MATCH!

Phase Identification from Powder Diffraction

User Manual

CRYSTAL IMPACT

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Version 1.9

Dr. Holger Putz

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Contents

Welcome!

Basics

MATCH! is an easy-to-use software for phase identification from X-ray powder diffraction data, which has become a daily task in material scientists work. Typically, an identification of the phases present in an unknown sample/powder proceeds as follows:

1. The X-ray diffraction pattern of the unknown sample is measured with highest possible accuracy and signal/noise ratio. The result is a file containing intensity vs. 2theta data (the so-called "raw data"), sometimes also including experimental conditions.

2. This diffraction data file is now imported into the search-match software.

3. As the diffraction data generally are raw (profile) data, the so-called "raw data processing" has to be carried out. This includes

   - stripping of the alpha-2-radiation (if present),
   - data smoothing,
   - background subtraction,
   - peak searching,
   - profile fitting and
   - correction for errors.

   The goal is to obtain a list of peaks (2theta and intensity values) with highest possible precision. It is extremely important that this step is performed as accurate as possible in order to obtain reasonable results in the search-match process later on!

4. If additional information is available about your sample (like chemical class, composition, density, color etc.), you should use it as restraints for the search-match calculation.

5. Once the list of peaks is available, the actual search-match process can be performed: The software compares each diffraction pattern in the reference pattern database to the pattern of the unknown sample. It calculates a numerical value indicating the degree of the agreement, the so-called "figure-of-merit" (FoM).

6. When the search-match has been finished, the so-called "candidate entries" are ranked according to their FoM values. The entries with the highest FoM are the ones that are most likely to be present in the sample. The ranked list of entries is then presented to the user.

7. The user analyzes the candidate entries at the top of the list and selects those that are most likely to be present in the sample ("matching entries/phases").

8. Finally, there should be a Rietveld refinement of the phases selected as "matching" against the original raw (profile) data. A successful refinement is generally taken as the proof that the phase identification is correct and complete.

You will learn in the tutorial sessions in the next chapter how to carry out these steps (in fact steps two to seven) using MATCH!.

i Paragraphs which are formatted like this one provide further details and/or additional information in the current context. You might skip these paragraphs if you have little time or do not want to go too much into detail at the moment.
However, it is especially this information which will give you a deeper understanding of the underlying concepts, thus enabling you to successfully explore MATCH! on your own later on. Hence, if you cannot work through these "info" paragraphs right now, we recommend to at least reserve some time later on and work through the tutorial sessions again, now including these paragraphs.

Installation

Before you install MATCH!, you should check the following

Minimum system requirements:

- Personal Computer with Microsoft Windows 98, ME, NT 4.0, 2000, XP or Vista operating system

- Microsoft Internet Explorer 5.01 or higher

- 128 megabytes of RAM (256 megabytes or more recommended)

- Hard disk with minimum 600 MB of free disk space

- Graphics resolution of 1024 x 768 pixels with 32,768 colors ("High Color")

- DVD drive

You might also want to read the license agreement conditions on page 62 to which you have to agree before installing the software.

Please insert the MATCH! DVD into your DVD-drive and wait a few seconds; an installation selection program will start automatically. If the selection program does not start automatically, please run "autostart.exe" in the main directory of the DVD.

Afterwards, please click on the button with the MATCH! logo next to "Install Match!". The actual MATCH! installation program will start and lead you through the setup process. Simply follow the instructions on the screen. Please note the terms of the "End User License Agreement", which will appear in the second dialog box!

Online Update

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

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

By default, MATCH! checks the Crystal Impact webserver for a new version automatically each time it is executed. If you would like to disable this feature (e.g. if you are not permanently connected to the internet), you can do so on the "General" page of the "Tools/Options" dialog, simply by removing the hook in front of "Automatically check for online updates". Please note that the box "Save as defaults" in the corner on the lower left-hand side of the dialog must also be checked in order for the change to be effective!

Even if you have disabled the "Automatic update checking" option, you can update your software online by selecting the "Online update" command from the "Help" menu. The procedure will be the same as the one described above for the automatic update.

Reference Databases

As has already been mentioned, 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.

A free-of-charge reference database called "IUCr/COD/AMCSD" is by default installed automatically along with Match![1]; it can be used straight away after the installation. This reference database contains powder diffraction patterns calculated from crystal structure data provided by the IUCr journals[2], taken from the "Crystallography Open Database" (COD[3]) and from the "American Mineralogist Crystal Structure Database" (AMCSD[4]).

In this context, we would like to thank Pete Strickland (IUCr), Armel Le Bail (COD) and Bob Downs (AMCSD) for their kind permission to download and distribute their data free-of-charge!

All entries of the "IUCr/COD/AMCSD" 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 (p. 6).

You can download additional or updated reference databases free-of-charge from

http://www.crystalimpact.com/match/download.htm#refdb

It is essential that you understand that both size and quality of the reference database have an extremely large influence on the results of your phase identifications! A phase cannot be identified if there is no corresponding entry of sufficient quality in the reference database!

In this context, please read the chapter "Reference Pattern Databases" starting on p. 28, where you will also learn how to use a different reference database (e.g. the ICDD PDF database and/or own diffraction patterns).

Where to get Help

If you have any questions when operating MATCH!, simply press the "F1" button on your keyboard. This will open MATCH!'s very detailed **online help**, where you will get context-sensitive information for your question/problem.

The online help can be consulted in a variety of different ways:

- context sensitive by pressing "F1" (e.g. if you do not know what you should select/enter in a certain dialog)

- continuous "in-depth" reading guided by the links (starting e.g. at the "Welcome" page; select "Help Contents" from the "Help" menu)

- index based ("Help Index"; e.g. if you are searching for a certain function/feature)

- searching for arbitrary keywords (free-text searching)

More information about what you can do if you have questions or encounter problems when using MATCH! is given on p. 61.

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[1]If you are using the normal Match! demoversion, only data from the AMCSD are installed. You can e.g. download and install the full IUCr/COD/AMCSD database from the Match! web page, or from a "Crystal Impact Software DVD" distributed at various meetings, e.g. the ECM- or IUCr-conferences.

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

[3]http://sdpd.univ-lemans.fr/cod

[4]R.T. Downs, M. Hall-Wallace, "The American Mineralogist Crystal Structure Database", American Mineralogist **88**, 247-250 (2003). http://rruff.geo.arizona.edu/AMS/amcsd.php

Tutorial

You are now certainly eager to get things running and start identifying phases with MATCH!. The four sessions of 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 sessions described in this chapter, we strongly recommend to restore the default (factory) settings of MATCH!, just in case a colleague has used MATCH! and changed them previously. In order to do so, please start MATCH![5,6] if it is not already running. Afterwards, select the "Restore factory settings" command from the "Tools" menu, which will reset all options to the original ones selected by Crystal Impact. Finally, please select the "Save as defaults" command (also from the "Tools" menu) in order to make the changes permanent. MATCH! will now operate exactly like it has just been installed[7].

Please note that all tutorial sessions have been carried out using the AMCSD as reference database. If you use the IUCr/COD/AMCSD, the ICDD PDF or your own diffraction data, the results may be a little bit different!

Basic Phase Identification

In this very first tutorial session you will perform a rather simple phase identification exercise. 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

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: 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. It will display a nearly completely empty screen (Fig. 1).

i The MATCH! screen is devided into three parts: In the large panel on the lower left hand side, the diffraction pattern is displayed. Above, the list of matching entries ("Results list") is placed. On the right-hand side, either the "Peak list" (as currently), the "Data sheet"or the "Phase Analysis Report" are displayed.

The first thing you have to do is to import the diffraction pattern into the MATCH! software. Please open the "File" menu, click on "Import", and select the command "Diffraction data". The "Select diffraction data" dialog opens (Fig. 2).

Please make sure that the file type at the bottom of the dialog is set to "All files (automatic detection) (*.*)" (so that the file format is determined automatically), then select the file "quickstart.rd" in the "Tutorial" subdirectory of the MATCH! program directory (e.g. "C:\Program Files\Match!\Tutorial"). Finally, please press "Open".

Now that the diffraction pattern has been imported, you can start the search-match process straight away (the raw data processing etc. will be performed automatically): Either click the corresponding toolbar button, press the combination "Ctrl+M" on your keyboard, or select the "Search-Match" command from the "Search" menu. After a few seconds, the result will be displayed; your screen should look similar to Fig. 4.

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

You now have to select the entries that you assume to be present in the sample, based both on the

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[5]In order to start MATCH!, press the Windows "Start" button, select the "Match!" folder of the "Programs" branch, and finally click on "Match!".

[6]If MATCH! has not been installed on your computer yet, you should read the chapter "Installation" on p. 2 and follow the instructions given there before you continue reading !

[7]Of course, you don't have to recreate the index files! However, please note that the settings concerning the current reference database will not be changed.
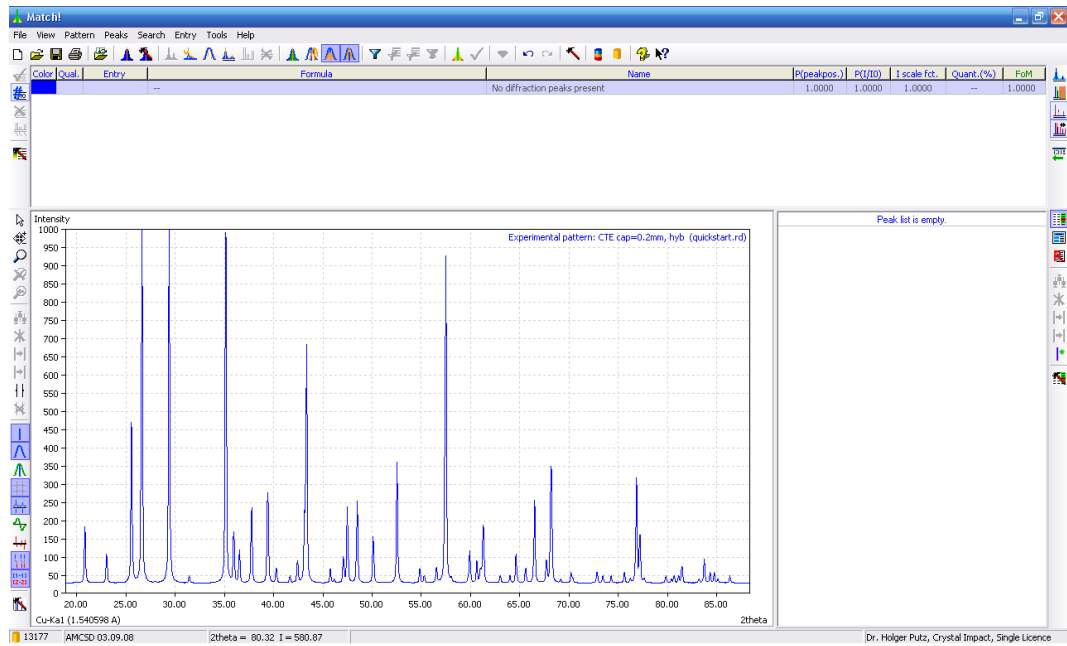
Fig. 1: MATCH! displaying an empty diffraction pattern, Peak list and Results list (answer set).

Fig. 2: In this dialog you select the file in which the diffraction data are stored.

"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 Al_2O_3 (Corundum). Please note the column "Quant. (%)" on the right-hand side of the Results list. Here, you can see if the corresponding entry contains the parameter I/I_c required for (semi-)quantitative phase analysis. If you are using the AMCSD or IUCr/COD/AMCSD reference database, 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/I_c parameter, so these entries would not be suitable for semi-quantitative phase analysis.

In order to select the first entry as matching, please press the space bar while the first entry Al_2O_3 (Corundum) is still marked in the Results list. Alternatively, you can also double-click on the corresponding entry. The selected phase will now be displayed in bold characters. 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. 5).

There are still several entries left in the Results list with good (high) figure-of-merit values, so obviously there are more phases present in the sample. Simply press the "cursor down" arrow button

Fig. 3: The diffraction data have been successfully imported.
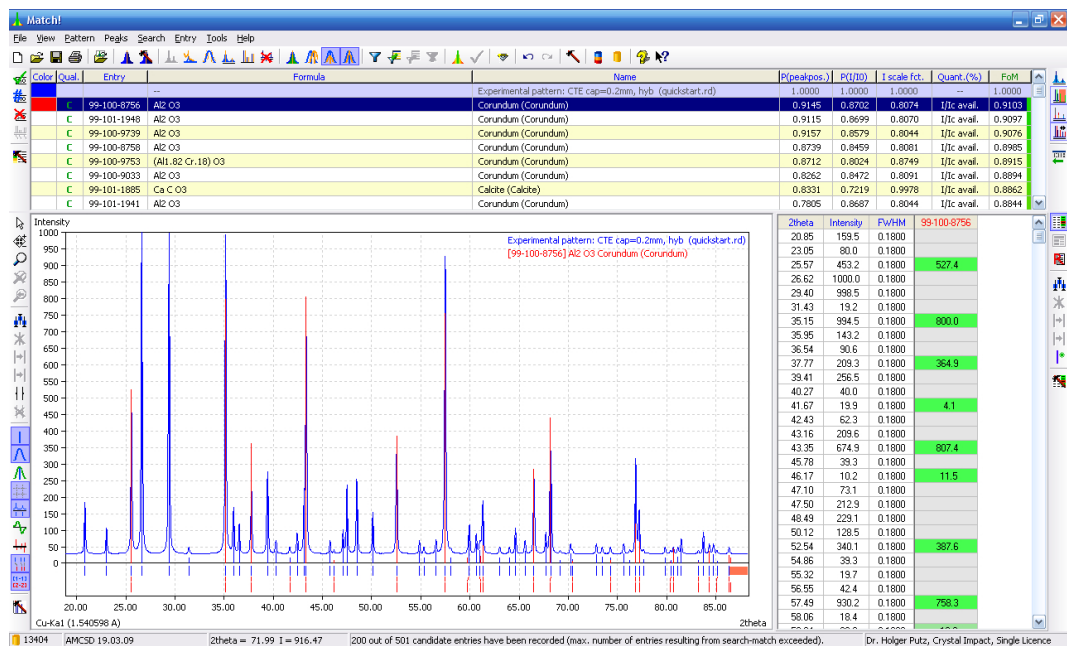
Fig. 4: The result of the search-match operation is displayed.

on your keyboard, in order to mark the next entry below the selected one.

Now you can clearly identify the second phase being Calcite (CaCO$_3$). Again, please press the space bar when the corresponding entry is marked, like you have done before for Corundum. By doing so, you have selected this entry as matching as well.

The next "unmatched" line in the Results list belongs to an entry describing the phase Quartz (SiO$_2$). Please move down the list ("cursor down" button on your keyboard) to mark the first Quartz entry, visually compare it to the experimental pattern, and finally press the space bar to select it.

As you see (Fig. 6), the next entry (Tungsten) has a very low figure-of-merit (FoM) value (indicated by the 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.

At this point the semi-quantitative phase analysis is also completed: Please have a look at the column
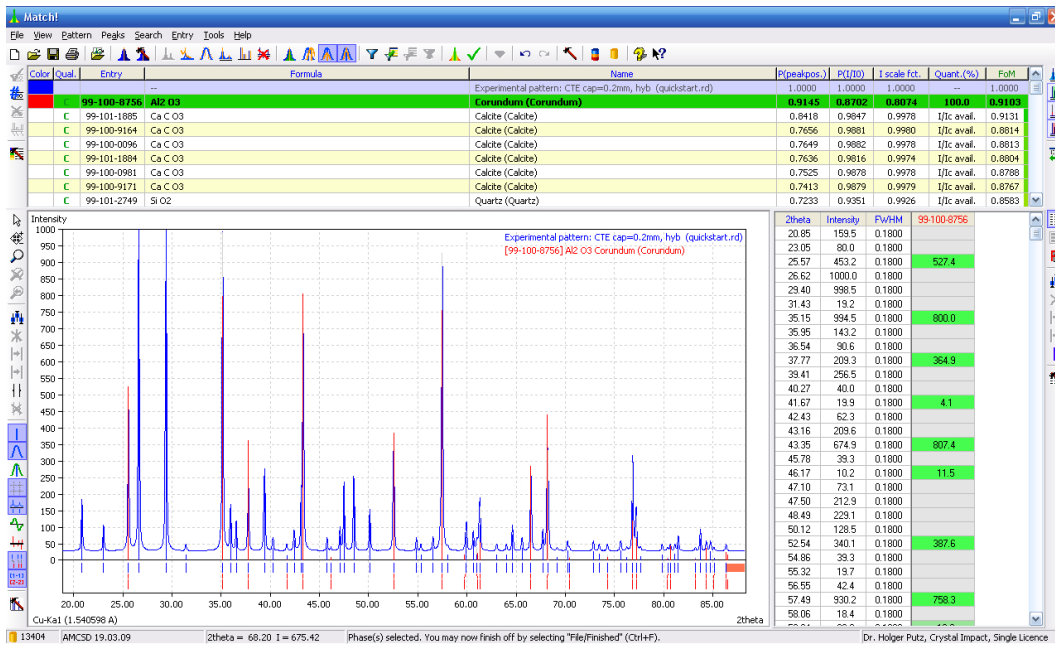
Fig. 5: The first phase (Al$_2$O$_3$, Corundum) has been selected as "matching".
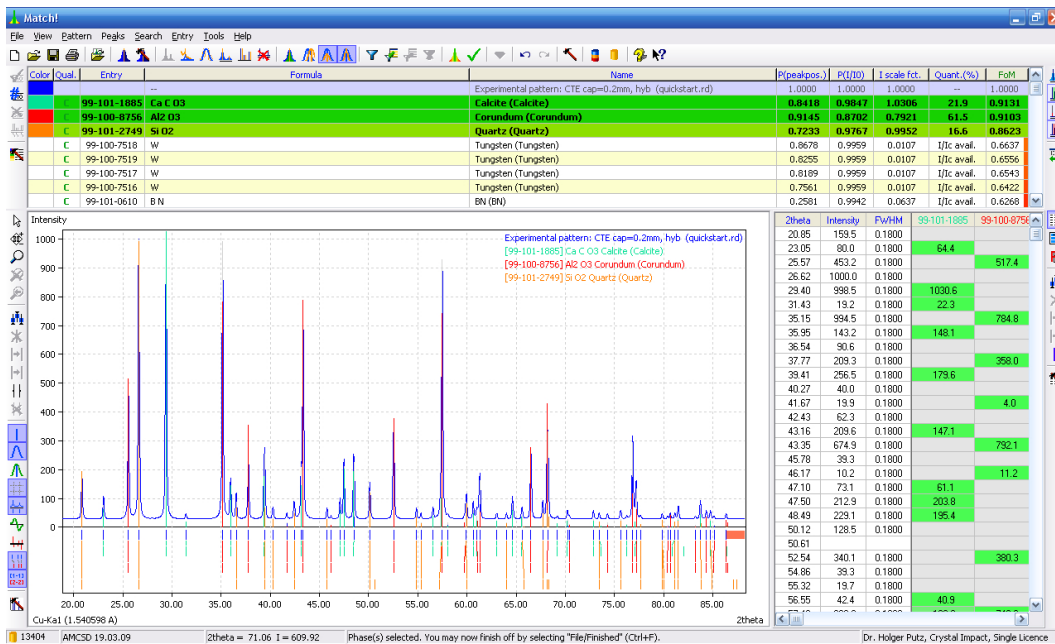
Fig. 6: The identification of phases in the unknown sample is complete. Note the column "Quant. (%)" in the Results list in which the weight percentage of the matching phases in the sample is given.

"Quant. (%)" in the Results list (to the left of the FoM column): Here you can see that your sample contains about 62% Corundum (weight-percentage), 22% Calcite and 16% Quartz.

There is nothing left to do but printing the report and saving the document. In order to finish your phase identification, either press the combination "Ctrl+F" on your keyboard, click the corresponding toolbar button, or select the "Finished" command from the "File" menu. This will open the dialog window shown in Fig. 7.

Please make sure that all settings correspond to Fig. 7, then press "OK". When the printer dialog is displayed, select your printer and press "Print". At the same time, the "Save file" dialog will be shown. Please enter a reasonable name (e.g. "result_quickstart") and click "Save". Afterwards, the MATCH! window will be closed automatically due to the "Quit Match!" option in the "Finish" dialog being active.
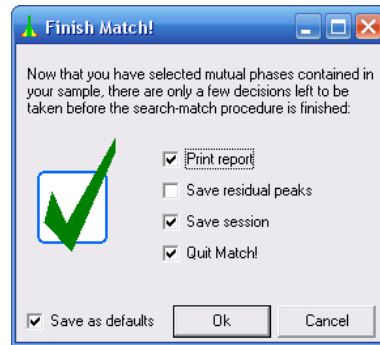
Fig. 7: Once you have selected the matching entries, there are only a few things left to do.

That's it!

Database Retrieval

An important aspect of phase identification is the application of additional knowledge about the sample, like chemical composition or density. It is always recommended to use any available information in order to limit the list of candidate entries. In this session, you will learn about database retrieval using the various restrainting options of MATCH!, enabling you to use information of this type.

Suppose that you are working on silicates, and you remember you once read a paper about an earth alkaline silicate forming an interesting network containing both Si and some earth-alkaline metal. The name of the journal was something like "European..."; unfortunately you cannot remember the rest. Can you find any corresponding information in the MATCH! reference database (e.g. AMCSD)?

Please start MATCH! if it is not already running; otherwise open a new document by selecting the "New" command from the "File" menu (or pressing the corresponding toolbar button). MATCH! will display the typical empty new document.

In order to perform a retrieval in the reference pattern database(s), you have to open the so-called "Restraints dialog": Please select the "Restraints" command from the "Search" menu, press "Ctrl+R" on your keyboard, or click on the corresponding toolbar button. The dialog will be opened (Fig. 8).
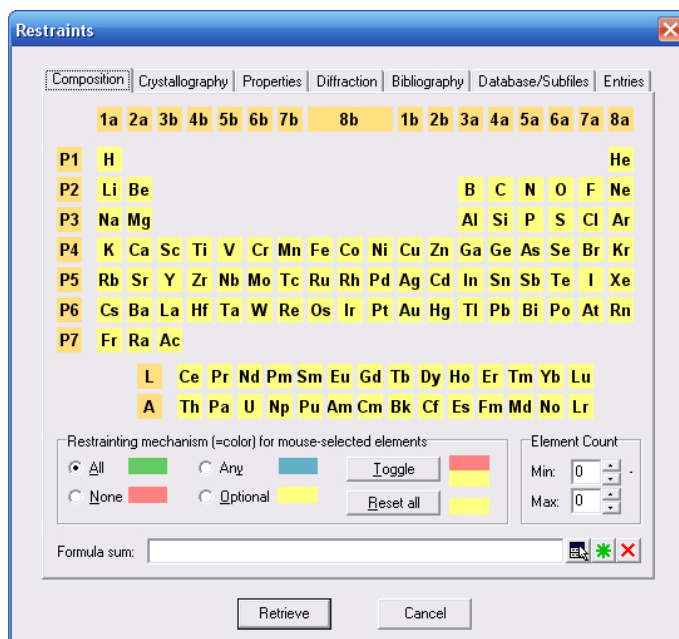
Fig. 8: In this dialog consisting of several tabsheets, you can enter the restrainting conditions for your reference database retrieval. For example, you can enter additional information about your sample, like chemical composition, crystallographic data (e.g. crystal system), physical properties (e.g. density), names (e.g. mineral names), peak position (ranges), bibliographic data or entry numbers.

There are two facts you remember about the entry you are interested in:

- It contains the elements Si and O as well as some alkaline earth metal.

- It is described in a journal the name of which starts with "European"

These facts have to be entered as search criteria in the Restraints dialog: The chemical composition ("alkaline earth silicate") has to be entered on the first page of it, e.g. in the "periodic table". You can define four states for each element, represented as colors:

green "All" elements with background in green have to be present in each resulting entry.

blue "Any" (at least one) of the elements with blue background has to be present in each resulting entry.

yellow The presence of elements with yellow background is "Optional". They may be present, but do not necessarily have to.

red "None" of the elements marked in red may be present, or, in other words, entries in which at least one of these elements is present are excluded from the resulting answer set.

By default, all elements are marked as "optional" (yellow). You now have to change the status of the elements given in your search criterion. At first, we will change the status of Si and O to "All" (green), since you know for sure that these elements are present: Please make sure that "All" (green) is selected in the "Restraining mechanism" box, then click on Si and O in the periodic table. The background color of the two elements will be changed to green; Si and O have to be present in all resulting entries. Since you don't know the alkaline earth metal for sure, you have to use a different restraining mechanism for it: "Any" (at least one) of the alkaline earth metals may/must be present, so please activate the corresponding "blue" restraining mechanism ("Any") and click on the group label "2a" at the top left. This will change the background color of all alkaline earth elements to blue. Your dialog should now look similar to Fig. 9.
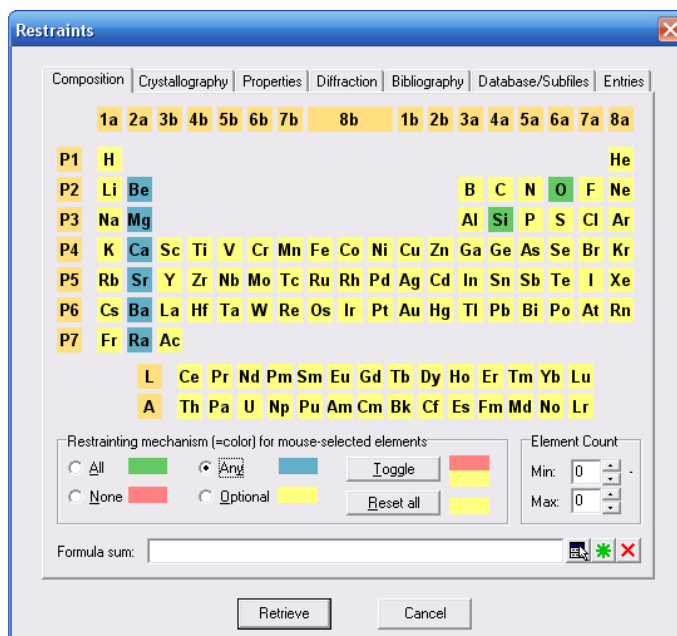
Fig. 9: Chemical composition restraints: The elements Si and O have to be present in the resulting entries, as well as any (at least one) of the alkaline earth elements. Other elements may be present as well.

At this point you have entered the facts you know about the chemical composition of the entry you are interested in; you now have to add the restraint that the entry must be described in a journal the name which starts with "European". This can be done on the "Bibliography" page of the Restraints dialog, so please select this page by clicking on the corresponding tabsheet header. Please click in the entry line next to "Journal" and enter *European* using your keyboard. Since you cannot remember the rest of the name, it is best to use the "text fragment search facility", so please click on (activate) the corresponding button with the green star to the right of the "Journal" input line. The dialog will now look similar to Fig. 10.

i The so-called "text fragment search" is generally useful if you don't know the exact phrase you are searching for, or if the phrase can be present in various contexts (e.g. author/co-author). If this option is active (button is pressed), the text in the input field does not have to completely match the values present in the database (as usual); it is sufficient that this text is **present** in the corresponding database value. **Please note that MATCH! will not distinguish between upper and lower case letters if you use the "fragment search" option, in contrast to its normal behaviour !**.
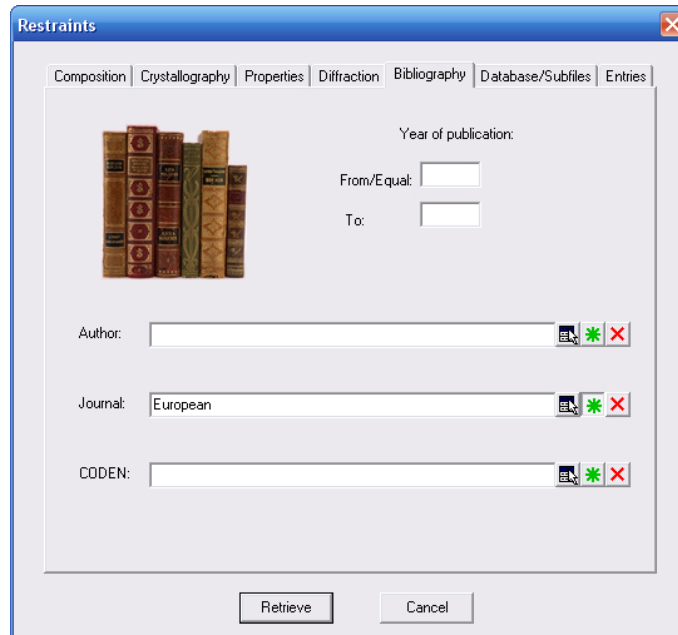
Fig. 10: Journal name restraints: The phrase "European" must be present (text fragment search) in the "Journal" database field of all matching entries.

All information you have about the entry you are searching for has now been entered, so please start the database retrieval by clicking "Retrieve" at the bottom of the dialog. A message window will be displayed indicating the number of entries that will result from the application of the restraints (Fig. 11).
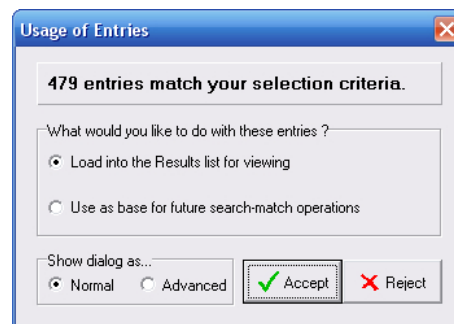

Fig. 11: This message window indicates that 479 entries will result from the application of the restraints you have entered. If you accept, these entries will be loaded into the Results list (for viewing) as well as into the so-called "restraints buffer", as restraints for future search-match operations. well as to form the new answer set.

Please accept the new answer set by clicking "Accept". MATCH! will display a progress windows while the new entries are loaded. Afterwards, the Results List contains the list of entries matching your restraints (Fig. 12).

A lot of entries (479) match your restraints; it will become a tedious work to inspect them all in order to actually find the one you are searching for. Fortunately, the moment you pressed the "Accept" button you saw this small sheet of paper on your desk on which you wrote down some more details during the talk: the space group is "P1 21/c 1", and the density is somewhere between 2.5 and 2.6 g/cm^3.

You now have additional criteria which should be able to limit the number of matching entries. As before, the criteria have to be entered in the Restraints dialog, so please open it again using the menu, Ctrl+R or the toolbar button. There are two additional facts now:

- Space group is P 1 21/c 1
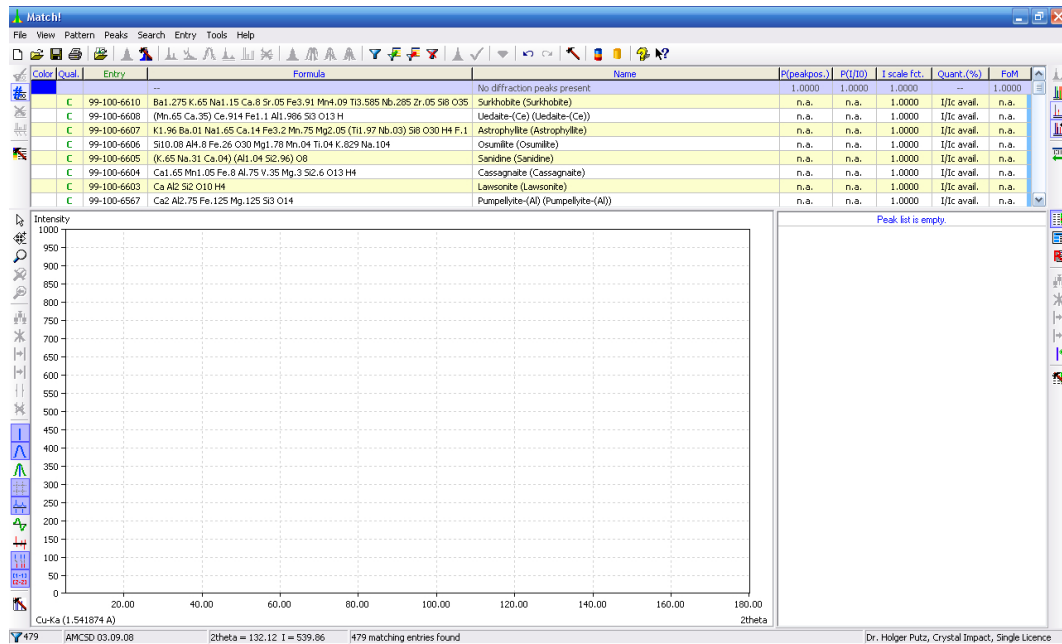
Fig. 12: 479 entries matching your restraints have been found.

- Density between 2.5 and 2.6 g/cm^3

The space group restraint has to be entered on the "Crystallography" page of the Restraints dialog, so please open this page by clicking on the corresponding tabsheet header. Since you don't remember exactly how the space group symbols are given in the reference database(s) (e.g. with or without spaces), you use the so-called "list selection box" facility of MATCH!: Please click on the button to the right of the "Space group" input line. The so-called "list selection box" for the database field "Space group" will appear, displaying a list of all values which are present for this field in your reference database (Fig. 13).
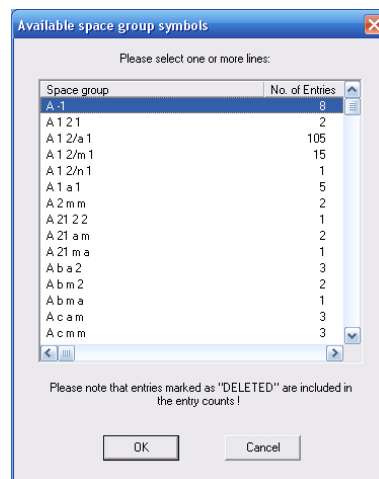
Fig. 13: The so-called "list selection box" for the database field "space group" has been opened, displaying a list of all values which are present for this field in your reference pattern database. To the right of each value, the number of entries which include this value are given.

Please scroll down the list until you reach the line "P 1 21/c 1". Mark this line (click on it using the left mouse button) (Fig. 14), then close the list selection box by clicking "OK". The value you have marked will be transferred to the input line of the space group database field.
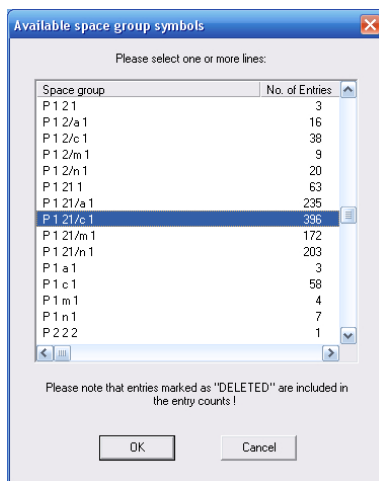
Fig. 14: The value "P 1 21/c 1" for the database field "space group" has been marked in the list selection box.

The basic aim of a "list selection box" is to provide the user with a quick and intuitive input facility for restrainting values. Besides this, a list selection box is generally the most appropriate way of entering the criteria, since the text strings of the database entries generally have to match **exactly** the one entered by the user in order to be accepted, the only exception being the **text fragment searching** (p. 10).

In order to select one or more values in the list selection box, simply mark the corresponding line(s) and close the list selection box afterwards by clicking "OK". The corresponding "values" will be copied to the input field automatically. If you would like to mark more than a single value/line, please click on the first line/value of interest, press the Shift key on your keyboard and keep it pressed until you have clicked on the final value/line. All values/lines in between the two lines will be marked as well.

You can easily **jump to a certain line** in the list by entering the first few characters (e.g. "gre" for "green") on your keyboard. MATCH! will automatically jump to the first line which starts with the characters you have entered. If you do not enter a character for longer than 1.5 seconds, this will reset the input buffer, so that you can start again with the first character.

Now you have to define the second new restraint, the density range. Please switch to the "Properties" page and have a look at the upper part of the dialog where the density values can be entered: There are three lines for density values; in each line you can define a density range (min./max.). You can search for calculated density values, measured values or any of them. Generally, it is recommended to use the third option, in which case entries having either a calculated or measured density within the defined range are accepted. In our case, the range for valid densities is 2.5-2.6 g/cm^3, so please enter the numbers in the corresponding fields (Fig. 15).

Now the two additional restraints you could extract from your notes have been entered; please press the "Retrieve" button at the bottom of the Restraints dialog to start the actual database retrieval. When the application of your new restraints to the reference database has been finished, you will be informed about the result similar to your first retrieval.

However, something is different compared to the previous retrieval: This time, the restraints buffer (and the answer set) already contain entries (the ones resulting from the first database retrieval). Hence, you now cannot only load the resulting entries into the Results list or use them for future search-match operations, but can also apply the newly found entries as restraints to the ones resulting from the first restrainting operation (composition and journal name).

In order to do so, please select the "Apply as restraints to current entries in Results list" option (Fig. 16)[8]. Afterwards, please press "Accept" to close the dialog. A single entry will remain in the Results list; it is the only entry in the reference pattern database which matches all four criteria (composition, journal, space group and density).

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[8]If you select the "Show dialog as Advanced" option at the bottom of the dialog, it will be enlarged and display more options. In the "Advanced" mode, you can e.g. perform additional logical operations like OR.
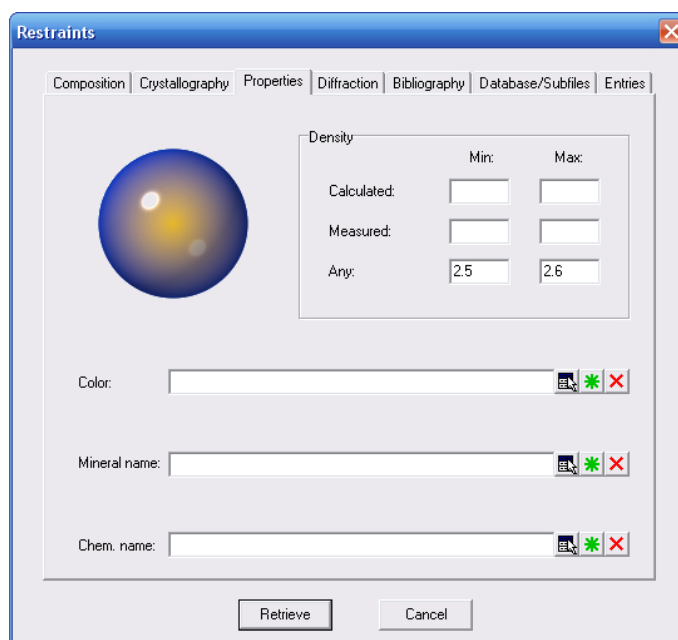
Fig. 15: Density restraints: All entries which contain either a calculated or measured density value between 2.5 and 2.6 g/cm^3 will be accepted.
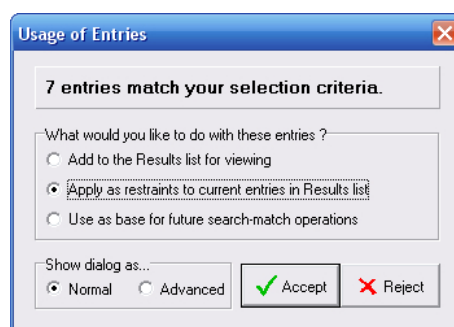

Fig. 16: 7 entries match the new restraints you have entered (space group and density). Since there are already entries present in the restraints buffer and the current answer set, you have selected to use these new entries as restraints to the previous entries, or, in other words, perform a logical "AND" operation on the two answer sets.

i   Each time you perform a reference database retrieval using the restraints dialog, the entries which match the conditions are taken as "restraints" for future search-match operations. This is achieved by copying them to a special buffer called "restraints buffer". The search-match routine will only consider these entries as possible candidates, or, in other words, only the diffraction patterns of the entries in the restraints buffer will be compared to the pattern of the unknown sample.

If the restraints buffer contains entries, this is indicated by a small funnel ("filter") symbol in the left corner of the status bar at the bottom of the Match! window. To the right of the filter symbol, the number of entries in the restraints buffer is indicated. If the buffer is empty, a colored hard disc symbol is displayed instead, along with the overall number of entries in the reference pattern database.

There are three commands (which can be accessed both in the "Search" menu as well as in the main toolbar) can be used to manage the restraints buffer:

"Answer set -> Restraints" copies the current answer set in the Results list to the restraints buffer, overwriting any entries which might have been present there before. As a result, only the entries which are currently present in the Results list will be considered in the next search-match calculation.

"Restraints -> Answer set" loads the entries from the restraints buffer into the Results list at the top of the Match! window, overwriting any entries which might have been present there before. This is especially useful if you would like to see or modify the entries currently present in the restraints buffer.

"Clear Restraints" empties the restraints buffer so that the next search-match operation will be performed on the full reference pattern database again.

Having finally found the entry you are interested in, you now want to view all of its details by

displaying its data sheet. Please mark (click on) the entry in the Results list, then select "Data sheet" from the "View" menu (or press the corresponding button in the toolbar to the right). The data sheet will be displayed in addition to the entry's diffraction pattern (Fig. 17).
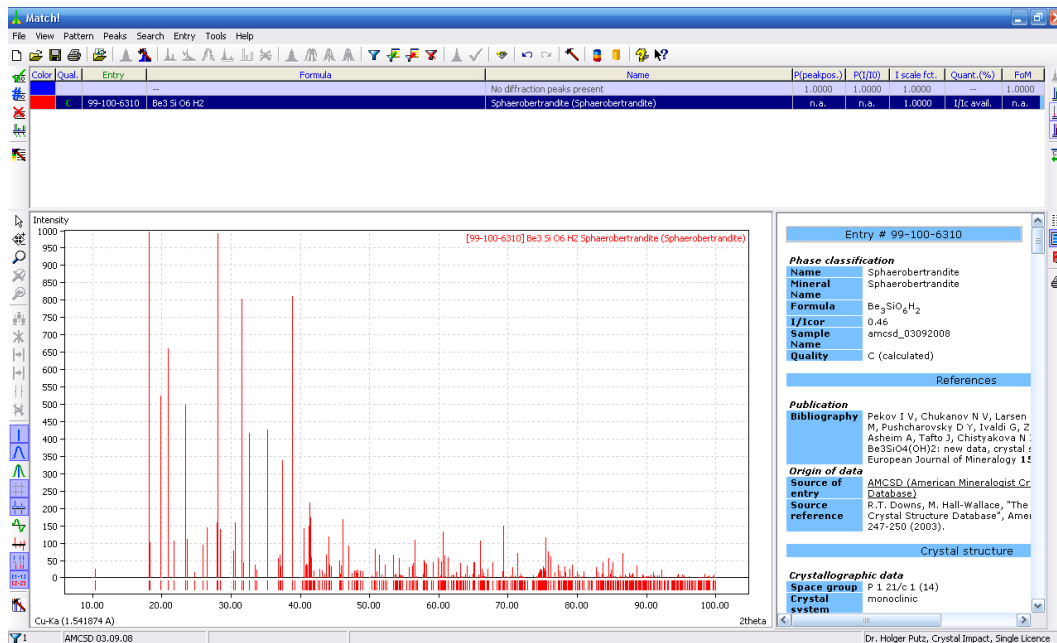

Fig. 17: This entry matches all four restrainting criteria you have entered.

You should probably print the data sheet in order to keep the data for reference purposes. Please click on the "Printer" button in the toolbar to the right and select your favourite printer afterwards.

Happy that you have found the crystal structure data you are interested in, you now would like to further investigate the interesting framework consisting of Si-O and Be-O polyhedra. Fortunately, you have the DIAMOND software for crystal structure visualization[9,10] available on your computer. All you have to do is export the entry data and import them into DIAMOND.

This can be done very easily: Simply click on the "View in Diamond" button in the toolbar at the top to transfer the complete entry data into DIAMOND. Here, the interesting framework structure can be visualized e.g. using polyhedra (Fig. 18).

You can also export one or more entries[11] into cif-file(s), e.g. in order to use the crystal structure data in a Rietveld refinement. In order to do so, please make sure that the corresponding entries are marked in the Results list, then select the "Entry data (CIF)" command from the "File/Export" submenu.

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[9] A demonstration version of this program can be installed from the Match! installation DVD.

[10] The full version of the Diamond software is available from Crystal Impact, http://www.crystalimpact.com/diamond

[11] If you are using a PDF database as reference, you can export up to five PDF entries, otherwise the number of exported entries is unlimited.
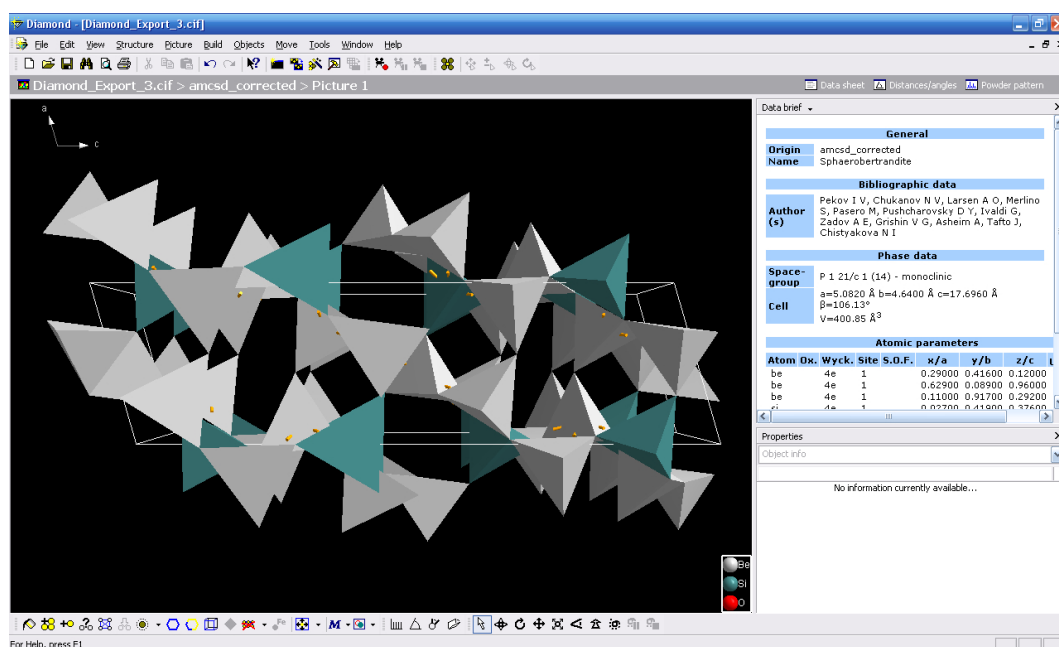
Fig. 18: The framework structure of the entry resulting from the database retrieval is visualized in DIAMOND using polyhedra.

Advanced Phase Identification

At this stage you already have got some practice, so we will come to a realistic example.

This example has been taken from the "Search-Match Round Robin - 2002", organized by J.-M. Le Meins, L.M.D. Cranswick and A. Le Bail in summer 2002[12]. We assume that the round-robin has already reached its second step: The elements present in the samples have been revealed. In the following, we will focus on the sample containing the elements Ca, Fe, Al, P, Si, O, C and H.

Please start MATCH! if it is not already running; otherwise open a new document by selecting the "New" command from the "File" menu (or pressing the corresponding toolbar button).

Once MATCH! is displaying the empty new document, you have to import the diffraction data. Please click on the appropriate toolbar button, then select the file "advanced_example.dat" in the "Tutorial" subdirectory of the MATCH! program directory and click "Open". Since this file does not contain the wavelength used in the diffraction experiment, the "Experimental Details" dialog will be displayed, in order to let you select the wavelength. Please accept the default wavelength 1.541874 Å (Cu Kα) by clicking "OK". MATCH! will now display the diffraction data (Fig. 19).
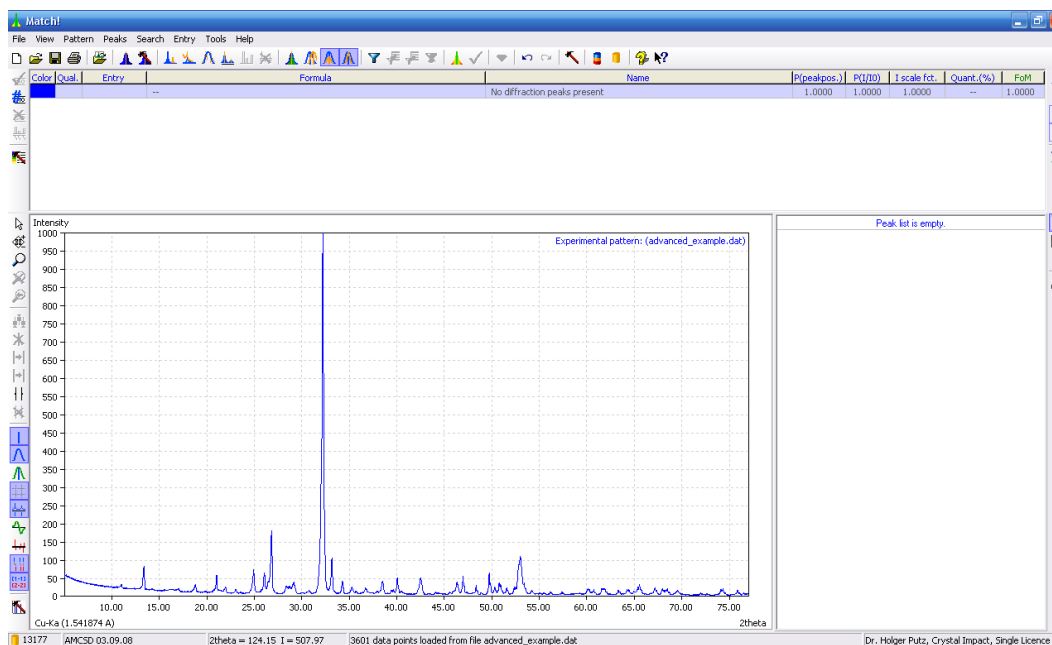
Fig. 19: MATCH! displaying the diffraction data from the "Search-Match Round Robin".

Unlike the first session, there is now additional information available about the sample: The elements present in the unknown sample are given to be Ca, Fe, Al, P, Si, O, C and H. We should use this information right away in the search-match operation. As has already been mentioned in the previous session, information restrainting the set of possible candidate entries is entered in the "Restraints" dialog. Please open it either by clicking on the corresponding toolbar button (in the main toolbar at the top), by pressing "Ctrl+R" on your keyboard, or by selecting the command "Restraints" from the "Search" menu.

Similar to the previous session, the chemical composition (in our case the elements present in the sample) is entered on the first tabsheet. Think a little bit about the details of the "composition" restraint: The elements given may be present, however, they do not necessarily have to be present all together in a single compound. All other elements of the periodic table must not be present according to the round-robin information.

This information now has to be entered on the first page of the restraints dialog; we will give here a short repetition of the usage of the periodic table: For each element you can define four states, presented as colors:

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[12]http://sdpd.univ-lemans.fr/smrr

green "All" elements with background in green have to be present in each resulting entry.

blue "Any" (at least one) of the elements with blue background has to be present in each resulting entry.

yellow The presence of elements with yellow background is "Optional". They may be present, but do not necessarily have to.

red "None" of the elements marked in red may be present, or, in other words, entries in which at least one of these elements is present are excluded from the resulting answer set.

By default, all elements are marked as "optional" (yellow). Since we have only relatively few elements which may be present at all, we will in the first step switch all elements to "None" (red) and change the state of our elements afterwards. Please press the "Toggle" button in the lower center of the dialog; all elements will be switched to "None" (red) (Fig. 20).
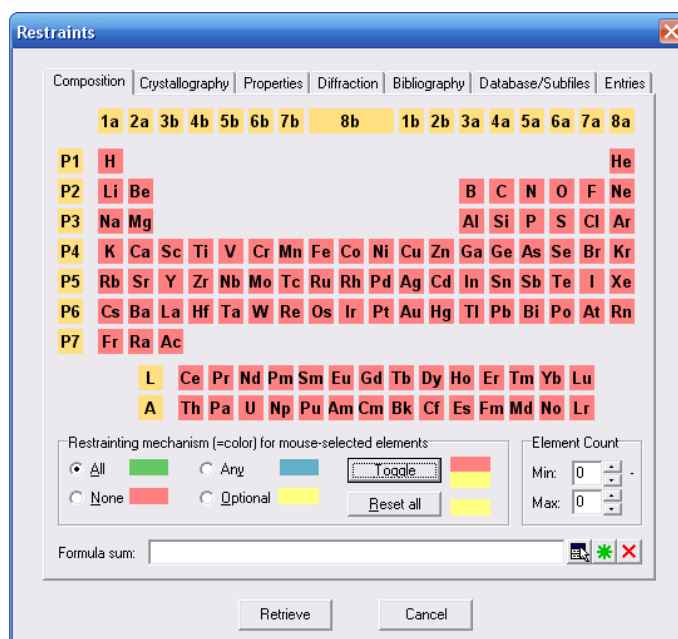
Fig. 20: The states of all elements have been switched to "None" (red background). None of these elements can be present in the resulting entries.

Now you have to change the status of the elements that are supposed to be present in the unknown sample. The elements that have been mentioned may be present optionally, so please mark the "Optional" (yellow) setting as "Restrainting mechanism", then click on the elements Ca, Fe, Al, P, Si, O, C and H. Your dialog should now look similar to Fig. 21.

All information you have about the unknown sample has now been entered, so please start the database retrieval by clicking "Retrieve" at the bottom of the dialog. A message window will be displayed indicating the number of entries that will result from the application of the restraints (Fig. 22).

Unlike the previous session, you now would like to use the resulting entries as restraints for the upcoming search-match run, so please mark the second option under "What would you like to do with these entries?" (Fig. 22). Afterwards, please accept the new answer set by clicking "Accept". MATCH! will display a progress windows while the new entries are loaded. Afterwards, the restraints buffer contains the list of entries matching your restraints. You should note the funnel/filter symbol which has appeared in the left corner of the status bar: The restraints buffer now contains 1369 entries; all subsequent search-match operations will consider only these entries and no longer the full reference pattern database (at least not until you perform a new retrieval or execute the "Clear Restraints" command from the "Search" menu).

There is one additional point you should note before starting the search-match operation:
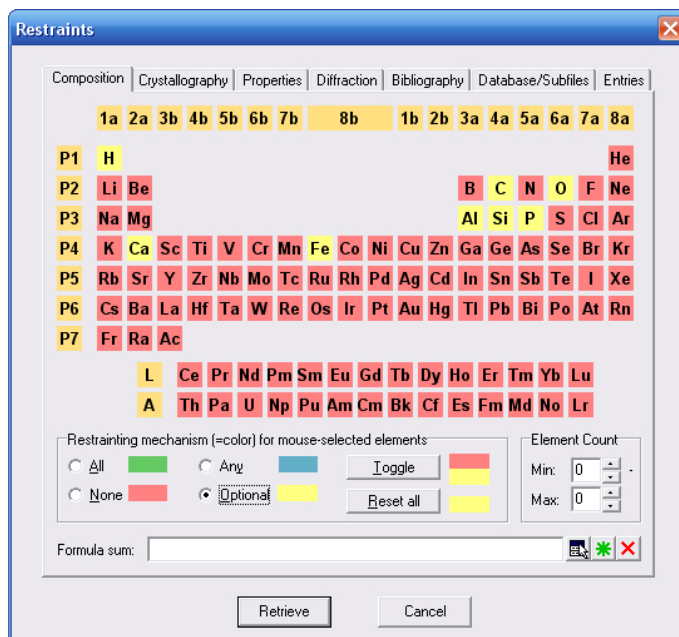
Fig. 21: You have finished entering the restraints for this example: The elements Ca, Fe, Al, P, Si, O, C and H may be present optionally in the resulting entries, the remaining elements are forbidden.
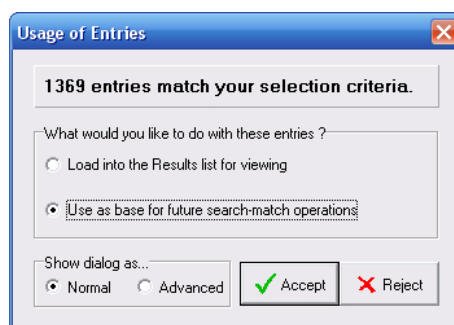
Fig. 22: This message window indicates that 1369 entries will result from the application of the restraints you have entered. The resulting entries will be used as base for future search-match operations.

Some of the peaks look rather broad, so it is probably a good idea to apply **profile fitting** for the determination of the peak parameters, instead of the default normal peak searching algorithm. You can select the method used for peak searching in the "Automatic Raw Data Processing Options" dialog (Fig. 23).

Using this dialog (which can be opened either from the "Pattern/Automatic" submenu, by pressing the key combination "Ctrl+Alt+A", or from the "Automatic"page of the "Tools/Options" menu) you can define which operations shall be carried out when the command "Automatic raw data processing" is executed. We will switch the peak searching from the default "normal" algorithm to "profile fitting" in order to obtain intensity values of higher precision. You could also switch the 2theta error correction from "zero point" to "specimen displacement", or even disable whole steps like "raw data smoothing" or "error correction".

For this tutorial session, we will modify the method for peak searching: Please open the dialog e.g. by selecting the "Configure..."command from the "Pattern/Automatic"submenu, then mark "Profile fitting" as the "Peak Searching Method" (instead of "Normal" which is the default (factory) setting).

i   Please note that marking "Profile fitting" as the "Peak Searching Method" will also mark the checkbox for "Background subtraction" automatically (and vice versa). The background is that our experiences show that using this option is adventageous for peak searching by profile fitting, while it may lead to a loss of information when using the normal peak searching.
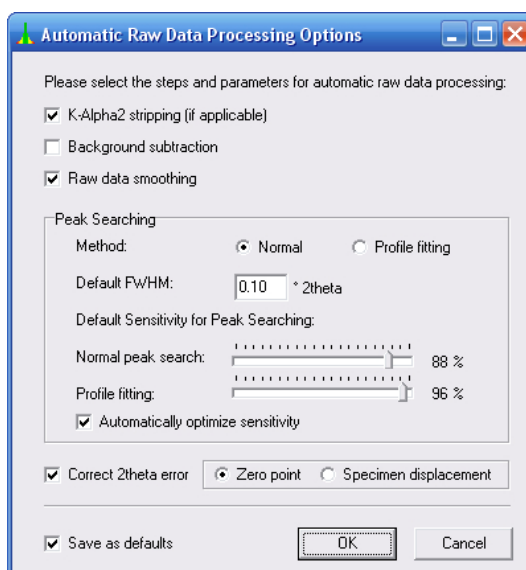
Fig. 23: In this dialog you can precisely define what MATCH! shall do when the command "Automatic raw data processing" (Ctrl+A) is called.

Afterwards, please uncheck (deactivate) the "Save as defaults" option at the bottom of the dialog, since we currently would like to use the profile fitting only for this session. Please compare your dialog to Fig. 24 and close it afterwards by pressing "OK".
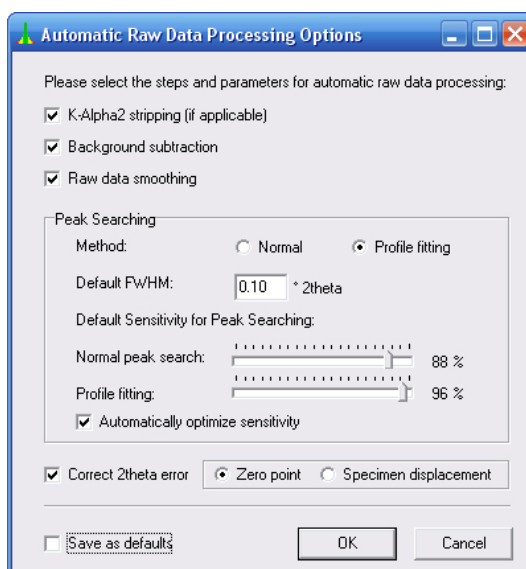
Fig. 24: We would like to use the more powerful (but a little bit more time-consuming) profile fitting for peak searching.

It is now time to perform the actual search-match process based on the entries resulting from the restraining operation. Similar to the previous sessions, you will let Match! perform the raw data processing automatically (using the profile fitting according to your recent selection). Please press the "Search-Match" toolbar button (or select the "Search-Match" command from the "Search" menu). After a few seconds, the result will be displayed; your screen should look similar to Fig. 25.

The first line in the Results list corresponding to the best-matching entry has already been marked automatically, so you can compare the diffraction pattern to the one of the unknown sample straight away. The agreement looks rather promising, you should select this entry/phase as "matching". In order to do so, simply press the space bar on your keyboard (alternatively, you can also double-click on the corresponding line in the Results list). As a result, the entry for the phase "Apatite" ($Ca_5P_3O_{13}H$) has been selected as a matching phase; all entries belonging to the same phase have
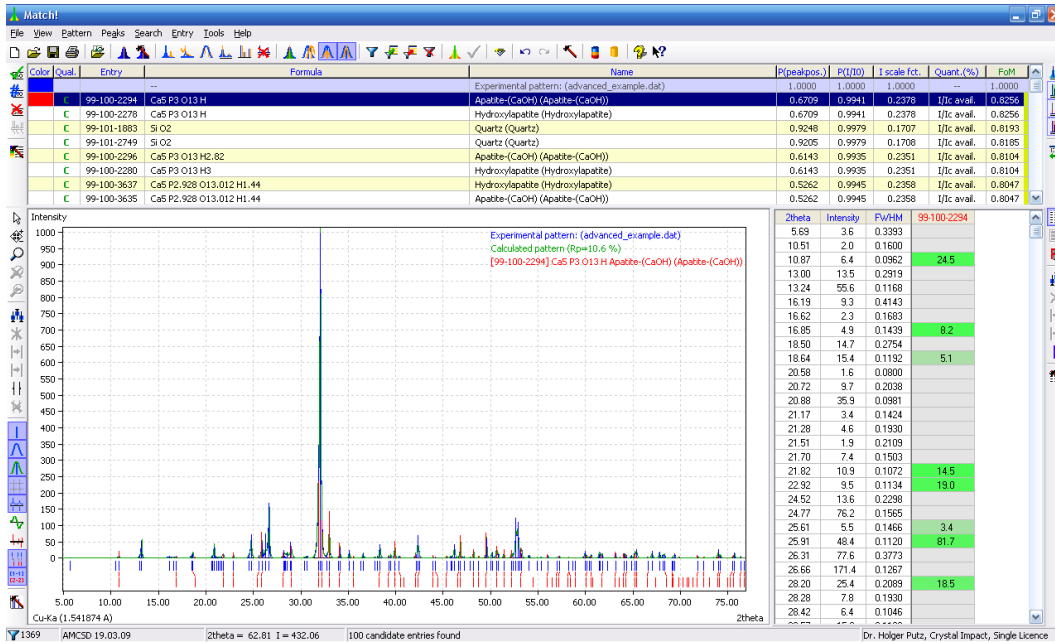
Fig. 25: The result of the search-match operation based on the entries resulting from the restrainting is displayed.

vanished (Fig. 26).
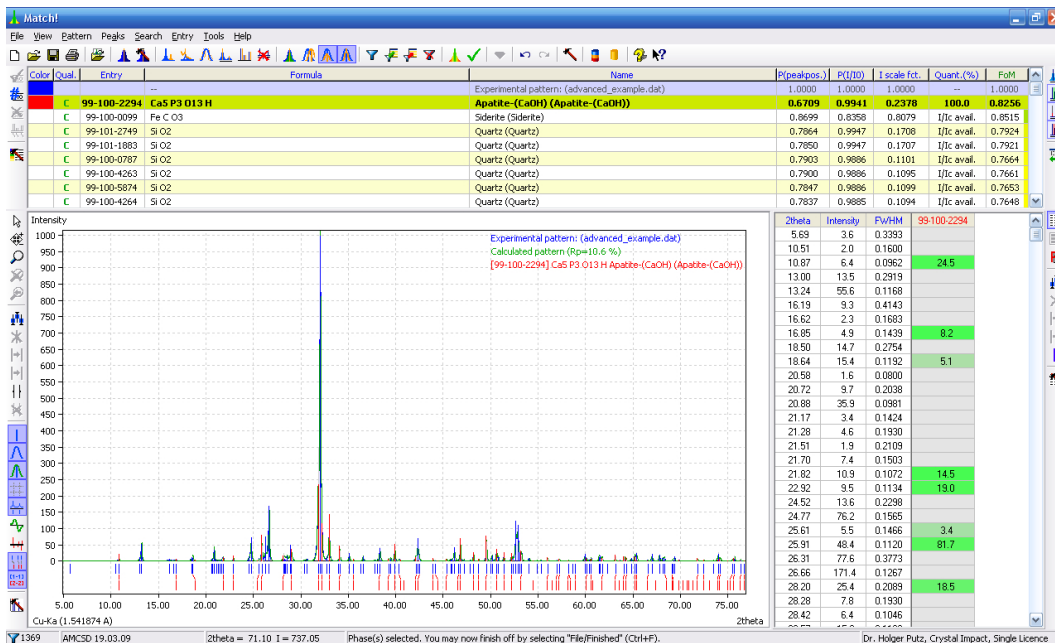
Fig. 26: The first phase (Apatite) has been selected as "matching".

Move the "cursor line" in the Results list down on step by pressing the "cursor down" button on your keyboard. The second-best matching phase is "Siderite" ($FeCO_3$), so please select this entry as well by pressing the space bar again (or by double-clicking on the corresponding line). The remaining entries belong to the phase "Quartz" (SiO_2), so please move the "cursor line" down again (press the "cursor down" button on your keyboard), and press the space bar (or double-click on the corresponding line) to select the "Quartz" phase as "matching" as well. Afterwards, no more candidate entries (not selected entries) are left; the phase identification has been finished (Fig. 27).

Please note that you have automatically also performed a semi-quantitative analysis by selecting the matching phases: The sample contains about 51% Siderite (weight-percentage), 39% Hydroxylapatite and 10% Quartz, as you can see in the "Quant." column close to the right-hand side of the
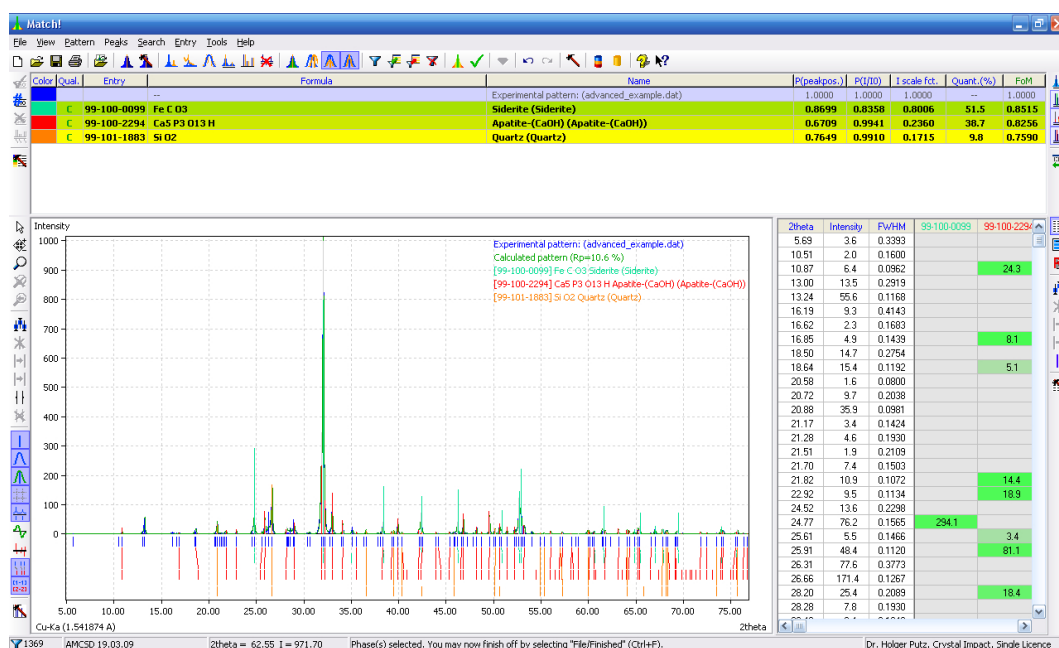
Fig. 27: Three matching phases have been identified to be present in the sample from the search-match round robin.

Results list.

Let us demonstrate one more important feature of Match! before we close this session: Before you decide if a Results list entry with a promising figure-of-merit (FoM) should be selected as "matching", it is generally advisable to carefully inspect the agreement between sample and reference diffraction pattern visually. For this, you can use MATCH!'s zoom and tracking features. Please activate the "Zoom" mode by clicking on the "Zoom" button (the magnifying glass) in the toolbar to the left of the diffraction pattern. Afterwards, move the mouse inside the diffraction pattern to the left border of the region you would like to zoom. Press the left mouse button and keep it pressed while moving the mouse to the right border, and finally release the button. MATCH! will zoom into the corresponding region, automatically adjusting the intensity axis so that the highest peak reaches to the top of the diffraction pattern pane (Fig. 28).
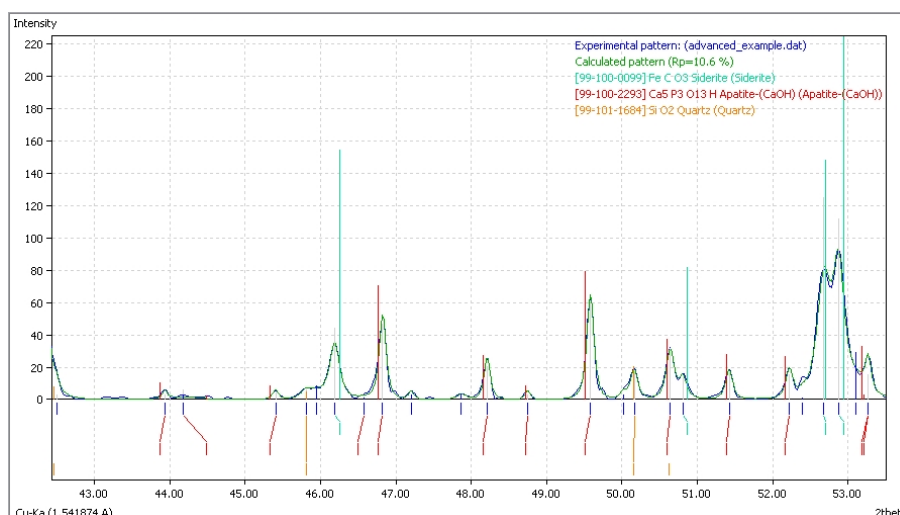
Fig. 28: After having zoomed into the diffraction pattern, you can easily check the agreement between sample and reference pattern.

You should also inspect other regions of the pattern for missing peaks. This can easily be done by using MATCH!'s zoom/track functionality. Please click on the "Zoom/Track" button in the toolbar to the left of the diffraction pattern. The mouse cursor inside the diffraction pattern will change.

You can now simultaneously zoom into interesting parts of the pattern as well as scroll through the pattern: If you move the mouse up and down while keeping the left mouse button pressed inside the diffraction pattern, MATCH! will zoom into (mouse up) or out (mouse down) of the region around the center of the pattern image. If you move the mouse to the left or right while keeping the left button pressed, you can scroll through the diffraction pattern to the left or right.

Please go ahead and try! Scroll through the entire pattern, focusing on interesting parts (e.g. where you suspect a missing peak), and zoom out on parts where there are no interesting details in order to scroll more quickly.

i If you would like to edit the peaks during your investigation, you can do so. Please read the corresponding chapters "Peak editing (diffraction pattern)" and "Peak editing (Peak List)" in the online help.

When you have finished inspecting the diffraction pattern, you can leave the "Zoom/Track" mode by clicking on the "Default" button in the toolbar to the left of the diffraction pattern. You should perhaps also restore the default viewing of the complete pattern by clicking on the "Zoom out" button in the left toolbar.

At this point, you have finished this tutorial session. If you like, you can now either open and print the report directly (menu "View/Report" or "File/Print..."), or open the "Finished" dialog and set the corresponding options similar to the first session.

Nevertheless, we should mention that there are small amounts of at least one more phase (Gormanite, Cu_2FeGeS_4) present in the sample which have not been identified in this session. There are two reasons for this:

For one, this phase is not present in the AMCSD reference database, so the application of a ICDD PDF reference database (in which this phase is contained) would have been necessary to detect this phase.

Besides this, a more detailed analysis of the diffraction pattern than we can describe in a tutorial session would have been required, since the amount of Gormanite in the sample is rather small.

Automatic Phase Identification

This tutorial demonstrates how all phase identification steps can be automated using MATCH!, making routine phase identifications from powder data much easier.

Generally, it is quite difficult to automate phase identification from powder diffraction data due to the crucial step "selection of matching entries from the list of candidates". As has already been mentioned, this selection requires some human experience in most "real-life" cases which can't easily be transferred to a computer program. However, in some specific situations a simple algorithm called "stair criterion" can be applied for the automatic selection of matching candidates.

i The stair algorithm works as follows: Starting with the entry revealing the highest figure-of-merit (FoM) value, MATCH! analyzes the differences between the FoM values of subsequent entries. If the difference between two entries is significantly higher than the average of the previous differences (the so-called "stair"), MATCH! assumes that all entries down to this FoM value are present in the sample.

Of course, this works only for really simple cases where only one or two dominant phases are present. Hence, this facility is only appropriate for simple cases and some routine applications.

There are two issues which help to apply the algorithm:

- The sample contains only one or two phases.

- The quality of the diffraction data is rather good.

If these assumptions apply to your "problem", MATCH! is able to perform a complete automatic phase identification which might proceed as follows: Immediately after you have imported the diffraction data file, MATCH! automatically processes the raw data, performs the search-match calculation, and selects the matching entries.

In order to setup the initial automatic steps it is necessary to first prepare MATCH! for the task and import the actual diffraction pattern of the phase to be identified later on (unlike the previous tutorial sessions). Please perform the following steps:

Please start MATCH!, or open a new document by selecting the "New" command from the "File" menu (or pressing the corresponding toolbar button). Afterwards, open the "Options" dialog either by using the corresponding command from the "Tools" menu, or by clicking on the button in the main toolbar at the top. Finally, select the "Automatic" page by clicking on the corresponding tabsheet header at the top (Fig. 29).

On this page of the dialog you can define which tasks or operations shall be carried out automatically under certain conditions. For example, you can let MATCH! process the raw diffraction data automatically once they have been imported. Automatic operations of this kind are quite useful for certain applications in which some steps do not need to be attended or executed by the user explicitly.

Please disable the "Save as defaults" box in the corner on the lower left-hand side of the dialog, so that the automatic processing you will define only applies to the current document/session. This option can be useful if you would like to setup MATCH! for your routine tasks; however, there is little sense in activating it while you are still learning how to use MATCH!.

Let's now have a look at the individual processing options which may be selected: MATCH! can automatically open the "Import Diffraction Pattern" dialog when MATCH! is executed[13]. This may be quite useful if you are using MATCH! in a routine phase identification procedure, however, we will not use this option here.

The next option lets MATCH! process the raw data automatically directly after they have been imported. There are several individual operations involved, so the corresponding options and parameters are adjusted in a separate dialog which can be opened by pressing the "Configure..." button. Please click this button now in order to open the "Automatic Raw Data Processing Options" dialog (Fig. 30).

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[13]Of course, this option is only of use if the "Save as defaults" checkbox at the bottom of the dialog is also marked.
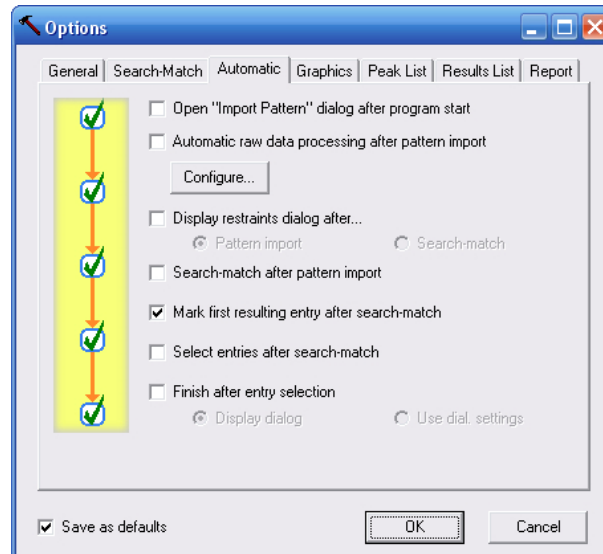
Fig. 29: On the "Automatic" page of the options dialog you can define which tasks shall be performed by MATCH! automatically in certain conditions. Note that the steps performed during the automatic raw data processing are adjusted in a separate dialog which can be opened by pressing the "Configure..." button.
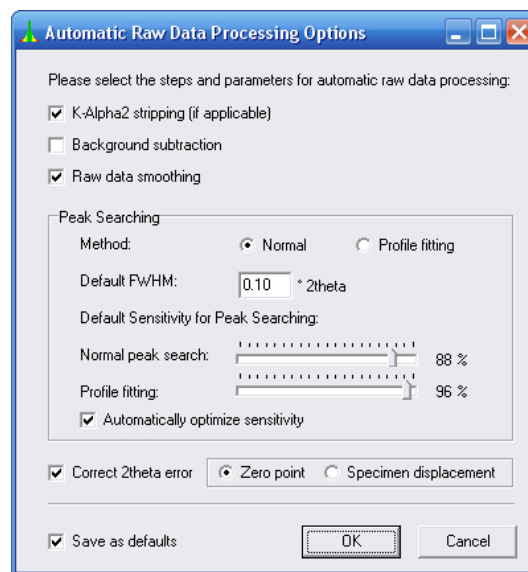

Fig. 30: In this dialog you can precisely define what MATCH! shall do when the command "Automatic raw data processing" (Ctrl+A) is called.

Using this dialog (which can also be opened either from the "Pattern/Automatic" submenu or by pressing the key combination "Ctrl+Alt+A") you can define which operations shall be carried out when the command "Automatic raw data processing" is executed. For example, you could switch the peak searching from the default "normal" algorithm to "profile fitting" in order to obtain intensity values of higher precision, or switch the 2theta error correction from "zero point" to "specimen displacement".

For this tutorial session, we will apply a single change so that the automatic raw data processing uses profile fitting for peak searching; Please mark "Profile fitting" as the "Peak Searching Method" (which will also mark the checkbox for "Background subtraction" automatically, as we have already mentioned). Please compare your dialog to Fig. 31 and close it afterwards by pressing "OK".

Being back on the "Automatic" page of the "Options" dialog, please mark the checkbox in front of "Automatic raw data processing after pattern import".
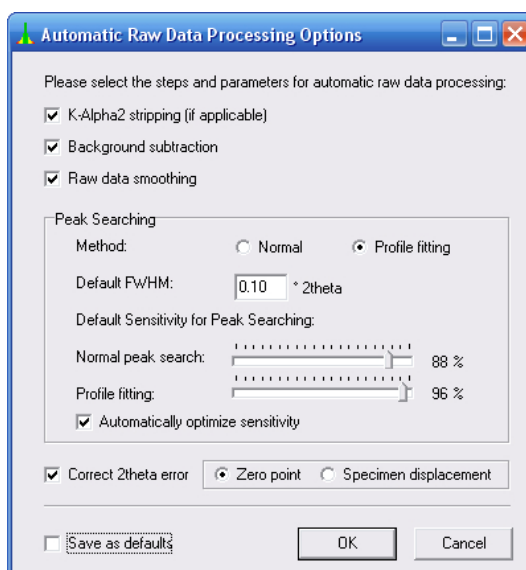
Fig. 31: We would like to use the more powerful (but a little bit more time-consuming) profile fitting for peak searching. Besides this, we would like MATCH! to optimize the peak searching sensitivity automatically.

The next operation which may be selected to be carried out automatically is to display the Restraints dialog (either after the pattern import or search-match), in case you would like to enter some additional restraints which may reduce the number of candidate entries. We will not use this feature at the moment, so please leave the corresponding checkbox empty.

In contrast to this, we certainly would like MATCH! to automatically perform a search-match calculation, and to select the matching phases afterwards, so please mark the corresponding next two options. Finally, you may let MATCH! open or use the settings of the "Finished" dialog you have seen at end of the first tutorial session. We will not do so at the moment.

Please make sure that your dialog page looks like Fig. 32; afterwards, close the dialog by pressing "OK".
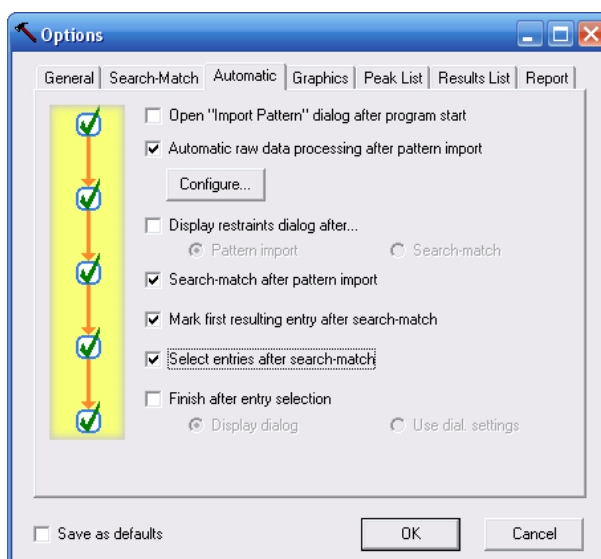
Fig. 32: These option settings will lead to a fully automatic phase identification once you have imported an experimental diffraction pattern.

MATCH! is now prepared for automatic phase identification, so let's try it:

The only thing you actually have to do is import the diffraction pattern[14], so please click the corresponding toolbar button. Please select the file "automatic.raw" from the "Tutorial" folder[15] and click "Open". That's it !

All remaining steps will be carried out by MATCH! automatically: You can see that the search-match will start right away once the raw data have been processed automatically. Afterwards, MATCH! will automatically select the matching phases according to the "stair criterion" (Fig. 33).
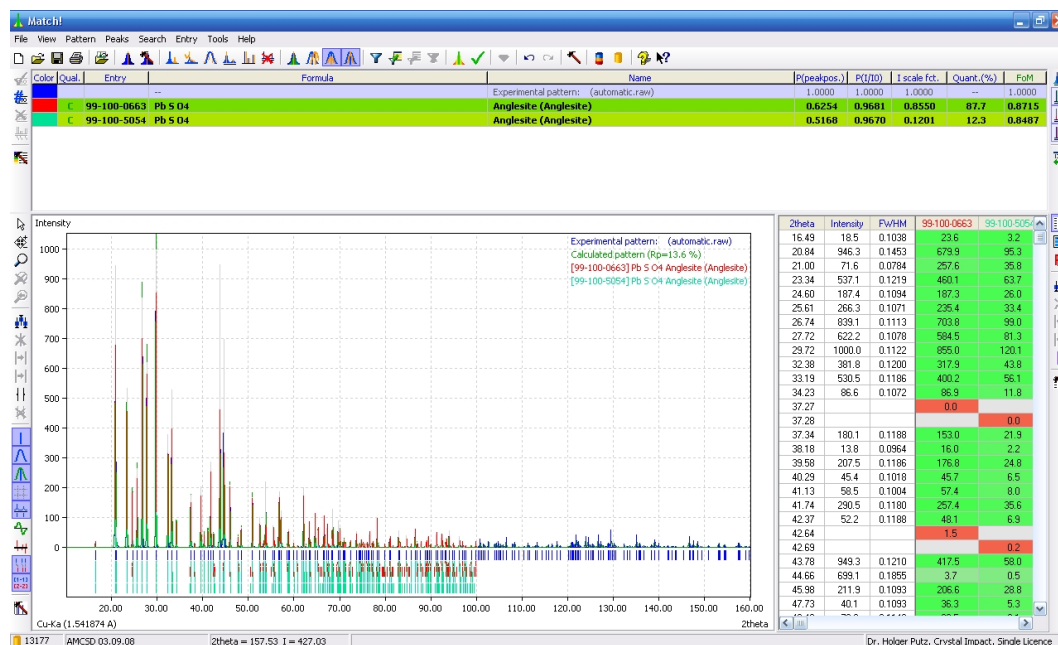
Fig. 33: MATCH! has automatically identified the sample as PbSO₄ (Anglesite).

As can clearly be seen from the two entries in the Results list which have been selected as "matching", the "unknown" sample is PbSO₄ (Anglesite).

Congratulations! You have finished the tutorial sessions and learned about the most important functions and features of Match!. Of course, not all functions could be included in the tutorials, so there is still a lot to discover while processing your own diffraction patterns. If you have questions or are looking for a certain functionality, we strongly recommend to have a look at the online help!

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[14]Note that you can also do the pattern import "automatically", by starting MATCH! from the command line and giving the file name of the diffraction pattern as a parameter; cf. p. 59.

[15]The "Tutorial" folder is placed in your MATCH! program directory, e.g. "C:\Program Files\Match!\Tutorial".

Reference Pattern Database

Overview

As has already been mentioned in the introduction to this manual, 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** called **"IUCr/COD/AMCSD"** is by default installed automatically along with MATCH![16]; it can be used straight away after the installation. This reference database contains powder diffraction patterns calculated from crystal structure data provided by the IUCr journals[17], taken from the "Crystallography Open Database" (COD[18]) and from the "American Mineralogist Crystal Structure Database" (AMCSD[19]).

  In this context, we would like to thank Pete Strickland (IUCr), Armel Le Bail (COD) and Bob Downs (AMCSD) for their kind permission to download and distribute their data free-of-charge!

  All entries of the "IUCr/COD/AMCSD" 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 (p. 6).

  You can download additional or updated reference databases free-of-charge from

  http://www.crystalimpact.com/match/download.htm#refdb

- You can use a **previous ICSD/Retrieve version (release 1993-2002)** that you might have available[20]. Match! can import the ICSD/Retrieve entries into a normal Match! user database and calculate reference powder diffraction patterns in a single step (p. 39).

- The classical reference pattern database is the so-called **"PDF" database** provided by ICDD[21]. 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 IUCr/COD/AMCSD 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. 38).

We have run several tests in order to evaluate the quality of the various reference databases mentioned above:

Compared to using the classical ICDD PDF database, our tests reveal a somewhat diverse performace when using the free-of-charge IUCr/COD/AMCSD reference patterns: When mineral samples were investigated, the results were generally very good, thanks to the excellent coverage of the AMCSD. Even for many samples other than minerals, the correct phases were identified in most cases,

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[16]If you are using the normal MATCH! demoversion, only data from the AMCSD are installed. You can e.g. download and install the full IUCr/COD/AMCSD database from the MATCH! web page, or from a Crystal Impact DVD distributed at various meetings, e.g. the ECM- or IUCr-conferences.

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

[18]http://sdpd.univ-lemans.fr/cod

[19]R.T. Downs, M. Hall-Wallace, "The American Mineralogist Crystal Structure Database", American Mineralogist **88**, 247-250 (2003). http://rruff.geo.arizona.edu/AMS/amcsd.php

[20]Of course, you must have a valid licence for ICSD/Retrieve! Please contact FIZ Karlsruhe (Germany) (e-mail: crysdata@fiz-karlsruhe.de) if you are in doubt whether your licence is still valid!

[21]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

however, we found some (few) samples where main phases were not recognized because the corresponding reference patterns were not present in the IUCr/COD/AMCSD reference database. In all cases, it was no problem to identify all phases when using the ICDD PDF-2 Release 2007 database.

According to our experience, it is optimal to combine the IUCr/COD/AMCSD database (which basically contains more recent entries) with a user database created from ICSD/Retrieve (which typically contains "older" entries). **Using such a combined reference database is the best solution if you do not have a recent ICDD PDF database available!**

Hence, if you are investigating mineral samples, you should be fine using the free-of-charge AMCSD or IUCr/COD/AMCSD reference database. For most other users, it is currently advisable to either add ICSD/Retrieve reference patterns to the IUCr/COD/AMCSD database, or use the conventional ICDD PDF-2 or PDF-4 database.

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 IUCr/COD/AMCSD or AMCSD), you first have to add it to the so-called "Reference Database Library". This is a table 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 (Fig. 34).
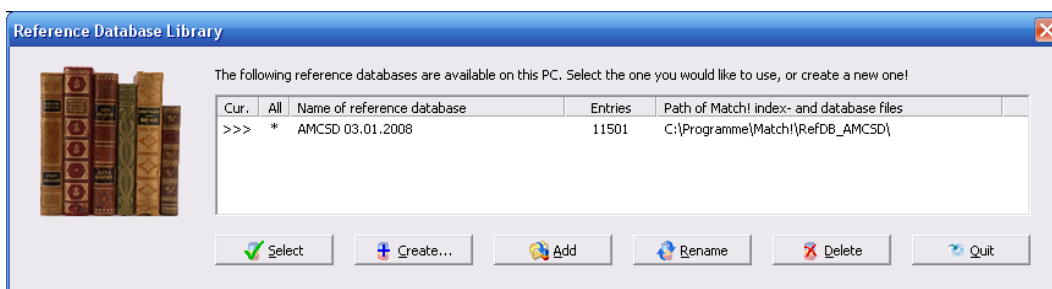
Fig. 34: Using the "Reference Database Library", you can manage the various reference pattern databases on your PC. In this case, the AMCSD database is installed for all users on this PC (column "All") and has been selected for being used in phase identification (column "Cur.").

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!

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 "Reference Database..." command from the Tools 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). In contrast to earlier versions of MATCH!, it is now perfectly possible to create a new reference database as a normal (standard) user, i.e. it is no longer 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 for all users. If a database is available to all users, this is indicated by a '*' sign in the column "All". Note that databases with this mark cannot be modified or deleted by

normal (standard) users!

You can manage your reference databases using the six 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 Results list and the Restraints buffer will be erased 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. from an existing Match! user database, or by importing entry data from cif files or the ICSD) (p. 30).

- **Add** a reference database that is stored "ready for usage" in a certain directory

- **Rename** an existing reference database

- **Delete** an existing reference database

- **Quit** the Reference Database Library.

Create a new Reference Database

MATCH! cannot use pattern sources like the PDF 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. 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. 35).

PDF-4 or PDF-2

In the following, we will demonstrate how to use 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-2 Release 2007 database (which of course already must be installed on your PC) (the procedure for using the corresponding PDF-4 is the same).

First, you 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 dialog. Afterwards, you must select which PDF database you would like to use. In our case, we would like to use the PDF-2/Release 2007, so please mark (click on) the corresponding line in the list below "ICDD PDF" now (Fig. 36).

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.

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. 37). Due to the large amount of data which have to be read and sorted[22], the creation of index files is a

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[22]The PDF-4+ Release 2007 contains more than 270,000 entries !
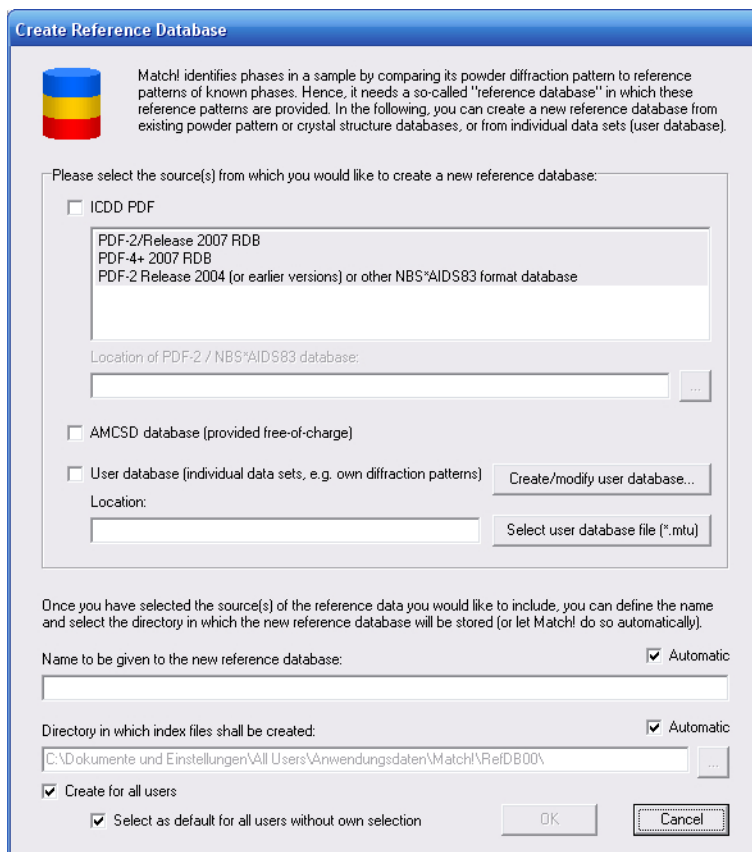
Fig. 35: Using this dialog you can create a new reference database for MATCH!.

rather time consuming process. The procedure may take between a few 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. 38).
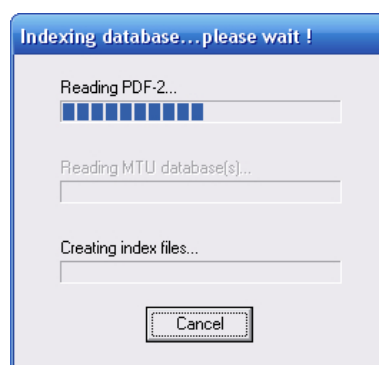
If the new reference database is the only one available in the Reference Database Library, it is selected for being used automatically. Otherwise, you have to select the new reference database manually: Simply mark (click) on the corresponding line in the table, then press "Select". The licence for the 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-2 reference database in phase identifications and database retrievals.

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

Old Format PDF-2

If you would like to use a 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. 39).

You now have to give the directory in which the PDF-2 database (to be exact: the file "pdf2.dat") is stored in the input box below "Location of PDF-2 / NBS*AIDS83 database". Normally, the corresponding dialog is opened automatically when you click on the line "PDF-2 Release 2004 (or earlier
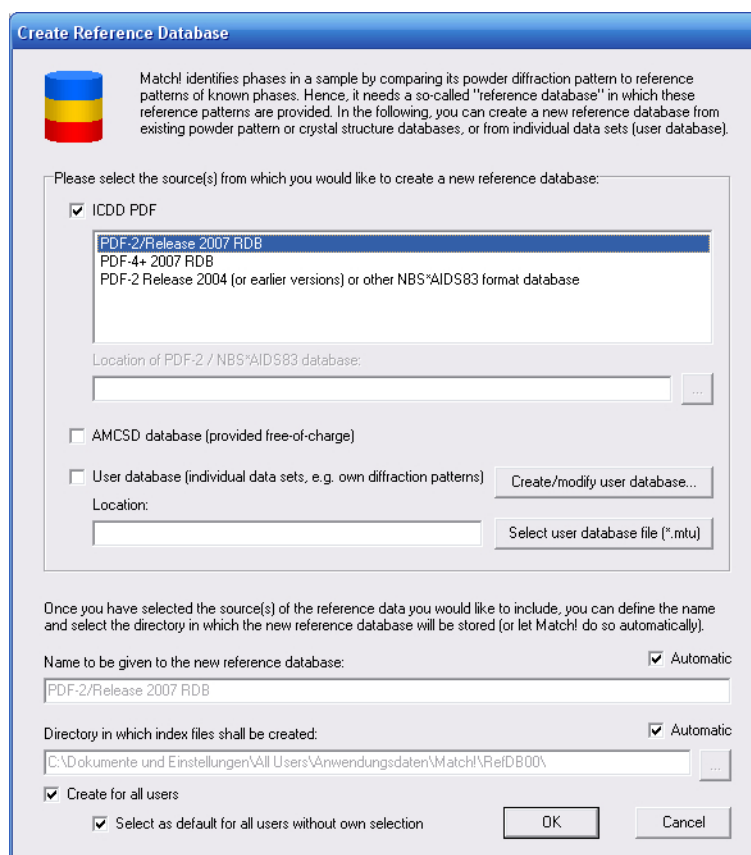
Fig. 36: You have selected to apply the ICDD PDF-2 Release 2007 database as MATCH! reference database.
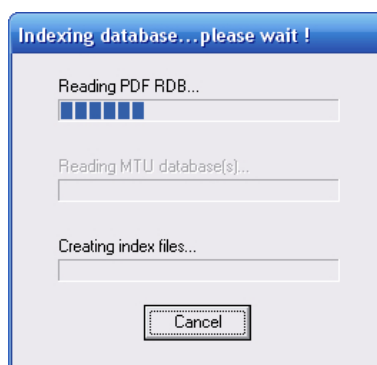
Fig. 37: This window shows the progress of the index file creation.
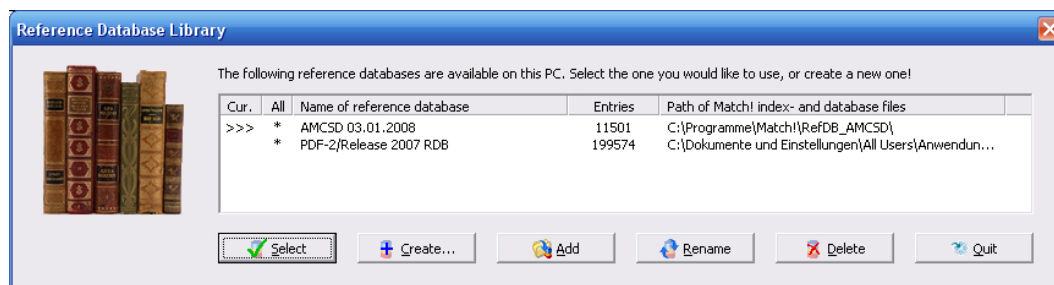
Fig. 38: The "PDF-2 Release 2007" reference database is now available in the list.

versions)". Alternatively, you can click on the "..." button to the right of this input line. This will bring up a dialog in which you can select if you would like to let MATCH! search for corresponding files on your PC automatically, or if you would like to select the file manually. Normally, the fastest
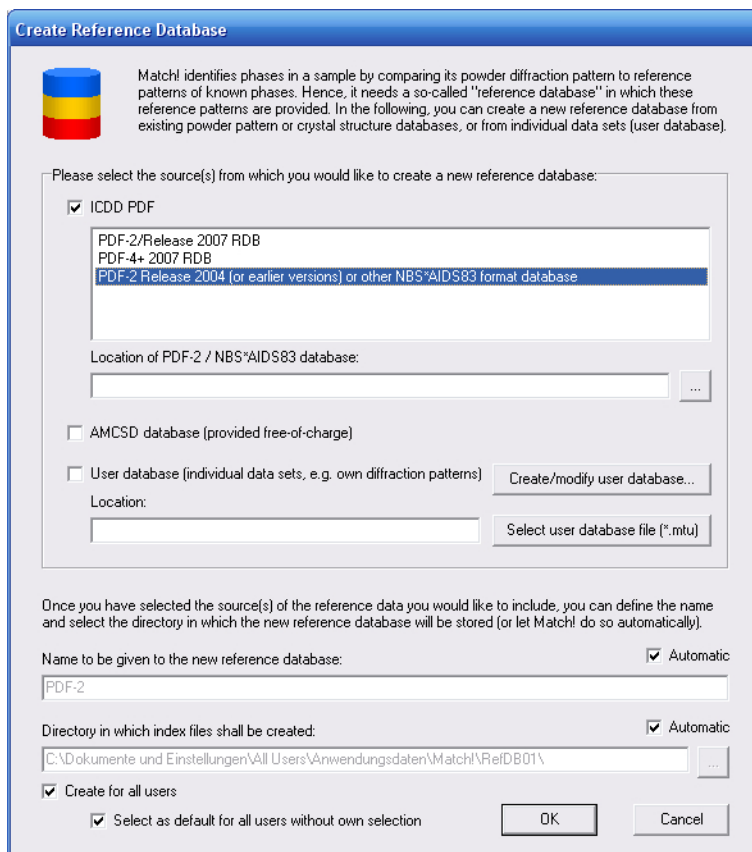
Fig. 39: You have selected to apply an ICDD PDF-2 database released before 2005 as MATCH! reference database.

method is to select the file manually (Fig. 40), so please mark the corresponding option and press "OK".
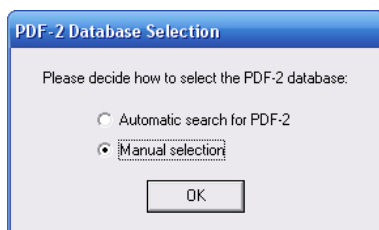
Fig. 40: You can either let MATCH! search your PC for the old-format PDF-2 database file, or you can select the file manually.

A "File Open" dialog will be displayed in which you have to select the file "pdf2.dat" in the directory where your PDF-2 database is stored. Afterwards, press "Open" to select the file/directory and return to the "Create Reference Database" dialog. The location of the PDF-2 database file will now 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 PC.

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). 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.
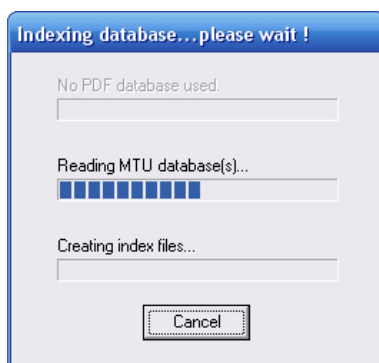

Fig. 41: This window shows the progress of the index file creation.

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 "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 PDF-2 reference database in phase identifications and database retrievals.

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[23].

If you have not already done so, please follow the instructions on p. 38 first, in order to create the mtu-file from your data. Afterwards, please return to this point and continue reading.

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. 42).

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.

i 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.

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[23]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 "Tools" menu.
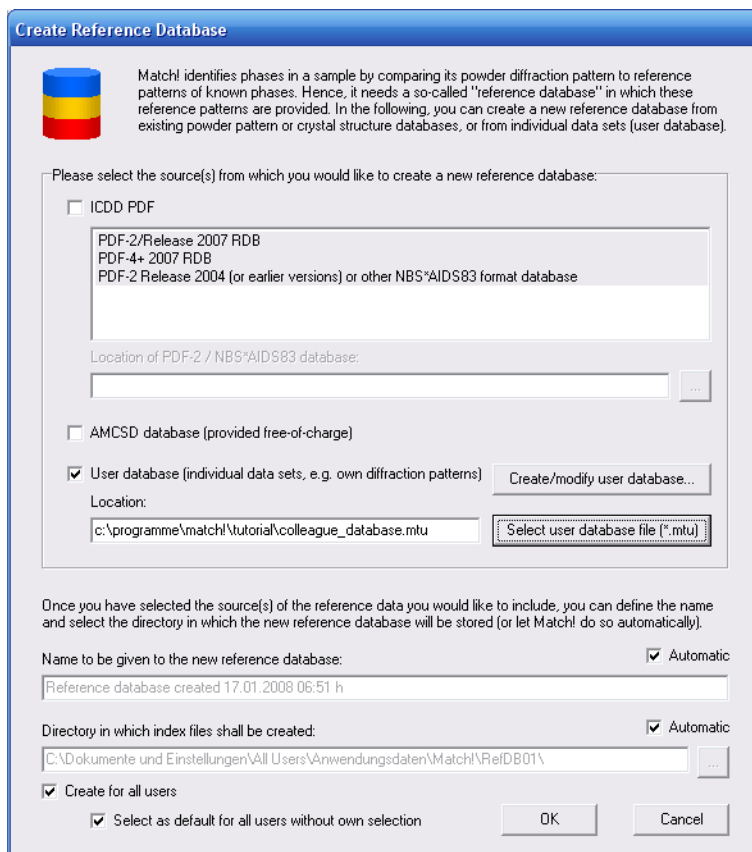
Fig. 42: The mtu-file based on which a new MATCH! reference database shall be created has been selected.

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.

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. 43). 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.

Fig. 43: 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 "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.

Select Reference Database

In order to select another existing reference database for being used in future search-match and restrainting 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 licence 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 Results list or Restraints buffer contain entries when you open the Reference Database Library, all these entries will be removed (i.e. the Results list and the Restraints buffer will be erased) 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 PC. 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 list 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), please note that you can only rename reference databases that are not marked with a '*' character in the column "All"!

- 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.

Delete Reference Database

In order to remove an existing reference database from the current PC, 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 not marked with a '*' character in the column "All"!

User Database

Overview

As has already been mentioned earlier in this manual, phase identification from powder diffraction data generally requires the availabilty of a so-called "reference pattern database". Up to now, this is the PDF database provided by ICDD in most cases. However, there are also alternative sources of reference patterns, like the IUCr/COD/AMCSD database delivered with MATCH!, the previous ICSD(Retrieve) versions, or even your own diffraction data. 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 IUCr/COD/AMCSD database can be downloaded "ready-to-use" from the Crystal Impact web page free-of-charge, the ICSD/Retrieve or your own diffraction patterns must be imported into so-called "user database entries" before they can be used with MATCH!.

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

- ICSD/Retrieve database (released 1993-2002)

- crystal structure data (typically CIF-files)

- own compounds measured on the laboratory diffractometer

- published in the literature

- your colleague's user database

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. 34). 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 pressing "Ctrl+U" on your keyboard, by selecting the command "User Database Manager" from the "Tools" menu, or by pressing the "Create/modify user database..." button in the "Create Reference Database" dialog.

The user database manager window (Fig. 44) 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 "tabsheets" in which the details of any entry marked in the entry list above are displayed and edited. You can switch between the individual tabsheets by clicking on the corresponding tabsheet header.

The first tabsheet (called "Summary") contains an extract of the database fields on the remaining tabsheets; the data can just be viewed here, but not edited. The second tabsheet "General" contains data required for the description of the phase, like formula sum, chemical name etc. On the third tabsheet "Crystal structure", crystal structure data can be entered in order to calculate the corresponding diffraction pattern on the subsequent tabsheet "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" tabsheet 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
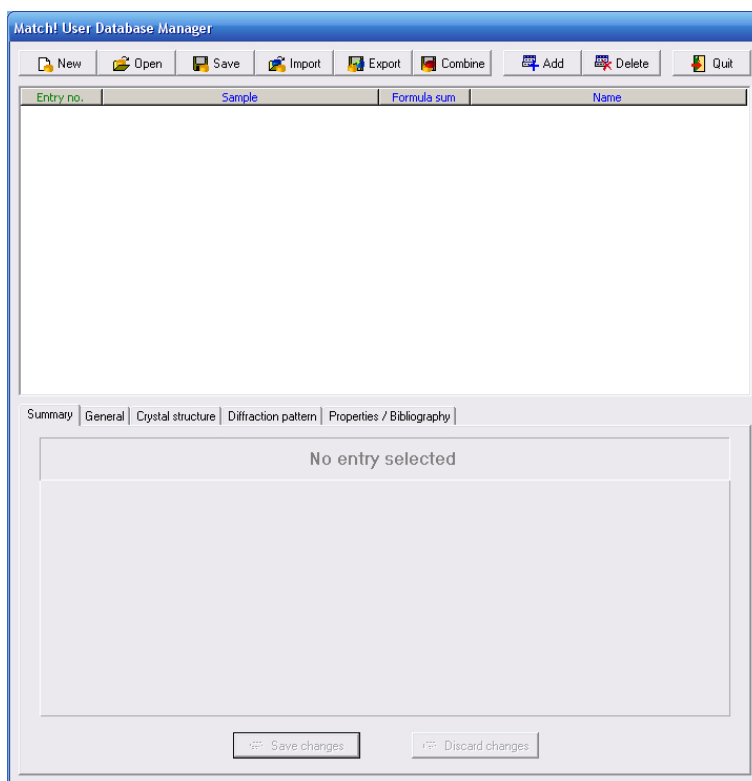
Fig. 44: The new user database is still empty.

by pressing the "Quit" button. Alternatively, you can also press the "Save" button at the top of the dialog window.

Calculate Patterns for Crystal Structures Imported from ICSD/Retrieve   If you have a valid licence[24] 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. 45).
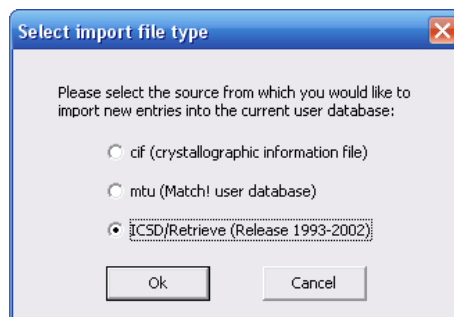
Fig. 45: In this dialog, you have to select the origin of the entry data to be imported (either CIF-files, MATCH! user database files or the ICSD).

Please mark the "ICSD/Retrieve" option as in Fig. 45, then press "OK". You now have to give

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[24]If you are in doubt whether your licence is still valid, please contact FIZ Karlsruhe (Germany) (e-mail: crysdata@fiz-karlsruhe.de).

the directory in which the ICSD/Retrieve database (to be exact: the file "ICSD.NEW") is stored. A dialog will open in which you can select if you would like to let MATCH! search for the latest corresponding file on your PC automatically, or if you would like to select the file manually. Normally, the fastest method is to select the file manually (Fig. 46), so please mark the corresponding option and press "OK".
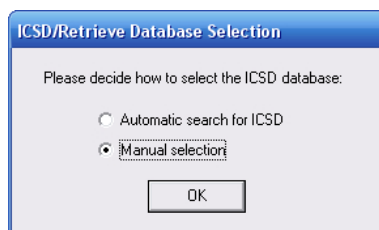
Fig. 46: You can either let MATCH! search your PC for the ICSD/Retrieve database file, or you can select the file manually.

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 licence for the ICSD/Retrieve version you are about to import (Fig. 47). The confirmation will be written to a protocol logfile.
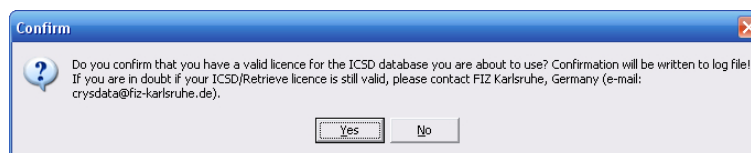
Fig. 47: Before you can use/import an ICSD/Retrieve database, you have to confirm that you have a valid licence for it.

If you have confirmed that you have a valid licence, 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 maximum 2theta angle, and the maximum number of peaks that shall be included in the database to be created (Fig. 48). Note that this is a convenient method to create a reference database for neutron diffraction data!

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 (Fig. 49).

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 occured 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 "IUCr/COD/AMCSD" reference database that is shipped along with MATCH!.
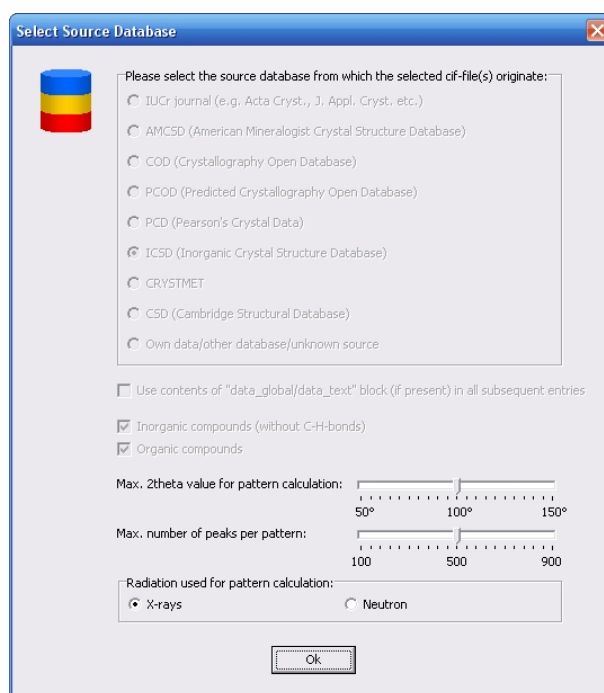
Fig. 48: There are several options that can be adjusted for the calculation of the reference powder diffraction pattern, like the radiation type and the upper 2theta limit.
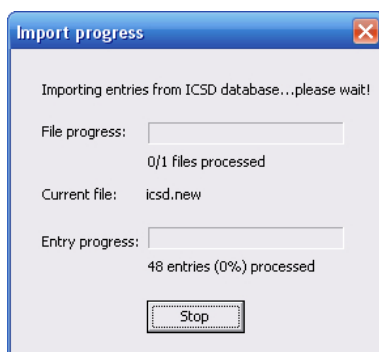
Fig. 49: The progress of the ICSD/Retrieve import is displayed in this window.

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_c 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. 50).
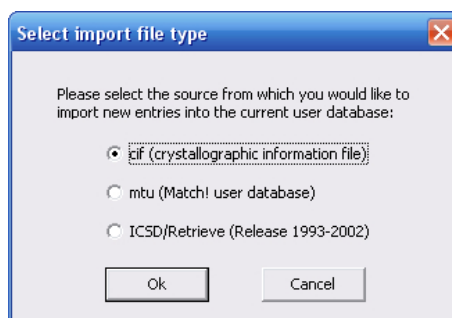
Fig. 50: In this dialog, you have to select the origin of the entry data to be imported (either CIF-files, MATCH! user database files or ICSD/Retrieve).

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[25]. Please mark the "Tutorial" subdirectory of the MATCH! program directory (Fig. 51), then press "OK".
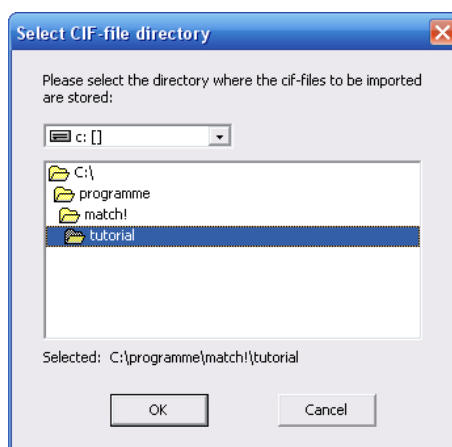
Fig. 51: Here, you have to select the directory in which the CIF-files you would like to import are stored.

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"[26], 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 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 from the AMCSD, so please mark the corresponding option (Fig. 52) and press "OK".

---

[25]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.

[26]The CIF-file has been taken from the American Mineralogist Crystal Structure Database (http://www.geo.arizona.edu/AMS/amcsd.php).
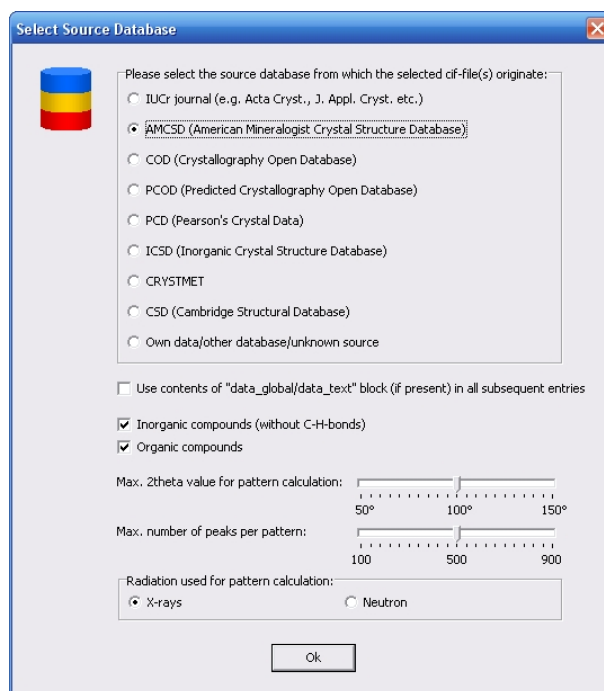
Fig. 52: The entry we would like to import has been taken from the AMCSD database.

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[27] (Fig. 53).

As has already been mentioned, it is possible to select more than a single CIF-file for being imported at a time, 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 IUCr/COD/AMCSD reference database containing more than 73,700 entries from CIF files provided by the IUCr, COD and AMCSD.

Import of Diffraction Data Another common way to add diffraction data to a MATCH! user database is the import of the corresponding peak data files. Currently, three peak data file formats are supported:

- 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:

---

[27] Of course, if the unit cell is large, the calculation of the diffraction pattern may take much longer...
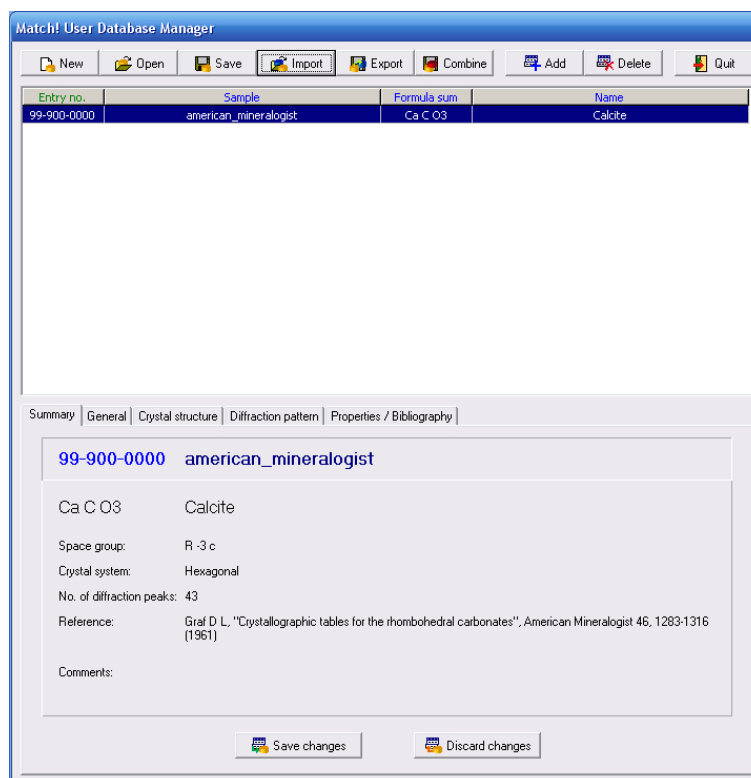
Fig. 53: The new entry "Calcite" has been imported from a CIF-file taken from the "American Mineralogist Crystal Structure Database".

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" tabsheet 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" tabsheet header in order to bring the corresponding tabsheet into front (Fig. 54).

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\Match!\Tutorial"). Finally, please press "Open". The diffraction data are now present in the "Diffraction pattern" tabsheet; they are displayed both as diffraction pattern picture as well as peak list (d-values/Intensities) in the table to the right (Fig. 55).

All that remains to do is to enter the phase information on the "General" tabsheet, so please activate this tabsheet now. As you see, the "Sample name" has already been taken from the diffraction data file[28]. Please press <Tab> to advance to the "Formula sum" input field, then enter "Ca C O3" (mind the blanks between the elements !). Afterwards, press <Tab> to advance. Enter "Calciumcarbonate" as "Chemical name", press <Tab>, 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 tabsheet. That's it ! Your diffraction data entry has been added to the user database, as can be seen from the entry list above (Fig. 56).

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.

---

[28]In fact, this is the reason why we imported the diffraction data BEFORE entering the phase description information !
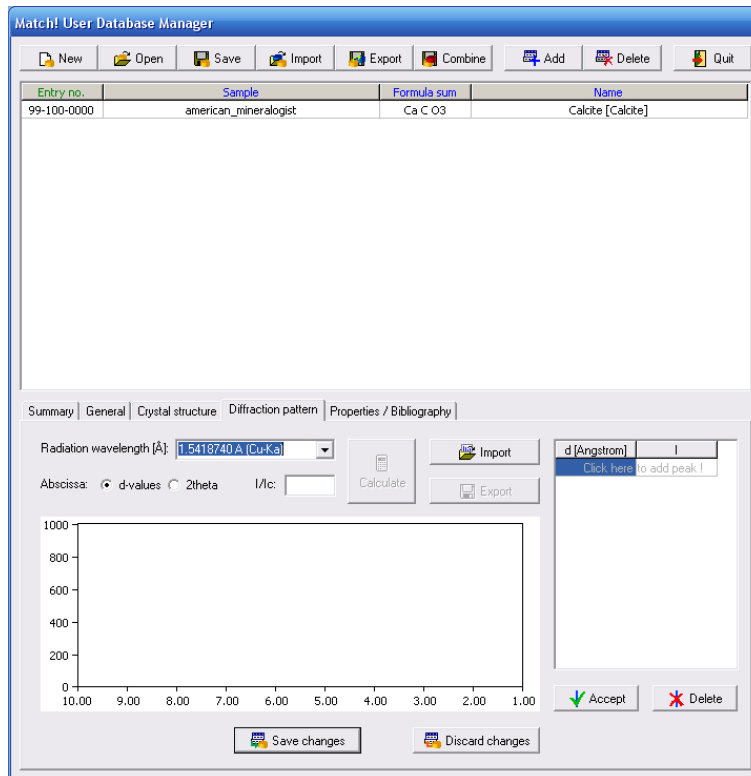
Fig. 54: The "Diffraction pattern" tabsheet is still empty.
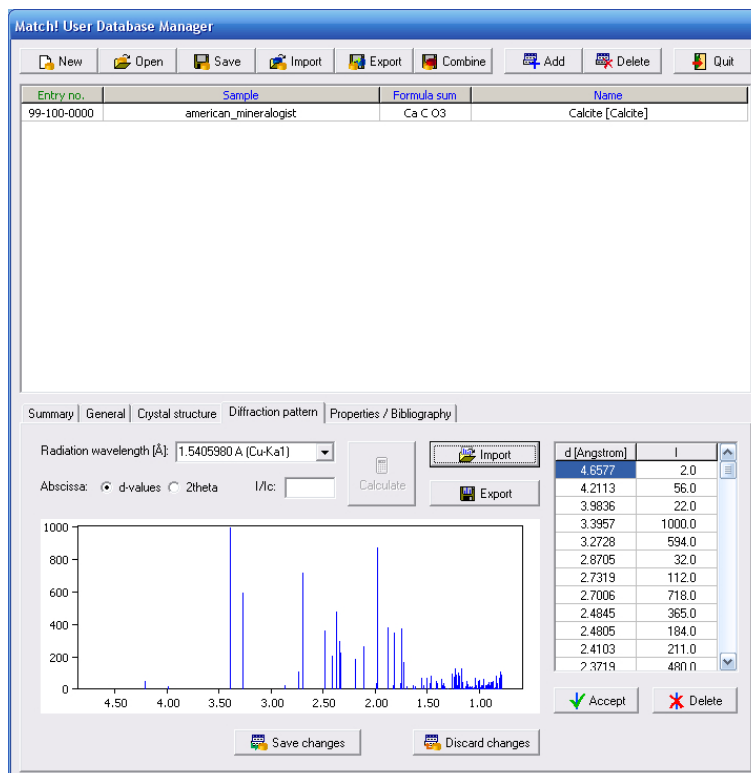
Fig. 55: Your "Aragonite" diffraction pattern has been imported from the file 'aragonite.udi'.

Here are the data extracted from a hypothetical scientific paper:

```
Title: Common Salt
```
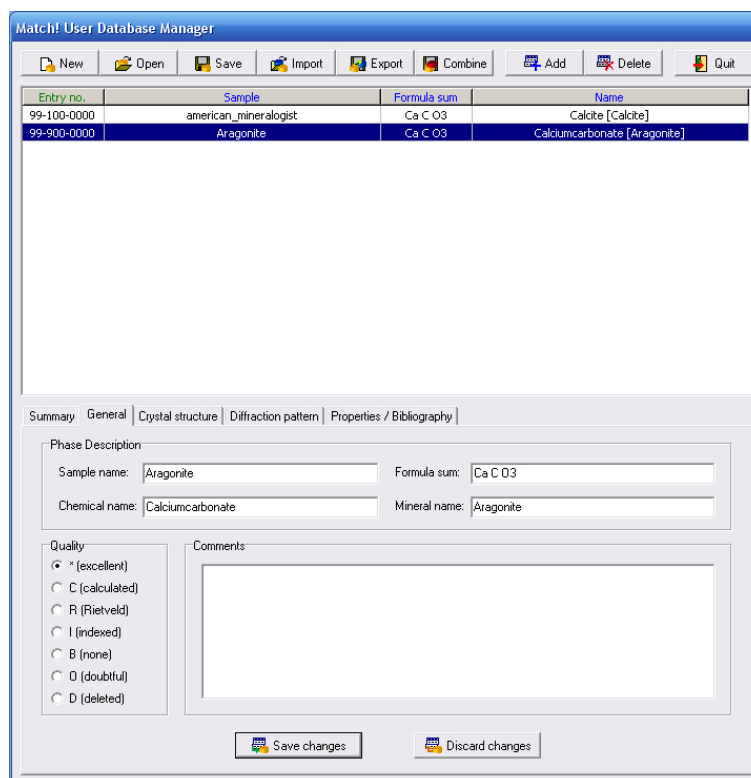
Fig. 56: Your diffraction pattern has been successfully added to the user database.

```
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 now 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 Result 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 radiobutton to the left. Your screen should now look similar to Fig. 57.

Fig. 57: The data on the "General" tabsheet have been filled in.

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 tabsheet into front. Afterwards, click on the first line in the table to the right (indicating "Click here to add peak¡‘), just below the "d [Angstrom]" header. Now enter the d-value of the first peak (3.2447), then press <Tab> to advance to the second column and enter the corresponding intensity (82.5). Finally, press <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.

Now the cursor has advanced to the "d-value" column of the second line, so you can 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. 58.

Please enter the peak data of the remaining eight peaks now in the same manner as above. When you have finished entering the data, please click on the "Accept" button below the peak table. Your screen should now look similar to Fig. 59.

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.

i 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 an IUCr journal, the entry number starts with "99-000-0000", for AMCSD entries the first entry number is "99-100-0000" etc. 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
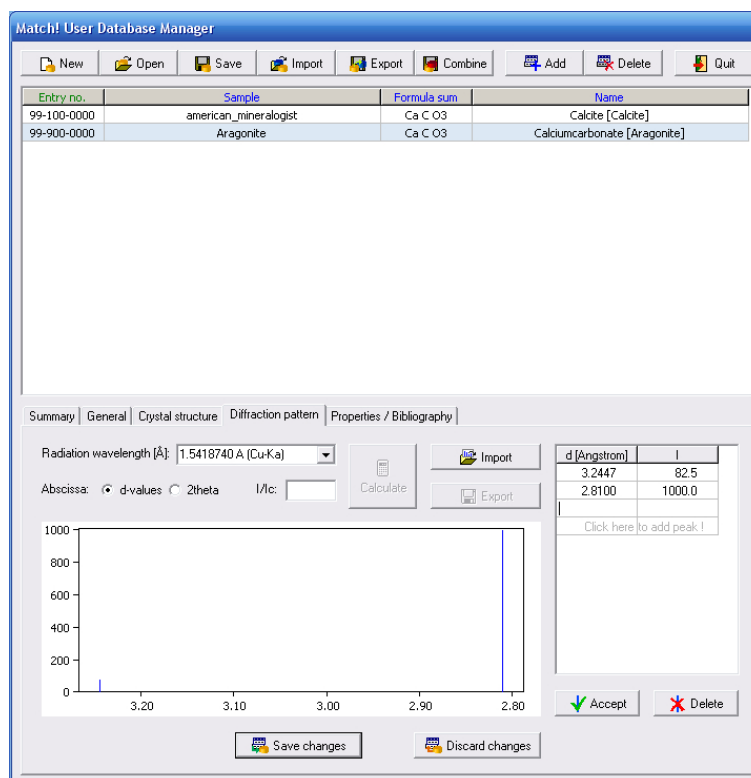
Fig. 58: The data of the first two peaks have already been entered; the User Database Manager is ready to receive the data of the third one.
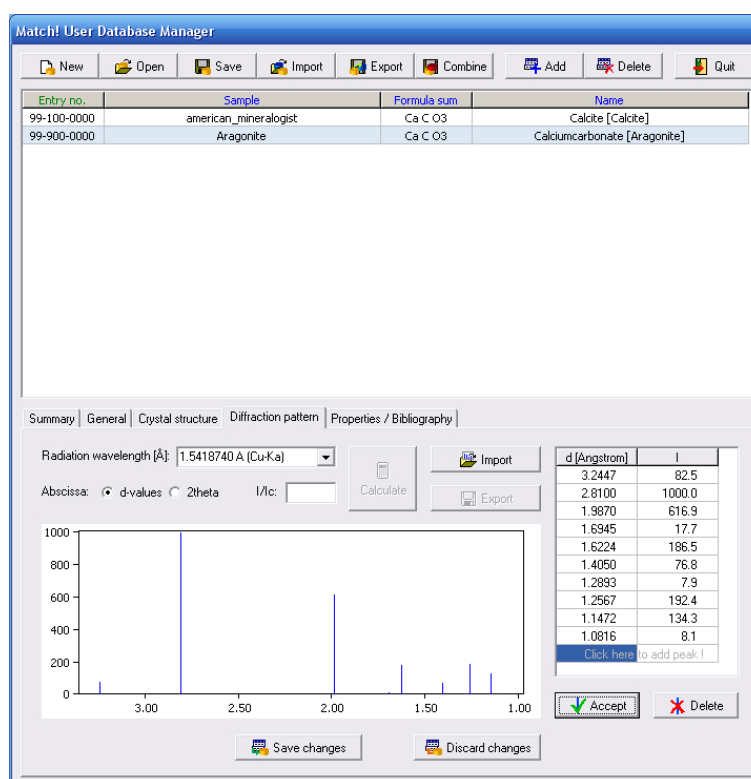
Fig. 59: All peak data have now been entered.

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: SiO$_2$

Chemical name: Silicondioxide

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" tabsheet 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 !) and press the <Tab> key again.

Afterwards, enter "Silicondioxide" 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. 60).

The next information extracted from the paper is the crystal structure, so please bring the corresponding tabsheet into front by clicking on the "Crystal structure" tabsheet header. The first thing you have enter is the crystal system "trigonal", so please click on (activate) the "Hexgonal/trig." radiobutton in the "Crystal system" group at the top left of the tabsheet.

Afterwards, you can select the space group in the corresponding combobox below. In this combobox, 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 combobox, 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 in the atomic parameter table to the right in the first line directly below "Element", 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_i and the site occupation factor "Occ.", so please press <Tab> three times in order to advance to the next line.

Now the coordinates of oxygen have to be entered: Please give "o" as element, "0.4145" as x, "0.2662" as y, and "0.7856" as z. Finally, click on "Accept atom" below the table to finish the input of the atomic parameters (Fig. 61).

Now that the crystal structure information is complete, we can advance to the diffraction pattern calculation: Please click on the "Diffraction pattern" tabsheet header. MATCH! will automatically display a message asking if you would like to calculate the diffraction pattern from the given crystal

Fig. 60: All data appropriate for the "General" tabsheet have been filled in.

Fig. 61: The complete crystal structure description has been entered: crystal system, space group, unit cell constants and atomic parameters.

structure data; please answer (click on) "Yes". After a few seconds, the diffraction pattern will be displayed (Fig. 62). Note that the I/I$_c$ value required for semi-quantitative phase identification has also been calculated automatically.
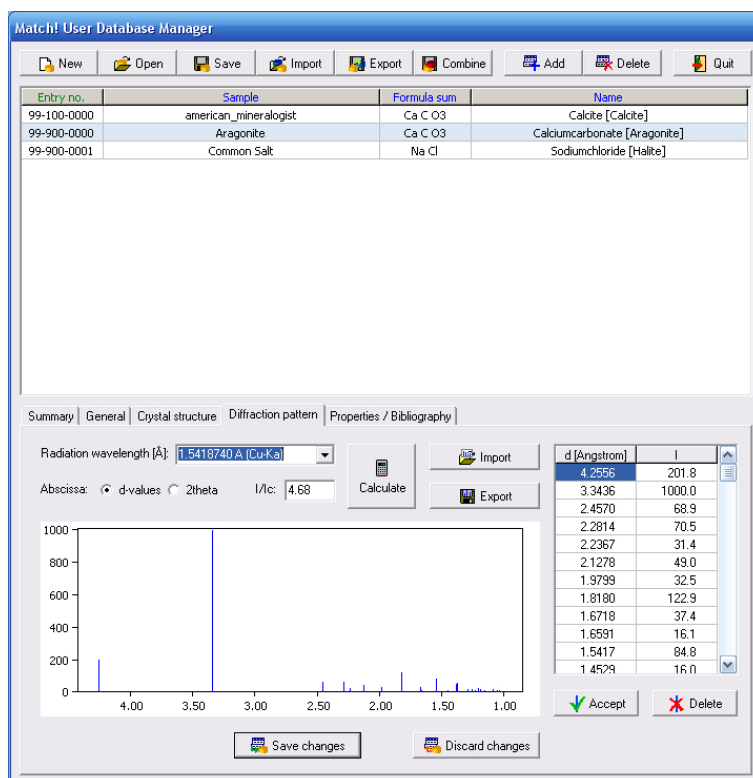
Fig. 62: The powder diffraction pattern (as well as the I/I$_c$ value and the density) has been calculated from the crystal structure data you have entered.

Finally, you have to enter the bibliographic data: Please select the ”Properties / Bibliography“ tabsheet, 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 Cr“. Your input will be automatically expanded to the next matching journal name. Once you have typed the ”r”, the correct journal ”Acta Crystallographica (1,1948-23,1967)” will be displayed.

Please press <Tab> two times (the CODEN will be automatically set 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 tabsheet should now be equivalent to Fig. 63.

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 tabsheet. 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) (Fig. 50). Please mark the ”mtu (Match! user database)“ option, 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.

Please select the file ”colleague-database.mtu” in the ”Tutorial” subdirectory of the MATCH! pro-
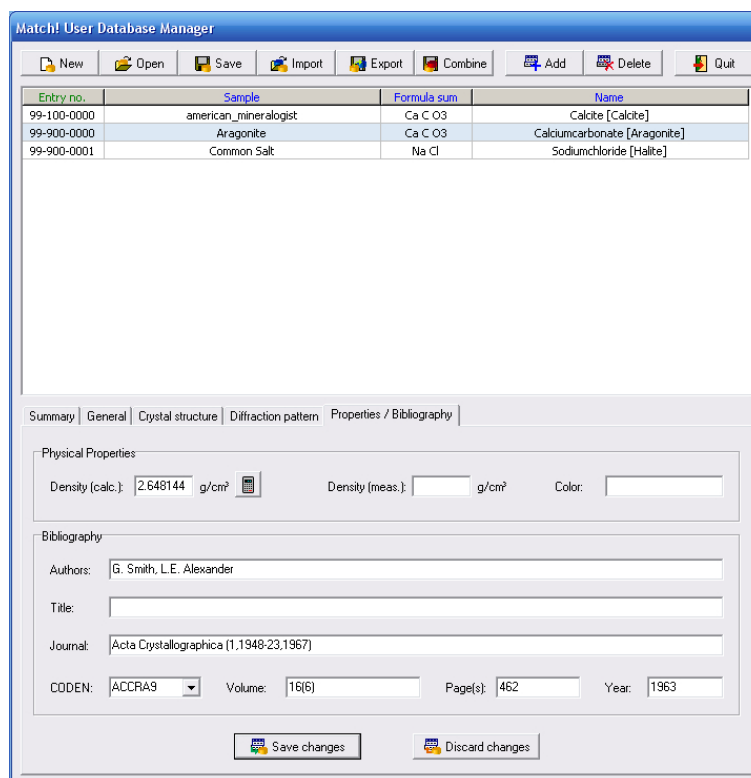
Fig. 63: You have successfully entered the bibliographic data; besides this, the density has been calculated from the given crystal structure data.

gram directory (e.g. "C:\Program Files\Match!\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).

i   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.

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! **licence is installed**.

If you know about potential sources of reference data that might be interesting for other users, please contact Crystal Impact (p. 61)!

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

Reference Manual

Supported File Formats for Diffraction Data

The following diffraction data formats are currently supported by MATCH!:

- ASCII profile (start, step, end, intensities; *.dat)

- ASCII profile (start, step, intensities; *.pro)

- ASCII profile (2 columns: 2theta/d intensity; *.dat)

- Bruker/Siemens DIFFRAC AT peak data (*.dif)

- Bruker/Siemens Raw data (*.raw)

- DBWS Raw data (*.rfl, *.dat)

- ENDEAVOUR peak list (2 columns: 2theta/d intensity; *.dif)

- INEL raw data (*.dat)

- Ital Structures raw data (*.esg)

- Jade/MDI/Scintag raw data (*.mdi),

- JEOL ASCII Export raw data (*.txt)

- PANalytical/Philips Peak data (*.udi)

- PANalytical/Philips Raw data (*.rd)

- PANalytical/Philips Raw data (*.udf)

- Rigaku raw data (*.raw)

- Scintag raw data (*.raw, *.rd)

- Shimadzu raw data (*.raw)

- Siemens Raw data (*.uxd)

- Sietronics XRD scan data (*.cpi)

- Stoe Raw data (*.raw)

- Stoe Peak File (*.pks)

- XRDML (PANalytical) Scan raw data (*.xrdml)

In the following, details about those file formats are provided which are not defined e.g. by the diffractometer manufacturers:

ASCII Profile Data (Start, Step, End, Intensities)

This is a common ASCII file format for raw (profile) data; files in this format can be edited using any conventional text editor. MATCH! expects the following format: In the first line, the 2theta start, step and final value are given. In the following lines, the intensity values for each step are given. The number of intensity values per line may vary.

Example:

```
5.000    0.020   77.000
 3410    3537    3406    3278    3425    3446    3430    3395    3346
 3485    3285    3222    3323    3269    3276    3238    3172    3223
 3129    3238    3137    3211    3075    3139    3098    3068    2978
 2984    2968    2998    2971    3035    2954    3003    2928    2797
 2831    2920    2907    2949    2769    2768    2798    2775    2833
<...>
```

ASCII Profile Data (Start, Step, Intensities)

This is another common ASCII file format for raw (profile) data; files in this format can be edited using any conventional text editor. MATCH! expects the following format: In the first line, the 2theta start and the step value are given. In the following lines, the intensity values for each step are given. The number of intensity values per line may vary.

Example:

```
3.201   0.029
272   257   250   280   225   268   258   270   285   265
272   261   272   254   261   260   243   254   242   266
259   278   227   273   280   266   259   311   292   303
 <...>
```

ASCII Profile Data (2 Columns: 2theta/d Intensity)

This is also a common ASCII file format for raw (profile) data; files in this format can be edited using any conventional text editor. MATCH! expects the following format: Each line contains a 2theta or d-value and the corresponding intensity separated by space(s) (commas will be ignored). You can also enter comment lines (which are ignored, too).

Example:

```
# This is a comment line.
# And here come the data:

10.000000,  685.562866
10.010000,  629.170715
10.020000,  637.972717
10.030000,  616.176697
10.040000,  612.602234
10.050000,  629.820190
10.060000,  630.793823
10.070000,  631.725220
<...>
```

DBWS Raw Data

Files in the DBWS format (file extension usually *.rfl or *.dat) are ASCII files an can be edited using any conventional text editor. MATCH! uses the following format: In the first line, the 2theta start, step and final value as well as a title are given. In the following lines, the intensity values for each step are given in Fortran 8F7 format.

Example:

```
5.293    0.030   42.523      1003
  600     600     600     600     600     600     600     600
  600     600     600     600     600     600     600     600
```

```
603    603    603    603    603    603    604    604
604    604    604    604    604    606    606    606
606    606    607    607    607    609    609    609
610    612    612    613    615    616    617    619
620    623    626    629    633    638    644    651
<...>
```

ENDEAVOUR Peak List Data

Peak lists that can be imported to or exported from ENDEAVOUR are simple two-column ASCII files (file extension *.dif). They can also be created or edited using any conventional text editor. MATCH! expects a line for each individual peak, containing the 2theta or d value and (separated by one or more spaces):

Example:

```
9.804231    42.6
8.207172    88.0
7.314649    17.3
6.254809    19.6
5.768748    35.6
5.424906    15.8
5.167478    24.2
```

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!:

Button(s)	Effect	Menu command
Ctrl+A	Automatic raw data processing	Pattern/Automatic/Autom. raw data proc.
Ctrl+B	Clear current restraints (buffer)	Search/Clear Restraints
Ctrl+C	Correct zero point error (2theta shift)	Pattern/Correct zero point
Ctrl+D	View data sheet	View/Data sheet
Ctrl+E	Load entry by giving its entry number	Entry/Load/Add
Ctrl+F	Finish Match!	File/Finished
Ctrl+H	Open online help at contents page	Help/Help Contents
Ctrl+I	Import powder diffraction pattern	File/Import/Diffraction data
Ctrl+K	Peak searching (conventional; second derivative)	Pattern/Peak searching/Peak search
Ctrl+L	View peak list	View/Peak list
Ctrl+M	Search-Match	Search/Search-Match
Ctrl+N	Open new (empty) Match! document / session	File/New
Ctrl+O	Open Match! document file (session)	File/Open
Ctrl+P	Print	File/Print...
Ctrl+R	Open restraints dialog (perform database retrieval)	Search/Restraints
Ctrl+S	Save current session (Match! document)	File/Save
Ctrl+T	Display analysis report	View/Report
Ctrl+U	Open user database manager	Tools/User Database Manager
Ctrl+X	Select current entry in Results list (if it has the input focus)	Entry/Select
Ctrl+Y	Redo last undo operation	-
Ctrl+Z	Undo last operation/command	-
DEL	Delete currently marked entries or peaks	Entry/Delete, Peaks/Delete
F1	Open help window for current situation (context-sensitive help)	-
F2	Increase peak search sensitivity for normal peak searching as well as profile fitting	Pattern/Peak searching/Increase sensitivity
F3	Decrease peak search sensitivity for normal peak searching as well as profile fitting	Pattern/Peak searching/Reduce sensitivity
F4	Optimize peak search sensitivity for normal peak searching as well as profile fitting	Pattern/Peak searching/Optimize sensitivity
F5	Perform profile fitting	Pattern/Profile fitting/Execute profile fitting
F6	Enable/disable fitting of 2theta values during profile fitting	Pattern/Profile fitting/Fit 2theta
F7	Enable/disable fitting of intensity values during profile fitting	Pattern/Profile fitting/Fit intensities
F8	Enable/disable fitting of FWHM values during profile fitting	Pattern/Profile fitting/Fit FWHM
Ctrl+Alt+A	Open dialog in which the individual automatic raw data processing steps can be configured	-

Ctrl+Alt+G	Open dialog in which the options for the diffraction pattern graphics can be adjusted	-
Ctrl+Alt+P	Open dialog in which the options for the peak list can be adjusted	-
Ctrl+Alt+R	Open dialog in which the options for the results list can be adjusted	-
Cursor up/down	Move the line mark in the Results list up/down (if it has the input focus)	-
Home	Jump back to the beginning of the Results list (if it has the input focus)	-
Space	Select current entry in Results list (if it has the input focus)	Entry/Select
Shift+Del	Delete all peaks	Peaks/Delete all peaks

Tips & Tricks

List Selection Box Handling

In the "Restraints" dialog, a 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 so-called "list selection box") by clicking on the 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.

Command line parameter

When invoking MATCH! from the "command line", you can give the path and name[29] of a diffraction data file as "command line parameter". Once MATCH! has started, the diffraction pattern will be imported automatically (using the automatic file format recognition), with optional further automatic processing (cf. p. 24).

Large number entries resulting from search-match

If your search-match calculation gives a large number of candidate entries, there may be two reasons for this:

1. Your diffraction pattern contains a large number of peaks. As a result, the probability that there is an acceptable agreement between reference peak positions and the experimental peaks is rather high, so a large number of 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.

2. 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. As a consequence, broad peaks (large average FWHM) result in large peak correlation windows, so a large number of 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 ("$\Delta 2\theta$") of the "Search-Match" page of the "Tools/Options" dialog, by deselecting the "Auto" check box below. Try to use/adjust a smaller value for "$\Delta 2\theta$", press <Ok>, and run the search-match again.

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[29] Note that if your path and/or file name contain blank characters, you have to put " characters in front and after the path/file name string.

Frequently Asked Questions (FAQ)

This section provides an overview over the most common questions along with the corresponding answers:

How can I manually load/add specific entries into the Results list, e.g. for comparison purposes?

There are two options for this:

- You can select the entry(s) to be added by entering corresponding selection criteria (e.g. the mineral name or the composition) using the "Restraints" dialog as usual:
  First, open the Restraints dialog and enter your selection criteria as described in the chapter "Database Retrieval" (p. 9). Once you have finished entering your criteria (e.g. mineral name) and pressed the "Retrieve" button at the bottom of the dialog, you will be informed about the result as usual.
  If there were no entries in the Results list previously, you can simply press "Accept" to load the selected entries into the Results list.
  If the restraints buffer (and the answer set) already contain entries, you have to decide in which way the entries resulting from the new restraining operation shall be logically combined with the ones that are already present in the Results list. **You should now select "Previous answer set" at the top and "OR" as the logical operation for the combination of the previous and the new entries.** By doing so, the entries resulting from the previous search-match (or retrieval) and the ones from the new one will be united in the new answer set. Finally, please press the "Accept" button.
  The selected entry(s) will be added to the Results list. If experimental diffraction peaks are present, the FoM and related values will be calculated as well. If the entry has not been found by the search-match code, it is very likely that its FoM (figure-of-merit) is rather low, in which case it can be found close to the bottom of the Results list.

- If you aready know the entry number (e.g. PDF number) of the entry of interest, you can easily load it simply by pressing the shortcut <Ctrl+E>[30], typing the entry number, and then pressing "OK". The corresponding entry will be added to the Results list. If experimental diffraction peaks are present, the FoM and related values will be calculated as well. If the entry has not been found by the search-match code, it is very likely that its FoM (figure-of-merit) is rather low, in which case it can be found close to the bottom of the Results list.

I would like to add own diffraction data to the user database. Does this affect my PDF installation ?

No. The user database is stored independent from the PDF database in a separate directory. MATCH! accesses the PDF in "read-only" mode; i.e. **your PDF is not affected in any way**. The combination of PDF and own (user database) entries is achieved by creating combined index files, which themselves are stored in a separate directory.

Is it possible to read document (*.mtd) or answer set (*.mta) files created by version 1.1 (or later) on a version 1.0 installation ?

No. Due to the new PDF entry numbering scheme supported since MATCH! version 1.1, the document structure has changed. In case of similar problems you should update the version 1.0 installation to the current version 1.x (which is free-of-charge; p. 61).

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[30]Alternatively, you can also select the "Load/Add" command from the "Entry" menu, or press the corresponding button in the toolbar on the upper left-hand side.

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 (which will 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 know how a command in a pulldown menu operates, press the **F1** key when the corresponding command is highlighted. This will open the help page for this command or its context.

- 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! webpage at:

  http://www.crystalimpact.com/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 - 2 28 - 9 81 36 44**

  or **write** to:

  Crystal Impact GbR
  Rathausgasse 30
  D-53111 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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In the same window, you can also determine the version of Match! you are currently using. This information is helpful if you would like to check for updates on the corresponding webpage:

http://www.crystalimpact.com/match/update.htm

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End-User License Agreement for

MATCH! - Phase Identification from Powder Diffraction -

between you and CRYSTAL IMPACT

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