the dialog with the (new) "Picture Start" page. This gives you options if and how to create a picture automatically (proposal or by scheme or from Auto Picture Creator settings). The status of what happens when a picture is started is now shown and changeable in the status bar.

**Picture Creation Assistant** (Picture/Picture Creation Assistant) You can choose a building scheme or initialize the assistant's first pages with Diamond's proposal. The packing diagram option as well as "Create all atoms" have been enhanced. On the picture design page, you can choose a design scheme.

**Connectivity dialog (Bonds page)** (Build/Connectivity) The evaluation now considers also bond parameters to extend the bonding spheres from mean bond lengths and effective radii. The dialog (and the distances histogram) have variable size. Indicators mark changed/updated bonding sphere boundaries in the table of atom group pairs. Distances from bond parameters appear as ticks in the distances histogram.

**Add All Atoms command** (Build/Add All Atoms and Connections) The command has been extended for connection parameters. Now it can also consider H-bond and contact parameters (optionally by checkmarks in a dialog).

**Coordination Spheres and Fixed Spheres commands** (Build/Coordination Spheres) The separate command "Fixed Spheres" as known from prior versions has been removed but merged with "Coordination Spheres". The extended "Coordination Spheres" dialog now offers "Generic", "Fixed size", and "Atomic environments" as sphere type – similar to the "Add Coordination Polyhedra" dialog. The new checkbox "Connect atoms" enables to have central and ligand atoms to be connected independent from the type of sphere. (Note: The command "Fixed spheres directly" - using the latest *RMin* and *RMax* - is still available from the dropdown menu next to the "Coordination Spheres Directly" toolbar button.)

**Connect Atoms dialog** (Build/Connect Atoms) The command now opens a dialog and offers additional connection methods: "Between atoms belonging to selected atom groups and/or sites" and "Around atoms currently selected in structure picture. Atomic environments and fixed sphere boundaries as alternative bonding sphere criterion.

**Broken-off bonds dialog** (Build/Broken-off Bonds) This new command and dialog offers functions to convert between normal and broken-off bonds or to delete all or selected broken-off bonds (together with the invisible atom at the broken-off end each).

**Complete Fragments dialog** (Build/Molecules/Complete Fragments) The command can be applied to all atoms or the currently selected atoms - as before - but also to atoms of selected atom groups or selected sites. (Tree view as in Coordination Spheres dialog or new Connect Atoms dialog.)

**Add Coordination Polyhedra dialog** (Build/Polyhedra/Add Coordination Polyhedra) The sphere criterion "Atomic environments" is also available here as well as "As is", which means the missing neighbouring atoms inside the sphere boundaries will not be complemented but a coordination polyhedron from the neighbouring atoms currently connected to the central atom is constructed each.

**Additive and subtractive selection** (Edit/Selection Mode submenu) The selection mode "additive selection" enables selecting objects by clicking on without loosing the other selections. "Subtractive selection" allows to individually switch off selections.

**Expand selection** (Edit/Expand Selection) This expands the current selection stepwise to the neighbouring (bonded) atoms and bonds. The first click selects the bonds, the second click each



selects the bonded neighbouring atoms, etc. Selection expansion is also available with the mouse wheel, see "Changing properties with the mouse wheel" above.

**Structure picture thumbnails preview** The picture thumbnail preview now offers three settings "Tiles", "Content", and "Details", where "Tiles" only gives the picture's title, whereas "Content" and "Details" give more information about the picture each. The pictures can also be grouped by structure data sets (multiple pictures for multiple structures in a document) as well as sorted for several criteria.

**Full screen view** (View/Full Screen) In this mode the document window occupies the full screen, while toolbars, docking windows, status bar and menu bar are hidden.

**Tables of connection parameters** (View/Table/Connection Parameters submenu) The connection parameters bonds, H-bonds, and non-bonding contacts (cf. "Structure/Connection Parameters...") can also be listed like e.g. the atomic parameters.

**Table of created molecules** (View/Table/Created Molecules) This new table lists all molecules in the structure picture, regardless if (still) fragmentated or (already) complete.



## Basic Software Handling

The following subsections give you a short introduction to the general handling of DIAMOND software and are especially dedicated to users with little knowledge in handling of general Windows software. More experienced users should continue reading on p. 2 where the usage of the DIAMOND software is described in detail in a series of tutorial sessions.

### Starting the Software



The DIAMOND software is generally<sup>25</sup> started by double-clicking on its symbol on the so-called "desktop" (the screen that is displayed right after the Windows operating system has been loaded). Alternatively, you can also press (click on) the Windows "Start" button (generally on the lower left-hand side of your screen) using the left mouse button, or Ctrl+Escape key, or the Windows key on your keyboard. Afterwards, please click on "Programs"<sup>26</sup> which will open the list of programs that are available on your computer. Now, select "Diamond 4" using the left mouse button, and finally click on "Diamond" which will start the software.

If there is no entry "Diamond 4" in the "Programs" list even if you press the space bar, the database and the software might not have been installed on your computer yet. In this case, please read the chapter "Installation" on p. 59 and follow the instructions given there before you continue.

Once DIAMOND has been started, it brings up a "splash screen" (with version number, copyrights, and license informations) and, with a few delay, the "application window" with the "Start" view. (Fig. 92).

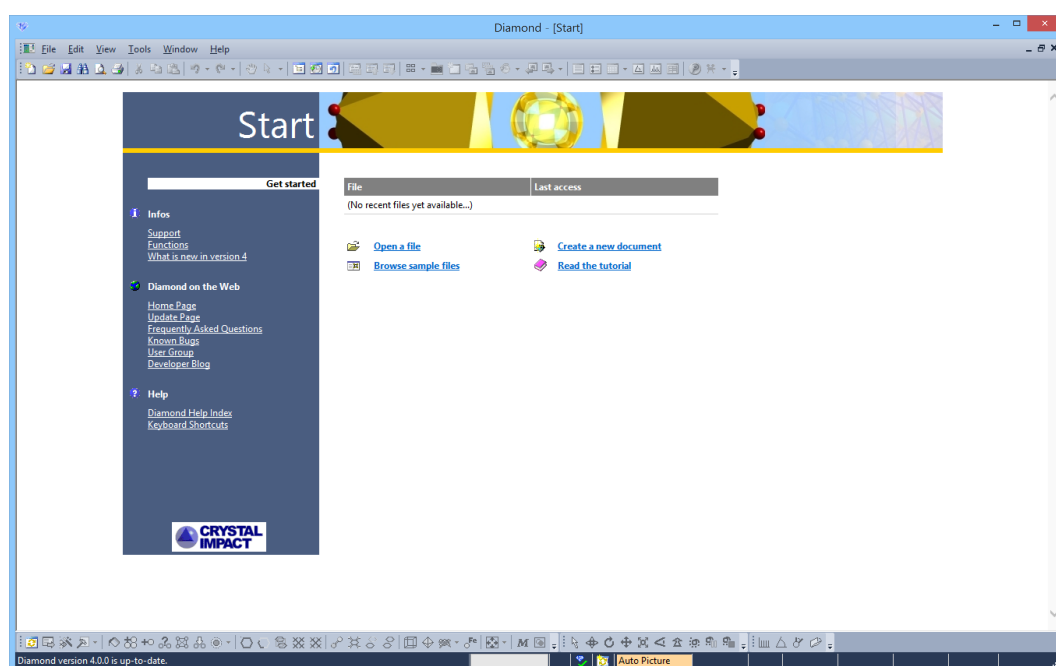


Fig. 92: DIAMOND has just been started.

### Application main window

The "application window" or "main window" of DIAMOND consists – like average Windows desktop software – of the typical user interface parts **title bar**, **menu bar**, **toolbars**, and **status bar**. The main part of the window is the **working area**. Here, you work with your structure pictures and other data.

<sup>25</sup>On Windows 8 or 8.1, the "Start Screen" (with the colored tiles) may be the default screen rather than the "Desktop". Diamond will start with a single mouse click or a finger tap on the "Diamond 4" tile. Or simply start typing "diamond" and select one of the search results in the right part of the screen.

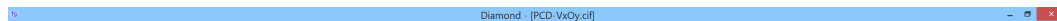
<sup>26</sup>The actual names and commands may vary depending on the language of your Windows operating system.



Note: The following refers to a typical DIAMOND working session with a document (file) open – rather than the "Start View" depicted above.

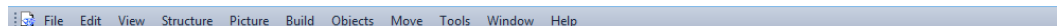
## Title Bar

The Windows title bar displays the name of the program ("Diamond") and the currently active document:



## Menu

Like most Windows applications, DIAMOND has a menu bar below the title bar:



To activate the menu use the left mouse button and click on an available item. Alternatively, you can press the Alt key, choose the appropriate entry using the cursor keys, and then press Enter. Some menu entries may be parents of another menu, a so-called "submenu".

**Please note that not all commands of the main menu are available, depending on which of the panes<sup>27</sup> has the input focus! In order to change the input focus, simply click into the pane you would like to switch to or use the View menu.**

You find all commands to activate a specified content in one of the panes in the View menu.

## Toolbars

A toolbar is a control bar which contains a row of button images, often called "icons". These buttons represent a lot of functions which are also available via menu commands, such as "New", "Open", or "Save". Additionally they contain buttons for commands that you else would reach only indirectly (e.g. via dialog boxes).

By default, there are two toolbars:

One at the top



and one at the bottom of the screen.



The toolbars are usually aligned to the top and the bottom of the window. However, the toolbars can be "docked" to any side (or sides) of the window. They can also be made to "float" in draggable "mini-frame windows", and you can resize floating toolbars.

You can shift, dock or "undock" a toolbar by dragging the corresponding toolbar with the left mouse button. You can also switch between docked and floating state by double-clicking into the interior of the toolbar (but outside the buttons on the toolbar). You can hide and re-display toolbars via the Toolbars command from the View menu.

## Status Bar

The status bar at the bottom of the screen displays various messages about the current state of the program.



<sup>27</sup>The distinct parts of the working area below the toolbar are also referred to as so-called "panes".



During lengthy processes, such as updating a large structure picture, the progress of the operation will be displayed here.

## Working Area

The working area is subdivided into so-called **”panes”** showing graphical as well as textual information. These panes are complemented by so-called **”docking windows”**. These kind of windows can float (like dialog windows) but also be docked at one of the sides of the application main window – or collapsed (with only the tile visible) or completely hidden (closed). Fig. 93 shows a typical situation when working with DIAMOND:

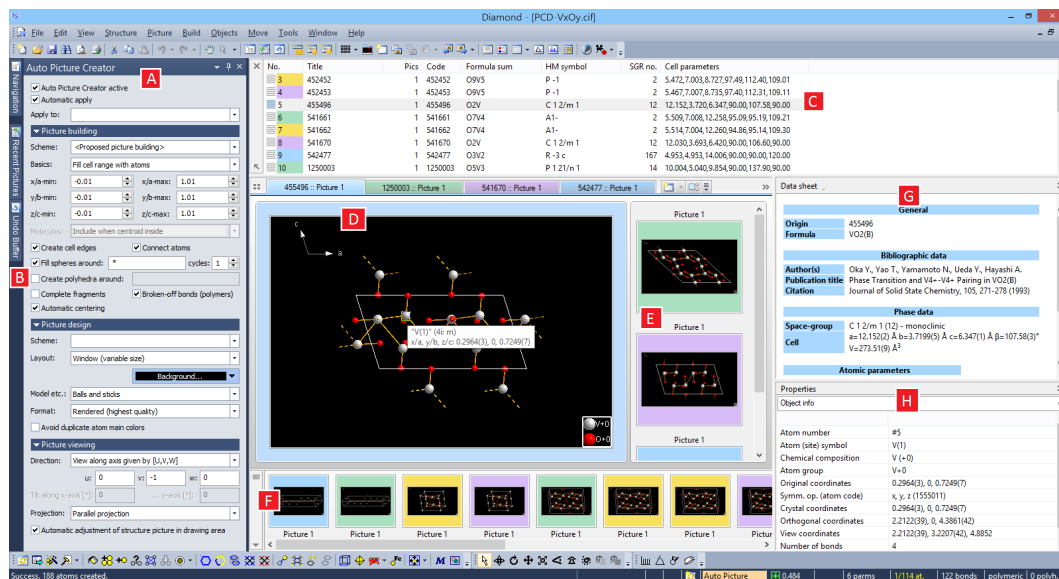


Fig. 93: Typical Diamond screen in action with several working areas.

**Auto Picture Creator (A)** This dialog in a dockable pane contains offers the most common settings in the categories picture building, design, and viewing and reflects changes automatically, provided "Automatic apply" is activated. (More information in the online help for "View/Auto Picture Creator". About getting online help, read below.)

**Collapsed docking panes (B)** Three more docking panes (Navigation tree, Recent pictures list, and Undo buffer) are collapsed in this example. They open when the mouse cursor hovers the vertical tab. To keep a docking pane open ("dock"), press the pin symbol in its title bar. (Cf. "View/Navigation", "View/Recent Pictures", and "View/Undo Buffer".)

**Structure table (C)** The list of structure parameter sets (here: 20 in document "PCD-VxOy.cif"). This table can collapse to a single-line "structure info bar". (Cf. "View/Structures/Show Table" and "View/Structures/Show Info Bar".)

**Picture Edit View (D)** The main structure picture, which has full access to all editing functions, with its title tab (together with more tabs for other "preferred" pictures). (Open the "What's New" page from the "Help" menu and read the article "Editing of a structure picture side-by-side with the other pictures' thumbnails in a multiple picture document".)

**Tabbed pictures overview (E)** Thumbnails of more ("preferred") pictures (selected by the user), for instance in order to compare with the picture in the Edit view.

**Picture Link Bar (F)** This contains thumbnails of the residual pictures - of the structure or of the whole document.

**Data sheet (G)** (Note: There is no more two separate views, "data sheet" and "data brief", as was in Diamond 3.) The data sheet is configurable as "comprehensive" (like the "data sheet" in Diamond 3) and "brief" (which is the default setting). (Cf. "View/Data Sheet".) Besides this,





the contents and order of the items in the data sheet can be configured ("customized") by the user.

**Properties pane (H)** - here with the properties of the selected atom, cf. info tip in structure picture. (Cf. "View/Properties".)

The contents of this area is described in detail on p. 4 during the first tutorial session.

### Context-sensitive menus

Each of the panes in the main window has a specific context menu. Unlike the pulldown menus from the main menu bar (File, Edit, View, etc.), these menus are context-sensitive and depend on the pane you are working with or you have clicked into and eventually the object you have selected. They are opened by clicking the right mouse button in the specific pane. If you e.g. right-click on an atom or a bond in a structure picture, there are several commands in the context menu to edit the design, add a label or change the model.

You can open such a context menu either

- by clicking with the right mouse button or
- by using the keyboard (Shift+F10 or the special context menu key on a Windows keyboard)

### Context-sensitive help

The following subsections describe where and how context-sensitive help is available for the several working situations in your DIAMOND session.

**Pressing F1 key** If neither a dialog box is open nor a menu item is highlighted, pressing of the **F1** key opens the help page at the index.

If a menu item is highlighted, help for that menu item (usually command) will be displayed. The menu item may be highlighted using the mouse or with the cursor keys.

If a dialog box is open, **F1** will show specific help for the usage of that dialog and the meaning of the controls in the dialog box.

**Entering Help Mode** A special mode, the "Help mode", is activated by pressing the **Shift+F1** key combination. This is a more versatile method of getting context-sensitive help. After this mode has been activated, the mouse cursor changes to a symbol consisting of standard arrow and question mark. In this mode, you will get context-sensitive help, if you click on a menu item or a symbol in a toolbar or on special parts of the main window, such as the status bar, system menu etc.

The Help mode can be cancelled by pressing the **Esc** key. The previous mouse cursor will be restored. The Help mode ends automatically, when you get help for a clicked item.



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