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**Citation of Match!**

If you like, you can add the following citation/reference in your paper:

Match! - Phase Identification from Powder Diffraction, Crystal Impact - Dr. H. Putz & Dr. K. Brandenburg GbR, Kreuzherrenstr. 102, 53227 Bonn, Germany, https://www.crystalimpact.de/match

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Welcome!

Welcome to the Match! software! This chapter contains some information that might help you when using the software for the first time, so please take a little bit of time to fully read it and understand its contents.

Match! is a software for phase identification from powder diffraction data. It compares the diffraction pattern of your sample to a database containing reference patterns of known phases, to find out which phases might be present in your sample. Additional knowledge about the sample like known phases, elements or density can be applied to restrict the number of suggested solutions. In addition to this qualitative analysis, a semi-quantitative as well as a quantitative analysis (using Rietveld refinement) can be performed as well.

As reference pattern database, you can apply the included free-of-charge COD database and/or any ICDD PDF product. In addition, it is possible to create a user database based on your own diffraction patterns. The user database patterns can be edited manually, imported from peak files, calculated from crystal structure data (e.g. CIF files), or imported from your colleague’s user database. Finally, you can import and use the data from any ICSD/Retrieve release between 1993 and 2002, if you have a valid license for it.

Throughout most chapters in this manual, the COD-Inorganics reference database that is installed along with Match! is used. If you would like to apply a different reference database (like the ICDD PDF), please read the chapter “Reference pattern database” starting on p. 72, in order to learn how to setup Match! accordingly.

If you have not yet installed Match! on your computer up to now, please follow the guidelines in the software maintenance chapter starting on p. 116. If you intend to run Rietveld refinement calculations with Match! using FullProf, you can already install FullProf right now (see p. 119), so that Match! can detect the presence of FullProf automatically when it is first run. However, it is also no problem to install FullProf and add the path to it in the Match! options later if required.

Once you have setup the software on your machine, please follow the chapter “Quick start” on p. 10 in which the basic usage of the program is demonstrated.

As soon as you have managed the “Quick start” chapter, please take a look at the chapter “Common operations” on p. 16 where you will learn about the most frequently used operations in Match!. Afterwards, you are ready to tackle your own phase identification projects. Typically, they will be more complicated than the simple quick start example, so we strongly recommend reading the chapter “Qualitative phase analysis” on p. 27 in order to get instructions how to perform tasks beyond the simple, automatic operation demonstrated in the “Quick start”. This is also recommended for more advanced users, because in these chapter many operations that you will use very frequently in phase identification are explained, in addition to a lot of background information that will provide you with a deeper understanding of the whole process.

If you are an experienced user and would like to get a quick overview on how to operate the software, please have a look at the chapter “Table of mouse button and key combinations” on p. 124 in the Appendix.

If you need help or are in doubt how to perform a certain operation, the first place to look at is the online help. There are two basic keyboard shortcuts you should always keep in mind in this context:

- F1 (<Cmd+?> on the Mac) will open the online help at the index page, so that you can easily search for information about a given keyword/issue.
- <Ctrl+J>1 will display a table of all mouse operations and keyboard shortcuts that can be used.

This manual can also be a valuable source of information. Finally, some tutorial videos are available on our web page

https://www.crystalimpact.de/match/videos.htm

where common operations are demonstrated in practice.

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1 On the Mac, you have to press Cmd+J instead.
Quick start

This tutorial will give you an introduction to the Match! software. You will perform a rather simple phase identification exercise and will be guided through the most important features of the software, so that you can start using it in your own projects right away. The basic aim of this chapter is to give you a first impression of the basic handling of the software: Pattern import, search-match, phase selection, quantitative analysis, report printing.

You are now certainly eager to get things running and start identifying phases with Match!. This chapter will show you the most important functions of Match!, enabling you to tackle your own phase identification problems straight away afterwards.

Before you follow the tutorial session described in this chapter, we strongly recommend to restore the default (factory) settings of Match!, just in case you or a colleague have used Match! on this machine/account earlier and changed these settings. To do so, please start Match! now (if it is not already running). Afterwards, select the “Restore factory settings” command from the “Options” menu, which will reset all options to the original ones selected by Crystal Impact. Please confirm (by clicking “Yes”) that you would like to do so, and confirm to keep your reference databases when you are asked for this. Match! will now operate exactly like it has just been installed.

When you run Match! for the first time (or have reset it to the factory settings), you will be asked which default level of automation (“user level”, “Beginner” or “Expert”) you prefer (Fig. 1).

In the “Beginner” mode Match! performs a nearly complete automatic processing of the initial steps: All you have to do is to select the diffraction data file you would like to analyze (you will be prompted automatically for it once the software has been started). Afterwards, Match! will automatically process the raw data, determine the peaks, and run the search-match calculation. All that remains to do is to select the “matching” phases (e.g. by double-clicking or dragging the corresponding entries from the candidate list on the left-hand side to the Match list to the right), and finally display the report containing e.g. the list of matching phases as well as their arbitrary amounts (e.g. by selecting “View/Report”).

In the “Expert” mode you have to perform nearly all actions manually. This mode is especially recommended for experienced users who would like to analyze more complicated samples.

You can customize the user level (“batch” behavior) in detail also later on the “Batch” tab of the “Options” dialog.

Two final remarks: Please note that this tutorial session has been carried out using the COD-Inorganics as reference database. If you use another reference database like the ICDD PDF or your own diffraction data, the results may be different! Besides this, all screenshots in this manual have been captured on a Windows 10 system. On other operating systems, their basic contents will be the same, although there may be slightly different window frames.

Let’s start with a very simple example so that you can draw your attention to the usage of Match! rather than to the actual phase identification problem. In fact, all you must do is to select the diffraction data file that you would like to analyze; Match! will do the rest.
Here we go: Suppose that you have obtained a high-quality powder diffraction pattern of a mineral sample. If you have not already done so, please start the Match! software now. Match! will display a nearly completely empty screen, as well as a “File/Open” dialog box (Fig. 2).

The Match! screen is divided into four parts: In the large panel on the upper left hand side, the diffraction pattern is displayed. Below, the list of candidate entries (“candidate list”) is placed. On the right-hand side, the dialog elements for the selection of restraints (like the periodic table) is displayed by default. They may be replaced either by the “peak list” or the “data sheet” for the currently marked entry. In the lower right-hand corner, the table of matching entries (the so-called “match list”) is located.

![Fig. 2: Match! has just been started. In its default “Beginner” setting, it opens a dialog in which you can select the diffraction data file you would like to analyze.](image)

The first thing you have to do is to select the diffraction data file you would like to import. In order to do so, please mark the file “quickstart.rd” in the “Tutorial” subfolder of Match!’s program directory, then press “Open”.

Match! will now run through the following steps automatically:

1) Import the diffraction data from the selected file

2) Process the imported raw data, i.e. strip the alpha2-contribution to the X-ray radiation (if required), detect the peaks and finally check/correct a potential 2theta error.

3) Run a search-match calculation.

Your screen should now look like Fig. 3.

---

2 If you do not know how the install or run the software, please have a look at the chapter “Installing and running Match!” starting on p. 83.
Fig. 3: Match! has run the raw data processing as well as the search-match calculation automatically.

The entry with the best (largest) so-called “figure-of-merit” has already been marked in the candidate list at the bottom left, so that you can evaluate its agreement with the experimental diffraction pattern in the diffraction pattern on the top left-hand side.

You now have to select the entries that you assume to be present in the sample, based both on the “figure-of-merit” values as well as the visual inspection of their agreement with the experimental pattern:

As you see, the entry with the best (highest) figure-of-merit belongs to the phase CaCO$_3$ (Calcite). To select the first entry as matching, please press the space bar while the first entry CaCO$_3$ (Calcite) is still marked in the candidate list. Alternatively, you can also double-click on the corresponding entry, or drag the corresponding entry from the candidate list to the Match list on the right-hand side (using your mouse). The selected phase will now be displayed in the Match list on the right.

The remaining entries belonging to the same phase as the selected entry have now vanished, because the corresponding peak intensities are now “occupied” by the selected phase/entry (Fig. 4).

You might note the column “I/Ic” on the right-hand side of the candidate list. Here, you can see if the corresponding entry contains the parameter I/Ic required for (semi-)quantitative phase analysis (p. 39). If you are using the COD as reference database (which is by default installed along with the Match! software), this parameter is available for all entries, since it has been calculated along with the diffraction pattern in the data import process. However, if you are using the ICDD PDF or other reference databases, there may be entries that do not contain the I/Ic parameter, so these entries would not be suitable for semi-quantitative phase analysis.
Fig. 4: The first phase (CaCO$_3$, Calcite) has been selected as “matching”.

There are still several entries left in the candidate list with good (high) figure-of-merit values, so there are more phases present in the sample obviously. The next best-matching entry has already been marked in the candidate list automatically, so you can clearly identify the second phase being SiO$_2$. Again, please press the space bar when the corresponding entry is marked, like you have done before for Calcite. By doing so, you have selected this entry as matching as well.

The next “unmatched” line in the candidate list belongs to an entry describing the phase Al$_2$O$_3$ (Corundum). Please compare it visually to the experimental pattern, then press the space bar to select it.

As you see (Fig. 5), the next entry has a rather low figure-of-merit (FoM) value (indicated by the orange-red bar on the right-hand side), so there is little chance that this phase is also present in your sample. Hence, it is highly probable that all (major) phases in the sample have been identified.
Fig. 5: The identification of phases in the unknown sample is complete. Note the column “Quant. (%)” in the candidate list in which the weight percentage of the matching phases in the sample is given.

At this point the semi-quantitative phase analysis is also completed: Please have a look at the column “Quant. (%)” in the match list: Here you can see that your sample contains about 60% (weight-percentage) Corundum, 23% Calcite and 17% SiO₂ (Quartz).

There is nothing left to do but display the report. In order to do so, either press the combination <Ctrl+R> on your keyboard (<Cmd+R> on the Mac), click the corresponding toolbar button, or select the “Report” command from the “View” menu. This will open the dialog window shown in Fig. 6.
Fig. 6: Once you have finished selecting the “matching phases” in the candidate list, you should display the Report providing the detailed results of the analysis.

As you see, the report contains a detailed analysis of your sample. The most important information is given at the top of the “Matched Phases” section: Here, you can see the list of matching phases, i.e. the phases that are most likely to be present in your sample, along with the corresponding arbitrary amounts (based on a semi-quantitative analysis). In our case, the sample consists of 59.8% Corundum (Al₂O₃), 23.6% Calcite (CaCO₃) and 16.7% Quartz (SiO₂).

Well, that’s it already! If you like, you can now print or save the report, simply by pressing the corresponding buttons at the bottom of the Report window.

The example you have just processed is rather artificial, and certainly most “real world’s” phase identification tasks are not so easy to solve. In this context, please note that by default Match! is running using the “Beginner” batch setup, in which as many steps as possible are run automatically. For more advanced users, it is certainly recommended to operate the software more “manually”, i.e. to select a “higher” user level (e.g. “Expert”).

To do so, simply close the report now (press “Quit”), then either press the button in the toolbar at the top, or select the “Batch options” command from the “Options” menu. Once the “Options”-dialog is displayed, bring the “Batch” page into front, and select your “user level” in the combo box at the top. In addition (or as an alternative), you can select each single step that shall be carried out automatically using the options below. Finally, please do not forget to mark the “Save as defaults” checkbox at the bottom before closing the dialog, to make your changes permanent.
Common operations

You should now be familiar with the basic usage of the Match! software demonstrated in the chapter “Quick start”. In this chapter, you will find more information about some frequently used functions and operations.

Several actions and operations that are used very frequently when working with Match! are summarized and described in the following sections:

Context menus

First of all, please note that many operations can be run (as well as options set) using so-called “context menus”. You can open the corresponding context menus and get access to the commands by right-clicking into the corresponding area of the screen. Try to do so in the diffraction pattern graphics, the candidate list, the match list and the peak list!

Mouse and keyboard shortcuts

A variety of operations like peak editing, zooming and tracking can be controlled using the mouse in combination with certain keyboard buttons. In addition, a lot of common commands cannot only be run from the menu but also by pressing key combinations like <Ctrl+I> (<Cmd+I> on the Mac) for the import of diffraction data.

You should look at the chapter “Table of mouse button and key combinations” on p. 124 in the Appendix. This table can also be displayed within the software by pressing <Ctrl+J>³. Knowing the keyboard shortcuts and mouse operations by heart will speed up your work and make it much easier!

Zooming and tracking/panning

To zoom into a certain area in the diffraction pattern graphics, press the left mouse button and keep it pressed while moving the mouse across the area you are interested in; Match! will adapt the graphics accordingly.

Alternatively, you can simply double-click the left mouse button, to focus into the area around the current mouse position. Double-click again in order to view the full pattern again.

Another available option is to use the mouse wheel for zooming: Move the mouse cursor to the region in the diffraction pattern you would like to focus on, and turn the mouse wheel away from you in order to focus right into this area (or out again, if you turn the mouse wheel into the opposite direction).

Once you have zoomed into the diffraction pattern, you can shift the pattern by keeping the “Shift” button on your keyboard (or the center mouse button/wheel) pressed while moving the mouse around (the so-called “tracking” or “panning”).

Finally, it is also possible to exactly define the area (intensity and 2theta) you would like to display. A corresponding dialog is now provided for this purpose (menu “View/Define zoom area…”).

Axis scaling

The scaling of the x- and y-axis in the diffraction pattern can be changed easily: Simply click on the axis label, and select the scaling you are interested in. As an alternative, you can make these selections on the “Options” page of the “Graphics” dialog; you can directly open this page either by pressing <Ctrl> + <Alt> + G (<Cmd> + <Alt> + G on the Mac), or by clicking on the corresponding button in the toolbar.

On the x-axis of the diffraction pattern graphics you can select 2theta, d-values or 1/d.

For the y-axis, you can select relative intensity (I rel.), count (cts), as well their corresponding logarithmic and square-root representations.

³ On the Mac, you have to press <Cmd+J> instead.
In order to make the current scaling permanent (i.e. to be used as default), please open the “Graphics options” dialog from the “Options” menu, mark the “Save as default” checkbox on the bottom left, then press “OK”.

**Colors, line styles and fonts**

You can define individual colors and line styles for experimental diffraction data, calculated patterns, reference patterns etc. It is also possible to define the fonts for text labels in the diffraction pattern as well as the dialog elements (texts on buttons, in dialog windows etc.).

All of this can be achieved in the “Colors and line styles” dialog that can either be opened from the “Options” menu, as well as by pressing the corresponding button in the toolbar. Note that you can make your changes permanent by marking the “Save as defaults” checkbox at the bottom of the dialog.
Raw data processing

Most important for a reliable analysis is the quality of the diffraction data on which it is based (e.g. peak positions and intensities for qualitative analysis/search-match). This chapter provides you with detailed information how to best process your raw diffraction data in order to achieve this goal.

Basics

One of the key functionalities in Match!, the qualitative analysis (often abbreviated as “search-match”) is to a large degree based on the Bragg peak data (d-values and intensities) of your sample’s diffraction pattern. Although the determination of the peak data from the raw data can be run automatically before a search-match calculation (as you have seen in the “Quick start” chapter), the computer is still not able to equal the “eye” of an experienced powder diffraction specialist who is normally much better e.g. in distinguishing between noise and peaks. Hence, with normal and especially with low quality diffraction data it is worthwhile to invest some time in a critical evaluation of the peak data with regard to the raw data. Match! offers several functions which make this procedure as comfortable as possible.

In the following, we assume that Match! is working in the “Expert” user level (so that it does not perform any operations automatically). You can switch Match! to this user level (e.g. if you have selected “Beginner” when running Match! for the first time) at the top of the “Batch” tab of the “Options” dialog (which can be opened from the “Options” menu).

Here are some suggestions for a reasonable workflow for raw data processing:

Trim diffraction pattern

After importing your raw diffraction data file into Match! (e.g. by pressing the ‘+’ button in the upper right corner of the pattern graphics, or by using the “File/Import/Diffraction data” command in the menu), take a critical look at your data. Sometimes there are areas (typically at low 2theta values) that contain effects which have nothing to do with your sample, e.g. cutoff or primary beam radiation.

If this is true, you should remove these “surplus” area(s) (“trim” your diffraction pattern), in order to focus on the analysis of your sample’s diffraction pattern. You can do so by moving the mouse cursor to the left (or right) of your diffraction pattern until it changes ( or ), press the left mouse button, and move the mouse to the right or left until the area you would like to remove has been marked. After releasing the mouse button, your diffraction data will be trimmed (i.e. the unwanted areas will be removed).

Alpha2 subtraction

If the radiation used in your diffraction experiment does not only contain the alpha1 but also the alpha2 component, you can now subtract the alpha2-contribution (menu “Pattern/Subtract alpha2”). However, please note that this is not mandatory: It is perfectly possible (even advisable) to perform a complete phase identification with the alpha2-contribution still present! Stripping the alpha2-contribution may even be a disadvantage if your data contains a significant amount of noise, because the noise will be increased, and surplus “ghost” peaks may be introduced in peak searching (see below).

Background definition

The contribution of the background radiation (simply called “the background”) is first determined automatically during the import of the diffraction data. It is displayed as an (by default) orange colored curve with small squares (control points) at the bottom of the raw (profile) diffraction data right after the import (Fig. 7).

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4 Don’t forget to mark the “Save as defaults” checkbox in the corner on the lower left-hand side of the “Options” dialog, if you would like to make this setting / user level permanent!
5 We recommend to switch over to the “Expert” user level for these tasks, as described in the “User levels” chapter on p. 25.
6 You must have fully zoomed out for this to work, i.e. your diffraction data limits must be equivalent to the limits of the pattern graphics.
There may be cases though in which the automatic determination does not give a satisfactory result, so that you would like to correct it. This should be done before running the peak searching command!

Maybe the automatically determined background does not completely detect all structures, either because the background is too “rigid” (in which case amorphous “humps” are not fully covered, leading to surplus peaks when using the automatic peak searching), or too flexible (in which case profile areas that belong to the peaks may be covered (i.e. hidden) by the background).

You can correct these issues by pressing <Ctrl+F2> (if you would like to increase the background flexibility) or <Ctrl+F3> (if the background shall be more rigid (cover less of the peak sockets), i.e. in order to decrease the flexibility) until the visual agreement between the orange curve and the estimated background is acceptable.

It is also possible to modify the shape of the background curve manually, simply by dragging around the control points of the background curve using the mouse. You can easily add more control points if required if a critical part of the curve cannot be modeled right yet, or delete surplus control points (e.g. on a straight line), by clicking the right or left mouse button if the mouse cursor is at the corresponding position (Fig. 8).

In order to do so, please make sure that the background curve is currently displayed. Afterwards, please note the small squares on the curve. These are the so-called “background control points” just mentioned. You can shift these points by first moving the mouse on top of them, pressing the left mouse button, and moving the mouse around.

If you would like to add more control points (e.g. to be able to model a certain critical range of the background curve more accurately), you can do so by first moving the mouse to the desired position on the background curve. The mouse cursor will change (a ‘+’ sign will appear on the top left of the cursor); you can now press the left mouse button in order to add a control point at the corresponding position of the background curve.

In order to delete a control point, simply move the mouse cursor on top of it, then press the right mouse button.

Please take a look at the chapter “Table of mouse button and key combinations” on p. 124, too, in order to learn how to modify the background control points using the mouse. You can also watch a corresponding tutorial video on our web page:

https://www.crystalimpact.de/match/video_working_in_graphics.htm

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You can toggle the displaying of the background curve e.g. by right-clicking in the diffraction pattern and selecting “Background” from the context menu that opens.
**Please note:** If you intend to strip the alpha2 contribution in your profile data using the corresponding command from the “Pattern”-menu, please make sure to do so first before you modify the background manually, because your manually defined background will be overwritten by the alpha2 stripping function.

**Raw data smoothing**

If the pattern looks very rugged, you might try to run one or two steps of “raw data smoothing” (menu “Pattern/Raw data smoothing”), but keep in mind that small peaks might be extinguished if you overdue it, resulting in a potential loss of minority or even minor phases.

**Peak searching**

The most important part of the raw data processing is the searching for diffraction peaks, since the peak positions and intensities are the actual input to the search-match calculation (i.e. the qualitative phase analysis). Match! uses the well-known second-derivative method⁸ to perform the peak searching.

In order to get an initial set of peak data (that can be fine-tuned later), run the automatic peak searching by selecting the menu command “Pattern/Peak searching”, or by clicking on the corresponding toolbar button 🔄. Alternatively, a peak search is also carried out automatically if the profile fitting command (menu “Pattern/Profile fitting”, as described on p. 24) is executed without any peak data present. As a result, the profile fitting can be used as an alternative to the normal peak searching, both manually as well as during the automatic raw data processing.

With very low-quality data, however, it may be better not to use the automatic peak searching and add the peaks manually (see below).

**Please note:** It is rather important to check (and maybe correct) the background (p. 18) before running peak searching, to get accurate results and reduce the risk of getting surplus peaks or missing small peaks because they are hidden by the background!

**FWHM**

If you use the normal peak searching functionality, Match! will try to determine the FWHM (Full Width at Half Maximum) separately for each peak automatically. If this is not possible, it will use the corresponding default value

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(which can be adjusted on the “Raw data” tab of the “Options” dialog). If you would like to obtain even more accurate FWHM values, you should apply profile fitting instead of or after the peak searching.

Integrated intensities
Normally, the intensity values that are calculated during the peak searching procedure are integrated intensities, taking into account both the height as well as the FWHM of each peak. You can view the integrated intensity values in the peak list on the upper right-hand side. An exception to this is the relative intensity scaling of the vertical axis, in which case the integrated intensity values are scaled to a maximum value of 1000.0.

Peak searching sensitivity
One task associated with peak searching is to decide which “hump” or structure in the raw data corresponds to a Bragg peak, and which is just an artifact or noise. Obviously, there must be a certain parameter “sensitivity” using which the software can make this decision.

When peak searching (in any variant just described) is carried out for the first time, a default sensitivity is used which takes the noise found in the raw diffraction data into account. This default sensitivity has been chosen to obtain good results with a large variety of diffraction patterns. However, it may nevertheless be necessary to adjust the sensitivity for your special data. Note that you can also modify the default peak search sensitivity values for peak searching and profile fitting separately on the “Raw data” tab of the “Options” dialog.

Peak detection issues
If some peaks are not detected, this may be caused by the fact that when detecting a new peak (based on a second-derivative minimum), Match! searches for a maximum in the raw data within two times the FWHM. This can cause shoulder peaks to be neglected if the default FWHM value is relatively large. You should adjust the default FWHM value on the “Raw data” tab of the “Options” dialog (maybe you have to deactivate the corresponding “Automatic” option in order to be able to modify the default FWHM value).

If peak positions are not determined exactly, this may be caused by a relatively large step width in your raw/profile data. To fix this problem, you could try to increase the resolution (i.e. decrease the step width) by interpolation, using the menu command “Pattern/Increase resolution...”. You should start by trying a small factor (e.g. 2 or 3) first, because otherwise the noise may be “fixed” (i.e. fluctuations are described by too many data points, so they are no longer detected as “random noise” but as a “signal”). Repeat the peak detection after increasing the resolution.

If far too many diffraction peaks are frequently determined during peak searching, we recommend enabling the raw data smoothing for the automatic raw data processing in the corresponding “Options” dialog page. Start with a single “Number of repetitions” and maybe increase this number if the result is not sufficient.

If there really is a lot of noise present in your raw data (so that raw data smoothing can hardly be avoided if you would like to keep the number of detected peaks at an acceptable rate), please apply the raw data smoothing gently and carefully!

Peak editing
Peak editing in the diffraction pattern
Now it is time to closely inspect your data: Match! offers a variety of keyboard shortcuts and mouse operation options for zooming and tracking; they are described9,10 in the chapter “Zooming and tracking” on p. 16. Zoom into the left-hand side (low 2theta region) of the pattern and inspect or edit peaks and their positions while slowly moving to the right (high 2theta region).

You can edit the peaks directly in the diffraction pattern using the mouse. Add, edit or delete peaks while scrolling through the enlarged pattern, and maybe fit individual peaks to the profile data to obtain accurate intensity values. Peaks can easily be added or edited using the mouse in combination with certain keyboard buttons9,10.

9 These features are also demonstrated in our tutorial video “Working in Match!’s Pattern Graphics” (https://www.crystalimpact.de/match/video_working_in_graphics.htm).
10 You should also have a look at the chapter “Table of mouse button and key combinations” on p. 82 in the Appendix.
Please note: Before you can start to edit the peaks in the pattern graphics using the mouse, you need to give the input focus to the diffraction pattern first, e.g. by clicking on it.

Take care that all maxima in the raw data that you estimate as being “real” diffraction peaks are “covered” by peaks, while at the same time using as few peaks as possible. Always keep in mind that the “empty” spaces between the peaks are as important to exclude non-matching phases as the peaks are important to find the matching ones! Hence, by only using the peaks you are certain about you can increase the separating power of the search-match calculation.

Add peak: If you would like to add a peak, please press the <Ctrl> button (<Cmd> on a Mac) first; the mouse cursor will change to \( \uparrow \). Keep the button pressed, move the mouse pointer to the corresponding 2theta position, and click the right mouse button. A peak will be inserted at the corresponding position. Once you have finished adding peaks, you can release the <Ctrl> keyboard button.

Depending on the (de-)activation of the profile fitting settings (2theta, intensity and/or FWHM, see below), the 2theta, intensity and/or FWHM value(s) of the new peak will be instantly optimized by automatic profile fitting, right after you have clicked the mouse button. If all three profile fitting options (2theta, intensity and FWHM) are active, it is enough to (right-)click somewhere in the peak area below the profile curve in order to add the peak.

If the calculated profile is currently displayed, the new peak data will be included in the profile and Rp-factor calculation automatically.

If no profile data are present, the top of the peak (i.e. the peak intensity) will be taken from the position of the mouse cursor. The FWHM of the peak will be set to the corresponding default value that can be defined on the “Raw data” tab of the “Options” dialog.

Please note: After adding the strongest peak you may want to run the “Scale relative intensities” command from the “Peaks” menu, in order to adjust the maximum relative peak intensity to a value of 1000.0.

Mark peak(s): There are several options to mark one or more peak(s):

- **Mark single peak:** Move the mouse cursor to a peak at or below the top of a peak (must be visible!). The mouse cursor will change to \( \uparrow \) or \( \downarrow \). Now, simply click the left button in order to mark the peak below the mouse cursor; marks at other peaks will be removed.

- **Mark selected peaks:** Move the mouse cursor to a peak at or below the top of a peak (must be visible!). The mouse cursor will change to \( \uparrow \) or \( \downarrow \). Press the <Ctrl> button on your keyboard (<Cmd> on the Mac), and keep it pressed while clicking on one or more peaks using the left mouse button in order to mark them, in addition to the peaks that are already marked. Finally, release the <Ctrl> button.

- **Mark range of peaks:** First, move the mouse cursor to the left of the left-most peak in the range you would like to mark. Press the <Ctrl> button on your keyboard (<Cmd> on the Mac), and keep it pressed while moving the mouse to the right until you have selected the range of peaks you would like to mark. Finally, release the mouse button and the keyboard button.

Marked peaks are indicated by a small triangle displayed at the top of the peaks in the pattern graphics. In the peak list, the corresponding lines are inverted.

Edit peak position: If you would like to edit a peak position (i.e. shift a peak on the 2theta axis), please move the mouse cursor close to the peak position (below the peak top), so that the mouse cursor changes to \( \uparrow \). Afterwards, press the right mouse button and move the mouse to the position inside the current viewing region where you would like to place the peak. Finally, release the mouse button. If the calculated profile and the Rp-factor are currently displayed, they will be updated with regard to the new peak position.

Edit peak position and/or intensity: You can also modify both peak position and intensity at the same time: Please move the mouse cursor close to the top of the corresponding peak until the mouse cursor changes to \( \downarrow \), then press the right mouse button and move the mouse to the intensity/2theta position where you would like to place the peak.
Finally, release the right mouse button. If the calculated profile and the \( R_p \)-factor are currently displayed, they will be updated with regard to the new peak position.

**Edit peak FWHM:** You can modify the FWHM (Full Width at Half Maximum) of marked peaks using the mouse: Mark one (or more) peaks as described above, then move the mouse over one of the marked peaks until the mouse cursor changes to \( \mathbf{\times} \), and finally turn the **mouse wheel** in order to modify the FWHM of the marked peak(s).

**Invert peak mark(s):** If you would like to mark all but a few peaks, you should use the “invert peak marks” facility: First, mark the few peaks you do not want to mark (see above), then press the **right mouse button** within the diffraction pattern (which will open the context menu), and select “Invert selection” from the menu.

**Delete peak(s):** To delete one or more peaks, you first have to mark the corresponding peaks in the diffraction pattern (see above). Once you have marked one or more peaks, there are several options to delete them:

- Press the **“Del” button** on your keyboard
- Press the **right mouse button** within the pattern graphics, and select the “Delete” command from the context menu
- Select the “Delete” command from the “Peaks” menu

If the calculated profile and the \( R_p \)-factor are currently displayed, they will be updated with regard to the remaining peaks.

**Deactivate peak(s):** You can deactivate individual peaks of the unknown sample's pattern so that they are not taken into account during the search-match (i.e. figure-of-merit) calculation. This is e.g. useful if you are not sure about a certain peak and would like to check what would be the result of the search-match without this peak.

To deactivate one or more peaks, you first have to mark them (see above). Afterwards, please press the **right mouse button** within the diffraction pattern and select “Deactivate” from the context menu (or use the corresponding command from the “Peaks” menu). The candidate list will immediately reflect the change in the FoM-values of the entries. However, you should perhaps perform a completely new search-match operation to check if there are new matching entries! Please note that **deactivated peaks are displayed in light grey** in the diffraction pattern.

**Activate peak(s):** You can reactivate individual peaks of the unknown sample's pattern you have deactivated earlier. Please mark the corresponding peaks (see above), then press the **right mouse button** within the diffraction pattern and select “Activate” from the context menu (or use the corresponding command from the “Peaks” menu).

**Peak editing in the peak list**
You can edit the peaks directly in the peak list using the keyboard. (If the peak list is currently not displayed, please select the “peak list” command from the “View” menu or press <Ctrl+L>.)

**Add peak:** If you would like to add a peak, please select the “Add peak(s)” command from the “Peaks” menu or press the corresponding button \( \mathbf{+} \) in the toolbar at the top. The “Add Peak” dialog will be displayed.

Please select if your data are 2theta, d-values or 1/d on the right-hand side of the dialog first. Afterwards, write the peak 2theta/d-value, the intensity and the FWHM in the corresponding fields. If you do not want to provide the FWHM value for each separate peak, you can activate the corresponding option below.

If you press the “**Add peak**” button afterwards, the peak will be added to your peak list, however, the dialog will remain open so that you can enter the next peak.

If you realize that you have accidentally entered a wrong peak after you have pressed the “Add” button, you can remove the corresponding peak again by pressing the “Delete previous” button.

Once you have finished entering peaks, please press the “**Quit**” button. The dialog will be closed.

**Edit peak position:** If you would like to edit a peak position of the experimental pattern, please activate the corresponding field in the **first** column of the peak list by double-clicking on it. The field will switch to the “**Edit**
mode. You can now enter the new value for the peak position. When you are finished, press <Return> or click on another field. Both the diffraction pattern and the candidate list will be updated immediately.

**Edit peak intensity:** This works similar to the editing of the peak positions: Activate the corresponding field in the second column of the peak list by double-clicking on it; the field will switch to the “Edit” mode. You can now enter the new value for the peak intensity. When you are finished, press <Return> or click on another field. Both the diffraction pattern and the candidate list will be updated immediately.

**Edit FWHM:** This works similar to the editing of the peak positions and intensities: Activate the corresponding field in the third column of the peak list by double-clicking on it; the field again in order to switch to the “Edit” mode. You can now enter the new FWHM value for the peak. When you are finished, press <Return> or click on another field. Both the diffraction pattern and the candidate list will be updated immediately.

**Mark peak(s):** You can mark individual peaks simply by clicking on the corresponding line(s) in the peak list using the left mouse button. If you keep the <Shift> or <Ctrl> button (<Cmd> button on the Mac) on your keyboard pressed while doing this, you can select more than one individual peak. The lines of the marked peaks are displayed inverted. Note that marked peaks are also indicated in the diffraction pattern by a small triangle displayed at the top of the peaks.

**Invert peak mark(s):** If you would like to mark all but a few peaks, you should use the “invert peak marks” facility: First, mark the few peaks you do not want to mark, then press the right button to open the peak list's context menu, and select the “Invert selection” command from this menu.

**Delete peak:** In order to delete one or more peaks, you first have to mark the corresponding peaks (see above). Once you have marked one or more peaks, please execute the “Delete” command from the “Peaks” menu, or right-click in the peak list (in order to open the context menu) and select the command from the context menu.

**Deactivate peak(s):** You can deactivate individual peaks of the unknown sample’s pattern so that they are not taken into account during the search-match (figure-of-merit) calculation. This is e.g. useful if you are not sure about a certain peak and would like to check what would be the result of the search-match without this peak.

To deactivate one or more peaks, you first have to mark them (see above). Afterwards, please open the peak list's context menu (by pressing the right mouse button on one of the marked peaks), then select the “Deactivate” command from this menu. The candidate list will immediately reflect the change in the FoM-values of the entries. However, you should perhaps perform a completely new search-match operation in order to check if there are new matching entries! Please note that deactivated peaks are displayed in light grey color.

**Activate peak(s):** You can reactivate individual peaks of the unknown sample's pattern you have deactivated earlier. Please mark the corresponding peaks, then open the context menu (press the right mouse button on one of the marked peaks) and select the “Activate” command from this menu.

Please note: After editing the strongest peak you may want to run the “Scale relative intensities” command from the “Peaks” menu, in order to adjust the maximum relative peak intensity to a value of 1000.0.

**Profile fitting**

While the normal peak searching algorithm is very fast and produces peak data appropriate for many “routine” problems, there may nevertheless be cases in which a more accurate determination of the peak parameters (d-value/2theta and intensity) is required, e.g. if a diffraction pattern contains “shoulder” peaks. In these cases, profile fitting may be applied.

During the profile fitting calculation, Match! tries to optimize the peak parameters (intensity, FWHM (“Full Width at Half Maximum”), and optionally 2theta) in order to obtain a reasonably good agreement between calculated and experimental diffraction pattern (profile data). This is achieved by using the peak data as parameters in a constrained least-squares refinement.

Profile fitting requires the presence of peak parameters (2theta, I, FWHM). If no peaks are currently present when the profile fitting command is executed, a special variant of the peak searching algorithm will first be applied internally. There are two major differences to the normal peak searching algorithm:
- There is no a priori minimum intensity for detected peaks, i.e. all potential peaks are taken into account at first. When the profile fitting calculation has finished, the peak data will be examined. Peaks revealing too low FWHM values will then be eliminated.

- The FWHM values of the individual peaks are already estimated during the peak searching, in contrast to the normal routine in which the same default FWHM value is used for all peaks.

If no peaks are currently marked/selected, the parameters of all peaks will be fitted, otherwise only the parameters of the marked peaks. Besides this, the user can select which parameter(s) (2theta, I, FWHM) shall be varied in the profile fitting. This can be achieved by clicking the corresponding buttons in the toolbar, by pressing the corresponding function keys <F6>, <F7> and <F8>, or alternatively be selecting the corresponding options in the “Pattern/Profile fitting” submenu:

<table>
<thead>
<tr>
<th>Peak parameter to be fitted</th>
<th>Toolbar button</th>
<th>Keyboard shortcut</th>
</tr>
</thead>
<tbody>
<tr>
<td>2theta</td>
<td></td>
<td>F6</td>
</tr>
<tr>
<td>intensity</td>
<td></td>
<td>F7</td>
</tr>
<tr>
<td>FWHM</td>
<td></td>
<td>F8</td>
</tr>
</tbody>
</table>

In other words: It is not only possible to perform a peak search followed by profile fitting for all peaks, but you can also fit individual parameters of individual peaks.

The default setting is to optimize intensity and FWHM values, and to leave the 2theta values resulting from the peak searching untouched. The reason is that the peak positions (2theta values) obtained by the second-derivative method for peak searching are generally extremely accurate.

The actual profile fitting calculation can be executed once the peaks and/or the parameters which shall be fitted have been selected. This is achieved simply by pressing the <F5> key on your keyboard, by pressing the corresponding button in the main toolbar, or by selecting the corresponding command in the “Pattern/Profile fitting” submenu. When the calculation is finished, the success is announced in the status bar at the bottom. Besides this, the Rp-factor which has been reached is given.

Profile fitting of the complete pattern (i.e. for all peaks) is implemented in Match! as an iterative process, where peaks are modified or eliminated in each so-called “pass” of the profile fitting. The profile fitting will stop either if convergence has reached (Rp-factor could not be reduced compared to the last pass), or if a maximum number of passes (currently 10) has been carried out.

When a combined peak searching/profile fitting calculation is carried out for the first time, a default sensitivity is used which takes the “noise” found in the raw diffraction data into account. This default sensitivity has been chosen to obtain good results with a large variety of diffraction patterns.

If you have the impression that the calculation either yielded too many or too few peaks, you might want to adjust the peak searching sensitivity for profile fitting on the “Raw data” tab of the “Options” dialog for your special data.

Normally, the intensity values resulting from the profile fitting procedure are integrated intensities, taking into account both the height as well as the FWHM of each peak. You can view the integrated intensity values in the peak list on the upper right-hand side. An exception to this is the relative intensity scaling of the vertical axis, in which case the integrated intensity values are scaled to a maximum value of 1000.0.

**Correction of 2theta errors using the mouse**

Once you have investigated the whole pattern and have settled on a set of peaks, check and (if necessary) correct the specimen displacement error as well as the zero point, using the corresponding commands in the “Pattern” menu. Use the histograms to decide on a certain correction value, and do not hesitate to come back and try a different correction if the search-match calculation did not give a reasonable result. Match! also offers a variety of tools for correcting 2theta errors using the mouse:
In addition to the 2theta correction functions “Zero-point” and “Specimen-displacement” that are available in the “Pattern” menu, it is also possible to directly adjust the experimental diffraction pattern manually using the mouse.

**Zero-point correction**
To shift the experimental diffraction data on the 2theta (x-) axis (zero-point correction), move the mouse into the diffraction pattern graphics, then press the <Ctrl> as well as the <Alt> buttons on your keyboard (<Cmd> and <Alt> on the Mac). The mouse cursor will now change into .

While keeping the <Ctrl> (<Cmd>) and <Alt> buttons pressed, turn the mouse wheel away from you in order to shift the experimental data to higher 2theta values, or towards you in order to shift to lower angles. The changes will be automatically applied to the candidate list as well as the peak correlations to reference diffraction patterns.

In order to restore the original 2theta values, simply press the mouse wheel button while keeping the <Ctrl> and <Alt> buttons pressed.

**Specimen-displacement correction**
The procedure to apply a specimen-displacement correction to the experimental pattern is pretty similar to the zero-point correction:

In order to shift the experimental diffraction data on the 2theta (x-) axis with cos(theta)- (Bragg-Brentano geometry) or sin(2theta)- (asymmetric geometry) dependence (specimen-displacement correction), move the mouse into the diffraction pattern graphics, then press the <Shift>, the <Ctrl> and the <Alt> buttons on your keyboard (<Shift>, <Cmd> and <Alt> on the Mac). The mouse cursor will now change into .

While keeping the <Shift>, <Ctrl> (<Cmd>) and <Alt> buttons pressed, turn the mouse wheel away from you in order to shift the experimental data to higher 2theta values, or towards you in order to shift to lower angles. The changes will be automatically applied to the candidate list as well as the peak correlations to reference diffraction patterns.

In order to restore the original 2theta values, simply press the mouse wheel button while keeping the <Ctrl> and <Alt> buttons pressed.

**Specimen-displacement correction for asymmetric geometry**
In addition to the specimen-displacement correction for Bragg-Brentano geometry just mentioned, a correction for asymmetric geometry is also available. The geometry (as well as the parameter Ω for the asymmetric geometry) can be adjusted at the bottom of the “Raw data” processing tab of the “Options” dialog.

**Correction of 2theta errors using internal standard**
To correct potential 2theta errors, you can also use an internal standard if you know that a certain phase is present in the sample. Simply press <Ctrl+F> (<Cmd+F> on the Mac) (or click into the corresponding field “Find phases/entries” to the right of the toolbar at the top), then type the name, the formula sum or the entry number of the known compounds, and finally press <Return>. Match! will make sure that the corresponding entries are displayed in the candidate list at the bottom of the screen, and then automatically highlight the first entry matching your criterion (e.g. name or formula sum). As a result, the corresponding diffraction pattern will be displayed in the pattern graphics above. You can now adjust the 2theta axis according to the highlighted internal standard, simply by pressing <Ctrl+T> (<Cmd+T> on the Mac).
Qualitative phase analysis

Once the raw data processing (p. 18) of your powder diffraction data has been accomplished, you are ready to determine the phases that are present in your sample, i.e. to perform a qualitative analysis.

“Qualitative analysis” means the determination of the phases that are present in your sample. Typically, this analysis is based on the Bragg peaks (positions and intensities) found in your sample’s powder diffraction pattern.

Due to this, the most important prerequisite for a successful qualitative analysis is to determine all diffraction peaks (and also the background curve!) in the raw (profile) data as accurately as possible. The quality of your analysis strongly depends on the quality of the peak data that are derived from your initial raw data: On the one hand, it is important not to miss any peaks, to identify all (even minor) phases in the sample. On the other hand, any surplus peaks might bring up wrong phases (“false positives”) to the top of the candidate list.

As a guide, you can use the diffraction profile calculated from the experimental peak data as well as the background: It should be in reasonable agreement with the experimental diffraction pattern/profile throughout the whole pattern. You may want to display the difference plot in the pattern graphics in order to check for remaining differences between experimental and calculated diffraction data.

If you have additional information about the sample, for example if you already know that certain elements are present or can be excluded, you should follow the guidelines given in the chapter “Instant usage of additional information (“restraints”)” on p. 34 to define them.

If you already know that one or more compounds are present in your sample, you can learn in the chapter “Search for specific phase/entry” on p. 31 how to apply this information.

Search-match

During the “search-match” calculation, Match! compares the Bragg peak data (d-values and intensities) of your sample’s diffraction pattern to a so-called “reference database” (like the PDF or the COD) in which peak data of a large number of compounds are stored. Afterwards, the results are sorted according to their “similarity” (figure-of-merit (“FoM”) values) and presented in the candidate list.

You can run the search-match calculation e.g. by pressing <Ctrl+M> (<Cmd+M> on the Mac), by pressing the button in the toolbar, or by running the “Search-match” command from the “Search” menu. Match! will now calculate figure-of-merit (FoM) values for all entries in the current answer set (i.e. for the whole reference database if you did not enter any selection criteria, like elements etc.)

Figure-of-merit calculation

As has already been mentioned, the qualitative analysis in Match! is based on the so-called “figure-of-merit” (FoM), a numerical value describing the quality of the agreement between a certain reference database pattern and the pattern of the unknown sample.

The calculation of the figure-of-merit is to a large degree based on the peaks found in the unknown sample's diffraction pattern. In a first step, Match! tries to correlate the database pattern's peaks to the peaks in the unknown sample's pattern. Depending on the command used to run the search-match, Match! will either try to correlate all peaks (menu command “Search/Search-Match”, shortcut <Ctrl+M>) or the marked peaks only (menu command “Search/Search-Match (marked peaks only)”; shortcut <Ctrl+Shift+M>.

Afterwards, it calculates the FoM as a weighted sum of a variety of different pattern agreement criteria:

- 2theta-value differences of correlated peaks

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If no peak data but profile data are available when you run the “Search-match” command, Match! will automatically perform the raw data processing and determine the peak data.
- Intensity differences of correlated peaks
- Difference between the number of correlated peaks and the total number of peaks in the unknown pattern.
- Difference between the number of peaks which have been correlated in relation to the number of peaks which should have been correlated.
- Intensity scaling factor for the database entry’s peaks which gives the best agreement with the unknown pattern regarding the peak intensities.

Depending on the kind of problem, some of these factors should be weighted to a larger or smaller degree. For instance, the “difference between the number of correlated peaks and the total number of peaks in the unknown pattern” favors entries which cover as much of the unknown pattern’s peaks as possible, thus favoring single phases. The corresponding weighting factor should be reduced in the search-match options (which can e.g. be displayed by pressing the button in the toolbar) if the possibility that the unknown sample contains more than a single phase cannot be excluded.

Search-match results evaluation
When the search-match calculation has finished, you should investigate the resulting entries in the candidate list, and finally select the matching phases, just as it has been described in the “Quick start” chapter. Typically, the phases that are more likely to be present can be found close to the top of the candidate list, as indicated by their higher FoM-values. However, there may be reasons to disregard entries despite they have a large FoM-value, e.g. if they contain elements that cannot be present in the sample.

Search-match based on marked peaks only
Normally, the search-match calculation in Match! is based on all diffraction peaks (at least on those that are not located in excluded ranges or that are disabled). However, it is also possible to run the search-match based on marked peaks only, by first marking one or more peaks and then running the “Search-Match (marked peaks only)” command in the “Search” menu (or pressing the keyboard shortcut <Ctrl+Shift+M>). Typically, the intention for this is to find/prefer phases who show a diffraction peak close to the marked peaks.

A common **strategy for qualitative analysis** using individually marked peaks goes like this:

1. Process your raw diffraction data carefully, until the profile calculated from the experimental peak data as well as the background is in reasonable agreement with the experiment. It is also essential to eliminate any potential 2θ axis errors (e.g. zero point or specimen displacement error) in this step.
2. Start with a full search-match calculation (menu command “Search/Search-Match”, shortcut <Ctrl+M>, toolbar button and the selection of a first (typically major) phase. The latter can e.g. be performed by double-clicking on the corresponding line in the candidate list.
3. Afterwards, a common strategy is to focus on experimental peaks that are not covered by identified phases yet. In order to make this easier, you can activate the “Show uncorrelated peaks” option, e.g. by pressing <Ctrl+Shift+K> or by using the menu command “View / Pattern / Uncorrelated peaks”.
4. Mark (click on) a peak that cannot be “explained” with the already selected phase(s), i.e. which has not been correlated to an identified phase yet.
5. Run the menu command “Search/Search-Match (marked peaks only)” (or press the keyboard shortcut <Ctrl+Shift+M> or the toolbar button ). Wait until the update of the candidate list (figure-of-merit values) has been completed.
6. Investigate the entries/phases at the top of the candidate list as usual and select one (or more) phases that you assume to be present, based on the results for the marked peak(s).
7. Match! will automatically run a new full search-match calculation (for all peaks) at this point, in order to update the figure-of-merit values for all reference database entries with regard to the new “situation” (list of selected phases as well as the peak intensities covered by them).
8. Repeat the steps 4-7 until the profile calculated from the selected phases (and the background) is in reasonable agreement with the experimental diffraction profile, so that it is rather likely that all phases in the sample have been identified.

If no reasonable phase is found when running a search-match calculation for one (or more) marked peaks, this could be due to one of the following reasons:

- Check if potential 2θ-errors (e.g. zero point or specimen displacement) have been eliminated.
- Check the value of the parameter “2theta window for peak correlation” in the search-match options. This parameter value is used to determine if a certain reference diffraction pattern contains a peak at the position of the marked peak(s) or not.
- Consider that there may be no suitable phase (entry) present in the current reference database.
- The phase may be still unknown.

Please pay attention to the following hints, too:

- You can mark all peaks that have not been correlated to known phases yet using the menu command “Peaks/Mark uncorrelated peaks”.
- If only raw (profile) but no peak data are present when a (full) search-match calculation is run, Match! will automatically execute the automatic raw data processing before the actual search-match is started.
- If you mark more than a single peak and run the command “Search-Match (marked peaks only)”, the entries that contain one or the other marked peak(s) will be united (logical OR), because you cannot estimate if several peaks belong to the same or different phases at this stage.
- If the current FoM-values (ranking) in the candidate list is based on a search-match for marked peaks only, this is indicated by the following means:
  - The data of the corresponding peaks are displayed in bold font in the peak list.
  - A ‘*’ character will be added to the column headers “P(2theta)”, “P(I/I0)”, “I scale fct.” and “FoM” in the candidate list.
  - The peaks that were used in this calculation are displayed in the pattern graphics with an increased line width.
  - A blue button is displayed in the status bar at the bottom. If you click on this button, the search-match calculation will be repeated for all peaks.
- The user can restrict the comparison with the pattern of the unknown sample to certain groups of database entries, by applying additional restraints (like chemical composition, color, density, crystallographic data, quality marks, PDF subfiles etc.), in order to keep the number of possible candidate phases as low as possible.
- A variety of options and parameters can be adjusted which affect the FoM-calculation. If your search-match calculation does not give a reasonable result, you should “play around” with the parameters a little bit to check how the results could be influenced (e.g. by reducing the effect of intensity differences in order to compensate for textural effects).
- You can clear the FoM values and all other results of a search-match calculation by running the “Reset search-match results” command from the “Search” menu. This might be useful e.g. if you are applying restraints and would like to check which entries would be present without the minimum figure-of-merit criterion.
- The FoM should only be one guide for the user to select the matching entries from the list of candidate entries, however, it should not be the only one. With most “real-live” samples it is definitely necessary to also visually compare the diffraction patterns using the diffraction pattern graphics and the peak list.
Direct searching for individual peaks

In addition to using the search-match functionality just described, you can also search the reference database for entries that have peaks at certain 2θ (or d-value) peak positions (or in ranges). This can be achieved on the “Peaks/Ranges” page of the Restraints tab. There are two different tabs/approaches available for this:

- **Ranges**: You can define 2θ ranges in which accepted diffraction patterns (entries) must have at least one peak, or in which accepted entries **must not have** a peak (depending on “Mode”).

- **Strong lines**: Here you can define one or more peak positions for up to three strongest peaks, similar to the well-known Hanawalt- or Fink-searching.

All this can be accomplished on the “Peaks/Ranges” sub-tab of the “Restraints” tab on the right-hand side of the windows. See also the chapter “Searching for entries (restraints and additional entries)” below.

**Ranges**

On this tab you can select entries that contain one or more peaks in certain ranges. For example, it is possible to search for entries that contain at least one peak in each of the ranges 23.07..23.09°, 43.1..43.3° and 50.1..50.2° (Fig. 9). This is sometimes useful if e.g. a few experimental peaks are still uncorrelated after you have run a search-match calculation and identified the matching phases based on the FoM-values.

![Fig. 9: You can search for entries containing peaks in certain ranges on the “Peaks/Ranges” sub-tab of the “Restraints” tab. In this case, 354 entries contain at least one peak in each of the range 23.07..23.09°, 43.1..43.3° and 50.1..50.2°.](image)

In a similar manner, it is also possible to exclude all entries that contain at least one peak in one of the ranges given (using the “Mode” option at the top of the “Peaks/Ranges” sub-tab).

**Strong lines**

On the “Strong lines” tab you can enter positions of peaks (“lines”) that must be present among the three strongest peaks in a diffraction pattern. In addition to the peak position (given as d-value) you can define a tolerance and select if you would like to search for this peak as the strongest (1.), second-strongest (2.) and/or third-strongest peak (or any combination of them) (Fig. 10).
Once you have entered the d-value to be searched for (and maybe the tolerance and strongest lines order), please press the **Add line** button in order to add this line position to the table below and apply it as selection criterion.

You can of course enter more than a single line position, so that you can work with this feature similar to the Hanawalt- or Fink-indices.

**Please note:** You can quickly open the “Strong lines” selection criteria page by pressing <Ctrl+H> (<Cmd+H> on the Mac) and entering the first line position straight away.

### Searching for entries (restraints and additional entries)

#### Search for specific phase/entry

Sometimes you would like to quickly view a certain entry/phase from the reference database, e.g. if you know that this phase is present in your sample.

The easiest way to do so is to press <Ctrl+F> (<Cmd+F> on the Mac), type the name (formula sum or entry number) of the phase you are looking for in the corresponding input line at the top right, and press <Return>. Match! will instantly display and mark the best-matching entry in the candidate list at the bottom left, and at the same time display its diffraction pattern in the graphics pane.

You can now use the commands from the “Entries” menu e.g. in order to select this entry as “matching” (by pressing the <Space> bar), to use it as an internal 2theta standard (by pressing <Ctrl+T>), to **load it as an additional experimental pattern** (by pressing <Ctrl+Shift+T>), or to display the complete entry data (data sheet) by pressing <Ctrl+D>.

The “search for specific phase” feature is extremely useful in a variety of situations:

- Sometimes you already know that one or more phases are present in your sample and would like to quickly select these phases before getting into the details of determining the remaining phases.
In other cases, you have the suspicion that a certain compound might be present and would like to quickly view a corresponding reference pattern in order to check it.

Maybe you would like to quickly find and highlight a certain phase, in order to use it as an internal standard for the correction of 2theta-errors?

Finally, this is also a convenient way to quickly display the data sheet of a certain compound.

Here is a quick example: Suppose that you have imported your experimental diffraction data, run the raw data processing, and performed a first search-match run, in order to calculate the figure-of-merit (FoM) values of the candidate entries. Now you are ready to perform your actual phase identification. Your screen might look like Fig. 11:

Fig. 11: That’s what the screen looks like having imported and processed the raw data, as well as run the search-match calculation. Now, you would like to find and display the diffraction pattern of quartz. In order to do so, simply press <Ctrl+F> on your keyboard (<Cmd+F> on the Mac), type ‘quartz’, and press <Return>. The best matching ‘quartz’ entry will automatically be highlighted in the candidate list and displayed in the diffraction pattern (Fig. 12).
Fig. 12: Once you have pressed <Ctrl(Cmd)+F> and entered your selection criterion ("quartz" in this case), the best-matching corresponding entry will automatically be highlighted in the candidate list.

The best matching entry for 'quartz' has already been marked in the candidate list, so you can instantly use it as an internal standard for the correction of the 2theta-error. In order to do so, simply press <Ctrl+T>. The new (corrected) 2theta values of the experimental peaks will be taken into account automatically in all 'views' of the data, resulting for example in an automatic update of the candidate list.

Due to the correction, the overlap between the experimental and the 'quartz' reference pattern has become better, resulting in an increased figure-of-merit (FoM) value for this phase/entry. As a result, it will now be displayed closer to the top of the candidate list (Fig. 13).

Fig. 13: In the candidate list, the best-matching entry corresponding to the criterion "quartz" has been marked automatically.

Now you can easily select the 'quartz' entry as matching: Since it is still marked in the candidate list, simply press the space bar to do so. Once the entry has been transferred to the Match list on the right-hand side, the candidate list will instantly be updated, and the next best matching entry (Siderite in this case) will be highlighted (Fig. 14).

Fig. 14: The best-matching entry for “quartz” has been selected as “matching”.

The best matching entry for 'quartz' has already been marked in the candidate list, so you can instantly use it as an internal standard for the correction of the 2theta-error. In order to do so, simply press <Ctrl+T>. The new (corrected) 2theta values of the experimental peaks will be taken into account automatically in all 'views' of the data, resulting for example in an automatic update of the candidate list.

Due to the correction, the overlap between the experimental and the 'quartz' reference pattern has become better, resulting in an increased figure-of-merit (FoM) value for this phase/entry. As a result, it will now be displayed closer to the top of the candidate list (Fig. 13).

**Table 1.**

<table>
<thead>
<tr>
<th>Color</th>
<th>Qual.</th>
<th>Entry</th>
<th>Formula</th>
<th>Candidate phase</th>
<th>$\theta$ (2theta)</th>
<th>$\theta$ (002)</th>
<th>I scale fit.</th>
<th>I/\sigma</th>
<th>FoM</th>
</tr>
</thead>
<tbody>
<tr>
<td>E</td>
<td>96-913-1907</td>
<td>CuO Cl H O2S P5</td>
<td>Apatite (CaF)</td>
<td>0.4746</td>
<td>0.9499</td>
<td>0.4336</td>
<td>1.59</td>
<td>0.002</td>
<td></td>
</tr>
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<td>0.002</td>
<td></td>
</tr>
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<td>0.9999</td>
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<table>
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<th>Entry</th>
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<th>$\theta$ (2theta)</th>
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<th>I/\sigma</th>
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<th>I/\sigma</th>
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<table>
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<th>Matched phase</th>
<th>$\theta$ (2theta)</th>
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</tr>
</tbody>
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<table>
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<tr>
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<th>Qual.</th>
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<th>$\theta$ (2theta)</th>
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<td>0.198</td>
</tr>
</tbody>
</table>
In practice, you could now compare and select the next best matching entry as well, simply by pressing the space bar again and so on, until you have identified all phases in the sample.

**Instant usage of additional information ("restraints")**

It is very easy to directly use any kind of additional information about the sample (like the elements that can or must be present). The aim is to restrict the entries in Candidate list to those that match certain criteria ("restraints").

All corresponding selections are made on the “Restraints” or “Additional entries” tabs on the upper right-hand side, and the results are instantly reflected in the candidate list at the bottom of the screen (and of course also apply to the entries that are investigated during the search-match calculation). This technique is called “perpetual restraining” and is also used in other software products, e.g. “Pearson’s Crystal Data”.

For example, if you would like to keep only compounds (i.e. entries) that contain the elements Si and O, simply click on these two elements on the “Composition” sub-tab of the “Restraints” tab, so that the color of these elements switches to green. Your Candidate list at the bottom will instantly be updated accordingly.

You can also use other selection criteria, like the name, the formula sum, crystallographic data, physical properties, peak positions, bibliographic data etc.

For example, suppose that you know that the element oxygen (O) must be present in all matching phases. In order to use this information, simply click on the corresponding button in the periodic table on the upper right-hand side; Match! will instantly apply this additional information to the current answer set (table “candidate list” at the bottom; Fig. 15).

As you see, Match! uses the same perpetual restraining mechanism that you may already know from “Pearson’s Crystal Data”: While entering your selection criteria, any modification will instantly be reflected e.g. in the table of resulting entries and the entry count.

As an example, we assume that you would like to enter the additional information that the element Si must be present. In order to do so, simply press on the element “Si” in the periodic table on the upper right-hand side. The candidate list at the bottom is instantly modified: All entries for CaCO$_3$ (Calcite) that were present before are now...
gone, and the number of entries matching your selection criteria (displayed to the right of “Restraints” on the tab control) has been significantly reduced (from 1632 to 399; Fig. 16).

In a similar manner, it is also possible to add specific entries to the table of candidate entries (candidate list): Simply click on the tab “Additional entries”; this will bring up a totally equivalent set of tab sheets like the “Restraints” set. You can now define precisely which entries you would like to add to the candidate list even though they do not match the “Restraints” criteria.

Add entries that match certain criteria to candidate list (“additional entries”)
If you are missing certain phases in the candidate list, you can add them using the “Add, entries” tab on the right-hand side. Similar to the restraints just mentioned, the selection criteria are entered on sub-tabs of the “Add, Entries” tab on the right-hand side. The same selection criteria are available for restraining and adding of entries.

Note that adding specific entries does not necessarily mean that they are immediately marked/displayed in the candidate list (like it would be the case when using the “Find phases/entries” functionality mentioned above)! Adding entries just makes sure that they are present in the current answer set. If the number of entries in the current answer set is sufficiently low (i.e. below the “Max. number of entries” which can be defined on the “candidate list” tab of the “Options” dialog), the additional entries are present somewhere in the candidate list, typically at its bottom because their figure-of-merit is normally rather low.

Saving of selection criteria (presets)
If you are frequently using the same restraints (selection criteria), you will instantly know what this feature is about: You can easily save the current selection criteria and recall them later on with just two mouse clicks. Of course, it is possible to save several sets of selection criteria.

You will find the corresponding control elements at the bottom of the “Restraints” (and also “Additional entries”) tab to the right of “Preset.” (Fig. 17).
Fig. 17: Using these buttons at the bottom of the periodic table, you can easily save and recall all kinds of restraints/additional entry settings.

In order to save the current selection criteria, simply press the “Save” button. Afterwards, you have to enter a name using which you can easily identify this set of selection criteria later on (“Silicon compounds” in our example).

Your selection criteria will then be stored in your personal settings (e.g. Windows registry). If another person is using the same computer, he can store his own selection criteria independent from yours (of course assuming that he is using his own account on this machine...).

If you would like to recall a certain set of selection criteria, simply press the “arrow down” button of the combo box to the left of the “Save” button and select the name of the desired selection criteria from the list that opens.

That's it! The selection criteria that have been loaded will instantly be applied to the table of candidate entries (candidate list), and of course also to the entries that are investigated during the search-match calculation.

Background information on searching and restraining

Using the entry searching and restraining facilities of Match! is rather straightforward in most cases, however, there may be circumstances in which an in depth knowledge of the logical concepts behind the “Restraints”, “Additional entries” and “Find phases/entries” functionality may be helpful:

First of all, the candidate list in the bottom left corner of the Match! program window displays a list of all entries in the current answer set, the entry number of which is always displayed in the status bar at the bottom to the left of the reference database name (in the corner on the lower right-hand side).

Right after you have started Match! or run the “File/New” command, the “current answer set” contains all entries from the current reference database. Typically, these are 40,000 to 400,000 entries, so it would take a lot of time and memory (and wouldn't even make much sense) to load and display the entry data of all reference database entries into the candidate list. Hence, Match! displays a message instead, asking you to do something in order to delimit this large amount of entries in order to find out which entries you are actually interested in, e.g. to import diffraction data and run a search-match, or to enter selection criteria (restraints).

For example, if you import diffraction data and run a search-match calculation, a figure-of-merit value (FoM) is calculated for each entry, so the criterion “Minimum FoM” (which can be adjusted in the lower left-hand corner of the “Search-Match” tab of the “Options” dialog) can be applied to restrict the answer set to only those entries whose figure-of-merit is above this user defined value, in order to select the entries that best match your diffraction pattern. Another possibility to delimit the full amount of reference database entries to the ones you are interested in is to enter selection criteria (e.g. name) on the “Restraints” tab on the right-hand side. This tab offers a large amount of selection criteria like elements that must or must not be present.

Some of these selection criteria are text fields, like e.g. “Name”. If you enter some text here, only reference database entries that exactly contain this text in the corresponding database field are accepted to be included in the answer set. In order to help you here, Match! can display a list of all corresponding values in the reference database so that you can directly select from this list. This “List selection box” is displayed by pressing the corresponding button to the right of a text field input line. You can also use the wild card character '*' to tell Match! to disregard text before and/or after the fragment you have entered (e.g. “*corundum*”), however, Match! still distinguishes between capital and small characters within the fragments (case-sensitive comparison).

Once you have delimited the full amount of reference database entries in one or the other way, you have obtained an answer set (a set of selected entries below the full reference database), the entries of which can now be displayed in the candidate list. However, there is another limitation for this, i.e. the “Max. number of entries” setting at the top of the “Candidate list” tab sheet of the “Options” dialog. Normally, the candidate list will only be filled with entries if the current answer set does not contain more than this number of entries. If the number of answer set entries is
larger than this value, a corresponding message “Too many matching entries” is displayed in the candidate list instead of the entries, instructing you to further delimit the current answer set e.g. by entering additional entries.

So far for the candidate list, the current answer set and the “Restraints” tab.

The “Add. Entries” (additional entries) tab does something different: While normally the current answer set (→ candidate list) only contains entries that match all “Restraints” criteria as well as the “Minimum FoM” criterion (if applicable), the “Add entries” tab allows you to add specific entries regardless of these criteria. This may be useful for example if you know that a certain phase/entry is present in your sample but has not been assigned a figure-of-merit value larger than “Minimum FoM” in the last search-match calculation. Hence, you most probably would like to add this entry to the answer set/candidate list, in order to check what caused the low FoM value, like missing/undetected peaks, a strong 2theta shift, or a very low intensity scaling factor.

In order to do so, you can enter selection criteria (e.g. name) on the “Add. Entries” tab, just like on the “Restraints” tab. The number of entries that match these selection criteria is displayed in brackets behind “Add. Entries” on the tab; these entries are then added to the ones selected by “Restraints” and/or the “Minimum FoM” criterion. Typically, you will find these additional entries at the bottom of the candidate list because their figure-of-merit values are low (quite often close to 0.0).

As you can imagine from these explanations, the usage of the “Add. Entries” tab only makes sense if the current answer set does not already contain the full reference database (in which case there would be no more entries that could be added). Hence, the “Add entries” tab is inactive in this case in some earlier versions of Match!.

The “Find phases/entries” functionality in the top right corner of the Match! window is pretty much some kind of mixture between these two facilities (“Restraints” and “Add. Entries”): Once you have entered some criterion (e.g. name) in the corresponding line at the top and pressed <Return>, Match! searches for matching entries in the reference database. It then checks if these entries are present in the current answer set. If this is not the case, it adds these matching entries, using the “Add. Entries” mechanism, by automatically entering the corresponding entry numbers on the “References” sub-tab of the “Add. entries” tab.

Afterwards, Match! locates the first of these matching entries (typically the one with the highest FoM-value) in the candidate list (answer set) and makes sure that it is marked and hence displayed in the powder diffraction pattern.

Hence, this functionality is some kind of abbreviation to the much more detailed “Add. Entries” mechanism and at the same time quickly locates the entry(s) of interest in the candidate list. In order to account for this “quick searching” character of the functionality, it is not required that the name entered in the “Find phases/entries” field is matched exactly (like it is the case on the “Add. Entries” and “Restraints” tab). Instead, it is sufficient that an entry to be regarded as “matching” contains the entered name as a fragment, also neglecting small and capital letters (case-insensitive comparison, in contrast to the criterion “Name” on the “Restraints” and “Add. Entries” tabs).

This latter feature is something that might have caused some misunderstanding in some cases: For example, the current “COD-Inorg” reference database contains 26 entries with name “Corundum” and 1 entry with name “corundum”, i.e. with a small letter at first position. As has already been mentioned, this difference does not matter when using the “Find phases/entries” line, so 27 entries are added using the “Add. entries” mechanism.

However, this mechanism does not delimit the current answer set, like it would be the case if you used “Restraints”, it just makes sure the corresponding entries are present (maybe among others) in the current answer set, and marks/displays the first one of these entries. If the current number of entries in the answer set is larger than the corresponding parameter (so that normally nothing would be displayed), Match! uses an internal “work-around” mechanism to nevertheless display a subset of entries (that also contain the ones matching the “Find phases/entries” criterion) in the candidate list.

If you use the wild card expression “*corundum*” on the “Restraints” or “Add. Entries” tab, Match! nevertheless still distinguishes between capital and small characters. As has already been mentioned, there is only 1 entry with a small ‘c’ and 26 with a capital ‘C’ at the beginning (“corundum” vs. “Corundum”), so that’s why you find a single entry when you enter “*corundum*”, 26 entries when you enter “*Corundum*”, and 27 entries when you give “*orundum*” instead.
Unification of candidate list

The “Unify phases” command (which can be executed either by selecting the corresponding command from the “Entries” menu, or by pressing <Ctrl+U> (<Cmd+U> on the Mac)) checks the candidate list for entries that describe the same phase. If any of these “duplicate entries” are detected, Match! removes all but the best-matching entry for this phase. As comparison criteria, Match! uses the composition as well as the powder diffraction pattern similarity (R-factor).

This command is especially useful if run before the selection of matching phases, in order to prevent multiple entries for a certain phase block the candidate list or even appear in the Match list.
Quantitative phase analysis

Once you have finished the qualitative analysis (i.e. you have found out which phases are present in your sample; see the previous chapter for details), you can determine the amounts (weight %) of the phases that are present. Depending on the method you apply, you can do so for all crystalline phases and/or (in some cases) also for the amorphous phase(s)\textsuperscript{12}.

Match! provides the following methods for quantitative analysis:

1. Semi-quantitative analysis using the “Reference Intensity Ratio”-(RIR)-method (p. 39)
2. Rietveld refinement\textsuperscript{13,14,15} (p. 40, p. 48)
3. Degree-of-crystallinity (DOC) analysis (p. 40)
4. Internal standard (p. 44)

These methods (that can be used alone or in combination, e.g. Rietveld + internal standard) are now explained and demonstrated in detail in the following sections. In addition, two commands for calculating peak/profile areas (that might be used for your own calculations) are also described in this context.

**Semi-quantitative analysis using the “reference intensity ratio”-(RIR)-method**

<table>
<thead>
<tr>
<th>Most suitable for...</th>
<th>Difficulties may arise in case of ...</th>
<th>Cannot be applied if...</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quick analysis</td>
<td>High accuracy required</td>
<td>No I/I\textsubscript{c} value is available for one (or more) of the selected phases (can be solved by using the I/I\textsubscript{c}=1.0 option)</td>
</tr>
</tbody>
</table>

Match! can perform a semi-quantitative analysis of the sample using the so-called “Reference Intensity Ratio method” (RIR-method)\textsuperscript{16}. This analysis is based on the comparison of the intensity scaling factors of the identified phases with reference to a “virtual” Corundum standard. “Virtual” means that Corundum must not be really present in your sample. Instead, so-called “I/I\textsubscript{c}”-factors for all phases are required, relating the intensity of the highest peak of a phase to the highest peak of Corundum, if both phases were present in a sample with the same amounts.

In Match!, the semi-quantitative analysis is performed automatically if at least two entries have been selected as matching. The quantity (weight %) of each selected phase/entry is displayed in the “Quant.(%)” column of the match list and of course also in the report. However, the analysis can only be carried out if all entries which have been selected as matching contain I/I\textsubscript{c} factors\textsuperscript{17}. As an exception, you can activate an option on the “General” tab of the “Options” dialog to let Match! use an I/I\textsubscript{c} factor of 1.0 which might be helpful in some “emergency” situations. Normally, if only one of the selected entries does not contain an I/I\textsubscript{c} factor, the values for the remaining selected entries will not be displayed either.

You can check if an entry contains an I/I\textsubscript{c} factor before selecting it by taking a look at the column “I/I\textsubscript{c}” in the candidate list (in which a corresponding value must be given).

\textsuperscript{12} If more than a single amorphous phase is present, you can only determine the sum of the amorphous phases.


\textsuperscript{14} N.V.Y. Scarlett, I.C. Madsen, “Quantification of phases with partial or no known crystal structure”, Powder Diffraction 21(4), 278-284 (2006).


\textsuperscript{17} All entries from free-of-charge COD reference database provided by Crystal Impact contain calculated I/I\textsubscript{c} values.
Manual adjustment of individual amounts for multiple-phase samples

Normally, the (semi-quantitative) amounts of the phases are calculated based on the corresponding automatically determined intensity scale factors of the selected entries. However, it is possible to modify these intensity scale factors manually (and hence also the amounts of the individual phases). You can do so in two different ways:

- One option is to mark the phase/entry you would like to adjust the quantity of in the match list on the right-hand side. Afterwards, you can simply move the mouse cursor close to the top of one of the corresponding peaks in the diffraction pattern, press the left mouse button, and keep it pressed while moving the mouse up or down. The amount (intensity scale factor) of the marked entry/phase will now follow the mouse movements: Moving the mouse up (i.e. away from you) increases the amount of the marked phase, while moving the mouse towards you reduces the amount. The amounts of the remaining (non-marked) phases will be adjusted automatically.

- Alternatively, you can mark the phase/entry in the match list (similar to the previous option), move the mouse cursor in the match list to the column “Quant. (%)” of the corresponding entry, and use the mouse wheel in order to adjust the amount for this phase.

Rietveld refinement

<table>
<thead>
<tr>
<th>Most suitable for...</th>
</tr>
</thead>
<tbody>
<tr>
<td>Careful analysis</td>
</tr>
<tr>
<td>Increased accuracy required</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Difficulties may arise in case of ...</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low quality data</td>
</tr>
<tr>
<td>Quick analysis required</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Cannot be applied if...</th>
</tr>
</thead>
<tbody>
<tr>
<td>No crystal structure data are available for one (or more) of the selected phases</td>
</tr>
</tbody>
</table>

Rietveld refinement (see the chapter on p. 48) tries to mimic the experimental diffraction pattern as closely as possible, by fitting a model containing the crystal structure data of the phases, along with a large variety of other parameters. The calculation basically consists of a least-squares refinement of selected parameters like scale factors, unit cell parameters, peak shape parameters and background. In addition, potential errors can be modeled, like zero-point, specimen displacement or preferred orientation.

Once the Rietveld refinement has converged, the weight fractions of the individual phases are calculated from the refined scale factors, along with the density values and unit cell volumes calculated from the known crystal structures of the phases. **The resulting weight fractions will be copied to the match list automatically after a successful Rietveld refinement calculation**, replacing any values resulting from the RIR calculation is present.

Although the main output of Rietveld refinement (at least with regard to quantitative analysis) are the scale factors of the phases (similar to the RIR-method described above), the accuracy is much higher, because the whole profile is used for the calculation and not just the heights of 1..N peaks. In Rietveld refinement, effects like peak broadening, asymmetry, preferred orientation etc. can be investigated and taken into account in the quantitative analysis.

Degree-of-crystallinity (DOC) analysis

<table>
<thead>
<tr>
<th>Most suitable for...</th>
</tr>
</thead>
<tbody>
<tr>
<td>Determination of amount of amorphous compound(s)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Difficulties may arise in case of ...</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elemental composition of amorphous phase is not similar to crystalline compounds</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Cannot be applied if...</th>
</tr>
</thead>
<tbody>
<tr>
<td>No ’empty sample holder’ diffraction pattern is available</td>
</tr>
</tbody>
</table>

This analysis requires that an additional “empty sample holder” diffraction pattern is available that has been recorded using the same experimental conditions as the sample’s pattern. This additional pattern is used to subtract the background contribution caused by the instrument from the one of the sample.

The DOC analysis works best if the crystalline and amorphous parts have similar elemental composition. If the sample consists of crystalline fractions and an amorphous fraction of different chemical compositions, the amounts of each of the individual crystalline phases may be estimated using appropriate standard substances as described below; the amorphous fraction is then deduced indirectly by subtraction.
If this prerequisite is met, it is neither necessary to determine the experimental peaks nor to select the matching phases (qualitative analysis) for the DOC analysis. Instead, it is sufficient to subtract the instrumental background from the sample’s diffraction pattern, re-determine the background, and then calculate the area below the background curve and compare it to the area of the whole pattern.

**Workflow for DOC analysis**

1. Collect the sample’s diffraction pattern as usual; the 2theta range should be large enough to see both the start and end of the amorphous part.

2. Collect an “empty sample holder” diffraction pattern with the same experimental conditions.

3. Import the sample’s diffraction pattern into Match!.

4. Define/check/modify the background so that it clearly separates the diffraction peaks from the background (Fig. 18).

5. Import the “empty sample holder” diffraction pattern as an additional pattern (menu “Pattern / Insert/overlay…”).

6. For a better visual comparison, you could switch over to “Counts” representation on the y-axis (e.g. by clicking on the corresponding y-axis label), so that the two patterns are scaled identically (Fig. 19).

7. Run “Quantify/Degree of crystallinity (DOC) / New analysis”

8. In the dialog that opens, make sure that the option “Use addition pattern” is marked as well as the correct additional pattern is selected.

9. Mark the option “Full pattern” under “Subtract full ‘empty sample holder’ pattern or background only”.

10. If you like to see the “real” diffraction pattern of the sample after subtraction of the instrument background, mark the option “Add result as a new experimental pattern”. Your dialog should now look similar to Fig. 20

11. Press “OK”. The result of the DOC analysis will now be displayed (Fig. 21). It will also be included/displayed in the report.
Fig. 18: Your sample’s diffraction pattern has been imported for degree-of-crystallinity analysis (DOC).

Fig. 19: The “empty sample holder” pattern (representing the instrument’s contribution to the background) has been imported as an additional experimental pattern, and the y-axis scaling has been switched over to “Counts”.
Fig. 20: Settings for DOC analysis: The “empty sample holder” data shall be taken from the additional pattern “Empty_sample_holder_Cu_Ka”, the full “empty sample holder” pattern shall be used (and not just the automatically determined background), and the result (pattern difference) shall be added as an additional experimental pattern for visual comparison.

Fig. 21: Result of the degree-of-crystallinity (DOC) analysis. In this case, the degree-of-crystallinity is 87.25%, and the amount of the amorphous phase(s) is 12.75%.
Internal standard

<table>
<thead>
<tr>
<th>Most suitable for...</th>
</tr>
</thead>
<tbody>
<tr>
<td>Careful analysis</td>
</tr>
<tr>
<td>Increased accuracy required</td>
</tr>
<tr>
<td>No separation of background from amorphous phases possible/required</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Difficulties may arise in case of ...</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low quality data</td>
</tr>
<tr>
<td>Quick analysis required</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Cannot be applied if...</th>
</tr>
</thead>
<tbody>
<tr>
<td>No known amount of a suitable standard compound can be added to the sample</td>
</tr>
<tr>
<td>The amount of more than a single amorphous or unidentified phase shall be determined individually</td>
</tr>
<tr>
<td>Amounts of amorphous and non-identified crystalline phases shall be determined separately</td>
</tr>
</tbody>
</table>

If you can add a known amount of a suitable compound (“internal standard”) to your sample before recording the diffraction pattern, this information can later on be compared to the result of a Rietveld (or RIR) quantitative analysis. The corresponding correction factor (obtained from the relation “known amount of phase A added to sample” / “amount of phase A resulting from RIR- or Rietveld analysis”) can then be used to correct the amounts of the remaining phases, rather than normalizing the sum to 100%. As a result, absolute phase quantities are obtained. The difference to 100 weight-% gives the amount of amorphous (and unidentified crystalline) phases in the sample.

There are a few conditions that the internal standard compound must fulfill though:

- It must be 100% crystalline.
- It should be a highly symmetric structure generating few but intense diffraction peaks.
- The internal standard compound must not react chemically with the sample.
- The internal standard amount must not exceed the amount resulting e.g. from Rietveld refinement (or RIR analysis), because this would result in the sum of all phase amounts being larger than 100%.

When these requirements are fulfilled, a quantitative “internal standard” analysis is performed as follows:

**Workflow for “internal standard” analysis**

First of all, add a known amount of a suitable “internal standard” compound to your sample and record its powder diffraction pattern. Import the corresponding diffraction pattern into Match! and perform the raw data processing and qualitative analysis as described above (example given in Fig. 22).
Afterwards, we recommend performing a “quantitative analysis”, by running a Rietveld refinement of the scale factors, unit cell parameters, peak shape parameters and background, in order to get reasonable starting values for the amounts of the crystalline phases (Fig. 23). If you cannot run a Rietveld analysis, you can use the results of the semi-quantitative “RIR” analysis that is performed automatically by Match! (see above).
Fig. 23: A Rietveld refinement calculation of scale factors as well as unit cell, peak shape and background parameters has been run.

Verify that the amount of the internal standard compound (in this case Zincite, ZnO) is over-estimated (larger) in the Rietveld (or RIR) analysis (here 22.2%), compared to the amount added to your original sample (in this case 15%). If the latter is larger than the amount resulting from the Rietveld refinement, this would cause the amounts of the remaining phases to be increased in the calculation. As a result, the sum of all phase amounts would be larger than 100%.

Mark the phase you would like to use as internal standard in the match list (here Zincite), then run the command “Internal quant. standard” from the “Quantify” menu (or from the match list’s context menu). In the dialog that opens, please enter the amount (weight %) of the standard phase in the sample (here 15%), then press “OK”.

Fig. 24: In this dialog you provide the amount of the internal standard phase that you have added to your sample.

The result of the “internal standard analysis” will now be displayed both in the match list (Fig. 25) as well as in the report. In our example, the original sample (without standard) contains 28.2% Quartz, 14.5% Calcium carbonate, 11.1% Albite, 7.9%, and 38.3% of amorphous (or unidentified) phase(s).

Fig. 25: The result of “internal standard” analysis is given in the match list.

If you would like to return to the “normal” quantitative analysis with the identified crystalline phases adding up to 100%, you can do so by running “Quantify / Reset internal standard”.

Calculate profile integrals

You can instruct Match! to calculate the intensity integrals of various profile areas by selecting the command “Calculate profile integrals...” from the “Quantify” menu. A new dialog will open and display a table of the following different profile areas (Fig. 26):

- Overall diffraction profile
- Background radiation
- Diffraction peaks
- Peak area belonging to selected phases
- Peak area belonging to each individual selected phase
- Unidentified peak area

Fig. 26: You can calculate various profile areas using the “Integrated profile areas...” command in the “Quantify” menu.

For each profile area, the **integrated counts** as well as the **relative amount** is given. The **profile integrals** are also given at the bottom of the match list as well as the report.

**Calculate peak residuals**

The peak residuals are the remaining experimental peak intensities after subtracting the intensities covered by the identified phases. You can ask Match! to calculate the **residual peak intensities** by selecting the “Calculate peak residuals...” command from the “Quantify” menu. A new dialog will open and display a table of 3 different peak intensities (Fig. 27):

- Overall peak intensity
- Peak intensity belonging to selected phases
- Unidentified peak intensity

For each peak intensity type, the **integrated counts** as well as the **relative amount** is given.

Fig. 27: Calculation of peak residual intensity values
Rietveld refinement

Basics

Before we start: An excellent introduction to Rietveld refinement suitable even for absolute beginners is the very clearly structured document “Lesson 5: Rietveld Refinement” of Nicola Döbelin’s Lecture Handouts\textsuperscript{18}.

Rietveld refinement is a tool that tries to model a full powder diffraction profile based on crystal structure data, specimen and instrument effects, by fitting a large variety of corresponding functions parameters. It was first introduced by Hugo Rietveld in 1967 and 1969. The parameters are varied using a least-squares procedure, in order to minimize the difference between the calculated and the experimental powder diffraction pattern. Details of the method are available in the literature\textsuperscript{19,20,21}.

One of the key issues of Rietveld refinement is that the method is rather sensitive to problems and errors in the model, resulting in non-convergence and other issues. Hence, it has become a common agreement for many scientists that a successful phase identification should be proven by a successful Rietveld refinement converging at low R- and $\chi^2$-factors.

Well, in practice things are not always that easy, but running Rietveld refinements on your diffraction pattern will at least give you a good chance to think and learn more about your experiment and sample.

Rietveld refinement in Match!

Today a variety of excellent programs for Rietveld refinement are available, so there is little need to invent the wheel again and again. Match! uses the well-known Rietveld program “FullProf\textsuperscript{22,23}” to actually perform the calculations. However, with Match! you do not have to interact with FullProf directly; instead, you can use the Match! user interface to define (“turn-on”) the parameters, setup the calculations and evaluate the results.

When you run Match! for the first time, the software tries to automatically determine the path to the FullProf software. If this is not possible, you will be asked if you would like to manually select this path. Finally, if this is not successful, you will be asked if you would like to download and install FullProf from the Crystal Impact web site.

This “checking for FullProf” procedure is carried out only once. If there is no valid path to FullProf available at its end (e.g. because you have pressed the “Cancel” buttons), you won’t be asked again until you try to run a Rietveld refinement calculation. However, you can download and install FullProf manually later on by selecting the “FullProf download” command from the “Tools” menu. As an alternative, you can define or modify the path to FullProf any time on the “Rietveld” tab of the “Options” dialog (which can be opened e.g. from the “Options” menu). Once you have defined the path to FullProf, you are ready to run Rietveld refinement calculations from within Match!.

In order to do so, you first have to perform the normal phase identification procedure, i.e. import (raw/profile!) diffraction data, find the peaks, run a search-match and select one or more “matching phases”. Afterwards, please select e.g. the “Rietveld (FullProf)” command from the “Options” menu (or press “Ctrl + Shift + R” on your keyboard), to bring up the “Parameter Turn-On” dialog (Fig. 28).

If any of the entries you have selected as “matching phases” does not contain a full crystal structure data set (e.g. if the atomic coordinates are missing), you will be prompted to import suitable crystal structure data from cif-files. The background is that it is not possible to run Rietveld refinements without complete structural models. Once complete crystal structure data sets are available for all matching phases, the “Parameter Turn-On” dialog will be displayed. Please note: You can eliminate all entries that do not contain a full crystal structure description from the candidate list using the menu command "Entries/Delete incomplete entries".

\textsuperscript{23} http://www.ill.eu/sites/fullprof/index.html
Match! will also switch to the “Rietveld” tab on the upper right-hand side of the Match! window automatically where the results and viewing options will be available after the refinement calculation.

Fig. 28: The “Parameter Turn-On Dialog” in its default state: The “Automatic Rietveld Refinement” option is active, so the Rietveld refinement can be run directly by pressing the “Run FullProf” button at the bottom left.

In order to introduce users that are new to Rietveld refinement to this method, we have implemented four different approaches to define (“turn-on”) the options and parameters for the calculation. The method that is easiest to use (“Automatic Rietveld Refinement”) is available simply by marking the corresponding checkbox at the top of the “Parameter Turn-On” dialog, while the three remaining facilities “Beginner”, “Advanced” and “Expert” are present as tabs in the main part of the dialog. The parameters on the three tabs are linked to each other, so that you can start turning on parameters e.g. on the “Beginner” tab and finish as an “Expert”.

We will now discuss the four approaches of using the “Parameter Turn-On” dialog in more detail:

1. **Automatic Rietveld refinement**
   
   The easiest way to setup a Rietveld refinement calculation is to activate the “Automatic Rietveld refinement” option at the top of the “Parameter Turn-On”-dialog. If this option is active, all remaining options are disabled. Afterwards, you can run the automatic refinement calculation by pressing the “Run FullProf” button on the lower left-hand side. The calculation(s) will be run automatically; at the end, the result will be displayed on the “Rietveld”-tab on the upper right-hand side of the Match! window.

   You can create own parameter sequences to be used in automatic Rietveld refinement; this will be described in the chapter “Configuring automatic Rietveld refinement calculations” below.

2. **Beginner**
   
   The next step for learning how to do Rietveld refinement is to deactivate the “Automatic Rietveld refinement” option, and to use the options (checkboxes) on the “Beginner” tab. On this tab, a selection of Rietveld parameters is available, along with a suggested order in which they shall be turned on in successive calculations (Fig. 29).
Fig. 29: On the “Beginner” tab of the “Parameter Turn-On” dialog, the available parameters are grouped according to the suggested order in which they shall be included in the refinement.

For example, in the first calculation only the scale factors and specimen displacement parameters are recommended for refinement. If this first refinement calculation is successful, the unit cell and first background parameters can be activated in addition to the first parameters, and another refinement calculation is performed. If this is successful, the W and atomic coordinate parameters are added etc.

In fact, this is just the order in which the calculations are carried out during the automatic refinement. However, you now have more control and can stop at certain points or repeat steps if you like. This order is taken from the excellent book edited by R. A. Young.

3. Advanced

Once you are familiar with the principal procedure and main parameters, you are ready for more detailed options and parameters. Hence, we have introduced the “Advanced” tab, on which a reasonable number of parameters is grouped according to their effect: “Peak positions”, “Peak intensities” and “Profile shape”.

You can e.g. address specific problems e.g. concerning the positions of the peaks by marking one or the other parameter on the “Peak positions” tab for refinement (Fig. 30).
Fig. 30: On the “Advanced” tab of the “Parameter Turn-On” dialog the available parameters are grouped according to the topic they take an effect on, like peak positions, peak intensities and profile shape.

Another new feature on the “Advanced” tab (that is also available on the “Expert” tab) is the possibility to define constraints for a certain parameter. In order to do so please press the “…” button to the right of the corresponding parameter (e.g. “Shift on 2theta-axis”). A new dialog window will open (Fig. 31) in which you cannot only modify the parameter value or mark the parameter for being optimized, but also define constraints by entering the limiting numerical values in the “Minimum value” and/or “Maximum value” fields.

Fig. 31: Using this dialog (which can be opened by pressing the “…” button to the right of a certain numerical parameter) you can modify the value of the parameter as well as define constraints for it.

At this stage you should also note the table of “Active parameters” on the right-hand side of the “Parameter Turn-On” dialog. Here you can get an overview over the parameters that are currently marked for being varied in the next refinement calculation. Please note that the parameter names given in the left-most column are the original full
parameter identifiers used in FullProf. If you double-click on a certain line of the table, the parameter modification
dialog just mentioned will be opened, so that you can modify parameter settings directly without having to search
for the corresponding “…” button or tab.

Once you have defined the parameters you would like to refine, please press the “Run FullProf” button at the bottom
in order to run the Rietveld refinement calculation.

4. Expert
This is the most comprehensive but also the most demanding option for setting up the Rietveld refinement
parameters. All FullProf parameters that are currently supported by Match! are available here. You can adjust global
settings like “Zero” or “Lambda” on the “Global” tab, as well as select or modify parameters for individual phases
(e.g. unit cell parameters or atomic coordinates). For each phase of the Match list, a separate tab is available. All
parameters belonging to a certain phase are distributed to subtabs like “Quant.”, “Profile” or “Crystal structure”.

Pattern calculation
Before we leave the “Parameter Tun-On” dialog please note that there is a fifth way of using the “Parameter Turn-
On” dialog: If you do not mark any of the “vary” checkboxes (i.e. if the table of “Active parameters” on the right-
hand side is empty), you can instruct FullProf to calculate the powder diffraction pattern (based on the current
settings and parameter values) simply by pressing the “Run FullProf” button. When the calculation has finished,
you can e.g. export the calculated pattern using the menu command “File/Export/Profile data (Rietveld)”.

Buttons in “Parameter Turn-On” dialog
There are a couple of buttons located at the bottom of the “Parameter Turn-On”-dialog:

- **Run FullProf**: Once you have selected the parameters you would like to optimize, the Rietveld refinement
calculation is started by pressing this button.

- **Clear**: By pressing this button you can turn off all parameters, i.e. uncheck the “vary” checkboxes of all
parameters. This will also erase the “Active parameters” table.

- **Reset**: You can reset all parameters to their original values (the ones before the first Rietveld refinement) by
pressing this button.

- **Export**: Match! offers a large variety of FullProf variables and options. Nevertheless, it may be useful in special
situations to use FullProf directly (without Match!). For this purpose you can export the input files required
(*.pcr, *.dat and *.bac) as a starting point for the FullProf calculation by pressing this button. You will be asked
to provide the path where the FullProf input files shall be stored. Afterwards, the files will be created in the
specified directory.

Running the calculation
When you have selected all parameters you would like to refine, the Rietveld refinement calculation is started by
pressing the “Run FullProf” button at the bottom left of the “Parameter Turn-On” dialog. As soon as the calculation
has finished, the results (e.g. R-factor, chi², FullProf comment) will be displayed in the “Rietveld” tab to the right of
the Match! window. You will also be informed if the calculation was successful (reached convergence) or not.

Results viewing
When the FullProf calculation has finished there are several facilities to view and evaluate the results of a refinement
calculation:

First of all, the convergence, the weighted average Bragg R-factor, the final reduced chi² and the comment from
FullProf are displayed at the top of the Rietveld tab. Below, there are several buttons using which more detailed
information is available:

The “View results” button displays a table in which you can compare the parameter values before and after the
refinement calculation. If FullProf has detected correlated parameters during the calculation, you can display them
by pressing the “Display correlated parameters” button below.

To the right, you can display the original FullProf files resulting from the calculation, simply by selecting the file you
would like to view in the “Display result file” combobox. A window will open where you can view and maybe copy
the contents of the selected file. This facility is especially useful if the result of a calculation is not to your satisfaction and you would like to view more details of the calculation.

Finally, you can copy the FullProf result files to a user-defined directory by pressing the “Save resulting files” button. If you do not save the FullProf files using this button, they will be deleted when you open or create a new Match! document.

Configuring automatic Rietveld refinement calculations

Using the "Define Parameter Sequence for Automatic Rietveld Refinement" dialog (Fig. 32) you can select which parameters shall be refined in which order (cycle) during the automatic Rietveld refinement procedure.

![Fig. 32: In this dialog you can select which parameters shall be refined in which Rietveld refinement calculation](image)

You can define parameters for a maximum of 10 subsequent refinement cycles.

The dialog can be opened by pressing the “Configure..." button at the top of the "Rietveld Parameter Turn-On" dialog (Fig. 28). In the top row of the dialog window, the dialog elements for the control of the current parameter sequence are placed:

- **New**: By pressing this button, the parameter sets for the 10 refinement cycles are erased, so that you can start from scratch to create a new parameter sequence. You will be asked if you would really like to do so after pressing the New button.

- **In the Preset combo box**, you can access all parameter sequence sets that you have already created. Simply click on the combo box and select the name of the parameter set you would like to open.

The "Standard" parameter set is always present in this combo box. This set contains the default/factory automatic refinement procedure; it cannot be deleted.

- **By pressing the Save button you can store the current parameter sequence set using a user-defined name, so that you can recall this setting later on in the "Preset" combo boxes both of the "Define Parameter Sequence..." as well as the Rietveld Parameter Turn-On" dialog. After pressing the button, you will be asked to enter a reasonable name for the parameter set. Once you have pressed "OK", the new parameter sequence preset will be added to the "Preset" combo box.

- **If you press the Default button**, the current parameter sequence set will be selected as the new default parameter sequence for automatic Rietveld refinements. The current parameter sequence must have been saved in advance for this purpose; otherwise a corresponding hint/message will be displayed.
• Pressing the Delete button removes the current set from the "Preset" list. Hence, if you would like to remove a parameter set, you have to select it from the "Preset" combo box first, and then press the "Delete" button.

Please note: The parameter set called “Standard” contains the factory parameter set; it cannot be deleted.

In the 10 boxes (parameter lists) (labeled "#1", "#2" etc.) below, you can select which parameters shall be varied separately for each refinement cycle. Match! runs the Rietveld refinements in the order as they are indicated at the top of the boxes, i.e. it starts with "Refinement #1", then runs "Refinement #2" etc. In each refinement cycle, all parameters that are present in the corresponding list (box) will be varied.

For every refinement cycle parameter box, a set of associated dialog elements is available:

• The "->" (arrow right) button at the top right of each parameter box copies the parameters of the corresponding box into the next box. This may be useful if you would like to add more and more parameters in each subsequent cycle, which is a common strategy in Rietveld refinement.

• In order to Add a new parameter to a parameter box, simply select it from the combobox at the bottom of the corresponding parameter list. It will instantly be added to the list.

• By pressing the ⌼ button at the bottom right of each parameter box you can delete the marked parameters from the corresponding parameter box. If no parameter is currently marked, all parameters will be removed from the box.

Once you have finished editing the Rietveld refinement parameter sets, please press the Close button to return to the “Rietveld Parameter Turn-On” dialog.

Rietveld options

On the “Rietveld” page of the “Options”-dialog you can make some adjustments for Rietveld refinement. First of all, you can define the directory in which the FullProf Suite is installed. In addition, you can select which tab (“Rietveld user level”; Beginner, Advanced, Expert or Previous) you prefer for being displayed first when the “Parameter Turn-On”-dialog is opened. It is also possible to make the “Automatic Rietveld refinement” option default. In addition, you can instruct Match! to keep the previous selection of parameters to be refined when you open the parameter turn-on dialog the next time (“Save parameter selection for next calculation”). Finally, you can decide if you would like to automatically display the profile data resulting from the Rietveld refinement (as well as the corresponding difference plot) when a refinement calculation has converged.

The Rietveld options page can also be displayed directly from the “Rietveld”-tab on the right-hand side of the Match! window by pressing the “Options” button.

Tips for Rietveld refinement

With Match! we have tried to get you into Rietveld refinement as gently as possible by offering different approaches with increasing difficulty level, from the “Automatic refinement” option to the “Expert” facilities. Nevertheless, Rietveld refinement is a complex subject that can require quite some experience. We would like to provide you with some hints and facts you should keep in mind in order to avoid running into problems at an early stage.

First of all, Rietveld refinement uses a local optimization method (least-squares refinement). This means that the method will try to reach the next minimum available from the starting point. You cannot expect from the method to investigate large parts of the cost function hypersurface! In practice this means that your starting model (e.g. crystal structure data, scaling factors, profile parameter values etc.) should be as close to the final model as possible, in order to reach convergence. You should avoid to give the system any “room” for getting stuck in a false minimum or being blown up by a singular matrix.

A reasonable strategy for performing a Rietveld refinement is not to vary all parameters straight away from the beginning, but to introduce them one after the other in a certain reasonable order. For example, there is little sense in trying to refine your atomic coordinates as long as the scaling factors of the phases are far off their optimum values!
On the “Beginner” tab of the “Parameter Turn-On” dialog you can see “our” suggestion for the order of parameter introduction into the calculation: You start by refining the scale factors of the phases and maybe the specimen displacement. Once you have run the corresponding Rietveld refinement and reached convergence, you can add the unit cell parameters and the first background parameter, and perform the second Rietveld refinement etc.

If a calculation does not converge, you should go back and try to find out which parameter causes the problem. Maybe you can keep it fixed or introduce some constraints for it.

In case of problems it is always advisable to take a look at the pattern graphics and compare the profile resulting from the Rietveld refinement (which has light-green color by default) to the experimental profile. Quite a lot of problems can be identified by this approach:

- Wrong scaling factor(s)
- Background is not correct
- Wrong or unidentified phase(s)
- Missing or surplus peaks
- 2theta error (e.g. zero point and/or specimen displacement)
- One or more unit cell parameters do not match
- Profile shape is not described correctly by the profile function applied, e.g. due to asymmetry

If you encounter convergence problems if only the scaling factor(s) of one or more phases are refined, you should check the crystal structure descriptions of the match list entries, especially the space group, setting and atomic coordinates. You could e.g. try to use a different entry describing the same phase, or display and investigate the crystal structure in the “Diamond” software (only available on Windows platforms).

If your successive Rietveld refinement calculations do no longer converge after activating the option/parameter “Atomic coordinates of all phases” on the “Beginner” or “Advanced” tab of the “Parameter Turn-On” dialog, you should try to activate the atomic coordinates of the atoms individually one after the other instead. This can be achieved on the separate “Crystal structure” tabs for each individual selected phase (tab “Expert”).

Another typical origin for convergence problems are parameter correlations. Correlated parameters can e.g. prevent a refinement calculation from converging by switching between two states, or by endless variations of one or more parameters that do not have any effect on the cost function (R-factor, $\chi^2$). As has already been mentioned above, you can press the “Display correlated parameters” button on the “Rietveld” tab to the right to display the correlated parameters detected by FullProf.

In addition, it might be extremely helpful to take a look at the FullProf output files (e.g. fpcalc.out, fpcalc.sum and fplog.log), especially at their lower part. Here you can normally locate the origin of severe problems. In order to display one of these files, simply select the corresponding file from the “Display result file” combobox on the right-hand side of the “Rietveld” tab, and/or press “Go!”.

If you really get stuck with your refinement, you might consider to vary individual parameters manually until you have reached a reasonable agreement between the pattern calculated by FullProf and the experimental pattern.

The background is that if the starting values of one or more important parameters (like the scaling factors) are too far off their optimum values, there may be little to no “contact” between the experimental diffraction pattern and the one calculated by FullProf. As a result, it may be very difficult for the Rietveld refinement to modify these parameters into the right “direction”, because there may be no real improvement when varying these parameters one or the other way. Keep in mind that “Rietveld refinement” is a local optimization, i.e. it tries to reach the next minimum!

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In order to improve this situation, it may be necessary to run a "manual refinement", i.e. to adjust some parameters manually until a reasonable agreement between calculated and experimental has been reached that may then be used as a starting point for the Rietveld refinement.

First of all, run some basic Rietveld refinement varying e.g. the scaling factors, and compare the resulting calculated pattern to the experimental one afterwards in the diffraction pattern graphics. Try to figure out which parameter should be changed in order to get a better agreement between the two curves. Afterwards, open the “Parameter Turn-On dialog”, disable the “Automatic Rietveld refinement” option at the top if necessary, and search for the parameter to be changed on the “Advanced” or “Expert” tab. Click on the “...”-button to the right of the corresponding parameter, and modify the “Current value” of the parameter in the dialog that is displayed. Do not activate the variation of this or any other parameter!

After you have modified the parameter(s) according to your assumptions, check again that no parameters are activated for Rietveld refinement (the “Table of active parameters” on the right-hand side must be empty), then press the “Run FullProf” button on the bottom left in order to instruct FullProf to recalculate the diffraction pattern based on the new parameter values. When the calculation has finished, compare the two curves mentioned above again, and think again of any parameters that may need some adjustment for a better agreement.

Repeat these steps until a reasonable agreement between calculated and experimental diffraction pattern has been achieved, then continue by running a normal Rietveld refinement starting at this point.

If all these hints do not help to obtain a reasonable refinement, or if you have special requirements, you might consider to move on to using FullProf directly, so that you really have all possibilities this program package offers. In order to do so, you can press the “Export” button in the “Parameter Turn-On” dialog to export FullProf files (pcr, dat and bac), so that you have a starting point for your journey into the world of FullProf.
Unit cell determination (indexing)

Basics

Within Match!, “indexing” means the derivation of unit cell parameters from given peak positions in a powder diffraction pattern. It is a mandatory step in crystal structure solution from powder diffraction data, e.g. using our software package “Endeavour”. Knowing the unit cell can also be very useful in phase identification, considering that cell parameters can be used as restraints.

Quite a lot of indexing programs are available today\(^\text{25}\); Match! can use two of the most prominent: Treor90 and Dicvol.

Prerequisites

In principle, you can download and install Treor and/or Dicvol separately on your PC, however, these programs are also included in the FullProf Suite\(^\text{26}\). Hence, there is no need to bother with this if you have already installed FullProf on your computer (e.g. for Rietveld refinement, p. 67). Match! will automatically locate the Treor90 and Dicvol06 programs included in this package, so you are ready to setup and run indexing calculations straight away. If this does not apply, you should take a look at the indexing options, in order to learn how to setup, the paths to the indexing programs.

Setting up and running indexing calculations

All that is required to run an indexing calculation are either experimental peaks or raw diffraction data. If only raw (profile) but no peak data are present when the indexing command is run, Match! will automatically execute the raw data processing before the actual indexing calculation is started.

Before running the “Indexing” command, you should mark the peaks to be taken into account in the indexing calculation. If you do not mark any peaks, Match! will automatically use the 20 strongest peaks (if present) that are not yet covered by selected phases for indexing, and whose relative intensity is larger than the corresponding minimum value (which can e.g. be adjusted using the red bar on the y-axis of the diffraction pattern graphics)\(^\text{27}\).

You can run indexing either using the corresponding command from the "Tools" menu, or simply by pressing the corresponding button \(\square\) in the main toolbar. Depending on the current settings and situation, this will either bring up a dialog asking which indexing method (Treor or Dicvol) you would like to use, run the default indexing program, or display the table of indexing results that are already present (and from which also new calculations can be run).

Once you have run the indexing command and maybe selected an indexing program, the corresponding parameter settings dialog will be displayed. The available parameters are different for Treor and Dicvol, so please see the corresponding chapters below for a detailed description of the two programs and their parameters.

Please note:

- Indexing can only be successful if all peaks that are considered belong to a single phase.
- It is strongly recommended to check (and maybe correct) 2theta errors (p. 25) before trying indexing.
- Criterion for the best cell: Maximum figure-of-merit, minimum number of unindexed lines

Results viewing

When the calculation has finished, you may be presented with one (or even a table of) potential solution(s). Please mark and/or confirm the solution(s) you would like to accept. You will then be taken to the “Indexing results” dialog (see below) where you can evaluate the solutions (i.e. unit cells), inspect peak data, select crystal system and space

\(^{25}\) http://www.ccp14.ac.uk/solution/indexing/

\(^{26}\) http://www.ill.eu/sites/fullprof/index.html

\(^{27}\) You can also adjust the corresponding parameter “minimum relative intensity for automatic peak usage” on the “Indexing” tab or the parameter “minimum relative intensity for peak correlations” on the “Search-Match” of the “Options” dialog. The values of these two parameters are identical.
group, and maybe add the solution as a new manual entry to the match list (e.g. to proceed with structure solution (p. 67)).

**Indexing results dialog**

The "Indexing results" dialog (Fig. 33) presents the solutions (e.g. unit cells) of all indexing calculations that have been accepted for the current experimental pattern up to now. It will either be displayed after an indexing calculation has been run, or if the "Tools/Indexing" command is run (or the corresponding toolbar button is pressed) when at least one indexing solution is already present for the current experimental pattern.

The "Indexing results" dialog provides an overview over all unit cells that have been found for the current experimental pattern so far, along with the corresponding peak data.

**The "Indexing results" dialog is organized as follows:**

The table at the top (the so-called "solution list") displays the main results of the indexing calculations (e.g. unit cell parameters, cell volume, number of (un-)indexed peaks, figure-of-merit, name of the indexing program used etc.). To its right, the parameters that were used for the marked indexing calculation are displayed. Below the parameter listing, a couple of buttons allow the refinement of the unit cell parameters, viewing of the original output files, the copying and export of the solution list, deleting marked solutions as well as adding solutions (unit cells) manually.

If a solution (unit cell) is marked in the solution list, the corresponding calculated peak positions are displayed as vertical bars in the main pattern graphics. (Depending on your screen size and resolution, you may have to adjust the position of the "Indexing solutions" dialog window to view the important parts of the pattern graphics.)

In the lower half of the dialog, the most prominent dialog element is the peak table on the left-hand side. Here, all peaks that are somehow involved (both experimental as well as calculated) in the indexing calculation marked in the solution list are listed. A color-coding on the left provides a quick overview regarding the influence of each peak, e.g. if it has been indexed (green) or not (red).

The main controls are located on the lower right-hand side of the dialog. Here, you can adjust, copy and export the pattern graphics and the peak table, setup and run new indexing calculations, select crystal system and space group, export or add a solution to the match list. Both peak table and control elements refer to the solution that is currently marked in the solution list at the top.

**Solution list and its controls**

The so-called "solution list" provides an overview over the unit cells (indexing calculation results, "solutions") that have been found so far for the current experimental diffraction pattern ("anchor pattern"). When a line in the solution list is marked, the peak data involved in this solution are displayed in the peak table at the bottom left. At the same time, the peak positions calculated from the current unit cell (and space group) will be displayed as vertical bars in the main diffraction pattern graphics. By default, these bars will have a light-orange color; you can change this color on the “Pattern graphics” page of the “Colors and line styles” dialog. The peak positions just mentioned are only
displayed as long as a solution is marked or the "Indexing solutions" dialog is displayed; they will vanish when the dialog is closed.

The parameters that have been used in the indexing calculation resulting in the marked solution are displayed in the parameters panel on the top right-hand side of the window.

Below, you can refine the unit cell by pressing the Refine button. A least-squares refinement of the currently marked unit cell parameters will be performed, based on all marked, indexed or at least correlated peaks. The result will be added as a new line to the solution list.

The View output button can be used to display the original Treor or Dicvol output file for the currently marked solution/calculation.

The Add button allows the user to manually add a “solution” (i.e. set of unit cell parameters) to the solution list. This can be useful e.g. to check how a certain unit cell you may have in mind relates to the experimental data or the solutions resulting from the indexing calculations. When you press the “Add” button, a new dialog will be displayed in which the unit cell parameters as well as the crystal system can be entered. After accepting the parameters by pressing <OK>, the new unit cell will be added to the table of solutions and can be handled just like the results from the “normal” indexing calculations.

By pressing the Del(ete) button you can remove the currently marked solution from the solution list. The Copy button (for copying the current solution list into the clipboard) gives also access to the Export and Print functionality for the solution list.

If you would like to edit the parameters of a manually added unit cell, you can do so by double-clicking on the corresponding line in the solution list.

Peak table
In the peak table, all peaks that are currently present in the experimental data as well as the marked solution are listed. For each peak, the following information is given as separate columns:

The “C(olor)” represents the status of each peak in the currently marked indexing solution:

- Indexed peak
- Experimental peak correlated to calculated peak, not used for indexing
- Unindexed peak
- Experimental peak not used for indexing, not correlated to calculated peak (maybe impurity phase)
- Calculated peak, not observed in experimental data
- Calculated peak, outside exp. 2theta range

The meaning of the individual colors is also displayed as a tooltip if you keep the mouse pointer over one of the colored panels.

If the checkbox “Use” is marked, the corresponding peak will be marked and included in the next indexing calculation.

In addition, the following peak parameters are given: “2theta” value of the experimental peak, “2theta calc.” 2theta value of the peak calculated from the current unit cell (solution), “d”-value of the experimental peak, “d calc.” d-value of the peak calculated from the current unit cell (solution), “h, k, l” Miller indices of the peak, referring to the current unit cell (solution), “I exp.” intensity value (I rel.) of the experimental peak.
Pattern graphics
Using this panel you can control some displaying options of the main pattern graphics: If you mark any of the three checkboxes Miller indices (hkl), d-values and/or 2theta, the corresponding information will be displayed at the top of each calculated (or reference database) peak.

By pressing the Copy button you can copy the current contents of the main pattern graphics to the clipboard (e.g. to paste it into some Word or PowerPoint document). You can also Export the current pattern graphics to a file by pressing the corresponding button.

Peak table control panel
In the “Peak table” panel you can toggle the display of the calculated peaks in the peak table on the lower left-hand side. Disabling the calculated peaks may sometimes be useful if a large number of them prohibits the inspection of the (un)-indexed peaks.

You can Copy, Export or Print the peak table: Pressing the “Copy” button gives access to all three commands.

New calculation
Here you can quickly setup and run a new indexing calculation: First, use the Select peaks button to mark the experimental peaks you would like to use for indexing (if you have not already marked the peaks otherwise, e.g. in the “Use” column of the peak table or directly in the pattern graphics or peak list). Afterwards, start the indexing calculation by clicking on Run.

If you click on the “Run” button, either the default indexing program will be run or the “Select indexing program” dialog will be displayed, depending on the corresponding options setting. If you keep the “Run” button pressed for about 1-2 seconds, you can directly select if you would like to run Treor or Dicvol.

Crystal structure
Using the dialog elements in this panel you can add more information about the crystal structure of the marked indexing solution (unit cell): You can select the crystal system and the space group from corresponding drop-down boxes.

If you mark the checkbox “Use extinctions to restrict space grps.”, only space groups that are in agreement with the observed peaks in the current experimental pattern are available in the “Space group” drop-down box.

This procedure works using systematic absences as follows: First, Match! calculates the powder diffraction pattern for all space groups that are in agreement with the current crystal system. Afterwards, Match! checks for every calculated pattern if there are peaks for which the intensity value in the calculated pattern is zero while there is a correlated experimental peak with an intensity > 0.0 (i.e. for which the correlated experimental peak is observed). If this applies, the space group does not fit to the experimental data and is removed from the list.

Export
By pressing this button, you can export the current solution (unit cell parameters and space group) to a cif-file, e.g. for importing it in some other program for crystal structure solution or visualization.

Add to match list
By pressing this button, you can add the current solution (unit cell parameters and space group) as a new manual entry (p. 106) to the match list. From there, you can e.g. run a crystal structure solution calculation (p. 67) using Endeavour.

Since an indexing calculation only reveals the peak positions that are in agreement with the resulting unit cell parameters but not the peak intensities, you have to select which peak intensity values shall be copied to the manual entry in the match list:

- **Full exp. intensities**: The full relative intensity values of the indexed experimental peaks will be used, i.e. the peaks that have been used for indexing or have been correlated to the indexing result.

- **Residuals**: The peak residuals are calculated by subtracting the peak intensities covered by the matching entries from the experimental peak intensities. Like with the previous option, the remaining intensity values
will be used both for the ‘indexed’ peaks (i.e. the peaks that have been used for indexing) as well as those that have been correlated to the indexing result.

- **No intensity values**: The peak intensities in the new manual entry will be left undefined.

**Close**
This button closes the "Indexing results" dialog. At the same time, the peak positions of the marked solution will vanish from the pattern graphics.

You can display the dialog again either by running the “Indexing” command from the “Tools” menu, or pressing the corresponding button in the main toolbar. Your indexing results will still be present, of course.

**Indexing using Treor90**

**Basics**
Treor90\(^{28,29}\) is a well-known program for indexing powder diffraction patterns. Treor can be used by Match! to derive unit cell parameters from the peak positions of marked experimental peaks. As an alternative to Treor, Dicvol (see below) can also be used for this purpose.

**Setting up and running Treor90 indexing calculations**
All that is required to run an indexing calculation are either experimental peaks or raw diffraction data. If only raw (profile) but no peak data are present when the indexing command is run, Match! will automatically execute the raw data processing before the actual indexing calculation is started.

Before running the “Indexing” command, you should **mark the peaks** to be considered in the indexing calculation. If you do not mark any peaks, Match! will automatically use the 20 strongest peaks (if present) that are **not yet covered by selected phases** for indexing, and **whose relative intensity is larger than the corresponding minimum value** (which can e.g. be adjusted using the red bar on the y-axis of the diffraction pattern graphics)\(^{27}\).

You can run indexing either using the corresponding command from the “Tools” menu, or simply by pressing the corresponding button in the main toolbar. Depending on the current settings and situation, this will either bring up a dialog asking which indexing method (Treor or Dicvol) you would like to use, run the default indexing program, or display the table of indexing results that are already present (and from which also new calculations can be run).

Once you have run the indexing command and selected Treor as the indexing program to be used, the Treor90 parameter settings dialog will be displayed (Fig. 34).

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Fig. 34: In this dialog, you can define unit cell and parameter limits for the Treor90 indexing calculation.

The following parameters are available:

**Crystal system(s) to be checked**: You can select if you would like to investigate either triclinic or non-triclinic crystal systems. If you mark “non-triclinic”, you can include or exclude cubic, tetragonal/hexagonal, orthorhombic and/or monoclinic cells.

**Unit cell parameter restrictions**: In this section, you can define maximum value for the cell lengths as well as the maximum unit cell volume.

**Additional limits**: You can define the minimum figure-of-merit as well as the maximum number of unindexed peaks for a solution to be accepted. Increasing the maximum number of unindexed peaks will increase the probability to get a solution (unit cell), so this may be a way out if you do not get a reasonable result with the standard settings. You should keep in mind though that you must check afterwards why the unindexed peaks are present in your pattern (maybe they belong to an impurity phase or are just artifacts). Note that by ignoring unindexed peaks it is quite easy to get artificial unit cells that have nothing to do with reality!

**Known formula weight and density**: If you know the arbitrary formula weight and density of your compound, and if the expected number of molecules or formula units in the unit cell is integer, you can enter the corresponding values as well as the max. density deviation as additional criteria to restrict the cell volume and hence the search space of the program. The value for the max. density deviation should be the maximum expected density deviation plus about 5-10%. The choice of the value should also take the quality of your diffraction data into account.

**Results viewing**

When the calculation has finished, Treor will select the most promising indexing result (unit cell) automatically. Match! will display the result and ask you to confirm or reject this solution. You will then be taken to the “Indexing results” dialog (p. 58) where you can evaluate the solutions (i.e. unit cells) that you have found up to now, inspect peak data, select crystal system and space group, and finally export the solution or add it as a new manual entry to the match list (e.g. in order to proceed with structure solution).

If you would like to take a look at the original Treor90 output file, you can do so by marking the corresponding solution in the solution list and clicking the “View output” button on the upper right-hand side.

**General hints on indexing from the Treor documentation**

- The standard procedure is to start with the high symmetries: cubic, tetragonal, hexagonal and orthorhombic (in one job). Next the monoclinic symmetry should be tried (more than one job may be needed). Successively increasing the number of base line sets and cell volume.
- The cell volume parameter may be estimated from the d-value of the 2th line (cf. keyword TRIC)
- Warning: If the true unit cell has a small volume, for example 250 Å³ and VOL=2000 is used, the correct solution may be lost in the trial process.
Warning: Estimation of the unit cell volume from the relations $\text{VOL(moniclinic cell)} = 20 \times D(20)^3$ and $\text{VOL(orthorhombic)} = 31 \times D(20)^3$ are much less reliable than the corresponding relation for the triclinic symmetry $\text{VOL(TRICLINIC)} = 13.39 \times D(20)^3$. Reason: Triclinic structures have no systematic extinctions!

- Generally, the first 20-30 lines should be used. Remaining lines may be used in later final refinements.
- You should not accept unindexed lines unless you are able to explain them.
- On the other hand, you should not put in uncertain (doubtful) lines in this program. They may be tested later by any refinement program.
- The output list will be interrupted as soon as a unit cell that will satisfy the criteria 'minimum figure-of-merit' and 'maximum number of unindexed lines' are fulfilled.
- Although the trial cells will be ordered according to priority rules (max. number of indexable lines and min. volume), it is not a guarantee that the first refined cell gives a correct solution.
- The main rule is that if all the first twenty lines are indexed and the de Wolff figure-of-merit $M(20)$ is greater than 9, then the indexing problem is in principle solved. This does not mean that the cell is reduced, that a cell axis may not be double etc.
- Unit cells obtained by this program should be carefully checked...
  - if the de Wolff figure of merit $M(20)$ is less than 10 or more than one line is unindexed within the 20 first observed lines, the solution is probably meaningless. Try next step in the strategy (see above).
  - for common factors in the quadratic forms. For example, a tetragonal pattern may have $H^2 + K^2 = 5 \times N$, i.e. the $a$-axis is $2.3607$ (square root of 5) times shorter than given on the output list. Obviously, if for example all $H,K$ or $L$ are even, the corresponding cell axis should be divided by two. This may occur if a too large VOL parameter has been given.
  - if the unit cell obtained is centered, derive a primitive cell.
  - reduce the primitive cell and derive the conventional cell.
  - Hexagonal and tetragonal cells are sometimes indexed as orthorhombic. For example: $a = b \times 1.7321$, i.e. a possible hexagonal cell.
  - Check for geometrical ambiguities (see reference list). It is also strongly recommended to check cubic, tetragonal and hexagonal solutions by an orthorhombic test.

Indexing using Dicvol

**Basics**

Dicvol06 is a well-known program for indexing powder diffraction patterns. Dicvol can be used by Match! to derive unit cell parameters from the peak positions of marked experimental peaks. As an alternative to Dicvol, Treor (see above) can also be used for this purpose.

**Setting up and running indexing calculations**

All that is required to run an indexing calculation are either experimental peaks or raw diffraction data. If only raw (profile) but no peak data are present when the indexing command is run, Match! will automatically execute the raw data processing before the actual indexing calculation is started.

Before running the “Indexing” command you should mark the peaks to be considered in the indexing calculation. If you do not mark any peaks, Match! will automatically use the 20 strongest peaks (if present) that are not yet covered by selected phases for indexing, and whose relative intensity is larger than the corresponding minimum value (which can e.g. be adjusted using the red bar on the y-axis of the diffraction pattern graphics). You can run indexing either using the corresponding command from the “Tools” menu, or simply by pressing the corresponding button in the main toolbar. Depending on the current settings and situation, this will either bring up a dialog asking which indexing method (Treor or Dicvol) you would like to use, run the default indexing program, or display the table of indexing results that are already present (and from which also new calculations can be run).

Once you have run the indexing command and selected Dicvol as the indexing program to be used, the Dicvol parameter settings dialog will be displayed (Fig. 35).

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Fig. 35: In this dialog, you can define unit cell and parameter limits for the Dicvol indexing calculation.

The following parameters are available:

**Crystal system(s) to be checked**: You can include or exclude cubic, tetragonal, hexagonal, orthorhombic, monoclinic and/or triclinic cells. Normally, you should **start by excluding monoclinic and triclinic crystal systems**.

**Unit cell parameter restrictions**: In this section, you can define maximum values for the cell lengths, minimum and maximum monoclinic cell angle, as well as minimum and maximum unit cell volume.

**Additional limits**: You can define the minimum figure-of-merit as well as the maximum number of unindexed peaks (in the Dicvol manual also called "impurity tolerance" N_IMP) for a solution to be accepted. Increasing the maximum number of unindexed peaks will increase the probability to get a solution (unit cell), so this may be a way out if you do not get a reasonable result with the standard settings. You should keep in mind though that you must check afterwards why the unindexed peaks are present in your pattern (maybe they belong to an impurity phase or are just artifacts). Note that by ignoring unindexed peaks it is quite easy to get artificial unit cells that have nothing to do with reality!

In addition, you can define the max. peak position deviation (in degrees 2theta), i.e. the maximum 2theta difference between an experimental and its corresponding calculated peak. If the 2theta difference is larger than this value, peaks are not regarded as being correlated (i.e. indexed).

**Known formula weight and density**: If you know the arbitrary formula weight and density of your compound, and if the expected number of molecules or formula units in the unit cell is integer, you can enter the corresponding values as well as the max. density deviation as additional criteria to restrict the cell volume and hence the search space of the program. The value for the max. density deviation should be the maximum expected density deviation plus about 5-10%. The choice of the value should also take the quality of your diffraction data into account.

**Results viewing**

When the calculation has finished, a table of the unit cells (solutions) found by Dicvol will be displayed. Please mark one or more solutions you would like to keep, then press <OK>. You will then be taken to the “Indexing solutions” dialog (p. 58) where you can evaluate the solutions (i.e. unit cells) that you have found up to now, inspect peak data, select crystal system and space group, and finally export the solution or add it as a new manual entry (p. 106) to the match list (e.g. in order to proceed with structure solution (p. 67)).

The **crystal system and space group suggested by Dicvol** are also copied to the individual solution(s) in Match!. They can be seen in the corresponding dialog elements on the right-hand side of the “Indexing results” dialog if a corresponding line is marked in the solution list at the top. You can of course modify these suggestions using the corresponding dialog elements.
If you would like to look at the original Dicvol output file, you can do so by marking the corresponding solution in the solution list and clicking the “View output” button on the upper right-hand side.

**General hints on indexing from the Dicvol documentation**

- Be careful in using the impurity tolerance: spurious lines increases the risk to miss the correct solution!

- It is recommended to use a two- or three-stages procedure (i.e. triclinic lattices should preferably be studied separately), for example:

  1. search in high symmetries down to orthorhombic: Line 2: n,itype,1,1,1,0,0,0
  2. search in monoclinic symmetry: Line 2: n,itype,0,0,0,0,1,0
  3. if necessary, search in triclinic symmetry: Line 2 : n,itype,0,0,0,0,0,1

  Note that for solutions with Monoclinic and Triclinic symmetries the program provides the reduced cell. If various equivalent solutions are found, only one of them is listed in the output file.

- Trigonal symmetry case with rhombohedral lattice: the pattern is indexed with an hexagonal lattice, having a unit cell volume three times greater.

- Please, spend time to ensure the quality of your collected data. With accurate data, the success rate of Dicvol06 is very high. Peak positions should be extracted with a profile fitting software. An interactive program should be preferred, since automatic extractions can miss lines (low intensity, shoulder, ...).

- With bad data, the chance to obtain the correct solution is small and the calculation can be time-consuming.

- With modern X-ray powder diffractometers (the use of monochromatic radiation is recommended), absolute errors on peak positions lower than 0.02 degrees 2theta can be routinely obtained. For indexing purposes, errors should not (ideally) exceed 0.03 degrees in 2theta.

- With high resolution powder diffraction data (conventional or, particularly, synchrotron X-ray sources), the absolute error is usually less than 0.02 degrees (or even 0.01 degrees with ultra-high resolution) in 2theta; consequently, a maximum peak position deviation of 0.02 (or even 0.01) is recommended; the convergence of the dichotomy procedure will be improved. However, be sure that this condition is true for all lines used as input data. (Remember that all mathematical solutions within the input limits and error bounds are found, the greater they are the greater is the number of mathematical solutions).

- The maximum number of unindexed lines (also called "number of impurity lines", N_IMP) can be used in case of expected spurious lines (i.e. impurity lines, as well as observed lines out of the input error). N_IMP acts at all successive levels of the dichotomy algorithm. As soon as an indexing solution is retained, a least-squares refinement of lattice parameters is carried out. For this refinement a larger error on observed lines is considered. Then, a line rejected at the last dichotomy level can, by chance, be accepted with the refined lattice parameters.

- Note that the program Dicvol06 is executable from 7 lines- 8 lines if the 'zero-shift' is refined - (though it is not recommendable since LS refinement instabilities can be expected).

- Long and short axis cases (dominant zone cases): if such cases are expected, the number N of lines used for searching the solution should, generally, be greater than 20.

- The minimum value for a linear lattice parameter has been fixed to 2.5 angstroms.

- Reliability of indexing solutions: read paragraph 8 of ref. 5 and refs 7 and 8.

- Note that with the option Dicvol04 (option =0), as soon as a solution is found, only solutions with smallest volumes will be subsequently retained. If (for some reasons!) you are not satisfied by the solution, you can run again the program with an input lower volume limit slightly greater than that of the found solution (the exhaustive search is then extended to a higher volume).
• Note that the search is exhaustive within the limits on the input data. In particular, the search is constrained by the higher and smaller bounds on parameters, volumes, selected FoM and absolute errors on peak positions. Please act on these parameters when using Dicvol06.

• A lattice metric singularity occurs when unit cells defining two lattices have an identical set of calculated d-spacings. This can be observed with high symmetry lattices, simple relations exist between the parameters of the two cells, as well as particular cell-volume ratios. A typical case is: an hexagonal cell \([a, c, \text{volume } v]\) can be indexed with an orthorhombic cell \([\text{parameters: } a/2, a \sqrt{3}, c, \text{volume } v/2]\). Due to the strategy used in Dicvol, based on an analysis through decreasing symmetry, all cells should be, in principle, displayed in the output file (except if a solution is rejected by the input maximum volume).

• Possible space groups: look at the hkl conditions in the output list of the reviewing of the complete input data provided after a solution is found from the first N lines.
Crystal structure solution using Endeavour

Basics
After collecting a set of peaks belonging to a presumably unknown phase in your sample/diffraction pattern, you should first try to index them (p. 48). Once you have been successful and obtained a promising set of unit cell parameters, you can store the result (peak data and unit cell parameters) in a manual entry (p. 106) in the match list. Afterwards, you can try to solve/complete the crystal structure (i.e. determine the atomic parameters) based on this manual entry, e.g. using our software Endeavour31,32 (which is available for Windows only, unfortunately).

Match! can forward the data you have collected (peak data, unit cell parameters and maybe space group) from the manual entry to Endeavour and run it. Once the calculations have finished and a promising structural model has been found, you can export the resulting crystal structure from Endeavour to a cif-file, and then re-import this into the manual entry just mentioned, e.g. in order to run a Rietveld refinement (p. 48).

Method
Endeavour uses a so-called “direct-space method” to solve a crystal structure: It starts by placing the atoms at random positions in the unit cell and then moves them around, trying to minimize the R-factor (difference between experimental and calculated diffraction pattern) and the potential energy (details can be found in ref. 31 and 32). For this, it needs to know which atoms (elements and maybe oxidation states/charges) are present in the unit cell.

Hence, in order to be able to apply Endeavour, you should at least know the composition (formula sum or molecule structure) of the unknown compound, e.g. from XRF experiments or chemical analysis. In addition, you also need the number of formula units per unit cell (Z). Endeavour can help you with the latter if you have at least a rough idea of the density of the material and/or of the space filling percentage.

Space group determination
What is still missing for a full description of the crystal structure is the space group:

Before adding a solution as a new manual entry to the match list in the “Indexing results” dialog, you can ask Match! to determine potential space group candidates, by activating the checkbox “Use extinctions to restrict space grps.” in the “Crystal structure” section of the dialog.

Once you have done so, only space groups that agree with the observed peaks in the current experimental pattern are available in the “Space group” drop-down box. This function works by checking systematic absences as described on p. 60.

Depending on the type of compound (individual atoms or molecules) and the symmetry it is sometimes advantageous to already use the space group information in the Endeavour crystal structure solution calculation. In other cases, it is better to run the crystal structure solution without space group restrictions (i.e. in space group P 1) and determine the space group from the resulting structural model afterwards. Endeavour can do the latter using the SFND/RGS function in the program KPlot33,34 developed by R. Hundt and co-workers.

Running Endeavour
If you are running a Windows version of Match! and have installed Endeavour on your computer, Match! will determine the path to the software automatically; you can also select it manually on the “General” tab of the “Options”-dialog.

32 Crystal Impact GbR, Endeavour 1.7, Internet: https://www.crystalimpact.de/endeavour, E-mail: info@crystalimpact.com, Bonn 2009.
To run an Endeavour calculation, please mark the corresponding entry in the match list that contains the data to be used (at least peak data and unit cell parameters) first. Afterwards, you can either run the "Structure solution (Endeavour)..." command from the "Tools" menu (or the context menu of the match list), or press the corresponding button in the Match! toolbar.

A new windows will open showing some instructions how to run the structure solution calculation in Endeavour, and how to get the resulting crystal structure data back into Match!. You can disable the future displaying of this information window by marking the corresponding option.

After confirming the dialog window by pressing <OK>, Endeavour will be run, and the current crystal structure and diffraction data will be transferred to it.

When the Endeavour program window is displayed, please press the “F7” button (or run “Structure/Start solution...”) to open Endeavour's structure solution wizard. It will take you step by step through the input of any missing information (like the elements and composition) and finally run the actual structure solution calculation.

**Reimporting Endeavour result into Match!**

Once the structure solution calculation(s) has finished and a promising solution has been found, you can transfer it back to Match!, e.g. in order to run a Rietveld refinement. To do so, please mark the solution in the configuration list on the upper right-hand side of the Endeavour program window, then click into the structure picture to shift the focus. Run the “File/Save As/Save Structure As...” command, select the file type “CIF (*.cif)”, and choose/enter an appropriate directory and file name.

In Match!, please right-click on the manual entry you would like to import the crystal structure to, select “Edit manual entry” from the context menu, and finally press the “Import from cif-file” button on the upper right-hand side of the dialog that opens.

As an alternative, you could also run the command “File/Import/Crystal structure (CIF)”, in order to add the solved structure as a new manual entry to the match list.
Crystallite size estimation

Match! can estimate the crystallite size $L$ (average in Å) in your sample using Scherrer's formula$^{35,36}$:

$$L = \frac{K \times \lambda}{FWHM \times \cos \theta}$$

where $K$ is the so-called "Scherrer constant" (typically $=0.94$ for FWHM of spherical crystals with cubic symmetry), $\lambda$ is the wavelength of the radiation and $\theta$ is the diffraction angle of the peak.

As you can see, the main "input" to the formula are the FWHM values (FWHM = Full Width at Half Maximum) of the peaks.

Before the FWHM values from the diffraction pattern can be correlated to the crystallite size, it is necessary to separate the contribution of the instrument to the peak broadening (FWHM) from the actual contribution of the sample. The FWHM values of the latter are then used in the Scherrer formula to calculate an estimate for the crystallite size of the corresponding phase/compound.

In order to separate the instrument contribution to the FWHM of the experimental peaks from the sample contribution, you first have to create a so-called "instrumental standard" that contains your instrument's contribution to peak broadening. For this, you have to record a powder diffraction pattern from a sample/compound for which it is known that it does not contribute to the diffraction peak profile (so that the peak broadening is almost entirely caused by the instrument). In this compound/compound, the crystallite size should be larger than 500 nm while the particle size should be less than 10 µm. In addition, the standard material should be defect and strain free. Finally, the standard should have a similar mass absorption coefficient than the nano-crystalline specimen as well as a similar atomic weight and packing density$^{37}$.

A “standard” as it is used in Match! consists of a list of peaks from the diffraction pattern of a suitable standard compound (e.g. LaB$_6$, CeO$_2$, Si, etc.) that has been recorded using the same instrument and setting than the compound for which you would like to determine the crystallite size. The most important data are the peak positions and their FWHM values, both of which should have been obtained from a profile fit calculation of the peak data to the standard's diffraction pattern. At least one peak position and FWHM value must be entered in order to create a valid standard.

Before you can run the crystallite size estimation calculation, please make sure first that a suitable instrumental standard is present:

In order to create a standard for crystallite size estimation in Match!, the first thing you have to do is to import the powder diffraction pattern of a suitable standard (see above). Afterwards, run the peak searching (if it is not performed automatically), then mark click on the individual peaks and run a profile fitting calculation for them until the agreement between the experimental diffraction profile and the one calculated from the experimental peak is fairly good. You can display the resulting peak parameters in the peak list if you like.

Now you are ready to add these peak data as a new instrumental standard for crystallite size estimation:

Run the "Crystallite size estimation..." command from the "Tools" menu. If you do so for the very first time (no standards are present up to now), a dialog displaying some background information will be displayed, asking if you are ready to add/enter the peak data of your new standard now. Please accept by clicking on "Yes".

Afterwards, Match! will detect that experimental peak data are currently present, so it will ask if you would like to add these peak data as a new instrumental standard. Again, click on "Yes" to do so. The "Add/edit instrumental

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broadening standard" dialog will be displayed (Fig. 36), providing a variety of commands and options to handle instrumental standards:

![Add/edit instrumental broadening standard dialog](image)

Fig. 36: In this dialog, you can define and/or edit the instrumental standards required for crystallite size estimation.

Detailed information about this dialog is available in the online help (which can be displayed by pressing the Help button at the bottom). For the current, all you have to do is to accept the new standard by pressing the OK button. You will be asked if you would like to save the current data/standard. Please click "Yes" and enter a reasonable name (e.g. the formula sum, like LaB6 in this case) for the new standard. Close the “Estimate crystallite size” dialog for the current, too.

Now that a suitable instrumental standard is present, you can create a new document (File/New) and prepare your sample's diffraction pattern for the analysis:

Import the diffraction pattern of your sample for which you would like to perform the analysis, run the peak searching (or add the peaks manually), then mark (click on) the individual peaks and perform profile fitting calculations for them until the agreement between the experimental diffraction profile and the one calculated from the experimental peak is fairly good. You can display the resulting peak parameters in the peak list on the right-hand side if you like. As has already been mentioned above, the main input to the crystallite size estimation calculation (Scherrer formula) are the FWHM values of the peaks along with the peak positions, so it is worthwhile to invest a little bit of time in this step, in order to obtain reasonable results.

Now you are ready to perform the actual crystallite size calculation. In order to do so, simply run the "Crystallite size estimation..." command from the "Tools" menu. Match! will open the corresponding dialog (Fig. 37), automatically subtract the instrumental peak broadening contribution (using the default instrumental standard mentioned above), and then present a table of the individual peak data and the resulting crystallite size estimation values.
Fig. 37: The “Estimate crystallite size” dialog, displaying a table of all peaks in the current diffraction pattern, along with their data, correlated phases and resulting crystallite size information. An average for all peaks for which the column “Use” is checked is also given.

The average crystallite size is given at the bottom right of the peak data table. It is calculated from all peaks for which the checkbox **Use** is marked in the table above. When you open the “Estimate crystallite size” dialog to perform the analysis for the first time, Match! will automatically mark the checkboxes for all peaks in the range 30-50° (which is typically most suitable for crystallite size analysis) for which all required FWHM data are available.

More information about the details and dialog elements in this dialog is available in the online help which can be opened by clicking the **Help** button on the lower right-hand side.
Reference pattern database

Overview

Match! identifies phases in a sample by comparing its powder diffraction pattern to reference patterns of known phases. Hence, it needs a so-called “reference database” in which these reference patterns are provided. Match! is extremely flexible in this context, with several options for obtaining/using a reference database:

- A free-of-charge reference database for inorganic compounds is by default installed automatically along with Match!; it can be used straight away after the installation. This reference database contains powder diffraction patterns calculated from crystal structure data taken from the “Crystallography Open Database” (COD), which itself provides crystal structure data published by the IUCr journals, the “American Mineralogist Crystal Structure Database” (AMCSD), and various other sources. In this context, we would like to thank Pete Strickland (IUCr), Armel Le Bail and Saulius Gražulis (COD), as well as Bob Downs (AMCSD) for their kind permission to download and distribute their data free-of-charge!
  
  All entries taken from the COD reference database contain atomic coordinates, based on which the corresponding powder diffraction patterns have been calculated. Besides this, for all entries, I/Ic-values have been calculated, so that a semi-quantitative analysis can be carried out.
  
  You can download additional or updated reference databases free-of-charge from https://www.crystalimpact.de/match/download.htm#refdb

- The classical reference pattern database is the so-called “PDF” database provided by the ICDD. There are several PDF database products available (e.g. PDF-2, PDF-4+, PDF-4/Organics, PDF-4/Minerals), all of which can be used with Match!
  
  According to our knowledge, the PDF is the largest and most comprehensive source of reference diffraction patterns.

- Many users also have diffraction patterns of own compounds that are not (yet) present in the COD or PDF databases. Hence, it is desirable to use these patterns in phase identification in addition to the “normal” patterns. This can be achieved using the so-called “user database” (p. 83).

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38 The Match! installer contains only data from the “Inorganics” subset of the COD. You can download and install the full COD reference database from the Match! web page https://www.crystalimpact.de/match/download.htm#refdb.


43 http://www.crystallography.net/cod/

44 International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, United Kingdom. http://journals.iucr.org


46 International Centre for Diffraction Data, 12 Campus Boulevard, Newtown Square, PA 19073-3273, U.S.A. Phone: +1-610-325-9814; Fax: +1-610-325-9823; E-mail: info@icdd.com, Internet: www.icdd.com

47 Please note that ICDD’s relational database products (PDF-4, PDF-2) are currently only available for the Windows platform. However, on Mac OS X or Linux, you can use the “old” PDF-2 database releases before 2005, if you have a valid license for it.
You can use an ICSD/Retrieve version released between 1993 and 2002 that you might have available\textsuperscript{48}. Match! can import the ICSD/Retrieve entries into a normal Match! user database and calculate reference powder diffraction patterns in a single step (p. 100).

You cannot only use one or the other of the above-mentioned reference databases but also combinations of them. For example, you can combine diffraction patterns of your own compounds with the COD database that is installed with Match! (p. 81).

When selecting your reference database, you should always keep in mind that there may be unforeseen phases in your samples, in which case it is extremely useful to have a large pattern database available in which even diffraction patterns of “strange” phases are present.

**Reference Database Library**

If you would like to apply a different reference database than the one that is installed along with Match! (typically, the COD or the “Inorganics” subset of the COD), you first have to add it to the so-called “Reference Database Library”. This is a table (in fact two tables) of all reference databases that are currently available to the user. Each row in the table corresponds to one reference database, for which the name, the number of entries, and the location/path of the database/index files are displayed. There are two tables, one for reference databases that are available to all users, and another one that can only be accessed by the current user (Fig. 38).

Fig. 38: Using the “Reference Database Library”, you can manage the various reference pattern databases on your PC. In this case, a COD “Inorganics” database (REV140301) is installed for all users on this PC (upper table) and has been selected for being used in phase identification (column “Cur.”). Besides this, the PDF-4+ Release 2015 is also available for all users. In addition, there is another COD version that has been combined with user data; this reference database is only available to the current user.

Thanks to the “Reference Database Library”, Match! is capable of handling more than a single reference pattern database at a time: You can switch between all reference databases you have created (i.e. created index files for) while keeping your diffraction data in memory, thus enabling you to compare phase identification results from various reference databases. Of course, it is not necessary to perform a re-indexation of a reference database when switching between them!

\textsuperscript{48} Of course, you must have a valid license for ICSD/Retrieve! Please contact FIZ Karlsruhe (Germany) (e-mail: crydata@fiz-karlsruhe.de) if you are in doubt whether your license is still valid!
The “Reference Database Library” dialog is opened automatically at program start if you did not install a reference database along with Match!. It can also be opened by selecting the “Select/create reference database” command from the “Database” menu, or by pressing the corresponding button in the toolbar.

As has already been mentioned, the “Reference Database Library” contains a list of all reference databases that are available for the current user (see below). For each available reference database, the name, the number of entries, and the directory in which it is stored are displayed. The database you are currently using is identified by an “>>>”-arrow to its left.

On a multi-user machine, each user may have individual reference database(s). It is perfectly possible to create a new reference database as a normal (standard) user, i.e. it is not necessary to have administrator privileges for this task. However, please note that a standard user can create reference databases only for himself, while an administrator can create databases also for all users. If a database is available to all users, it is listed in the upper table. Note that databases in this table cannot be modified or deleted by normal (standard) users!

You can manage your reference databases using the buttons at the bottom of the “Reference Database Library” dialog:

- **Select** another reference database for search-match or database retrieval purposes (of course without the need to perform a complete new indexation!). Please note that the current contents of the candidate list will be updated if you select a new reference database, in order to avoid problems like a certain entry being present in one reference database while missing in another one.

- **Create** a new reference database (e.g. as a working-copy of the COD, from an existing Match! user database or by importing entry data from cif-files or the ICSD).

- **Add** a reference database that is stored “ready for usage” in a certain directory.

- **Rename** an existing reference database.

- **Shift** the position of a classical PDF-2 database that is used in the marked reference database to a new directory.

- **Delete** an existing reference database.

- **Quit** the Reference Database Library.

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**Create a new reference database**

Match! cannot use pattern sources like the PDF or COD database directly; it requires the presence of so-called “index files”. These files contain sorted extracts of the original data, thus enabling a much faster processing of diffraction pattern comparison and database retrieval tasks. In other words, creating a new reference database basically means to create index files for an existing source database.

If you would like to create a new reference database, please press the “Create” button in the Reference Database Library dialog. This will bring up the “Create Reference Database” dialog in which you can select the source(s) of the reference powder patterns. You can either mark one source or create combined reference databases by marking more of them, e.g. the “COD” and “User database”. It is also possible to define a name for the new reference database, and to select the directory in which all files of this new reference database shall be stored (Fig. 39).

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49 Not yet available in current beta version!
Using this dialog you can create a new reference database for Match!

PDF-4 or PDF-2
Using the ICDD PDF database products with Match! is easy: Simply install the PDF database on your Windows PC according to the instructions given by ICDD, then launch Match!). Match! will automatically detect newly installed PDF database products at program startup (at least if the corresponding option is set) and ask if you would like to index one of them straight away. If you agree by clicking “Yes”, the database indexing will be performed immediately. You will then be asked if you would like to use the new reference database straight away. You can do so by clicking “Yes” again. That's it!

Please note:
- Even if you click “No” in the last step, you can switch over to the new PDF reference database later in the Reference Database Library.
- You can also check for new/updated PDF database products from within Match!, by running the “Database/Check for new PDF databases...” menu command.

You can also perform the indexing of a PDF database manually, of course. In the following, we will demonstrate how to apply an existing ICDD PDF-4 or PDF-2 database as a Match! reference database:

Let us assume that you would like to add the ICDD PDF-4+ Release 2015 database (which must have been installed on your PC in advance, of course); the procedure for using the corresponding PDF-2 is the same.

Once you have pressed the “Create” button in the Reference Database Library as just described, Match! will automatically check for available PDF relational database products (like the PDF-4+ or the PDF-2). If at least one PDF RDB is found, the checkbox “ICDD PDF” in the upper part of the dialog will be checked automatically, with the first PDF that has been found already selected in the drop-down box below “ICDD PDF”. If you would like to select a different PDF version, you have to click on the drop-down box and mark the corresponding line. In our case, we

50 The ICDD PDF relational database products (like PDF-4+, PDF-2 starting with release 2005 etc.) are currently only available for the Windows platform. Hence, you cannot use these databases if you are running Match! on a Mac or Linux machine.
would like to use the PDF-4+/Release 2015, with the corresponding line already having been selected automatically (Fig. 40).

If you like, you can change the name of the new reference database at the bottom of the dialog (deactivate the corresponding “Automatic” checkbox first!), and/or change the location (directory) in which the index files for the new reference database shall be stored. Normally, Match! will automatically create a suitable name and select an appropriate directory.

In case you have administrator privileges, you can also select if you would like to make the new reference database available to all users (or only to you), and if you would like to make it the default Match! reference database for new users on your PC.

Please note that on Windows it is not sufficient to run Match! from an administrator account; you have to explicitly use the command "Run as administrator" (which is available e.g. in the context-menu (click right mouse button)) in order to enable the two options "Create for all users" and "Select as default for all users without own selection"!

On Linux, you have to use "su" or "sudo" in order to run Match! with "root" privileges and enable these two options.

Once you have made your selections, press the “OK” button at the bottom to start the creation of the index files. A small window will be display the progress of the indexation (Fig. 41). Due to the large amount of data which have to be read and sorted, the creation of index files is a rather time-consuming process. The procedure may take between about 30 minutes to an hour or even more, depending especially on the drive access and processing speed of your computer.

When the indexation has finished, a corresponding message will be displayed. Afterwards, the new reference database will appear in the list of the Reference Database Library, ready for being selected (Fig. 42).

Fig. 40: You have selected to apply the ICDD PDF-4+ Release 2015 database as Match! reference database.

Fig. 41: This window shows the progress of the index file creation.

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The PDF-4+ Release 2010 contains more than 300,000 entries!
Fig. 42: The “PDF-4+ 2015 RDB” reference database is now available in the list for all users.

If the new reference database is the only one available in the Reference Database Library, it is selected for being used automatically. Otherwise, you have to select the new reference database manually: Simply mark (click) on the corresponding line in the table, then press “Select”. The license for the PDF database is checked, then the new reference database is marked as selected, indicated by the “>>>” arrow on the left-hand side of the corresponding line.

You can now leave the Reference Database Library by pressing “Quit” and apply the PDF-4+ reference database in phase identifications and database retrievals.

If you would like to use the PDF-2 or any other current ICDD PDF database product, this can be done in a similar way than the procedure just described for the PDF-4+.

Old format PDF-2
If you would like to use an ICDD PDF-2 database in the old format (i.e. release before 2005) as reference database, you can do so as follows:

Similar to current PDF-2 or PDF-4 versions, you first have to tell Match! that you would like to use an ICDD PDF database, by marking the checkbox “ICDD PDF” in the upper part of the “Create Reference Database” dialog. Afterwards, please mark (click on) the line “PDF-2 Release 2004 (or earlier versions)” in the list below “ICDD PDF” (Fig. 43).
Fig. 43: You have selected to apply an ICDD PDF-2 database released before 2005 as Match! reference database.

You now have to give the directory in which the PDF-2 database (to be exact: the file named “pdf2.dat” or similar) is stored in the input box below “Location of PDF-2 / NBS*AIDS83 database”. You can easily select this file/directory by clicking on the “...” button to the right of this input line.

A “File Open” dialog will be displayed in which you have to select the file “pdf2.dat” (or similar) in the directory where your PDF-2 database is stored. Afterwards, press “Open” to select the file/directory. A new dialog will open in which you have to explicitly confirm that you have a valid license for the PDF-2 database you are about to use. If you confirm the validity of the license, the location of the PDF-2 database file will be displayed in the corresponding input box.

If you like, you can now change the name of the new reference database at the bottom of the dialog (deactivate the corresponding “Automatic” checkbox first!), and/or change the location (directory) in which the index files for the new reference database shall be stored. Normally, Match! will automatically create a suitable name and select an appropriate directory.

In case you have administrator privileges, you can also select if you would like to make the new reference database available to all users (or only to you), and if you would like to make it the default Match! reference database for new users on your computer.

Please note that on Windows it is not sufficient to run Match! from an administrator account; you have to explicitly use the command “Run as administrator” (which is available e.g. in the context-menu (click right mouse button)) in order to enable the two options “Create for all users” and “Select as default for all users without own selection”!

On Linux, you have to use “su” or “sudo” in order to run Match! with "root" privileges and enable these two options.

Once you have made your selections, press the “OK” button at the bottom to start the creation of the index files. A small window will display the progress of the indexation (Fig. 44). The procedure will take a few minutes, depending especially on the drive access and processing speed of your computer. When the indexation has finished, a corresponding message will be displayed. Afterwards, the new reference database will appear in the list of the Reference Database Library, ready for being selected.

Fig. 44: This window shows the progress of the index file creation.
If the new reference database is the only one available in the Reference Database Library, it is selected for being used automatically. Otherwise, you have to select the new reference database manually: Simply mark (click) on the corresponding line in the table, then press the “Select” button at the bottom. The new reference database will be marked as selected, indicated by the “>>>” arrow on the left-hand side of the corresponding line.

You can now leave the Reference Database Library by pressing “Quit”, and apply the PDF-2 reference database in phase identifications and database retrievals.

**Create a working-copy of the COD**

If you would like to apply modifications to the COD reference database that is installed along with the Match! software, you first must create a working-copy of it, because as a standard user you do not have write permission to the original database.

In order to do so, please click the “Create” button in the “Reference Database Library” dialog first. In the dialog that opens, please make sure to only mark the “COD database” checkbox (remove the hook in front of “ICDD PDF” if required), and adjust all settings according to Fig. 45.

![Fig. 45: Instructions to create a working-copy of the COD-Inorganics reference database installed with Match!](image)

Once you have finished and clicked “OK”, a copy of the COD reference database will be created. A small window will display the progress of the process (that will typically take only a few seconds to complete). Afterwards, a corresponding message will be displayed, and the new reference database will appear in the list of the Reference Database Library, ready for being selected.

**Create reference database from user data or ICSD/Retrieve**

As has already been mentioned, it is also possible to use own diffraction patterns or the ICSD/Retrieve database in phase identification. Before you can do so, you have to store/convert the corresponding diffraction patterns and/or crystal structure data sets into a so-called “user database” file (file extension *.mtu), using the so-called “User Database Manager” dialog.

If you have not already done so, please follow the instructions on p. 83 first, in order to create the mtu-file from your data. Afterwards, please return to this point and continue reading.

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52 You can open the “User Database Manager” directly from the “Create Reference Database” dialog by pressing the “Create/modify user database...” button. Alternatively, the “User Database Manager” can also be invoked from the “Database” menu.
The procedure to use an existing user database file (*.mtu) as reference database is pretty similar to the one using an old PDF-2 version: First, you have to tell Match! that you would like to apply a user database, by marking the corresponding option in the middle of the “Create Reference Database” dialog. Afterwards, you have to select the location of the *.mtu file, by pressing the button “Select user database file (*.mtu)” to the right of the corresponding input line “Location:”.

A “File Open” dialog will be displayed in which you have to select the mtu-file in which your user data are stored. Afterwards, press “Open” to select the file/directory and return to the “Create Reference Database” dialog. The location of the mtu-file will now be displayed in the corresponding input box (Fig. 46).

![Fig. 46: The Match! user database file based on which a new Match! reference database shall be created has been selected.](image)

If you like, you can now change the name of the new reference database at the bottom of the dialog (deactivate the corresponding “Automatic” checkbox first!), and/or change the location (directory) in which the index files for the new reference database shall be stored. Normally, Match! will automatically create a suitable name and select an appropriate directory.

If you create a new reference database for an existing user database (mtu-file), the selected mtu-file will be copied to the directory in which also the index files are stored. Hence, it does not matter if you change or delete the original user database file later on; this will not affect the reference database.

In case you have administrator privileges, you can also select if you would like to make the new reference database available to all users (or only to you), and if you would like to make it the default Match! reference database for new users on your PC.

Please note that on **Windows** it is **not** sufficient to run Match! from an administrator account; you have to explicitly use the command "Run as administrator" (which is available e.g. in the context-menu (click right mouse button)) in order to enable the two options "Create for all users" and "Select as default for all users without own selection"! On **Linux**, you have to use "su" or "sudo" in order to run Match! with "root" privileges and enable these two options.

Once you have made your selections, press the “OK” button at the bottom to start the creation of the index files. A small window will display the progress of the indexation (Fig. 47). The procedure will take a few minutes, depending especially on the number of entries as well as the drive access and processing speed of your computer. When the indexation has finished, a corresponding message will be displayed. Afterwards, the new reference database will appear in the list of the Reference Database Library, ready for being selected.
If the new reference database is the only one available in the Reference Database Library, it is selected for being used automatically. Otherwise, you have to select the new reference database manually: Simply mark (click on) the corresponding line in the table, then press “Select”. The new reference database will be marked as selected, indicated by the “>>>” arrow on the left-hand side of the corresponding line.

You can now leave the Reference Database Library by pressing “Quit” and apply the new reference database in phase identifications and database retrievals.

Creating combined reference databases

You can create combined reference databases that e.g. contain diffraction patterns of your own compounds along with the COD or PDF data. To do so, simply mark the corresponding checkboxes in the “Create Reference Database” dialog (Fig. 46, p. 80).

If you would like to use a suitable name for the new reference database instead of the one that is suggested by Match! automatically, you can remove the hook in the checkbox “Auto” to the right of the line “Name to be given to the new reference database”, then edit the name.

Select reference database

In order to select another existing reference database for being used in future search-match and restraining operations, please mark (click on) the corresponding line in the Reference Database Library dialog. Afterwards, press the “Select” button at the bottom of the dialog. If the selected reference database is a PDF-2 (Release after 2004) or PDF-4 database, the validity of the license will be checked. Afterwards, the reference database will be marked as selected, indicated by the “>>>” arrow on the left-hand side of the corresponding line.

Please note:

- If your candidate list contains entries when you open the Reference Database Library, it will be updated if you select a different reference database. This is because the entries present in one reference database will most probably not be present in another database.

- The name of the currently selected reference database is displayed in the status bar at the bottom of the Match! window. This name is updated when the Reference Database Library is closed.

Add reference database

You can create backup copies of complete reference databases, simply by copying the complete contents of a reference database index directory. The name of a current reference database directory is given in the right-most column in the Reference Database Library dialog.

If you would like to use/restore a backup copy later on, you can simply copy it to an appropriate directory on your computer. Afterwards, click the “Add” button in the Reference Database Library. A “File Open” dialog will be displayed in which you can select the “Match! Reference Database” file (MatchRefDBInfo.mtn) that contains the information required to use the index files in the same directory. Please mark the file “MatchRefDBInfo.mtn”, then press “Open”.

In case you have administrator privileges, you will now be asked if you would like to make the new reference database available to all users (or only to you). Afterwards, the new reference database will appear in the corresponding table of the Reference Database Library, ready for being selected for usage.
**Rename reference database**

If you would like to rename an existing reference database, please mark (click on) the corresponding line in the Reference Database Library dialog. Afterwards, press the “Rename” button at the bottom of the dialog, and enter the new name in the input window that is opened. Once you press “OK”, the name of the currently marked reference database will be updated in the Reference Database Library list.

Please note:

- If you are a standard user (i.e. do not have administrator privileges), you can only rename reference databases that are listed in the table “Your personal reference databases”!

- The name of the currently selected reference database is displayed in the status bar at the bottom of the Match! window. This name is updated when the Reference Database Library is closed.

**Shift PDF-2 reference database**

If the reference database that is currently marked contains a PDF-2 database in the “old” format, you can shift the corresponding PDF-2 database file to a new location: First move or copy the corresponding file “pdf2.dat” (or similar) to the new location (e.g. using the Windows Explorer or file manager), then press this button, and select the file “pdf2.dat” at the new location. Match! will update the internal reference to this file, so that it knows where to find it when reading data e.g. for displaying them in an entry data sheet.

**Delete reference database**

In order to remove an existing reference database from the current computer, please mark (click on) the corresponding line in the Reference Database Library dialog. Afterwards, press the “Delete” button at the bottom of the dialog. Once you have acknowledged the warning message, you will be asked if you would also like to “physically” remove the corresponding index files. If you answer “No”, you can reactivate the corresponding reference database later on using the “Add” command. Once you press “OK”, the name of the currently marked reference database will be removed from the Reference Database Library list.

If you are a standard user (i.e. do not have administrator privileges), please note that you can only delete reference databases that are listed in the table “Your personal reference databases”!
User database

Overview
As has already been mentioned earlier in this manual, phase identification from powder diffraction data generally requires the availability of a so-called “reference pattern database”. In many cases, this is one of the PDF database products provided by the ICDD. However, there are also alternative sources of reference patterns, like the COD database delivered with Match!, your own diffraction data, or even data from the literature. The latter is especially appropriate when e.g. new compounds have been synthesized in a laboratory whose diffraction patterns and/or crystal structures have not yet been published.

While the COD reference database can be downloaded “ready-to-use” from the Crystal Impact web page free-of-charge, your own diffraction patterns (or other suitable data) must first be imported into a so-called “user database” (a file with extension “*.mtu”) before they can be used with Match!. Once you have created this user database file, you can select it in the “Create Reference Database” dialog.

User databases are typically created and maintained in the so-called “User Database Manager” which can e.g. be opened using the “User database manager” command in the “Database” menu, or simply by pressing the corresponding button in the toolbar.

The contents of user database entries may originate from a variety of sources:

- Own diffraction patterns
- Crystal structure data (typically CIF-files)
- Data published in the literature
- Your colleague’s user database
- ICSD/Retrieve database (released 1993-2002)

These user diffraction patterns have to be stored in a so-called “user database” (file with extension “*.mtu”) which can then be selected in the “Create Reference Database” dialog (p. 79). In the following, we will demonstrate how a user database (*.mtu-file) can be created using any of the data sources mentioned above.

Creating a user database
The central tool for the creation and maintenance of the user database is the so-called “User Database Manager”. It can be opened either by clicking on the corresponding toolbar button (in the main toolbar at the top), by selecting the command “User Database Manager” from the “Database” menu, or by pressing the Create/modify user database... button in the “Create Reference Database” dialog.
Fig. 48: User Database Manager: The new user database is still empty.

The user database manager window (Fig. 48) consists of three parts: At the top, there are nine buttons using which the basic actions (e.g. import or adding of entries) can be initiated. Below, in the upper half of the window, is the list of entries currently present. Finally, in the lower part of the window there is a set of so-called “tab sheets” in which the details of any entry marked in the entry list above are displayed and edited. You can switch between the individual tab sheets by clicking on the corresponding tab sheet header.

The first tab sheet (called “Summary”) contains an extract of the database fields on the remaining tab sheets; the data can just be viewed here, but not edited. The second tab sheet “General” contains data required for the description of the phase, like formula sum, chemical name etc. On the third tab sheet “Crystal structure”, crystal structure data can be entered in order to calculate the corresponding diffraction pattern on the subsequent tab sheet “Diffraction pattern”. Here, it is not only possible to calculate and view the pattern, but also to import (or export) diffraction data as peak list files, or to enter the diffraction data manually. Finally, the “Properties / Bibliography” tab sheet provides access to the physical property (e.g. density) as well as bibliographic database fields.

In the following subsections, we will create a small user database in order to demonstrate the various ways in which data can be entered into the database. Once you have entered your data, the modified user database has to be saved to a mtu-file before it actually can be used. You will be asked automatically to save your user database when you leave the User Database Manager dialog by pressing the “Quit” button. Alternatively, you can also press the “Save” button at the top of the dialog window.

**Import of Diffraction Data**

You can use your own diffraction patterns as reference for phase identification. For this you must import them into a Match! user database file first.

This is possible in two different ways:

- You can add the current experimental diffraction pattern (to be exact: the peak data) to a user database file (*.mtu).
In the User Database Manager, you can create a new entry and import the diffraction peak data from a peak list file.

These two methods are described in detail in the following:

**Add current experimental peaks to user database file**

In order to add the current experimental peaks as a new entry to a user database file (*.mtu), please run the command “Add peaks to user database” from the “Peaks” or the “Database” menu. A dialog will open in which you can select the user database file (*.mtu) to which the new entry shall be added to. (It is also possible to create a new user database file at this point, simply by entering a new file name in this dialog.)

Once you have selected the name of the user database file, a new dialog will open in which you can enter additional information for the new entry, like formula sum of the compound, chemical and/or mineral name etc. Please enter your data on the appropriate tab sheets following the guidelines given for the manual addition of entries in the chapter “Manual input and editing of entry data” on p. 102.

After closing the “Add New Entry Data” dialog by pressing “OK”, the entry will be added to the selected user database file.

**Please note:**

- If experimental peaks are marked, only the marked peaks will be copied to the new user database entry. This may be useful when identifying an unknown phase in a mixture with known phases, in which the peaks of the latter are covered by selected phases (command “Peaks/Mark uncorrelated peaks”). If no peaks are marked, all peaks will be copied.

- A corresponding command to add the current experimental peak data to a user database file is also available in the “Pattern” menus of additional experimental patterns, provided that they contain peak data.

**Import peak data into new user database entry**

As an alternative to adding peaks from the current experimental data as a new entry to a user database file (as described above), it is also possible to add a new entry in the User Database Manager, and to import peak data from a corresponding file into it.

When the User Database Manager is displayed, you can import the diffraction pattern of the entry you are currently editing from the following peak data file formats:

- Stoe peak files (*.pks)
- Philips/PANalytical peak data files (*.udi)
- Endeavour peak list files (2 columns: 2theta/d intensity; *.dif)

Of course, peak data files normally do not contain a lot of additional information (e.g. the composition), so we have to enter these data manually. We will start with the diffraction pattern import and enter the phase information afterwards.

Suppose that you have a diffraction pattern of the mineral Aragonite available in the Philips/PANalytical peak data format (aragonite.udi), and you would like to include the data from this file into your user database. This is a rather simple task:

Make sure that the “User Database Manager” is displayed, then click on the “Add” button at its top in order to add a new entry. The “General” tab sheet will be activated automatically, with the cursor in the first input field “Sample name”. However, we will import the diffraction data first and enter the phase information details afterwards, so please click on the “Diffraction pattern” tab sheet header in order to bring the corresponding tab sheet into front (Fig. 49).
Afterwards, please click on the “Import” button to the left of the peak data table. A dialog will open in which you have to select the diffraction data file you would like to import. Please mark “Philips/PANalytical Peak data (*.udi)” as “File type” at the bottom of the dialog, then select the file “aragonite.udi” in the “Tutorial” subdirectory of the Match! program directory (e.g. “C:\Program Files\Match3\Tutorial”). Finally, please press “Open”. The diffraction data are now present in the “Diffraction pattern” tab sheet; they are displayed both as diffraction pattern picture as well as peak list (2theta or d-values/Intensities) in the table to the right (Fig. 50).
Fig. 50: Your “Aragonite” diffraction pattern has been imported from the file “aragonite.udi”.

All that remains to do is to enter the phase information on the “General” tab sheet, so please activate this tab sheet now. Afterwards, please enter “Aragonite” as the “Sample name”, then press <Tab> to advance to the “Formula sum” input field. Enter “Ca C O3” (mind the blank characters between the elements!). Afterwards, press <Tab> to advance. Enter “Calciumcarbonate” as “Chemical name”, press <Tab> again, and give “Aragonite” as mineral name.

Finally, you might want to mark the quality of the data. In our case, the diffraction pattern is really excellent, so please click on “* (excellent)” in the “Quality” box on the lower left-hand side. Afterwards, press the “Save changes” button at the bottom of the tab sheet.

That's it! Your diffraction data entry has been added to the user database, as can be seen from the entry list above (Fig. 51).
Fig. 51: Your Aragonite diffraction pattern has been successfully added to the user database.

**Calculate Patterns for Crystal Structures Imported from CIF-Files**

The most convenient way to add entries to a user database is probably the import of crystal structure data from CIF-files, whereupon the corresponding powder diffraction patterns (as well as the I/I<sub>c</sub> values required for quantitative analysis) are calculated automatically.

Please click on the “Import” button at the top of the user database manager; a dialog will be displayed in which you can select if you would like to import entry data either from cif (crystallographic information files), from some other Match! user database (mtu-file), or from the ICSD (Fig. 52).

Fig. 52: In this dialog, you have to select the origin of the entry data to be imported (either CIF-files, Match! user database files or ICSD/Retrieve).
Please mark the “cif” option, then press “OK”. A new dialog is displayed in which you have to select the directory from which you would like to import CIF-files\(^{53}\). Please mark the “Tutorial” subdirectory of the Match! program directory (Fig. 53), then press “OK”.

![Select CIF-File directory](image)

**Fig. 53:** Here, you have to select the directory in which the CIF-files you would like to import are stored.

Another dialog will open, presenting a list of all CIF-files present in the selected directory (as well as all cif-files from all subdirectories if present). Here, you can actually select the CIF-files you would like to import. Please mark the file “calcite.cif”\(^{54}\), then press “OK”.

Again, a new dialog is displayed in which you can select the origin (e.g. source database) from which the CIF-files has been taken, e.g. the COD or AMCSD. Besides this, you can also adjust some settings concerning the calculation of diffraction patterns: the radiation type (X-rays or neutron), the wavelength, the maximum 2theta angle, and the maximum number of peaks that shall be included in the database to be created. Note that this is a convenient method to create a reference database for neutron diffraction data!

In our case, the entry has been taken directly from the original AMCSD, so please mark the corresponding option (Fig. 54) and press “OK”.

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\(^{53}\) The normal “File-Open” dialog cannot be used for this task due to a well-known Windows bug when a large number of files is selected.

\(^{54}\) The CIF-file has been taken from the American Mineralogist Crystal Structure Database (http://rruff.geo.arizona.edu/AMS/amcsd.php).
That's it! Everything else will be handled automatically: A new entry will be created; the data from the CIF-file will be imported into the corresponding data fields, and the diffraction pattern, the density and the $I/I_c$ value will be calculated from the imported crystal structure data. The new entry will be automatically added to the user database, so it will appear in the Entry list a few seconds later. Of course, if the unit cell is large, the calculation of the diffraction pattern may take much longer...
Fig. 55: The new entry "Calcite" has been imported from a CIF-file taken from the "American Mineralogist Crystal Structure Database".

As has already been mentioned, it is possible to select more than a single CIF-file for being imported at a time, e.g. by keeping the <Shift> or <Ctrl> button pressed while you click on the individual file names. In this case, all selected files will be imported automatically one after the other. If you import more than a single CIF-file at a time, a report of warnings and errors is displayed when the last file has been imported, compared to the import of a single CIF-file in which case any warnings and errors are reported directly. The “import of multiple CIF-files” functionality is rather powerful; it has been used by Crystal Impact to create the COD reference database containing about 177,000 entries from the COD CIF files.

**Manual Input of Diffraction Data**

The probably most flexible (but also the most tiresome) way is to enter the diffraction data manually. However, in many cases this is the only applicable way, if e.g. the data estimate from a printed publication. We will now add a (small) entry from scratch in order to demonstrate how this can be done.

Here are the data extracted from a hypothetical scientific paper:

**Title**: Common Salt  
**Formula Sum**: NaCl  
**Chemical name**: Sodiumchloride  
**Mineral name**: Halite  
**List of peaks (d Int.)**:

- 3.2447  82.5  
- 2.8100  1000.0  
- 1.9870  616.9  
- 1.6945  17.7  
- 1.6224  186.5  
- 1.4050  76.8  
- 1.2893  7.9  
- 1.2567  192.4  
- 1.1472  134.3  
- 1.0816  8.1

We will enter this minimal data set into the user database. Please click on the “Add” button at the top of the User Database Manager window, in order to add a new entry to the user database. The “General” tabsheet will be activated automatically, with the cursor in the first input field “Sample name”.
The four database fields at the top of the “General” tabsheet grouped as “Phase Description” are used later on to identify a certain entry in the Candidate list, so it is worth while to enter reasonable data here.

In our case, we will enter the publication title as sample name, so please type “Common Salt” (of course only the text between the quotation marks, not the quotation marks themselves!) and press <Tab> in order to advance to the next field “formula sum”.

Here we will enter the composition NaCl; however, it is important to insert a blank character between the elements according to the CIF- or PDF-standard. Hence, please enter “Na Cl” and advance to “Chemical name” by pressing the <Tab> key again.

Please enter “Sodiumchloride” as chemical name, then advance to the “Mineral name” field (<Tab>) and enter “Halite”. Finally, set the “Quality” to “* (excellent)” by clicking on the corresponding radio button to the left. Your screen should now look similar to Fig. 56.

The only data extracted from the paper which have not yet been entered so far are the diffraction data, so please click on the “Diffraction pattern” header to bring the corresponding tab sheet into front. You will enter the d-values of the peak, so please make sure that you click on the “d-values” radio button in the bottom left corner first.

Afterwards, please click on button “Add” below the peak data table on the right-hand side, enter the d-value of the first peak (3.2447), then press <Tab> to advance to the second column “Int.”. Please enter the corresponding intensity value (82.5), then press <Return> in order to finish the input of the first peak. The peak will appear in the diffraction pattern to the left of the table.

In the same way, you can now enter the data of the second peak (2.81, 1000.0) right away. Please do so, and do not forget to press the <Tab> key in between to advance to the next field! The second peak will also appear in the diffraction pattern; your screen should now look like Fig. 57.
Fig. 57: The data of the first two peaks have already been entered.

Please enter the peak data of the remaining eight peaks now in the same manner as above.
Fig. 58: All peak data have now been entered; the new entry has been saved.

So far, the data have been input but not yet saved to the database (the entry is not yet present in the list at top of the User Database Manager window). In order to do so, please click the “Save changes” button at the bottom of the User Database Manager; your entry will now appear in the entry list at the top. Your screen should now look similar to Fig. 58.

The entry numbers for the user database are assigned automatically according to the new ICDD PDF numbering scheme; they cannot be changed by the user.

The entry numbers depend on the origin of the data. If the entry has been imported from the COD, the entry number is calculated as 960000000 + COD file number + 1, e.g., the COD cif file 9000000.cif gets the entry number 96-900-0001. If the entry has been imported from the ICSD, the entry number is calculated as 980000000 + ICSD Collection Code (COL), e.g., the ICSD entry with COL=68860 gets the entry number 98-006-8860. Entries that have been entered manually start with the entry number 99-900-0000.

Manual Input of Crystal Structure Data

If a publication does not contain the powder diffraction pattern of a compound but the crystal structure data, you can enter them instead and calculate the diffraction pattern from these data afterwards. We will add a new entry “Quartz” in order to demonstrate how to do this.

The data extracted from the scientific paper are:

Title: alpha-quartz
Formula Sum: SiO₂
Chemical name: Silicon dioxide
Mineral name: Quartz
Crystal structure data:
Crystal system: trigonal
Space group: P 32 2 1
Unit cell: a = 4.914 c = 5.405 alpha = 90.0 gamma = 120.0
Atomic coordinates:
Si 0.4698  0.0000  0.6667
O 0.4145  0.2662  0.7856
Reference: G. Smith, L.E. Alexander, Acta Cryst. 16(6), 462 (1963)

Please enter these data in the User Database Manager as follows: Click on the “Add” button at its top in order to add a new entry. Like in the previous examples, the “General” tab sheet will be activated automatically, with the cursor in the first input field “Sample name”.

Please enter the title “alpha-quartz” as sample name and advance to the “Formula sum” field by pressing <Tab>. The composition is SiO$_2$, so please enter “Si O2” (mind the blank character between Si and O!) and press the <Tab> key again.

 Afterwards, enter “Silicon dioxide” as “Chemical name”, press <Tab>, and give “Quartz” as mineral name. Finally, set the “Quality” to “C (calculated)”, since the diffraction pattern will be calculated from the crystal structure data (Fig. 59).

Fig. 59: All data appropriate for the “General” tab sheet have been filled in.

The next information extracted from the paper is the crystal structure, so please bring the corresponding tab sheet into front by clicking on the “Crystal structure” tab sheet header. The first thing you have enter is the crystal system “trigonal”; please click on (activate) the “Trig./hexag.” radio button in the “Crystal system” group at the top left of the tab sheet.

Afterwards, you can select the space group in the corresponding combo box below. In this combo box, only space groups which belong to the crystal system selected above are displayed. The space group given in the paper is “P 32 2 1”, so please click on the “arrow down” to the right of the combo box, scroll down the list and select “P 32 2 1 (154)” (the number in brackets is the one given in the “International Tables of Crystallography”).
Once you have selected crystal system and space group, you can enter the unit cell constants. Depending on the crystal system and space group selection, only a few parameters have to be entered. In our case, please enter “4.914” for \(a\) and “5.405” for \(c\).

You are now ready to enter the atomic parameters: Please click on the “Add” button below the atomic parameters table on the right-hand side, enter “si” and press <Tab>. The cursor will advance to the next column “X”. Enter “0.4698” for \(x\), press <Tab>, then “0.0” for \(y\) (<Tab>), and finally “0.6667” for \(z\). There is no information given about the isotropic displacement factor \(B\) and the site occupation factor “Occ.”, so please press <Enter> to finish the input of the first atom’s parameters.

Now the coordinates of oxygen have to be entered: Please press “Add” below the atomic parameters table, then give “o” as element, “0.4145” as \(x\), “0.2662” as \(y\), and “0.7856” as \(z\). Finally, press <Enter> to finish the input of the atomic parameters (Fig. 60).

Fig. 60: The complete crystal structure description has been entered: crystal system, space group, unit cell constants and atomic parameters.

Now that the crystal structure information is complete, we can advance to the diffraction pattern calculation: Please click on the “Diffraction pattern” tab sheet header, then press the “Calculate pattern” button. After a short moment, the diffraction pattern will be displayed (Fig. 61). Note that the \(I/I_c\) value required for semi-quantitative phase identification has also been calculated automatically.
Fig. 61: The powder diffraction pattern (as well as the \( \frac{I}{I_c} \) value and the density) has been calculated from the crystal structure data you have entered.

Finally, you have to enter the bibliographic data: Please select the “Properties / Bibliography” tab sheet, click in the input line to the right of “Authors”, and enter “G. Smith, L.E. Alexander”. Afterwards, press <Tab> two times to advance to the “Journal” input line, and type “Acta Crystallographica (“. Your input will be automatically expanded to the next matching journal name. Once you have typed the “(“, the correct journal “Acta Crystallographica (1,1948-23,1967)” will be displayed.

Please press <Tab> two times (the CODEN will be set automatically to “ACCRA9”) to advance to the “Volume” input line, then enter “16(6)”. Press <Tab> again, and enter “462” as “Page(s)”. Finally, advance to “Year” (<Tab>) and give “1963”.

At this point, you have entered all data extracted from the scientific paper; your tab sheet should now be equivalent to Fig. 62.
Fig. 62: You have successfully entered the bibliographic data; besides this, the density has been calculated from the given crystal structure data.

All that remains to do is to actually add the entry data to the user database. Like in the previous examples, this is achieved by clicking the “Save changes” button at the bottom of the tab sheet. The new entry will be added to the entry list at the top.

**Add Entries from other User Databases**

If you are more than one Match! user in an institution, it is reasonable to share the own reference diffraction patterns, or, in other words, the user database entries. Match! is able to append another user's user database entries to your own. In fact, this is a rather simple task:

Simply copy your colleague's user database file (*.mtu) to your computer, then click the “Import” button at the top of the User Database Manager window. A dialog will be displayed in which you can select if you would like to import entry data either from cif (crystallographic information files) or from some other Match! user database (mtu-file). Please mark the “mtu (Match! user database)” option (Fig. 63), then press “OK”; a “File Open” dialog will be displayed.

For your convenience, we have prepared a (small...) user database in the “Tutorial” subdirectory of the Match! program directory, so you can import it right away.
Fig. 63: In this dialog, you have to select the origin of the entry data to be imported (either CIF-files, MATCH! user database files or ICSD/Retrieve).

Please select the file “colleague_database.mtu” in the “Tutorial” subdirectory of the Match! program directory (e.g. “C:\Program Files\Match3\Tutorial”). Afterwards, please press “Open”.

A message will appear indicating that 9 entries have been imported. Once you acknowledge by pressing “OK”, the new entries will appear in the entry list (Fig. 64).

Fig. 64: The 9 entries from your colleague's user database have been added to your user database.

Once you have finished adding or modifying entries\(^5\) to/in your Match! user database, please press the “Quit” button at the top of the User Database Manager. You will be asked if and where you would like to save your modified

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\(^5\) If you would like to modify an entry in the user database that is currently loaded / displayed in the User Database Manager, please mark the corresponding entry line in the table at the top, then edit the entry data at the bottom. Once you have finished, do not forget to press the “Save changes” button at the bottom in order to make the changes permanent.
user database. Please select/enter an appropriate file name and path and press “Save”. Once the user database has been saved, the User Database manager dialog will be closed.

Please note that new entry numbers are assigned automatically to the entries imported from your colleague’s user database. It is not possible to keep your colleague’s entry numbers when importing; this is necessary in order to avoid duplicates.

**Calculate Patterns for Crystal Structures Imported from ICSD/Retrieve**

If you have a valid license for an ICSD/Retrieve version released between 1993 and 2002, you can create a powerful reference database without additional costs, simply by importing the crystal structure data from the ICSD. During the import procedure, the corresponding powder diffraction patterns as well as the I/I_c values required for quantitative analysis are calculated automatically.

If you would like to do so, please click on the “Import” button at the top of the user database manager; a dialog will be displayed in which you can select if you would like to import entry data either from cif (crystallographic information files), from some other Match! user database (mtu-file), or from the ICSD (Fig. 65).

![Image of dialog box]

Fig. 65: In this dialog, you have to select the origin of the entry data to be imported (either CIF-files, Match! user database files or the ICSD).

Please mark the “ICSD/Retrieve” option as in Fig. 65, then press “OK”. You now have to give the directory in which the ICSD/Retrieve database (to be exact: the file “ICSD.NEW”) is stored. A “File Open” dialog will be displayed in which you have to select the file “ICSD.NEW”. Normally, this file is located in the “INDEX” subdirectory of your ICSD/Retrieve program directory. Once you have found and marked the file “ICSD.NEW”, please press “Open”.

A new dialog is displayed in which you have to confirm that you have a valid license for the ICSD/Retrieve version you are about to import (Fig. 66). The confirmation will be written to a protocol log file.

![Image of license confirmation dialog]

Fig. 66: Before you can use/import an ICSD/Retrieve database, you have to confirm that you have a valid license for it.

If you have confirmed that you have a valid license, a new dialog is displayed in which you can adjust some settings concerning the calculation of diffraction patterns: the radiation type (X-rays or neutron), the wavelength, the maximum 2theta angle, and the maximum number of peaks that shall be included in the database to be created (Fig. 67). Note that this is a convenient method to create a reference database for neutron diffraction data!

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57 If you are in doubt whether your license is still valid, please contact FIZ Karlsruhe (Germany) (e-mail: crysdata@fiz-karlsruhe.de).
When you have made your selections (if any), please press “OK”. That's it! The import of the entries from the selected ICSD/Retrieve database will now begin. The progress will be displayed in a small window.

Depending both on the number of entries in the ICSD/Retrieve database as well as the processing speed of your PC, the import procedure may take a day or even longer. When the import has finished, the new entries will be automatically added to the current user database, so they will appear in the Entry list a few seconds later. Any errors that might have occurred during the import will be displayed in your text editor.

Once the import has finished, please don't forget to press the “Save” button at the top of the user database manager, in order to save the entries imported from the ICSD/Retrieve to a so-called “user database file” (file extension *.mtu). As has already been mentioned, this user database file can then be selected in the “Create Reference Database” dialog to create a new “ICSD/Retrieve” reference database, probably in combination with the COD reference database that is shipped along with Match!.

**Add entry to reference database directly**

It is also possible to add a new entry to the current reference database directly, i.e. without having to use the User Database Manager and/or to run a new reference database indexing in the Reference Database Library. The corresponding command “Add to reference database” is available in the “Database” menu; it can also be run using the keyboard shortcut <Ctrl+Shift+A>. Both will open the “Add New Entry Data” dialog in which you can enter the entry data.

**Please note:**

- You must have **write access** to the directory in which the current reference database is stored. If this does not apply, a corresponding error message will be displayed.
- If you are currently using a pure ICDD PDF reference database, Match! will add a user database (i.e. create a combined reference database) automatically in which the new entry data will be stored. The original PDF database itself will not be affected by this, of course.

- Once you have added one or more entries to a reference database, it can no longer be used by Match! version 1. However, you can copy the actual user database file (user_database.mtu) from the reference database directory and create a new reference database from it in Match! version 1.

- If the current anchor pattern (bottom-most experimental pattern) contains peak data when the “Add to reference database” command is run, they will be copied to the new entry automatically.

Once the "Add New Entry Data" dialog is displayed, you can enter the information to be stored in the new entry:

**Import entry data from cif-file**
The easiest way to enter the new entry data is to import them from a cif-file. In order to do so, please click the corresponding button in the top right corner of the dialog, select the cif-file and finally press "Open". The entry data will be imported from the cif-file and displayed in the corresponding dialog elements afterwards. Afterwards, you can edit them using the dialog elements described below

**Manual input and editing of entry data**
You can enter or edit the entry data on the “General”, “Crystal Structure”, “Diffraction pattern” and/or the “Properties / Bibliography” tabs. The only mandatory information that needs to be given is the Formula sum on the “General” tab. However, we recommend to at least also enter the Chemical name and/or the Mineral name information, because they will be displayed in the "Candidate phase" column in the Candidate list later on.

**General information**
The four database fields at the top of the "General" tab sheet grouped as "Phase Description" are used later on to identify a certain entry in the Candidate list, so it is worthwhile to enter reasonable data here. As has already been mentioned, the Chemical name and/or the Mineral name information will be displayed in the "Candidate phase" column in the Candidate list later on.

Please note: When you enter the Formula sum in the corresponding field on the "General" tab sheet, please keep in mind that you have to use upper and lower-case characters in the element symbols, like in "Ca Si O3" (do not use "ca si o3" or "CA SI O3"). We also recommend inserting a blank character between the elements according to the CIF- or PDF-standard. Hence, please enter e.g. "Cu S O4 (H2 O)5" (and not "CuSO4(H2O)5").

You can add a Quality qualifier in the lower left corner if you can estimate the quality of your diffraction data (e.g. 'C' if they are calculated).

**Crystal structure data**
If you do not have a diffraction pattern available but crystal structure data, you can enter them on the “Crystal structure” tab sheet, so that the diffraction pattern can be calculated by Match!. The first thing you have to enter is the crystal system in the upper left corner. Once you have selected a crystal system, the "space group" combo box below will be filled with appropriate space groups, so that you can select your space group afterwards.

Please note:

- In the "space group" combo box only space groups which belong to the crystal system selected above are displayed.

- You can get additional information about the space group currently selected in the combo box by placing the mouse cursor over the combo box.

Once you have selected crystal system and space group, you can enter the unit cell parameters. Depending on the crystal system and space group selection, only a few parameters have to be entered.

You are now ready to enter the atomic parameters:
Please click in the atomic parameter table to the right in the first line directly below "Element", enter the first element and press <Tab>. The cursor will advance to the next field "X". Enter the coordinate x of the first atom, press <Tab>, enter y, press <Tab> again, and finally enter z. If there is any information given about the isotropic displacement factor B and the site occupation factor "Occ.", you can enter them in the corresponding remaining two columns; otherwise, please press <Tab> until the cursor has advanced to the next line. Once you have entered all atomic coordinates given in the described manner, you should press the <Return> on your keyboard to finish the input of the atomic parameters.

**Diffraction data**

There are four alternate ways in which the “Diffraction pattern” tab sheet can be filled:

1. **Copy of current peak list:** If the current anchor pattern (bottom-most experimental pattern) contains peak data, they will be copied to the new entry automatically when you run the “Add to reference database” command.

2. **Calculation of diffraction pattern from crystal structure data:** If a complete set of crystal structure data is present on the “Crystal structure” tab sheet (e.g. imported from a cif-file), Match! will automatically calculate the diffraction pattern from the given crystal structure data when you open the "Diffraction pattern" tab sheet. After a few seconds, the diffraction pattern will be displayed. Of course, you can also (re-)calculate the diffraction pattern by clicking on the corresponding button.

   **Please note:**

   - If diffraction data are already present (e.g. copied from the anchor pattern) when crystal structure data are imported from a cif-file or entered manually, the original diffraction data will be kept at first. You can overwrite them with the calculated data by pressing the “Calculate pattern” button on the "Diffraction pattern" tab.
   
   - Along with the diffraction pattern, also the I/I value (required for semi-quantitative analysis) as well as the density are calculated from the crystal structure data.

3. **Import of diffraction pattern:** If you have a peak data file (Stoe (*.pks), Philips PANalytical (*.udi) or Endeavour (*.dif)) available, you can import it by clicking on the "Import" button to the left of the peak data table.

4. **Manual input of diffraction data:** In order to enter the diffraction pattern (peak data) manually, you should first check the appropriate settings of the "Radiation wavelength" and "Abscissa" fields on the upper left hand side of the tab sheet. Afterwards, click on the "Add" button below the table to the right. Now enter the 2theta value (or d-value, depending on "Abscissa") of the first peak, then press <Tab> to advance to the second column and enter the corresponding intensity. Finally, press <Return> or <Tab> again in order to finish the input of the first peak; the peak will appear in the diffraction pattern to the left of the table. Continue entering the remaining peak data in a similar manner until you have finished.

**Physical properties and bibliographic data**

On the “Properties / Bibliography” tab sheet, both physical property data (density, color) and bibliographic information can be entered. If a complete set of crystal structure data is present on the corresponding tab sheet, you can (re-)calculate the density (which is an additional useful information for phase identification) simply by clicking on the "Calculate pattern" button on the “Diffraction pattern” tab sheet. We also strongly recommend to enter measured density and color if available.

Below, you can enter the bibliographic details, e.g. if the entry data originate from a scientific paper. When you enter the journal name, your input will be automatically expanded to the next matching journal name in the internal CODEN table. At the same time, the CODEN will be automatically set. This works also the other way round: If you know the CODEN for the journal, you can select it in the corresponding combo box in the lower left corner; the corresponding journal name will be set automatically.

Once you have finished editing the new entry data, please press "OK", in order to add the new entry to the reference database. After a few seconds, a message will be displayed indicating that the new entry has been added to the current reference database.
The new entry is now available for search-match and retrieval operations straight away.

**Edit reference database entry**

In order to edit an entry, please mark it in the candidate list first. Afterwards, you can either run the "Edit reference database entry" from the 'Database' menu, or select the corresponding command from the context menu of the candidate list (which can be opened by right-clicking on the corresponding line/entry to be edited). This will open the “Edit Entry Data” dialog in which you can modify the entry data.

**Please note:**

- You must have **write access** to the directory in which the current reference database is stored. If this does not apply, a corresponding error message will be displayed.
- You cannot edit ICDD PDF database entries.
- You can only edit a single entry at a time, i.e. only a single line must be marked in the candidate list in order to enable this command.
- Once you have edited one or more entries in a reference database, it can no longer be used by Match! version 1. However, you can copy the actual user database file (user_database.mtu) from the reference database directory and create a new reference database from it in Match! version 1.
- If the current anchor pattern (bottom-most experimental pattern) contains peak data when the “Add to reference database” command is run, they will be copied to the new entry automatically.

After the "Edit Entry Data" dialog is displayed, you can modify the entry information just like adding a new entry (see above). Once you finished editing the entry data, please press "OK". After a few seconds, a message will be displayed indicating that the modified entry has been saved in the current reference database.

When an updated entry is saved to the database, Match! in fact only updates the index files and appends the modified entry data as a new entry to the end of the database file. The original entry is still kept within the database file, in order to avoid shifting/copying a lot of data while the software is still in use. When the user closes Match!, the program checks if entries have been edited or deleted, and removes the surplus entry data from the database file before finally closing. This procedure may take a few seconds.

**Delete reference database entry**

You can delete one or more entries that is/are currently marked in the candidate list from the reference database under the following conditions:

- You must have **write access** to the directory in which the current reference database is stored. If this does not apply, a corresponding error message will be displayed.
- You cannot delete ICDD PDF database entries from the corresponding reference database.
- Once you have deleted one or more entries from a reference database, it can no longer be used by Match! version 1. However, you can copy the actual user database file (user_database.mtu) from the reference database directory and create a new reference database from it in Match! version 1.

In order to delete one or more entries, please mark them in the candidate list first, e.g. by keeping the <Ctrl> (or <Cmd>) button pressed while clicking on them. Afterwards, you can either run the "Delete reference database entry" from the "Database" menu, or select the corresponding command from the context menu of the candidate list (which can be opened by right-clicking on the corresponding line/entry to be deleted). You will be asked for confirmation. After a few seconds, a message will be displayed indicating that the entry has been deleted from the current reference database.

When one or more entries are deleted from a reference database, Match! in fact only updates the index files and appends the modified entry data as a new entry to the end of the database file. The original entries are still kept within the database file, in order to avoid shifting/copying a lot of data while the software is still in use. When the
user closes Match!, the program checks if entries have been edited or deleted, and removes the surplus entry data from the database file before finally closing. This procedure may take a few seconds.

**Copyright issues**

With Match!, it is perfectly possible to use data from various sources (e.g. ICSD/Retrieve or cif-files downloaded from the internet) as sources for creating an own reference pattern database. However, please note that before doing so, you have to check if this does not violate the copyright of the original data! **Crystal Impact shall not be liable for any copyright violations of Match! users!** In order to prevent copyright violations, **user databases created by Match! can only be used/read on PCs on which the same Match! license is installed.**

If you know about potential sources of reference data that might be interesting for other users, please contact Crystal Impact (p. 133)!
Advanced operations

Multiple diffraction patterns

In addition to the first (so-called “main” or “anchor”) pattern, it is possible to add more experimental diffraction patterns and display them on top of the main experimental pattern (Fig. 68). For example, this can be useful if you have collected several data sets and would like to use these different patterns to decide if a certain peak is present or not.

For this, you can either import additional patterns, by pressing <Ctrl+I> or clicking the ‘+’-button in the top right-corner of the pattern graphics, or mark a candidate list or match list entry and run the “Load as experimental” command from the “Entries” menu. The latter will calculate profile data from the peak data given in the marked entry, and add profile and peaks as a new “experimental” pattern to the pattern graphics.

By default, multiple diffraction patterns are stacked on top of each other. However, you can reduce the stacking distance between diffraction patterns manually step by step up to a complete overlap with the anchor pattern at the bottom. To do so, press the Ctrl- (Cmd-) key along with ‘-’ (or ‘+’ vice versa), run the corresponding command(s) from the View/Pattern menu, or move the mouse cursor to the right of the diffraction pattern until it changes to , then turn the mouse wheel up or down.

It is also possible to display a vertical line following the mouse cursor (by pressing <Ctrl+X>), so that you can compare e.g. peak positions between several stacked patterns very accurately.

Manual phases/entries

The match list on the lower right-hand side of the Match! window contains those entries/phases that are currently selected as "matching", i.e. that have been decided on as being present in the sample. Normally, match list entries correspond to entries in the current reference database. However, it is also possible to add so-called "manual entries" (or phases) directly from scratch, e.g. by importing crystal structure data or entering them manually. It is even possible to enter only partial crystal structure data sets (e.g. containing only unit cell parameters but no space group or atomic coordinates).
To **add a new manual entry** to the match list, please run the command "Add new manual entry" from the "Entries" menu, or use the corresponding command from the match list's context menu (which can be opened by right-clicking in the match list).

The procedure that follows is completely equivalent to adding a new entry to the reference database (p. 100), with the same dialog being used for data editing and the import of cif-files. The only differences are that for adding manual entries you do not need to have write permission for the reference database, and that the crystal structure data are accepted even if they are incomplete.

If you add **incomplete manual entries** to the match list (entries that contain peak positions but not intensities), the intensities of correlated experimental peaks will be occupied completely by these peaks if the "residual searching" option is active.

The **entry numbers of manual entries** are only virtual, of course, because manual entries are not added to the reference database normally. The numbers start with "99-999-9900" for the first manual entry. They are displayed in bold characters in the match list, so that you can distinguish them from the normal reference database entries. Manual entries are displayed just like normal match list entries in the pattern graphics. If only peak positions (but no peak intensities) are available (e.g. due to missing atomic parameters), the peaks will be displayed as vertical bars from the top to the bottom of the diffraction pattern.

Once you have added one (or even more) manual entries to the match list, you can edit them freely, e.g. to check the effect of different unit cell parameters or space groups. To do so, please mark the corresponding manual entry in the match list, then run the "Edit manual entry" either from the "Entries" menu or from the match list's context menu. Once you have closed the "Edit manual entry" dialog by pressing "Ok", the corresponding peak and other data will be updated.

Another option to add manual entries to the match list is to **create a copy of the reference database entry** that is currently marked in the candidate list. To do so, please mark the corresponding entry in the candidate list, then run the command "Select/add copy as manual 'matching' entry" either in the "Entries" menu or in the candidate list's context menu. Once the copy has been created in the match list, you can edit the entry data as you like.

Once you have created a manual entry in the match list, you can also **add it to the current reference database**. To do so, please mark the corresponding manual entry, then use the corresponding command either from the "Database" menu or from the context menu (click right mouse-button to open).

**Please note:** Manual entries that have not been added to the current reference database cannot be retrieved using e.g. the restraints or "find phases/entries" functionality, because their data are not present in the index files!

**User levels**

In addition to the option to set the automatic options for each individual step, you can also select among several so-called "user levels" at the top of the 'Batch' options page of the "Options"-dialog. The user levels define certain sets of automatic options that have shown to be reasonable. For example, the "Automatic" level lets Match! perform the complete phase identification procedure automatically, while on the "Expert" level you have to run every single step on your own. Of course, you can also save your own batch options settings as new 'user levels'.

When you run Match! for the very first time, you will be asked which default user level ("Beginner" or "Expert") you prefer:

In the “Beginner” mode Match! performs a nearly complete automatic processing of the initial steps: All you have to do is to select the diffraction data file you would like to analyze (you will be prompted automatically for it once the software has been started). Afterwards, Match! will automatically process the raw data, determine the peaks, and run the search-match calculation. All that remains to do is to select the “matching” phases (e.g. by double-clicking or dragging the corresponding entries from the candidate list on the left-hand side to the Match list to the right), and finally display the report containing e.g. the list of matching phases as well as their arbitrary amounts (e.g. by selecting “View/Report”).

In the “Expert” mode you have to perform nearly all actions manually. This mode is especially recommended for experienced users who would like to analyze more complicated samples.
You can customize the user level ("batch" behaviour) on the “Batch” tab of the “Options” dialog (which can quickly be opened by pressing the button in the toolbar) also later on. In addition to selecting user levels like “Beginner” or “Expert” you can also select individual batch steps according to your requirements.

**Batch processing and automatics**

Match! contains several kinds of automatic functions. You can define which steps the program should carry out if another step has been accomplished. For example, you can tell Match! to process raw data automatically immediately after they have been imported.

![Image of Match! Options dialog](image)

**Fig. 69:** On this page of the “Options” dialog (which can be opened from the “Options” menu), you can precisely define in which order automatic operations shall be carried out.

Match! is also capable of automatically selecting multiple matching phases, so the program is (at least in principle) able to automatically determine the components of a mixture of crystalline phases completely on its own. Well, from practice you will know that there may be cases in which minority phases are not identified with this approach, or that there may be other issues not recognized by the software, of course.

**Repeating similar analyzes**

If you often analyze samples that contain the same phases but in different amounts (wt%), you can create and use predefined sets of entries (so-called "predefined selections" or "answer sets") that can be loaded into the match list straight away.

To do so, please run a first analysis, so that the match list contains all required phases. Afterwards, please run the command "File/Export/Answer set (match list)", select an appropriate directory and file name, and finally press "Save".

As an alternative, you can also mark appropriate entries in the candidate list (maybe after using restraints or the "Find phases/entries" function). Afterwards, please run the command "File/Export/Answer set (cand. list)" (or use the corresponding command from the context menu), select an appropriate directory and file name, and finally press "Save".

You have now created a text file containing a list of entry numbers (a so-called "Match! answer set file", extension *.mta) that belong to the entries marked in the candidate or match list. This file can be used to directly select all matching phases during similar analyzes.
Any time you would now like to **run a similar analysis** in the future, please import the diffraction data as usual. Afterwards, please run the command "File/Import/Predefined phase selection" (or press <Ctrl+Shift+O> on the keyboard). Select the answer set file you have created in the step described above, then press "Open". The entries listed in the answer set file will be loaded into the match list straight away, with the peak searching and a single update calculation of the figure-of-merit values being performed automatically (if required). The amounts of the phases are then available in the match list straight away (if all entries contain the required \( \frac{I}{I_c} \) values, of course).

As an **alternative to using Match! answer set files** you can also **quickly add one (or more) specific entries** directly to the match list, by pressing <Ctrl+E> and entering either the name, the formula sum or the entry number. If more than a single entry matches your criterion, a new dialog will be displayed in which you can select the entry(s) you would like to add to the match list.

**Please note:** If you use own diffraction patterns (user database) in addition or even instead of the COD or PDF, it is important to keep in mind that the entry numbers are specific for a certain user database. If a colleague uses an own (different) user database, it is not possible (or at least not reasonable) to exchange answer set files with her/him.

### Controlling Match! using scripts

Match! cannot be only controlled using the normal graphical user interface; it is also possible to create a list of commands in a so-called “batch script file” to be executed by Match!. Using this feature, Match! can e.g. be controlled from external programs.

The batch scripting functionality is intended to be used as follows:

First of all, you should manually optimize the relevant parameters (like the peak searching sensitivity) on diffraction patterns similar to the ones you would like to use with batch scripting. Afterwards, once you have found reasonable values for all relevant parameter values that are appropriate for your diffraction patterns and samples, you should define them as "default values", by marking the “Save as defaults” checkbox on the lower left-hand side of the “Options”-dialog before closing the dialog by pressing “Ok”. You are now ready to use batch script files and commands for controlling the flow of the program. Match! will use the new default parameter values automatically.

A batch script file is typically created using a text editor; you can find a description of the format as well as a list of available commands below.

You can run a batch script e.g. from within Match! by selecting the corresponding command from the “File” menu. As an alternative, you can also run Match! from the command line, giving the name of the batch script file to be run as a command line parameter when the Match! program executable is invoked.

Here is a sample batch script that contains all of the commands that are currently available. You can create the corresponding file using any conventional text editor and save it e.g. as “batchscript.mbf”:

```bash
MATCH!_3_BATCH
!new_document
!use_ref_db("PDF-2 Release 2014")
set_default_wavelength(1.541874)
set_default_abscissa(2theta)
import("/Users/putz/Match/Samples/quickstart.rd")
!import_answerset("/Users/putz/Documents/ergebnis.mta")
!add_peak(26.62,1000.0,0.15)
strip_K_alpha2
!import_background("/Users/putz/Match/Samples/quickstart_background.bac")
subtract_background_automatic
smooth_exp_raw_data
find_peaks_normal(0.1,40.0,1)
!find_peaks_profile(0.1,96.0,1)
!correct_2theta_shift_automatic
!correct_2theta_spec_displ_automatic
!correct_2theta_shift(-0.14)
!correct_2theta_spec_displ(0.001)
!automatic_raw_data_processing
internal_standard(961011173)
!selection_preset("Silicon compounds")
```
search-match
!add_entry(96-900-7499)
!unify
!mark_first_entry
!import_selection_criteria("/Users/putz/Documents/selcrit.mss")
!select_matching_automatically
!select_first_entry_as_matching
!automatic_rietveld_refinement
!crystallite_size_estimation("LaB6",0.94)
!finish
!set_sample_id("TestID")
!set_sample_date_time("02.12.2010, 15:12 Uhr")
!view_report
!save_peak_residuals("/Users/putz/Documents/residuals.dif")
!save_document("/Users/putz/Documents/testdoc.mtd")
!close
!export_pattern_graphics("/Users/putz/Documents/pattern.jpg",JPG,1024,768,0)
!export_profile_data("/Users/putz/Documents/testprofile.dat")
!export_peak_data("/Users/putz/Documents/peaks.dif",DDIF2)
!export_background("/Users/putz/Documents/testbackground.dat")
!export_entry_data(96-900-7499,"/Users/putz/Documents/entry_969007499.txt",TXT)
!export_reference_pattern(96-900-7499,"/Docs/entry_969007499.pks",PKS)
!export_candidatelist("/Users/putz/Documents/resultslist.pdf",PDF)
!export_matchlist("/Users/putz/Documents/matchlist.htm",HTML)
!print_pattern_graphics(1024,768,1)
!print_peaklist
!print_entry_data(96-900-7499)

Note that the lines beginning with a ‘!’-character are comments and not run as commands. The keyword “MATCH!_3_BATCH” in the first line is mandatory; script files of the previous version 2 containing “MATCH!_2 BATCH” in the first line are also accepted.

You will find a complete list of commands available for batch script files along with their explanations in Match!’s online help (which can be opened by selecting the “Index” command from the “Help” menu).
**Tips & Tricks**

**Identification of minor phases**

The determination of minor phases will become easier if you pay attention to the following hints:

- Before you run a peak searching command, please check the background (which is normally determined automatically). If the background is too high (which may e.g. be the case if there is a lot of noise in your pattern), this may prevent small peaks from being detected. If the background is not visible, please right-click in the diffraction pattern graphics and select the "Background" command from the context menu that opens.

- Please take a careful look at the peaks, especially if they have been determined automatically. It may be necessary to increase (press <F2>) or reduce (press <F3>) the peak searching sensitivity, or even to restart from scratch and determine the peaks manually.

- You may try to skip the 'alpha2 stripping' step in the raw data processing. Stripping the alpha2 part of the radiation is not necessary for phase identification (search-match) and may increase the noise in the pattern.

- The parameter "Preference for single or multiple phases" on the "Search-Match" tab of the "Options" dialog is some sort of compromise between Match!'s ability to clearly distinguish between one or two phases that are present with significant amounts (setting "Single"), and its acceptance of minor phases (setting "Multiple"). The basic influence of this parameter is the degree to which the intensity scaling factor is taken into account in the calculation of the figure-of-merit (FoM) values.

- If you are missing some minor phases, you should try to increase the value of the "Preference for single or multiple phases" parameter.

- A common problem of the conventional "residual searching" approach is that when selecting a certain phase as "matching" also other phases can be eliminated from the Candidate list, e.g. if they contain some peaks at similar positions than the selected phase. Hence, it may be easy to "overlook" these phases, especially if they are minor or even trace phases.

In these cases, try to avoid using the automatic residual searching option: Residual searching works by subtracting the peak intensities of identified phases from the experimental diffraction pattern. You can disable the automatic residual searching by removing the hook in front of the "Residual searching" option on the "Search-Match" tab of the "Options" dialog. This is also recommended if you suspect a strong peak overlap of different phases to be present.

When selecting phases as matching, you can use a "unified phases" approach instead: Please turn the search-match option "Residual searching" off (on the "Search-Match" tab of the "Options"-dialog).

Import your diffraction data, determine peak positions and run the search-match calculation as usual.

Once the search-match calculation has finished and the Candidate list has been filled with entries, please run the menu command "Entries/Unify phases" (or press <Ctrl+U>). This will quickly eliminate all duplicate or multiple occurences of phases from the Candidate list.

Mark the best-matching entry/phase in the Candidate list and select it as "matching" as usual.

Since the "Residual searching"-option is not active, the phases selected as matching will be marked as "deleted" and hence be removed from the Candidate list.

- In certain circumstances, it may be difficult to identify minor phases if one or more of their three strongest peaks are not observed (or not found by the peak searching function). The background is that normally a reference pattern is only accepted as “candidate” if at least the three strongest peaks are observed (i.e. can be correlated to the experimental diffraction pattern).

If you are in doubt that you might be missing one or more minor phases, you should deactivate the option “Check 3 strongest peaks before running full match” on the “Search-Match” tab of the “Options” dialog.
Afterwards, please run a new search-match calculation, e.g. by selecting the “Search-Match” command from the “Search” menu. The drawback of deactivating this option is that the search-match calculation may take significantly longer.
Large number entries resulting from search-match

If your search-match calculation gives many candidate entries, there may be two reasons for this:

- Your diffraction pattern contains many peaks. As a result, the probability that there is an acceptable agreement between reference peak positions and the experimental peaks is rather high, so many entries may have an acceptable figure-of-merit (FoM) value. Please inspect the peaks carefully one by one, and delete all those peaks that you are not really sure about. Afterwards, run the search-match again.

- The "peak correlation 2theta window" is rather large. Normally, this window is adjusted by Match! automatically before the search-match calculation, based on the average FWHM (full width at half maximum) of the experimental peaks. Therefore, broad peaks (large average FWHM) result in large peak correlation windows, so many peaks (entries) is considered as "matching". You can disable the automatic determination of the 2theta peak correlation window size on the lower right-hand side ("Delta 2theta") of the "Search-Match" page of the "Options" dialog, by deselecting the "Auto" check box below. Try to use/adjust a smaller value for "Delta 2theta", press "Ok", and run the search-match again.

Exporting reference pattern (profile data)

In addition to the export of peak data of reference patterns, it is also possible to export them as raw (profile) data, by following these instructions:

1. Make sure that the reference database entry for which you would like to export raw (profile) data is displayed and marked in the candidate list or match list.

2. Right-click on the corresponding entry, then select the command “Load as experimental pattern (calculate profile)” from the context menu that opens (or simply press <Ctrl+Shift+T>).

3. The peak data of the marked entry will be added as an additional experimental diffraction pattern in the pattern graphics. In addition, its diffraction profile will be calculated automatically, using the default FWHM (full width at half maximum) value defined in the “Raw data processing” options.

4. If the new pattern is the first experimental pattern (anchor pattern), please run the menu command “File / Export / Profile data”.

5. Otherwise (if the new pattern is added as an additional pattern on top of an already existing anchor pattern), please click on the corresponding pattern menu button  in the top right corner of the additional diffraction pattern, then select the menu command “Export profile data”.

6. In the dialog that opens, please select an appropriate file type, directory and file name, then press “OK”.

Please note:

- It is possible to export combined diffraction patterns (calculated from several reference database entries), by first adding them as new experimental patterns separately (as described above), and then combining them, using the “Add to pattern below” command from the “Pattern menus” of the additional experimental patterns. Finally, you can use the “Export profile data” command for the resulting pattern.

- You can export the profile data in the following (ASCII text) formats:
  - start, step, end, intensities
  - 2 columns (2θ intensity)
  - 2 columns (d-value intensity)

Difficulties with FWHM values of newly added peaks

If the FWHM values of newly added peaks are much too high (the peak profiles are too wide), you should check the automatically determined default value for FWHM on the “Raw data” tab of the “Options” dialog (which can be opened from the “Options” menu). In certain circumstances it may also be reasonable to deactivate the automatic
fitting of the FWHM value, either using the menu command “Pattern / Profile fitting / Fit FWHM”, or simply by pressing <F8>.

Repeated usage/storing of restraints ("presets")

If you are frequently using the same set of restraints (e.g. elements, density, inorganics only etc.), you might get tired of selecting these restraints in the corresponding dialog repeatedly. Instead, it would be much easier if you could somehow store the entries that correspond to these restraints, to use them as a subset based on which you can run search-match operations later on.

You can easily save the current selection criteria, and recall them later with just two mouse clicks, using the so-called "selection criteria presets". You will find the corresponding control elements at the bottom of the "Restraints" (and also "Additional entries") tab to the right of "Preset". Of course, it is possible to save several sets of selection criteria.

To save the current selection criteria, simply press the "Save" button. Afterwards, you must enter a name using which you can easily identify this set of selection criteria later on. Your selection criteria will then be stored in your personal settings (e.g. Windows registry).

If another person is using the same computer, he can store his own selection criteria independent from yours (of course if he is using his own account on this machine...).

If you would like to recall a certain set of selection criteria, simply press the "arrow down" button of the combo box to the left of the "Save" button, and select the name of the desired selection criteria from the list that opens. That's it! The selection criteria that have been loaded will instantly be applied to the table of candidate entries (candidate list), and of course also to the entries that are investigated during the search-match calculation.

List selection box handling

On the "Restraints" and "Additional entries" tab sheets, a so-called "list selection box" can be opened in each case where a manual/keyboard input of a numerical or text value is required, i.e. in each case where an edit/input line is present. In these cases, you can open a list of all available values for the corresponding field (the list selection box) by clicking on the corresponding "table" button to the right of the input line.

You can easily select the value(s) you are interested in by clicking on the corresponding lines. Besides this, you can shorten the search for a particular value/line by rapidly typing the first few letters. For instance, if you are looking for an author "Stolpovskaya V.", you can simply type stolp without pausing between the letters, and the corresponding line will instantly be displayed.

If you made a mistake by typing a wrong letter, simply wait for two seconds (which will automatically clear the input buffer) and try again.

Creating cif-files for Rietveld refinement

If you are using a reference database that does not contain atomic coordinates for all entries, you might face the problem how to create a cif-file providing the full crystal structure data for Rietveld refinement. If you cannot export a reasonable cif-file e.g. from Pearson’s Crystal Data, you might want to use a crystal structure description from a corresponding scientific paper. However, in many cases there is no cif-file available for this paper, so you have to create one on your own by manually entering the data from the paper. The problem is that the cif-syntax is far from being trivial.

Fortunately, you can use the Match! User Database Manager to create the cif-file. In order to do so, please open it e.g. by selecting the corresponding command from the "Database" menu. Once the dialog is displayed, please press the "Add" button in the toolbar at the top of the window. The tabs at the bottom of the dialog will be activated, with the "General" tab in front. Please click on the "Crystal structure" tab to make it visible, then start to enter your crystallographic data by first marking the appropriate crystal system. Afterwards, select the space group from the corresponding combo box below, and fill in the unit cell parameters. Finally, press the "Add" button below the table of atoms to the right, and enter the element and coordinates of the first atom. Finish the input of the first atom's parameters by pressing <Return>, then repeat this step for the remaining atoms. Once you have finished entering the atomic parameters, press the "Save changes" button at the bottom of the dialog.
Make sure that the new entry is marked in the table at the top, then press the "Export" button in the toolbar at the top of the dialog. Select "CIF file (*.cif)" as "Files of type:", select an appropriate directory and file name, and press "Save".

That's it! You can now leave the User Database Manager by pressing the "Quit" button (you can save the new user database at this step if you like), and import the cif-file as a response to the corresponding question next time you try to run a Rietveld refinement.

**Match! crashes after splash screen on Windows 7 64-bit**

We have received two reports of Match! crashing right after displaying the splash screen (no program window is shown). In both cases, Windows 7 64-bit was used as operating system. At least in one case, the problem was caused by a wrong OpenSSL installation or configuration. This problem can be solved by (re-)installing OpenSSL as follows:

Download OpenSSL from [http://slproweb.com/products/Win32OpenSSL.html](http://slproweb.com/products/Win32OpenSSL.html). Normally, you should download the version Win32OpenSSL_Light-1_1_0d.exe. Run the installer, and install the main files to "C:\Program Files (x86)\OpenSSL" (or similar). Make sure to install the library files to the Windows system directory when you are asked to do so. When the installation has finished, please try to run Match! again.

Please contact us in case this should not fix the problem!
Software maintenance

If you intend to run Rietveld refinement calculations with Match! using FullProf later, you should install FullProf first (see below), so that Match! can detect the presence of FullProf automatically when it is first run. However, it is also no problem to install FullProf later and add the path to it in the Match! options.

Installing and running Match!

Installing from installation DVD-R

Windows
First please check the minimum system requirements:

- Personal Computer with Microsoft Windows XP, Vista, Windows 7, Windows 8/8.1 or Windows 10 operating system (separate versions are available for 64-bit and 32-bit)
- 2 GB of RAM
- Hard disk with minimum 500 MB of free disk space
- Graphics resolution of 1024 x 768 pixels (1280 x 800 pixels or more recommended)
- FullProf release January 2018 (or later) required for Rietveld refinement

Afterwards, simply insert the Match! DVD into your drive and wait until the AutoStart program is run automatically. If nothing happens after a reasonable amount of time, you can also run it manually in the DVD’s main directory. Click on the button or label corresponding to the version you would like to install (64-bit or 32-bit) to launch the installer.

Please note the terms of the “End User License Agreement”, which will appear in the second dialog box of the installer!

Once the installation has finished, you can run Match! e.g. by clicking the Windows “Start” button, then on “Match3/Match!” . Alternatively, you can run the software by double-clicking on the file “Match!.exe” in the directory where you have installed the program (e.g. “C:\Program Files\Match3”).

macOS
Before you install and run Match!, you should check the following minimum system requirements:

- Mac with Intel processor and macOS 10.10 “Yosemite” operating system (or later)
- 2 GB of RAM
- Hard disk with minimum 500 MB of free disk space
- Graphics resolution of 1024 x 768 pixels (1280 x 800 pixels or more recommended)
- FullProf release March 2018 (or later) required for Rietveld refinement

Afterwards, please copy the disk image “Match-3-osx-installer.dmg” from the DVD’s directory “Match!” to some temporary directory on your hard disk. Open the disk image in order to display its contents (e.g. by double-clicking on it), then run the installer “Match3.pkg” by double-clicking. Please follow the instructions on the screen, and note the terms of the “End User License Agreement”, which will appear in the second dialog box!

Once the installation has finished, you can run Match! e.g. by double-clicking on the corresponding desktop symbol “Match!”, or alternatively using the Finder (Folder “Applications/Match3”).

Linux
Before you install and run Match!, you should check the following minimum system requirements:
Afterwards, please use the corresponding installer (either Match-3-linux-x64-installer.run.zip for 64-bit or Match-3-linux-installer.run.zip for 32-bit) in the DVD's directory "Linux". Please copy the installer to some temporary directory on your hard disk, then check that the file access permissions show that the installer file can be executed. If this is not the case, please run the command

```
chmod a+x Match-3-linux-x64-installer.run <Return>
```

In addition, you need to install the software as "root" (administrator privileges required). To do so, either run a "su" command before running the installer, or use "sudo", e.g. by running

```
sudo Match-3-linux-x64-installer.run <Return>
```

When the installer is running, please follow the instructions on the screen, and note the terms of the "End User License Agreement", which will appear in the second dialog box!

Once the installation program has finished, you can run Match! e.g. by double-clicking on the corresponding desktop symbol "Match!", by selecting "(Computer/)Applications/Other/ Match!", or by running the script "Match.sh" in the directory where the software has been installed (which is "/opt/Match3" by default).

**Installing from download package**

**Windows**

First please check the minimum system requirements:

- Personal Computer with Microsoft Windows XP, Vista, Windows 7, Windows 8/8.1 or Windows 10 operating system (separate versions are available for 64-bit and 32-bit)
- 2 GB of RAM
- Hard disk with minimum 500 MB of free disk space
- Graphics resolution of 1024 x 768 pixels (1280 x 800 pixels or more recommended)
- FullProf release February 2018 (or later) required for Rietveld refinement

In order to install Match!, please download and run the corresponding installer from

https://www.crystalimpact.de/match/download.htm

Please note the terms of the "End User License Agreement", which will appear in the second dialog box!

Once the installation program has finished, you can run Match! e.g. by double-clicking the file "Match!.exe" in the directory where you have installed the program (e.g. "C:\Program Files\Match3"). Alternatively, you can run the software by double-clicking on the corresponding desktop symbol "Match!", or by clicking the Windows "Start" button, then on "Match3/Match!".

**macOS**

Before you install and run Match!, you should check the following minimum system requirements:
Mac with Intel processor and macOS 10.10 “Yosemite” operating system (or later)

- 2 GB of RAM
- Hard disk with minimum 500 MB of free disk space
- Graphics resolution of 1024 x 768 pixels (1280 x 800 pixels or more recommended)
- FullProf release March 2018 (or later) required for Rietveld refinement

In order to install Match!, please download the corresponding installer disk image (“Match-3-osx-installer.dmg”) from

https://www.crystalimpact.de/match/download.htm

Once the download has finished, please open the disk image in order to display its contents (e.g. by double-clicking on it), then run the installer “Match3.pkg” by double-clicking. Please follow the instructions on the screen and note the terms of the “End User License Agreement” which will appear in the second dialog box!

When the installation program has finished, you can run Match! e.g. by double-clicking on the corresponding desktop symbol “Match!”, or alternatively using the Finder (Folder “Applications/Match3”).

Linux

Before you install and run Match!, you should check the following minimum system requirements:

- Personal Computer with Linux 64-bit, e.g. Ubuntu
- 2 GB of RAM
- Hard disk with minimum 500 MB of free disk space
- Graphics resolution of 1024 x 768 pixels (1280 x 800 pixels or more recommended)
- FullProf release February 2018 (or later) required for Rietveld refinement

In order to install Match!, first please download the corresponding compressed installer file (“Match-3-linux-x64-installer.run.zip”) from

https://www.crystalimpact.de/match/download.htm

Once the download has finished, please decompress the zip-file into some temporary directory. Check that the file access permissions show that the file “Match-3-linux-x64-installer.run” can be executed. If this is not the case, please run the command

```
chmod a+x Match-3-linux-x64-installer.run
```

In addition, you need to install the software as “root” (administrator privileges required). To do so, either run a “su” command before running the installer, or use “sudo”, e.g. by running

```
sudo Match-3-linux-x64-installer.run
```

When the installer is running, please follow the instructions on the screen, and note the terms of the “End User License Agreement”, which will appear in the second dialog box!

Once the installation program has finished, you can run Match! e.g. by clicking on the corresponding desktop icon that has been created during the installation, or by running the script "Match.sh" in the directory where the software has been installed (which is "/opt/Match3" by default).
License installation

After you have installed the main software from a download package, the program will run in the evaluation mode, which basically means that it will stop functioning 60 days after the installation. You still need to install your personal license to transform the software into the fully personalized, unrestricted version.

To do so, simply copy the license file “yourlicense.lic” that you have received by e-mail into the directory where you have installed the program. The directories where the software is installed by default are:

- **Windows:** C:\Program Files\Match3
- **macOS:** /Applications/Match3
- **Linux:** /opt/Match3

You may need administrator privileges to perform this task!

Afterwards, please verify again that the license file is really present in the corresponding directory, then run Match!. Your license data should now be displayed at the bottom of the splash screen (at program startup), to the right of the status bar (at the bottom of the program window) as well as in the “About Match!” dialog which can be opened from the “Help” or system menu.

Installing FullProf

Match! can use the well-known software “FullProf” (J. Rodriguez-Carvajal, Physica B. 192, 55 (1993); http://www.ill.eu/sites/fullprof) to run Rietveld refinement calculations. If you would like to use this feature, you have to install FullProf (at least if it is not already present on your machine) using one of the following options (FullProf release February 2018 (or later) required):

Installing from installation DVD-R

If you have obtained your Match! software on DVD-R, you can install FullProf directly from this disk:

**Windows**

To install the Windows version of FullProf, please run (double-clicking) the corresponding installer (e.g. “Setup_FullProf_Suite_January2018.exe”) in the “FullProf_Suite/Windows” subdirectory of your installation DVD-R. Simply follow the instructions on your screen, keeping in mind not to use any blank or non-ASCII characters for the file and directory names!

**macOS**

Before you install and run FullProf, please verify that you are using macOS 10.8 “Mountain Lion” operating system (or later). You will find the installer packages required in the “FullProf_Suite/Mac_OS_X” directory of your installation DVD-R. In the following we will copy the installation instructions taken from the FullProf web page (with minor modifications):

The current version of FullProf for Mac works only for macOS’s starting with Mountain Lion (10.8) (or higher).

Double-click on the image “FullProf4Mac-v252.dmg” in the “FullProf_Suite/Mac_OS_X” directory of your installation DVD-R. Copy the bundle “FullProf4Mac” form the window that opens into your “Applications” directory.

**Linux**

You will find the installer package required in the “FullProf_Suite/Linux” or “FullProf_Suite/Linux_64-bit” directory of your installation DVD-R. In the following we will copy the installation instructions taken from the FullProf web page (with minor modifications):

General Mode (installation for all users of the system):

1. Activate the super-user mode
2. Create a directory in which you want to hold the programs of the FullProf_Suite. For instance: /usr/local/bin/FullProf_Suite in some Linux systems
3. Copy the file `FullProf_Suite_XXXXNNNN_Lin.tgz` (XXX=Month NNNN=year) from the “FullProf_Suite/Linux” subdirectory on your installation DVD-R to the directory just created in step 2.

4. Decompress the file .tgz with the following command:

   ```bash
tar -xzf FullProf_Suite_XXXXNNNN_Lin.tgz
   ```

5. Tell the users to activate the environment variable FULLPROF in their configuration file (see below).

**Local Mode (installation for a single user only):**

1. Create a directory in which you want to hold the programs of the FullProf_Suite. e.g.: `$HOME/FullProf_Suite`

2. For doing that you must execute the following commands:

   ```bash
   cd $HOME
   mkdir FullProf_Suite
   cd FullProf_Suite
   ```

3. Copy the file `FullProf_Suite_XXXXNNNN_Lin.tgz` (XXX=Month NNNN=year) from the “FullProf_Suite/Linux” subdirectory on your installation DVD-R to the directory just created in step 2.

4. Decompress the file .tgz with the following command:

   ```bash
tar -xzf FullProf_Suite_XXXXNNNN_Lin.tgz
   ```

5. Modify the configuration file to activate the environment variable FULLPROF (see below).

**Activation of the environment variable of the FullProf_Suite:**

The following steps are only required if you would also like to use the FullProf Suite programs without Match!, i.e. with its own user interface, editors etc.:

1. Depending of the SHELL of the user the commands are different. The aim is to create the environment variable FULLPROF. To know what is the shell one is using you should execute the command:

   ```bash
   echo $SHELL
   ```

   Generally it is one of the following: Bourne (sh, bash), Korn(ksh), C(csh)

2. From now we suppose we are using the Bourne of bash type. If you have another one you must consult how to do the equivalent commands we explain below.

3. Edit the setting file of the user. In our case it should be in the root directory of the user and the name is `.bashrc` or `.bash_profile`.

4. Add the environment variable FULLPROF, that has as value the absolute path of the directory in which we have installed the programs of the FullProf Suite.

   For instance:

   ```bash
   FULLPROF=/opt/FullProf_Suite
   ```

   or

   ```bash
   FULLPROF=/usr/local/bin/FullProf_Suite
   ```
5. Add the above directory to the PATH variable

PATH=$FULLPROF:$PATH

6. Export the defined variable

export FULLPROF

7. The changes will be effective on opening a new terminal window. To verify that everything is OK, just type in your terminal the command:

    echo $FULLPROF

The system will show the directory in which you have installed the programs.

After doing all the above steps all the programs of the FullProf Suite are available from whatever working directory. If you need to update the FullProf Suite you just have to do the steps 3 and 4 of the General or Local mode described above. Only in the case you decide to use another directory you have to redefine the environment variable. You can use the programs in console mode or use the toolbar (command tfp) to access the different programs.

If you need to update the FullProf Suite you just have to do the steps 3 and 4 of the “General” or “Local mode” described above. Only in the case you decide to use another directory you have to redefine the environment variable. You can use the programs in console mode or use the toolbar (command tfp) to access the different programs.

Depending of your installation you may need to install the libraries of OpenMotif version 2.3. Do that only in case one of the GUIs doesn't work and you see a message of the form: "libXm.so.3" not available or something similar.

**Installing from download package**

If you have obtained your Match! software by electronic delivery, you can download and install FullProf directly from the FullProf web page (where you will also find detailed installation instructions):


As an alternative, you can also download and install FullProf from the Crystal Impact web page

[https://www.crystalimpact.de/match/download.htm#download_fp](https://www.crystalimpact.de/match/download.htm#download_fp)

Simply follow the download and installation instructions given there for the platform you are using (Windows (32-bit, 64-bit or XP), Mac OS X or Linux).
When you run Match! for the very first time, you will be asked which default user level ("Beginner" or "Expert") you prefer:

In the “Beginner” mode Match! performs a nearly complete automatic processing of the initial steps: All you have to do is to select the diffraction data file you would like to analyze (you will be prompted automatically for it once the software has been started). Afterwards, Match! will automatically process the raw data, determine the peaks, and run the search-match calculation. All that remains to do is to select the “matching” phases (e.g. by double-clicking or dragging the corresponding entries from the candidate list on the left-hand side to the Match list to the right), and finally display the report containing e.g. the list of matching phases as well as their arbitrary amounts (e.g. by selecting “View/Report”).

In the “Expert” mode you have to perform nearly all actions manually. This mode is especially recommended for experienced users who would like to analyze more complicated samples.

You can customize the user level ("batch" behavior) on the “Batch” tab of the “Options” dialog also later on. In addition to selecting user levels like “Beginner” or “Expert” you can also select individual batch steps according to your requirements.

Online update

By default, Match! automatically checks the Crystal Impact web server for a more recent version each time it is executed. If a new version is found, you will be informed and guided to the corresponding web page from which you can download the new version.

You can also manually check for a more recent version, simply by selecting the "Check for updates..." command from the "Help" menu. The procedure will be the same as the one described above for the automatic update.

Uninstalling Match!

Windows

If you would like to uninstall Match!, please click on the Windows "Start" button, then click on "Programs", and finally select the command "Uninstall Match!" from the "Match! 3" subfolder.

If you are using Microsoft Vista or Windows 7 as operating system, please note that you need to run the uninstaller using administrator rights explicitly. In order to do so, please right-click on the command "Uninstall Match!" in the "Match! 3" subfolder, then select "Run as administrator" from the context menu.

Alternatively, you can also open the "Control Panel" from the "Settings" folder in the Windows "Start" menu. Afterwards, double-click on "Software" (on some operating systems called "Add/Remove Programs") in order to bring up the normal Windows software installation dialog. In the list, please mark "Match! 3", then click "Change/Remove". As soon as the uninstall program has been opened, please click "Ok" in order to remove Match!.

macOS

If you would like to uninstall Match!, simply remove the folder “Match3” from your “Applications” folder using the Finder.

Linux

If you would like to uninstall Match!, please switch over to "root" ("su" or "sudo"), then run "uninstall" in the Match! program directory (e.g. "/opt/Match3/uninstall").
Update permission time model

With Match! version 3, Crystal Impact has switched over to a **update permission time model for updates**, replacing the current “major/minor update model”. With the new model, **you can still use your software/license as long as you like** (if you have purchased a permanent license), just like it has been with the previous “major/minor update model”.

The major change in the new model is that **all updates and new versions that are released within a certain amount of time** (called your "**update permission time**") will be available for download and installation **free-of-charge**, even if major improvements have been implemented. Updates of versions that are released after your update permission time has expired cannot be installed and run. If you would like to use these more recent versions, you have to purchase an extension for your update permission time.

More information about the new update permission time model as well as some frequently asked questions and their answers are available on our web page:  

https://www.crystalimpact.de/subscription.htm
Appendix

Table of mouse button and key combinations

A variety of operations can be carried out directly in the diffraction pattern graphics using the mouse. In some cases, it is also necessary to keep one or the other button pressed on your keyboard, in order to invoke the appropriate command. Here is an overview what you can do inside the diffraction pattern using your mouse.

**Note:** If the mouse cursor or program does not react as expected, please make sure that the diffraction pattern graphics gets the input focus, simply by clicking into the diffraction pattern (at a position without any objects). Afterwards, please try your operation or mouse action again.

Please note that you have to replace “Ctrl” by “Cmd” if you are using a Mac!

<table>
<thead>
<tr>
<th>Effect/purpose</th>
<th>Cursor position in pattern graphics</th>
<th>Keyboard button(s)</th>
<th>Cursor shape</th>
<th>Mouse action</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Background mod.: shift control point</strong></td>
<td>Control point (small square) in background curve (must be visible!)</td>
<td>-</td>
<td></td>
<td>Press left button and keep it pressed while moving the mouse</td>
</tr>
<tr>
<td><strong>Background mod.: delete control point</strong></td>
<td>Control point (small square) in background curve (must be visible!)</td>
<td>-</td>
<td></td>
<td>Press right button in order to remove the background control point below the mouse cursor</td>
</tr>
<tr>
<td><strong>Background mod.: add control point</strong></td>
<td>Background curve (must be visible!)</td>
<td>-</td>
<td></td>
<td>Press left button to add a new background control point below the mouse cursor</td>
</tr>
<tr>
<td><strong>Mark single peak</strong></td>
<td>Peak below its top (must be visible!)</td>
<td>-</td>
<td></td>
<td>Click left button to mark the peak below the mouse cursor; marks at other peaks will be removed</td>
</tr>
<tr>
<td><strong>Mark selected peaks</strong></td>
<td>Peak below its top Ctrl (must be visible!)</td>
<td>-</td>
<td></td>
<td>Click left button to mark the peak below the mouse cursor, in addition to the peaks that are already marked</td>
</tr>
<tr>
<td><strong>Shift peak on 2theta axis</strong></td>
<td>Peak below its top (must be visible!)</td>
<td>-</td>
<td></td>
<td>Click right button and keep it pressed while moving the mouse to the left or right</td>
</tr>
<tr>
<td><strong>Mark range of peaks</strong></td>
<td>To the left of the leftmost peak in the range Ctrl</td>
<td>-</td>
<td></td>
<td>Press the left button, then move the mouse to the right until you have selected the range of peaks you would like to mark</td>
</tr>
<tr>
<td><strong>Mark single peak</strong></td>
<td>Top of a peak (must be visible!)</td>
<td>-</td>
<td></td>
<td>Click left button to mark the peak below the mouse</td>
</tr>
<tr>
<td>Effect/purpose</td>
<td>Cursor position in pattern graphics</td>
<td>Keyboard button(s)</td>
<td>Cursor shape</td>
<td>Mouse action</td>
</tr>
<tr>
<td>-------------------------------------------</td>
<td>------------------------------------</td>
<td>-------------------</td>
<td>--------------</td>
<td>-----------------------------------------------------------------------------</td>
</tr>
<tr>
<td><strong>Mark selected peaks</strong></td>
<td>Top of a peak (must be visible!)</td>
<td>Ctrl</td>
<td></td>
<td>Click <strong>left</strong> button to mark the peak below the mouse cursor, in addition to the peaks that are already marked.</td>
</tr>
<tr>
<td><strong>Add peak</strong></td>
<td>Anywhere</td>
<td>Ctrl</td>
<td></td>
<td>Click <strong>right</strong> button to add a peak at the current cursor position.</td>
</tr>
<tr>
<td><strong>Shift peak on 2theta axis</strong></td>
<td>Peak below its top (must be visible!)</td>
<td>-</td>
<td></td>
<td>Click <strong>right</strong> button and keep it pressed while moving the mouse to the left or right.</td>
</tr>
<tr>
<td><strong>Modify peak FWHM</strong></td>
<td>Peak below its top; peak must be marked and visible!</td>
<td>-</td>
<td></td>
<td>Mark a peak by left-clicking on it, then move the mouse over the peak (mouse cursor will change), and turn the <strong>mouse wheel</strong> in order to modify the FWHM (full width at half maximum) of the marked peak.</td>
</tr>
<tr>
<td><strong>Modify peak intensity and/or position</strong></td>
<td>Top of a peak (must be visible!)</td>
<td>-</td>
<td></td>
<td>Click <strong>right</strong> button and keep it pressed while moving the mouse in any direction.</td>
</tr>
<tr>
<td><strong>Select range(s) to be excluded</strong></td>
<td>Anywhere</td>
<td>Alt</td>
<td></td>
<td>Press the <strong>left</strong> button, then move the mouse to the right until you have selected the range you would like to exclude from FoM calculations.</td>
</tr>
<tr>
<td><strong>Delete range exclusion mark</strong></td>
<td>Inside a range marked to be excluded (grey background color)</td>
<td>-</td>
<td></td>
<td>Press the <strong>right</strong> mouse button inside a range marked to be excluded in order to re-use this range (delete the exclusion marking / grey background color).</td>
</tr>
<tr>
<td><strong>Trim pattern on left-hand side</strong></td>
<td>Left border of the diffraction pattern</td>
<td>-</td>
<td></td>
<td>Move the mouse cursor to the left border of the diffraction pattern until the mouse cursor changes, press the left button, and move the mouse to the right until you have marked the desired area to be trimmed.</td>
</tr>
<tr>
<td>Effect/purpose</td>
<td>Cursor position in pattern graphics</td>
<td>Keyboard button(s)</td>
<td>Cursor shape</td>
<td>Mouse action</td>
</tr>
<tr>
<td>----------------------------------------</td>
<td>------------------------------------</td>
<td>--------------------</td>
<td>--------------</td>
<td>-----------------------------------------------------------------------------</td>
</tr>
<tr>
<td><strong>Trim pattern on right-hand side</strong></td>
<td>Right border of the diffraction pattern</td>
<td>-</td>
<td></td>
<td>Move the mouse cursor to the right border of the diffraction pattern until the mouse cursor changes, press the left button, and move the mouse to the left until you have marked the desired area to be removed. Finally, release the mouse button.</td>
</tr>
<tr>
<td><strong>Zoom (select range)</strong></td>
<td>Anywhere</td>
<td>-</td>
<td></td>
<td>Click <strong>left</strong> button at the position where you would like to start selecting your zoom range, and keep it pressed while moving your mouse, until you have selected the desired zoom range, then release the button.</td>
</tr>
<tr>
<td><strong>Zoom</strong></td>
<td>Anywhere</td>
<td>-</td>
<td>Any</td>
<td>Move the mouse cursor to a point you would like to zoom into, then turn the mouse <strong>wheel</strong> away from you to zoom right into this position (or vice versa)</td>
</tr>
<tr>
<td><strong>Zoom</strong></td>
<td>Anywhere</td>
<td>-</td>
<td>Any</td>
<td>Double-click the <strong>left</strong> button at the position you would like to zoom into (only applicable if fully zoomed out; see below)</td>
</tr>
<tr>
<td><strong>Zoom out</strong></td>
<td>Anywhere</td>
<td>-</td>
<td>Any</td>
<td>Click the <strong>right</strong> button to open the context menu, then select “Full pattern” or “Previous zoom”</td>
</tr>
<tr>
<td><strong>Zoom out</strong></td>
<td>Anywhere</td>
<td>-</td>
<td>Any</td>
<td>Double-click the <strong>left</strong> button</td>
</tr>
<tr>
<td><strong>Tracking (shifting of the zoom range)</strong></td>
<td>Anywhere</td>
<td>Shift</td>
<td></td>
<td>Once you have zoomed into the pattern, press the <strong>Shift button</strong> on your keyboard or the mouse <strong>wheel</strong>, and keep it pressed while moving the mouse around</td>
</tr>
<tr>
<td>Effect/purpose</td>
<td>Cursor position in pattern graphics</td>
<td>Keyboard button(s)</td>
<td>Cursor shape</td>
<td>Mouse action</td>
</tr>
<tr>
<td>--------------------------------------------</td>
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</tr>
<tr>
<td>Vertical line at mouse cursor position</td>
<td>Anywhere</td>
<td>Ctrl+X</td>
<td>Any</td>
<td>Press &lt;Ctrl+X&gt; to toggle the display of a vertical line at the cursor position, e.g. to compare peak positions</td>
</tr>
<tr>
<td>Zero point shifting</td>
<td>Anywhere</td>
<td>Ctrl+Alt</td>
<td></td>
<td>While keeping the Ctrl and Alt button pressed, turn the mouse wheel to shift the positions of exp. peaks and raw data along the 2theta-axis</td>
</tr>
<tr>
<td>Correct specimen displacement</td>
<td>Anywhere</td>
<td>Ctrl+Alt+Shift</td>
<td></td>
<td>While keeping the Ctrl, Alt and Shift button pressed, turn the mouse wheel to shift the positions of exp. peaks and raw data along the 2theta-axis according to ( \Delta 2\theta = -2s\cos \Theta / R; T = -s/R )</td>
</tr>
<tr>
<td>Adjustment of difference plot size/height</td>
<td>2theta/d-axis</td>
<td>-</td>
<td></td>
<td>Move the mouse cursor to the 2theta- or d-value axis (x-axis) (mouse cursor will change), press the left mouse button, and move the mouse away from you to open/increase the size of the difference plot (or vice versa)</td>
</tr>
<tr>
<td>Adjust intensity scaling factor manually</td>
<td>Top of a peak of an entry marked in the match list</td>
<td>-</td>
<td></td>
<td>Move the mouse cursor to the top of a peak of the entry that is currently marked in the match list (mouse cursor will change), then press the left mouse button, and keep it pressed while moving the mouse up or down to adjust the intensity scaling factor (-&gt; quantity) of the corresponding selected phase</td>
</tr>
<tr>
<td>Adjust experimental pattern distance</td>
<td>To the right of the diffraction pattern graphics</td>
<td>Ctrl+‘-’; Ctrl+‘+’</td>
<td></td>
<td>Place the mouse cursor to the right of the diffraction pattern, then turn the mouse wheel up or down in order to decrease or increase the vertical distance between the experimental diffraction patterns. Only available if</td>
</tr>
<tr>
<td>Effect/purpose</td>
<td>Cursor position in pattern graphics</td>
<td>Keyboard button(s)</td>
<td>Cursor shape</td>
<td>Mouse action</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>at least two diffraction patterns are present</td>
</tr>
</tbody>
</table>
### Table of keyboard shortcuts and function keys

Many of the most common commands and procedures in Match! can also be invoked by pressing certain buttons on your keyboard. These so-called shortcuts are quite useful to speed up your work with Match!, especially if you know them by heart. Here is a list of all keyboard shortcuts in Match!.

Please note that you have to replace “Ctrl” by “Cmd” if you are using a Mac!

<table>
<thead>
<tr>
<th>Button(s)</th>
<th>Effect</th>
<th>Menu command</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ctrl+A</td>
<td>Automatic raw data processing</td>
<td>Pattern/Automatic/Autom. raw data proc.</td>
</tr>
<tr>
<td>Ctrl+Shift+A</td>
<td>Add new entry to the reference database directly, e.g. import from cif-file, use the current peak list or enter manually</td>
<td>Database/Add to reference database</td>
</tr>
<tr>
<td>Ctrl+B</td>
<td>Clear the current selection criteria (restraints)</td>
<td>Search/Reset restraints/additional entries</td>
</tr>
<tr>
<td>Ctrl+Shift+B</td>
<td>Enables the display of the radiation background and displays instructions how to manually modify the background using the background control points</td>
<td>Pattern/Background/Edit background</td>
</tr>
<tr>
<td>Ctrl+C</td>
<td>Copy the current diffraction pattern graphics into the clipboard, e.g. in order to paste it into other programs like Microsoft Word or Excel</td>
<td>Edit/Copy</td>
</tr>
<tr>
<td>Ctrl+Shift+C</td>
<td>Correct zero-point error (2theta shift)</td>
<td>Pattern/Correct zero-point error</td>
</tr>
<tr>
<td>Ctrl+D</td>
<td>View entry data sheet of the entry that is currently marked in the candidates- or match list</td>
<td>View/Data sheet</td>
</tr>
<tr>
<td>Ctrl+E</td>
<td>Load an entry into the match list directly by specifying e.g. its name, formula sum or entry number</td>
<td>Search/Add entry to match list directly</td>
</tr>
<tr>
<td>Ctrl+F</td>
<td>Find and display the best entry for the selection criteria you have entered</td>
<td>Search/Find phase/entry(s)</td>
</tr>
<tr>
<td>Ctrl+G</td>
<td>Find next (to be applied after having used “Find” (Ctrl+F)); find the next best entry in the candidate list for your selection criteria</td>
<td>Search/Find next</td>
</tr>
<tr>
<td>Ctrl+Shift+G</td>
<td>Find previous (to be applied after having used “Find” (Ctrl+F)); find the previous entry for your selection criteria</td>
<td>Search/Find previous</td>
</tr>
<tr>
<td>Ctrl+H</td>
<td>Search for strong lines in diffraction pattern (“Hanawalt (or Fink) search”)</td>
<td>-</td>
</tr>
<tr>
<td>Ctrl+I</td>
<td>Import (another) diffraction pattern file</td>
<td>Pattern/Insert/overlay…</td>
</tr>
<tr>
<td>Ctrl+J</td>
<td>Display mouse operations and keyboard shortcuts in online help</td>
<td>Help/Keyboard shortcuts and mouse operations</td>
</tr>
<tr>
<td>Ctrl+K</td>
<td>Peak searching using conventional method (second derivative)</td>
<td>Pattern/Peak searching/Peak search</td>
</tr>
<tr>
<td>Ctrl+Shift+K</td>
<td>Toggle graphics option “Show uncorrelated peaks”, displaying a light-orange rectangle</td>
<td>View/Pattern/Uncorrelated peaks</td>
</tr>
<tr>
<td>Button(s)</td>
<td>Effect</td>
<td>Menu command</td>
</tr>
<tr>
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<td>----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------</td>
<td>-----------------------------------</td>
</tr>
<tr>
<td></td>
<td>in the background of experimental peaks with a certain minimum intensity that have not been assigned to identified phases yet.</td>
<td></td>
</tr>
<tr>
<td><strong>Alt+K</strong></td>
<td>Add peaks manually by entering the peak parameters (open corresponding dialog)</td>
<td>Peaks/Add peak(s)</td>
</tr>
<tr>
<td><strong>Ctrl+L</strong></td>
<td>View tabular summary of all experimental and reference pattern peaks</td>
<td>View/Peak list</td>
</tr>
<tr>
<td><strong>Ctrl+M</strong></td>
<td>Run a new search-match calculation</td>
<td>Search/Search-Match</td>
</tr>
<tr>
<td><strong>Ctrl+Shift+M</strong></td>
<td>Run a new search-match calculation based on the currently marked peaks only</td>
<td>Search/Search-Match (marked peaks only)</td>
</tr>
<tr>
<td><strong>Ctrl+N</strong></td>
<td>Open/read Match! document from file, or import first diffraction pattern file</td>
<td>File/Open</td>
</tr>
<tr>
<td><strong>Ctrl+O</strong></td>
<td>Directly define the matching entries, by loading the corresponding entry numbers from a Match! answer set file (*.mta). This is especially helpful if series of similar samples have to be investigated.</td>
<td>File/Import/Predefined phase selection</td>
</tr>
<tr>
<td><strong>Ctrl+Shift+O</strong></td>
<td>Run a new search-match calculation based on the currently marked peaks only</td>
<td>Search/Search-Match (marked peaks only)</td>
</tr>
<tr>
<td><strong>Ctrl+P</strong></td>
<td>Open the “Print” dialog where you can select what you would like to print</td>
<td>File/Print…</td>
</tr>
<tr>
<td><strong>Ctrl+Q</strong></td>
<td>Close Match!</td>
<td>File/Quit (Mac: Match!/Quit)</td>
</tr>
<tr>
<td><strong>Ctrl+R</strong></td>
<td>Display phase analysis report</td>
<td>View/Report</td>
</tr>
<tr>
<td><strong>Ctrl+Shift+R</strong></td>
<td>Display the “Parameter Turn-On”-dialog in order to prepare and run a new Rietveld calculation</td>
<td>Tools/Rietveld (FullProf)</td>
</tr>
<tr>
<td><strong>Ctrl+S</strong></td>
<td>Save current session (Match! document)</td>
<td>File/Save</td>
</tr>
<tr>
<td><strong>Ctrl+Shift+S</strong></td>
<td>Save current session (Match! document) to a new file name/path</td>
<td>File/Save as…</td>
</tr>
<tr>
<td><strong>Ctrl+T</strong></td>
<td>Shift the experimental pattern on 2theta axis in order to obtain the best peak overlap with the reference pattern currently marked in the candidate list (internal standard)</td>
<td>Entries/Internal standard</td>
</tr>
<tr>
<td><strong>Ctrl+Shift+T</strong></td>
<td>Load the reference database entry that is currently marked in the candidate list as a new experimental pattern. This new pattern does not only contain the reference entry’s peaks but also a profile curve that is calculated from them, using the current default FWHM value.</td>
<td>Entries/Load as experimental</td>
</tr>
<tr>
<td><strong>Ctrl+U</strong></td>
<td>If there is more than a single entry for a certain phase present in the candidate list,</td>
<td>Entries/Unify phases</td>
</tr>
<tr>
<td>Button(s)</td>
<td>Effect</td>
<td>Menu command</td>
</tr>
<tr>
<td>----------------</td>
<td>------------------------------------------------------------------------</td>
<td>---------------------------------------------------</td>
</tr>
<tr>
<td></td>
<td>remove all but the best matching entry (FoM) for each phase</td>
<td></td>
</tr>
<tr>
<td>Ctrl+V</td>
<td>Paste (add) text data in clipboard as a new experimental diffraction pattern</td>
<td>Edit/Paste diffraction pattern</td>
</tr>
<tr>
<td>Ctrl+W</td>
<td>Finish Match!, i.e. run the finishing actions defined on the “Batch” page of the Options dialog</td>
<td>File/Finish</td>
</tr>
<tr>
<td>Ctrl+X</td>
<td>Toggle the displaying of a vertical line at the mouse cursor position inside the diffraction pattern (e.g. for peak position comparison)</td>
<td>View/Pattern/Cursor position</td>
</tr>
<tr>
<td>Ctrl+Shift+X</td>
<td>Toggle the displaying of a &quot;spectrum&quot; of X-ray line positions as vertical line at the mouse cursor position inside the diffraction pattern. This can be handy for the investigation of peaks resulting e.g. from alpha2 or beta radiation contributions.</td>
<td>View/Pattern/X-ray spectral lines</td>
</tr>
<tr>
<td>Ctrl+Y</td>
<td>Redo last undo operation</td>
<td>Edit/Redo</td>
</tr>
<tr>
<td>Ctrl+Z</td>
<td>Undo last operation/command</td>
<td>Edit/Undo</td>
</tr>
<tr>
<td>Ctrl+’-’</td>
<td>Decrease vertical distance between experimental patterns in diffraction pane (only available if two or more patterns are present/stacked)</td>
<td>View/Pattern/Reduce pattern distance</td>
</tr>
<tr>
<td>Ctrl+’+’</td>
<td>Increase vertical distance between experimental patterns in diffraction pane (only available if two or more patterns are stacked and the vertical distance has been reduced before)</td>
<td>View/Pattern/Increase pattern distance</td>
</tr>
<tr>
<td>Ctrl+’&lt;’</td>
<td>Switch back to the previously used zoom (pattern area)</td>
<td>View/Previous zoom</td>
</tr>
<tr>
<td>Del</td>
<td>Delete the currently marked item(s), e.g. peaks or candidate list entries</td>
<td>Edit/Delete</td>
</tr>
<tr>
<td>F1</td>
<td>Open help window</td>
<td>Help/Index</td>
</tr>
<tr>
<td>F2</td>
<td>Increase peak search sensitivity</td>
<td>Pattern/Peak searching/ Increase sensitivity</td>
</tr>
<tr>
<td>Ctrl+F2</td>
<td>Increase flexibility of automatically determined background curve, to follow the structures of the pattern more closely.</td>
<td>Pattern/Background/Increase flexibility</td>
</tr>
<tr>
<td>F3</td>
<td>Decrease peak search sensitivity</td>
<td>Pattern/Peak searching/ Reduce sensitivity</td>
</tr>
<tr>
<td>Ctrl+F3</td>
<td>Decrease flexibility of automatically determined background curve, to attribute</td>
<td>Pattern/Background/Decrease flexibility</td>
</tr>
<tr>
<td>Button(s)</td>
<td>Effect</td>
<td>Menu command</td>
</tr>
<tr>
<td>----------------</td>
<td>-------------------------------------------------------------------------</td>
<td>--------------------------------------------------</td>
</tr>
<tr>
<td>F4</td>
<td>Optimize peak searching sensitivity, to obtain the best overlap between experimental and calculated pattern</td>
<td>Pattern/Peak searching/ Optimize sensitivity</td>
</tr>
<tr>
<td>F5</td>
<td>Perform profile fitting</td>
<td>Pattern / Profile fitting / Profile fit</td>
</tr>
<tr>
<td>F6</td>
<td>Enable/disable fitting of 2theta values during profile fitting</td>
<td>Pattern / Profile fitting / Fit 2theta</td>
</tr>
<tr>
<td>F7</td>
<td>Enable/disable fitting of intensity values during profile fitting</td>
<td>Pattern / Profile fitting / Fit intensity</td>
</tr>
<tr>
<td>F8</td>
<td>Enable/disable fitting of FWHM values during profile fitting</td>
<td>Pattern / Profile fitting / Fit FWHM</td>
</tr>
<tr>
<td>Ctrl+Alt+A</td>
<td>Open dialog in which the individual automatic raw data processing steps can be configured</td>
<td>Pattern / Automatic / Configure…</td>
</tr>
<tr>
<td>Ctrl+Alt+G</td>
<td>Open dialog in which the options for the diffraction pattern graphics can be adjusted</td>
<td>Options / Diffraction pattern options…</td>
</tr>
<tr>
<td>Cursor up/down</td>
<td>Move the line mark in the candidate list up/down (if it has the input focus)</td>
<td>-</td>
</tr>
<tr>
<td>Space</td>
<td>Select current entry in candidate list (if it has the input focus) as “matching” (i.e. move it to the match list)</td>
<td>Entries / Select as matching</td>
</tr>
<tr>
<td>Shift</td>
<td>If you have zoomed into the pattern previously, you can now move the visible diffraction pattern section around (tracking) simply by moving the mouse</td>
<td>-</td>
</tr>
<tr>
<td>Shift+Del</td>
<td>Delete all peaks in the current experimental pattern</td>
<td>Peaks / Delete all peaks</td>
</tr>
</tbody>
</table>
Support

In case of trouble when using Match!, 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 (<Cmd+?> on the Mac) in order to open the online help, and examine the context sensitive help text. Especially read the items mentioned under Note: and See also: Check the help jumps, too, which are underlined like links in a web browser.

- Look for appropriate keywords in the Help Index, and use the free-text search facility of the online help.

- If you do not find a command, use the Help Index (Index tab on the Match! Application Help window) to get an alphabetic list of search items.

- Visit the Match! web page at:

  https://www.crystalimpact.de/match/update.htm

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

- If this page does not give you an answer, or if the trouble is caused by an error in the software (a "bug"), send an e-mail to support@crystalimpact.com

  Or – if you are not connected to the internet – send a fax to: ++49-228-9813644

  or write to:

  Crystal Impact GbR
  Kreuzherrenstr. 102
  D-53227 Bonn
  Germany

  Please describe how the bug can be reproduced as detailed as possible, and attach possibly required files (e.g. diffraction data)!
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