DIFFRAC.SUITE

User Manual

DIFFRAC.EVALUATION PACKAGE
DIFFRAC.EVA

Original Instructions

Innovation with Integrity

XRD

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DIFFRAC.EVA User Manual

Table of Contents

DIFFRAC.EVA

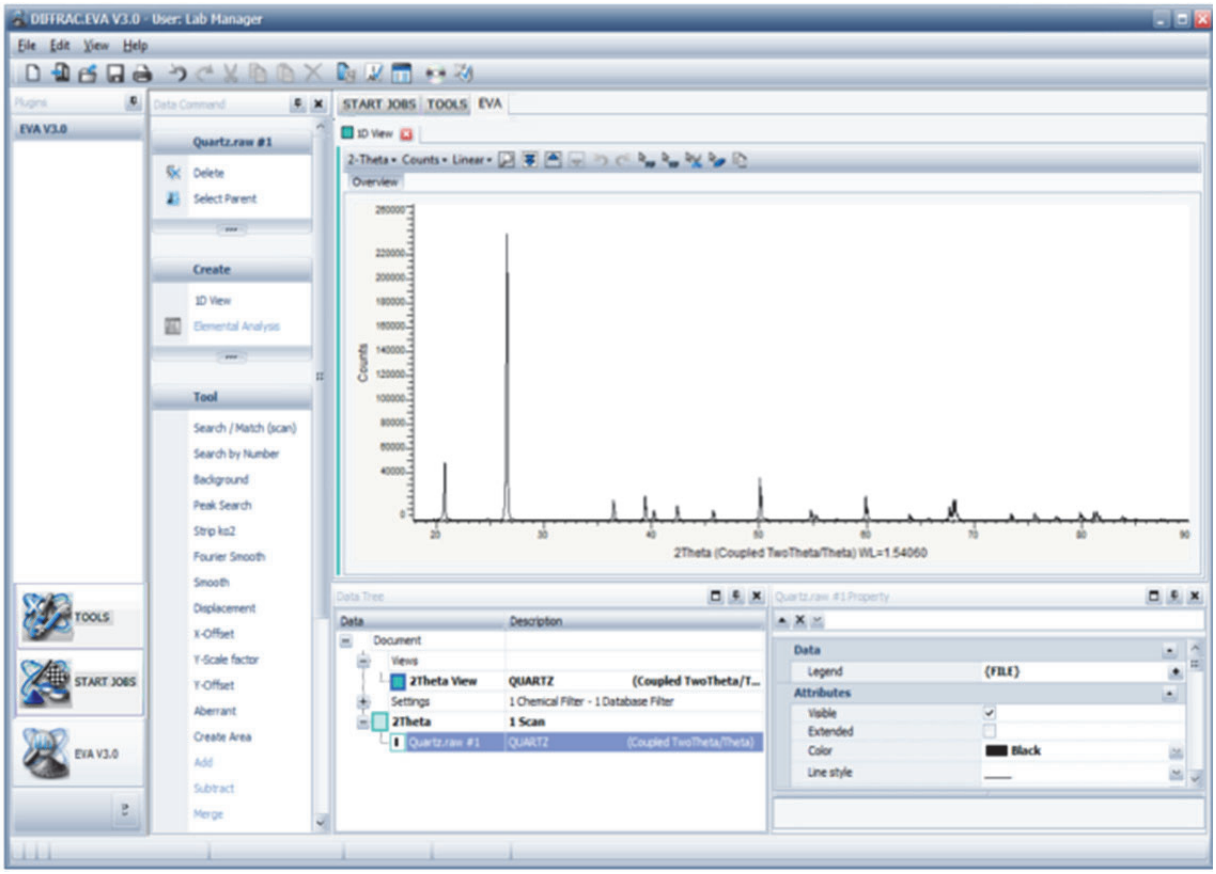
Introduction

DIFFRAC.EVA is a universal software to evaluate X-ray diffraction data. It provides general tools to evaluate peaks, background and areas. Tools to work with patterns and perform searches in phase databases are also provided.

DIFFRAC.EVA is a software module of DIFFRAC.SUITE. It is referred to as a plug-in because it is a part of the common framework of DIFFRAC.SUITE.

Each button in the framework's navigation bar corresponds to a plug-in. The Navigation bar can be displayed or be hidden by clicking **Navigation bar** on the **View** menu.

Here is an example:



DIFFRAC.EVA is usually installed as a single plug-in. In this case, the navigation bar is switched off by default.

In this manual the term "EVA" and "DIFFRAC.EVA" are synonymous.

About Licenses

The right to use DIFFRAC.EVA V4 is not limited to users who have either purchased this version or an update from an earlier version: all users of DIFFRAC.EVA can run it, but some features are disabled if their license is not up-to-date.
Newer versions will run while the functionality will be restricted to the licensed version. For example, the new features of V4 will be disabled when run with a license valid only for V1. However, this will not affect PDF updates. In contrast to DIFFRAC^{plus} EVA the capability of working with newer PDF versions will not be restricted to a license. It is sufficient to install the latest DIFFRAC.EVA version to use the latest PDF.

The features which may be disabled are clearly indicated in this manual and summed up in the appendix.

Introducing EVA

The program EVA is a versatile tool to analyze diffractograms.

An X-Ray diffractogram is saved as a raw file (file with the extension .BRML or .RAW). EVA creates an internal copy of the raw file. This copy as well as the user interface settings can be saved in an EVA document file with the extension .EVA. Thus, the original data (background subtraction, smoothing, angular shift...) can be adjusted without modifying the original raw file itself.

EVA uses five different kinds of data *objects* (called *EVA objects*): "Scans", "Patterns", "Peaks", "Areas" and "Levels".

Scans

A "scan" is a diffractogram resulting from the collection of scattered X-ray radiation when analyzing a sample with a powder X-ray diffractometer. The data are stored in a file with the extension .BRML or .RAW. EVA works with a copy of these data. The original file is never changed so the user can always come back to the initial point.

RAW and EVA files are recognizable by this icon .

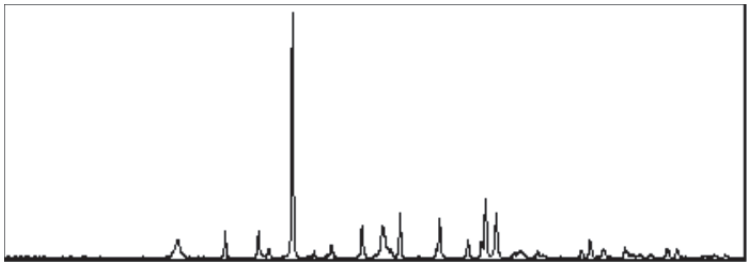


Fig.1: EVA displays a scan as a continuous line by default

Patterns

A pattern is the set of peaks of a given phase. It can be considered as the signature of this crystalline phase. It is sometimes called d-I list because it is no more than a list of d-spacings and relative intensities I of the corresponding peaks.

The reference patterns are stored in powder diffraction databases. They are displayed as stick diagrams.

The powder diffraction file (PDF) is a scientific database for powder diffraction data. It is the intellectual property of the International Centre for Diffraction Data (ICDD)[1]. This organization makes the PDF database available under license agreements.

You can find a reference pattern by its name or number, or by a search/match process. These possibilities are described in the section “Performing a Search on a Scan” on page 62.

The user can convert a set of peaks located by EVA into a pattern (called a DIF pattern) which will be displayed like any other reference pattern.

Patterns (DIF) are associated with this icon .

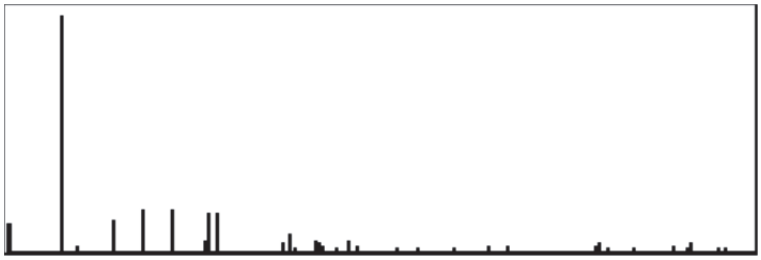


Fig.2: EVA displays patterns as stick patterns

[1] ICDD ® and PDF ® are registered trademarks of the JCPDS – International Centre for Diffraction Data

Peaks

Peaks result from an automatic peak search treatment on the scan (research of the minima of the second derivative, with filtering on breadth and height). They can be inserted and edited manually.

Once a peak list is created, it can be converted into a pattern (called DIF, for d-I file), and used in another EVA document or in other programs.

Information concerning each peak on the scan, including the scan's x unit (e.g. *d* or 2θ) and intensity can be displayed on the screen.

Peaks are associated with this icon  .

Areas

EVA can calculate the net intensity, full width at half maximum (FWHM), and many other significant values of a selected area. This set of results is called an Area. Areas are calculated by integration, not by profile fitting.

The area computation can be performed on all regions of interest and results are stored in the list of Areas. Two other DIFFRAC.SUITE components perform similar operations: DQUANT (quantitative analysis using pre-set angular regions) and TOPAS (a profile fitting program). This program can separate unresolved line clusters in single lines).

Areas are associated with this icon  .

Levels

This feature is useful when working with multi-range data. The multi-range data refer to several similar scans measured successively while one parameter varied (for example, 2θ scans with increasing temperature, or rocking curves with increasing 2θ). If the user considers the surface $I = f(2\theta, n)$ — or $I = f(\theta, n)$ for rocking curves — in which n is the number of the curve, the user can define iso-intensity level, with I=constant.

Levels are associated with this icon  .

Program Start

The Windows start menu contains a folder "DIFFRAC.EVA V4.0" which contains the shortcuts to start the DIFFRAC.EVA program, a folder Help which contains shortcuts to the documentation and a folder Tools which contains shortcuts to several helper programs.

The "DIFFRAC.EVA V4.0" folder contains an entry "DIFFRAC.EVA" which starts the program to work with files only. The software will not be connected with a database.

A second entry "DIFFRAC.EVA (database access)" starts and connects DIFFRAC.EVA with a DIFFRAC.MEASUREMENT CENTER database if available.

If DIFFRAC.EVA is installed for 21 CFR Part 11 mode the only available shortcut is "DIFFRAC.EVA (database access)".

Cluster Analysis

The Cluster Analysis is available from software version 4 and license level 4 up.

A cluster analysis, which is designed to match and analyze full profile diffraction and other numeric data, is integrated into DIFFRAC.EVA.

The cluster analysis has a dedicated user manual. See the DIFFRAC.EVA | Help folder in the Windows Start menu | All programs.

Overview

When EVA has been started and a scan file has been imported for the first time, the EVA main window appears as such:

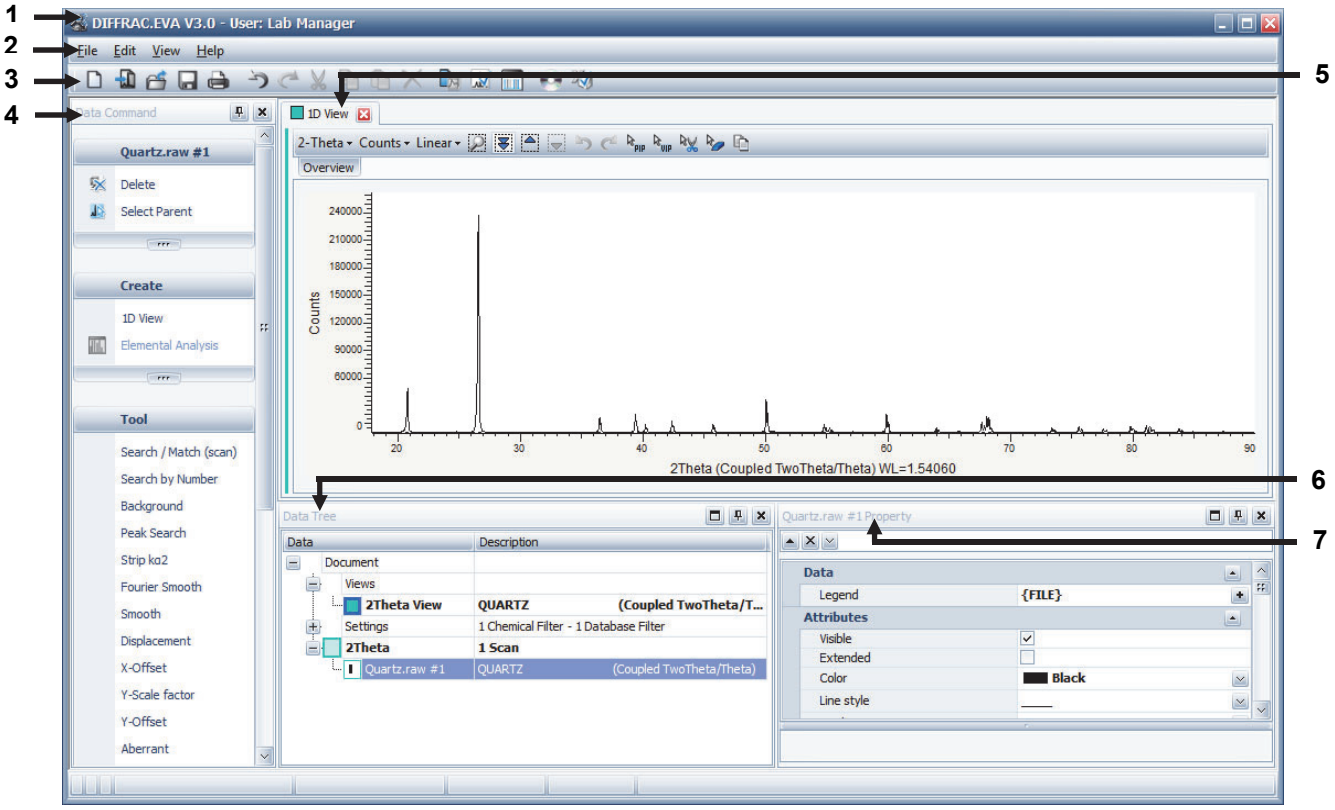


Fig.3: Exploring the screen

1	Title bar	**5**	View window
2	Menu bar	**6**	Data tree panel
3	Toolbar	**7**	Data/view property panel
4	Data command panel		

Title Bar

The title bar shows the name of the user currently connected at the top of the window.

Menu Bar

The menu bar gives access to commands.
Point to a menu name with the mouse to display the corresponding commands and click the desired command.

File Menu

Command	Shortcut	Function
New	CTRL+N	Create an empty EVA document
Import from Files		Import scans from RAW/BRML files
Import from Database		Import scans from database
Open	CTRL+O	Open an existing EVA document
Close		Close the current active EVA document
Save	CTRL+S	Save an open EVA document using the same filename. If it is the first time a new EVA document is saved, the name proposed by default is the file name of the first imported scan.
Save As…		Save an open EVA document with a specified filename; the default name is the current name.
Print Preview	CTRL+P	Display a print preview
Exit	Alt+F4	Exit from EVA

Edit Menu

Command	Shortcut	Function
Undo	CTRL+Z	Undo the last action
Redo	CTRL+Y	Reverse the action of the **Undo** command
Cut	CTRL+X	Cut the selected item
Copy	CTRL+C	Copy the selected item
Paste	CTRL+V	Paste an item from the clipboard
Delete		Delete the selected item

View Menu

Command	Shortcut	Description
Skins		Select a skin for the program
Language		Select the language for the program
Plugins		Select the desired plugin
Date Tree Panel	F2	Show/hide the Date Tree Panel
Data Property Panel	F4	Show/hide the Data Property Panel
Data Command Panel	F6	Show/hide the Data Command Panel
Navigation Bar		Show/hide the Navigation Bar

Tools Menu

The Save/Load Settings/Layout and Start AbsorbDX commands are available from software version 4.0 up.

Command	Description
Start AbsorbDX	Start the AbsorbDX program
Start FileExchange	Start the FileExchange program
Start DSRD Compiler	Start the DSRD Compiler program
ICCD RDB Databases	Display information about the databases and licenses
Settings	Display the EVA Settings dialog box
Save Settings…	Save the current EVA settings into a file
Load Settings…	Load EVA settings from a file
Save Layout…	Save the current workspace layout into a file
Load Layout……	Load a workspace layout from a file

Help Menu

The View User Manual/Tutorial commands are available from software version 3.2 up.
The View Cluster Analysis Manual/What's New/FAQ commands are available from software version 4.0 up.

Command	Description
View User Manual	Display the user manual
View Tutorial	Display the tutorial manual
View Cluster Analysis Manual	Display the cluster analysis manual
View What's New	Display the "What's new" document
View Manual Addendum	Display the manual addendum
View FAQ	Display the Frequently Asked Questions
About…	Display the About EVA box with information about version number, operating system, file versions and licensing

Toolbar

The toolbar permits easy access to commonly used tools.

Symbol	Description	Command	Shortcut
	Create a new EVA document	File | New	CTRL+N
	Import from files	File | Import from Files…	
	Import from database	File | Import from Database…	
	Open an existing EVA document in a new window	File | Open	CTRL+O
	Save the active EVA document to its current name and directory	File | Save	CTRL+S
	Replace the main window with a print preview window (Working pane displayed in printed format)	File | Print Preview	
	Reverse the last command or the last entry typed (undo)	Edit | Undo	CTRL+Z
	Reverse the action of the **Undo** command	Edit | Redo	CTRL+Y
	Cut the selected object(s) and moves it to the clipboard		CTRL+X
	Copy the selected object(s) to the clipboard		CTRL+C
	Paste the content of the clipboard		CTRL+V
	Delete the selected object(s)		
	Show/Hide Data Tree Panel	View | Data Tree Panel	F2
	Show/Hide Data Property Panel	View | Data Property Panel	F4
	Show/Hide Data Command Panel	View | Data Command Panel	F6
	Display information about the databases and licenses	Help | ICCD RDB Databases	
	Display the Settings dialog box	Help | Settings	

View Window

This window groups all the views: column views as well as graphical views or DB views.
Each view has its corresponding tab when they are stacked on each other.
Click a tab title to display the corresponding view.

To remove a view from the display, click the **Close** button in the corresponding tab heading.

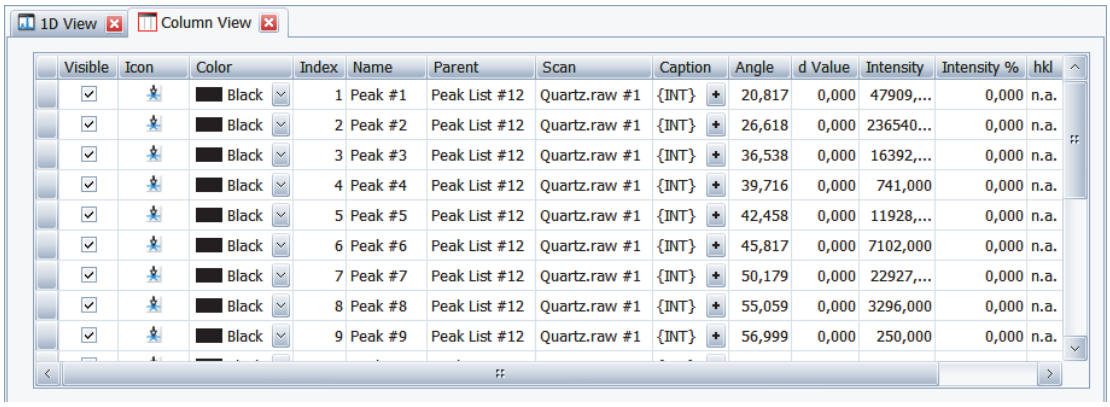


Fig.4: Example of a Column view

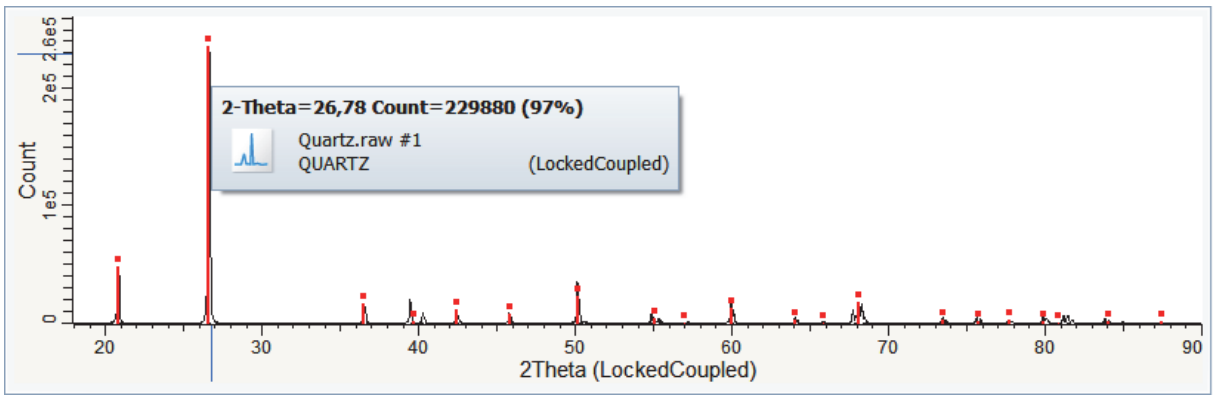
Graphical Views

There are two main types of graphical views: 1D views and 2D views.

1D View

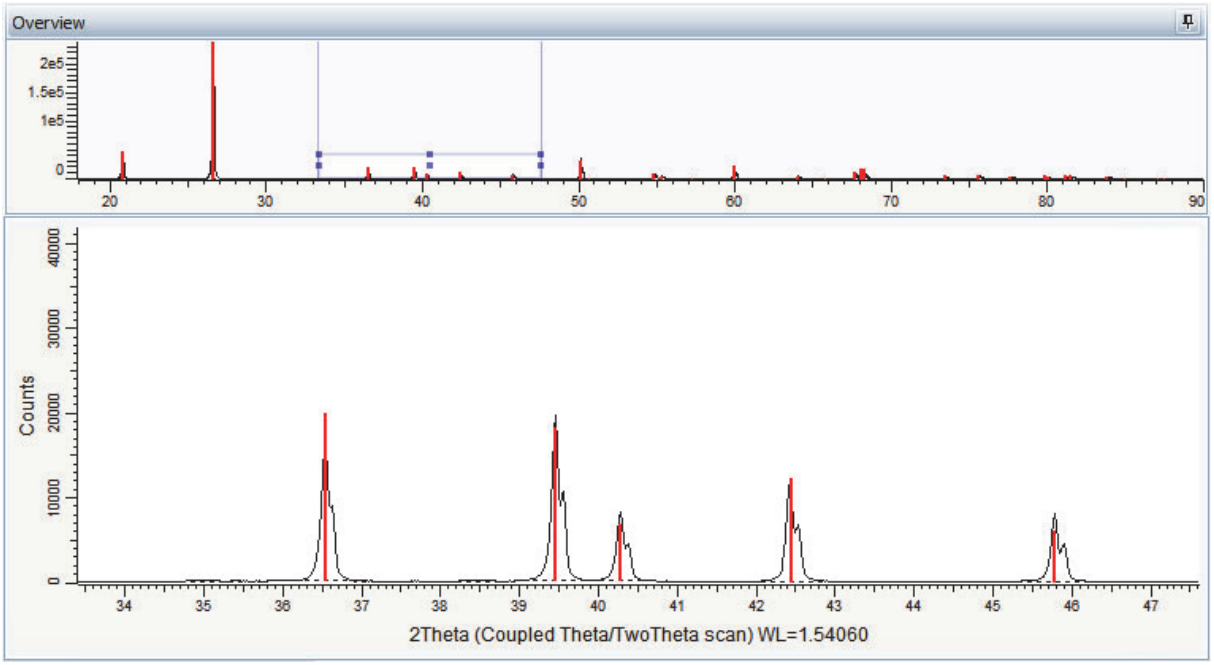
1D views are associated with this icon .

- General view



This is in the general view in which the scans are imported and the user can see the graphical results of the operations performed such as a pattern or some peaks.
A pop-up window containing information about an EVA object can be displayed by moving the mouse over it (without clicking). See the example in the figure above: the cursor is pointed to the scan and an automatic pop-up window displays the scan information.

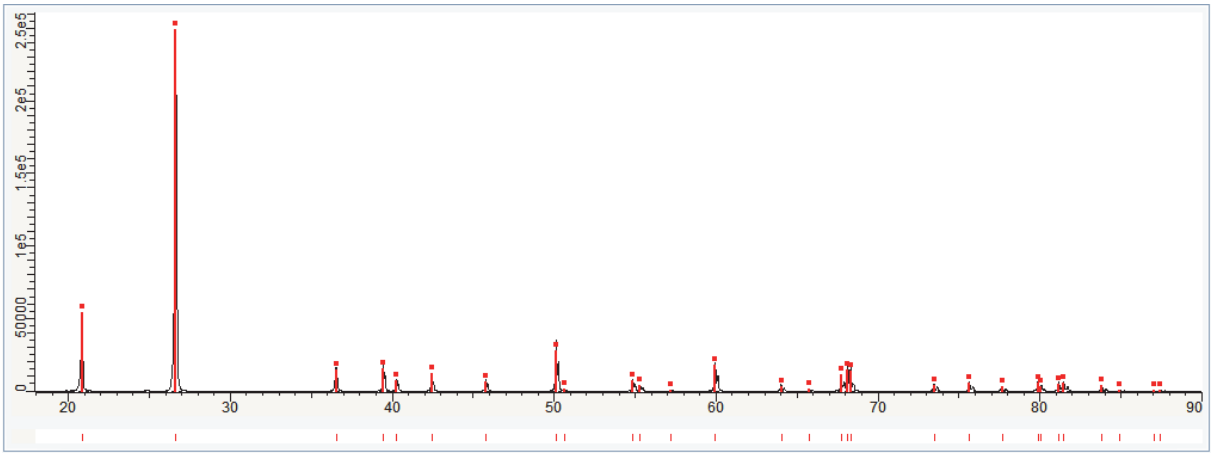
- Overview



The overview provides a useful view when zooming in. It gives a view of the whole scan while the zoomed area is displayed in the general view. Moreover, it allows adjustment to the zoom area when moving it left or right.

The overview window will be hidden using the automatic hiding feature: see section “Automatic Hiding Feature” on page 39 for a detailed description.

- Stick view

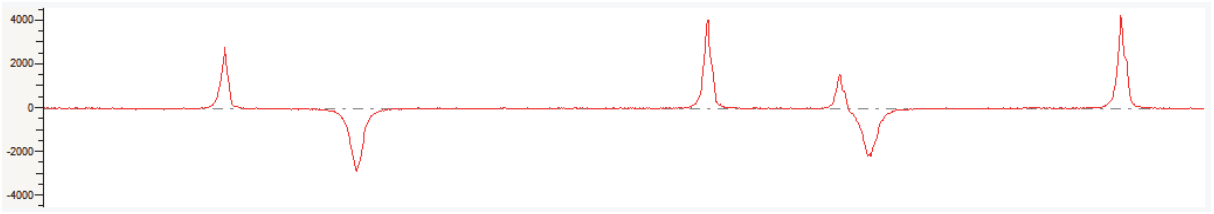


The stick view is displayed below the general view and shows the same X-range.
This view represents all the sticks of the general view as small sticks.

To display the stick view:

- select the **Display Stick View** check box in the View Property table.

- Extended view



The extended view is displayed below the general view and shows the same X-range. It is mostly dedicated to the display of difference curves.

In the extended view, the 0 line is in the middle. When this view is active, difference curves are automatically displayed in the extended view.

To use the extended view:

- select the **Display Extended View** check box in the View Property table to display the view itself.
- select the scan(s) to be displayed in the extended view and check the **Extended** check box in the corresponding Scan Property table.

To change the scale in the extended view, click it and drag up or down to zoom in or out.

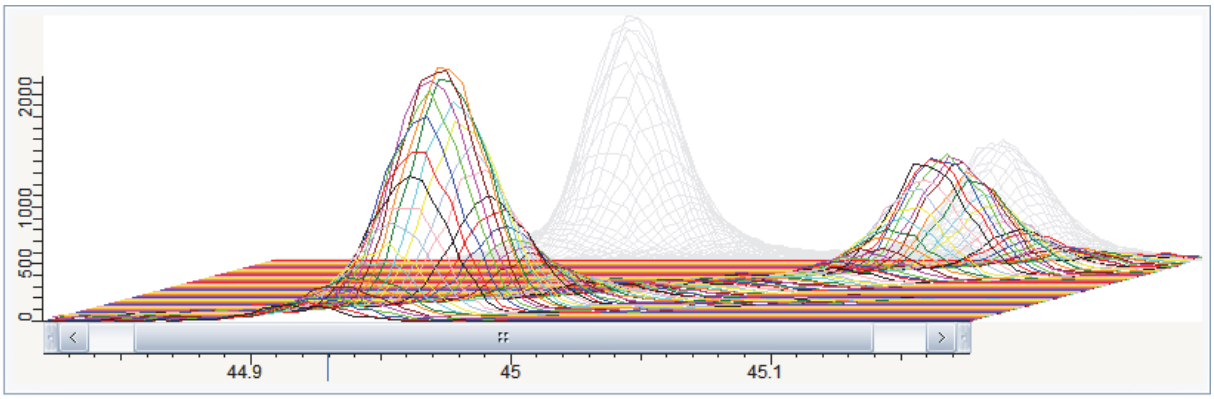
NOTE

This is the only way to display and print curves with negative values.

NOTE

The extended view is automatically displayed for the statistical error and the subtract tools in case there are negative values in the result.
The result scan is visible only in the extended view (property Visible = No and property Extended = Yes).

- Waterfall view

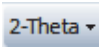
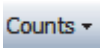
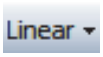


A waterfall view of a list of scans can be displayed by selecting the **Waterfall display** check box in the View Property table.
To zoom, proceed as usual but select the zone of interest in the shadow representation at the back.
By clicking on the X-axis or the Y-axis, a scroll bar can be displayed which permits the user to move through the view.

- View toolbar

The view toolbar gives access to graphical tools. It is displayed by default.

It can be hidden or the position can be changed (top, right, left or bottom) by selecting the corresponding option in the View Property table.

Icon	Tool	Description
	X-scale	To select the X-scale unit
	Y-scale	To select the Y-scale unit
	Y-scale projection	To select the Y-scale projection
	Zoom reset	Self-explanatory
	Zoom Base Always Zero	To set the bottom of the working area to I = 0 (recommended). In case of a logarithmic Y-scale in counts, the base is not zero but one. In case of a logarithmic Y-scale in CPS, the base is 1 divided by the counting time per step
	Zoom Always Fit Top	To adjust the top of the working area in order to fit the highest measured point available in the area
	Zoom Always Fit Bottom	To adjust the top of the working area in order to fit the lowest measured point available in the area
	Zoom Undo/Zoom Redo	Self-explanatory
	PIP Mode	To create a PIP view
	VIP Mode	To create a VIP view
	Residual Scan: Apply to all visible scans	Self-explanatory
	Residual Scan: Restore all visible scans	Self-explanatory
	Copy view picture to clipboard	To copy the view picture as Bitmap or as Metafile to the clipboard

2D View

2D views are associated with this icon .

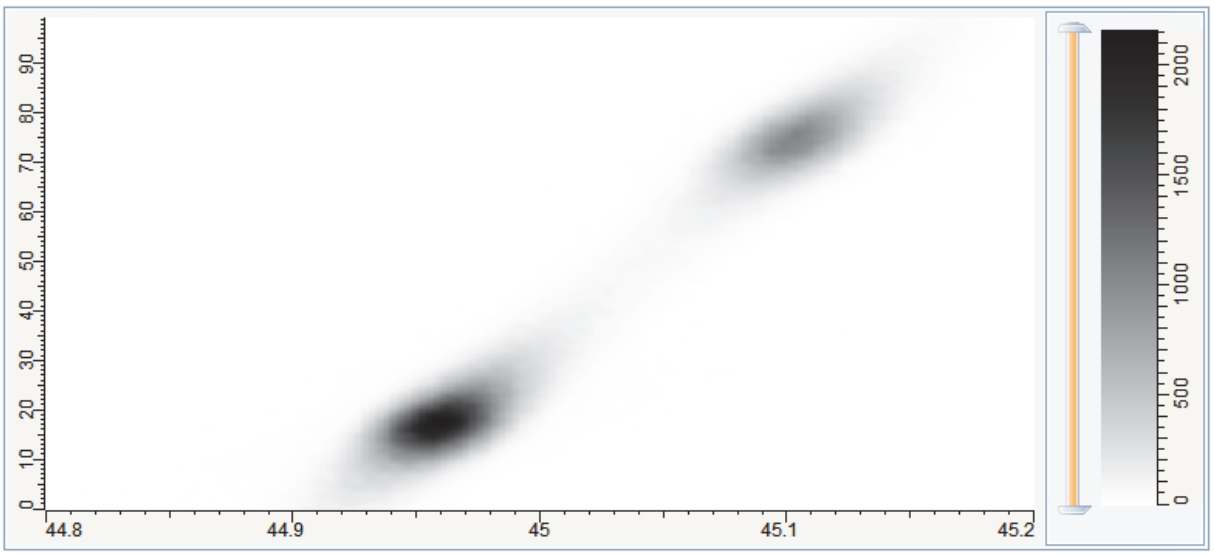


Fig.5: Example of 2D View

The 2D view shows the scans using the scans' axis for X and the scan number in the set of multiple scans for Y.
The user can customize the colors of the intensity map by right-clicking the color scale on the right and selecting the color set in the context menu.

Chart View

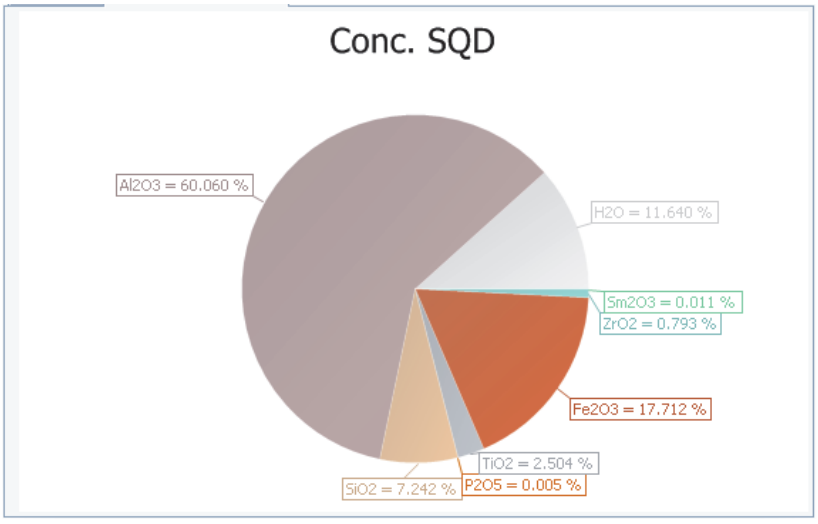


Fig.6: Example of Pie Chart View

The Chart view shows data as a Pie chart, a Bar chart or a Stack chart.
It can be created from all possible data list nodes: Scan list, Pattern list, Element list… The Legend (the horizontal axis for a bar or stack chart) and the Value (the y axis or the sector size for a pie chart) are selected in the Chart View Property table.

Frame View
The Frame view shows the 2-dimensional frame data measured by the detector. Additionally, multiple frames can be “merged” together for display and analysis.

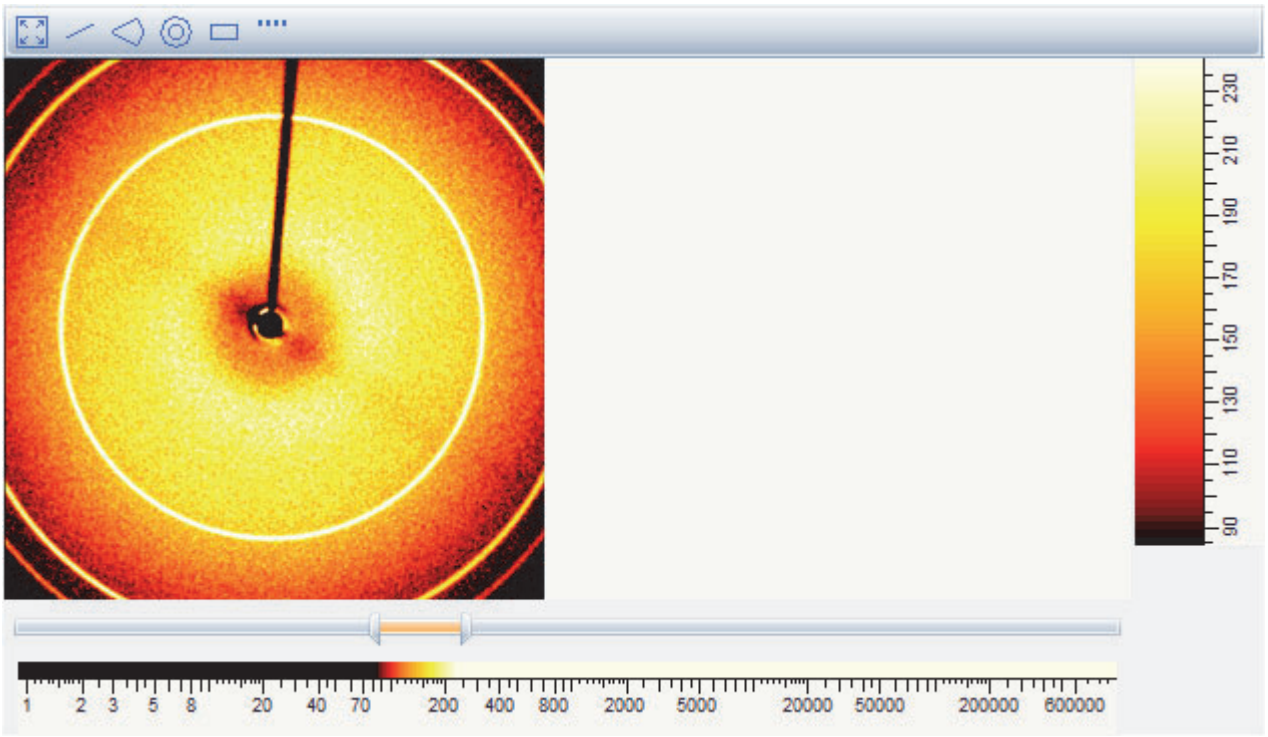


Fig.7: Example of a Frame View displaying a single frame

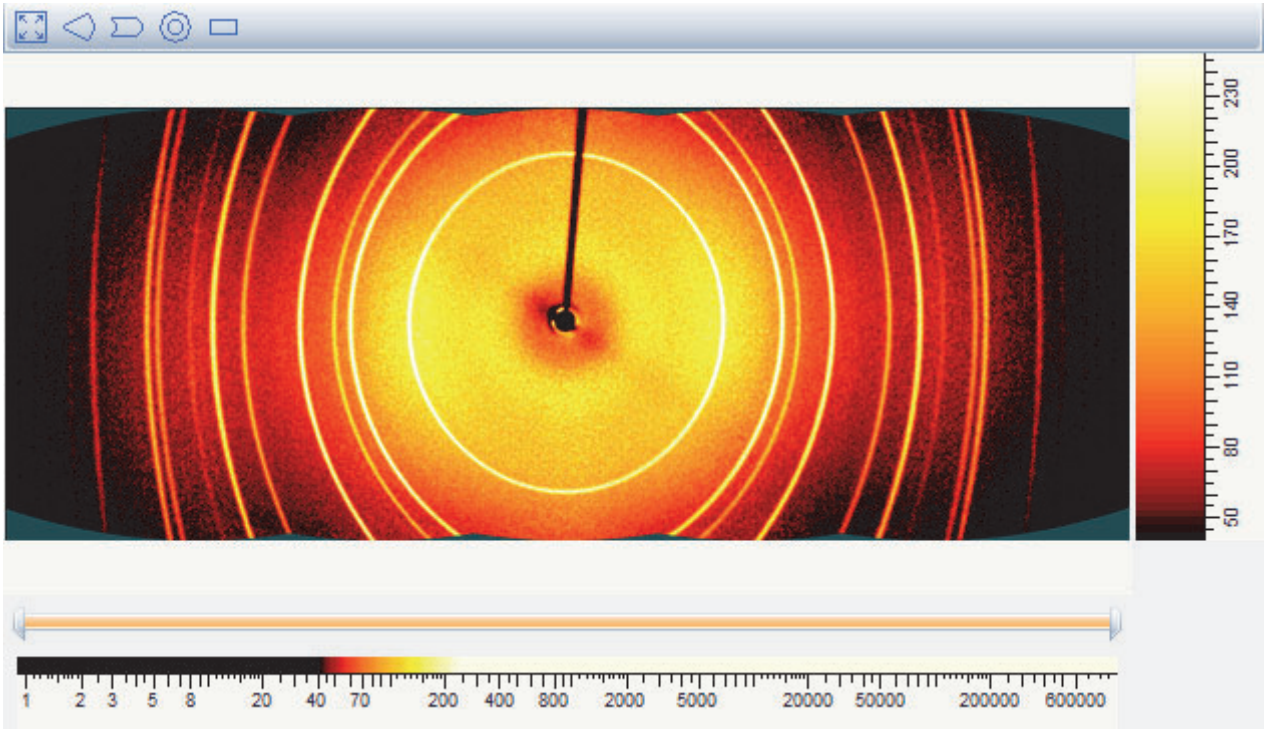


Fig.8: Example of a Frame View displaying five merged frames

Palette Range Control

A slider control below the frame display allows you to set the displayed colors of the frame's X-ray intensity values in a given range.

To adjust the minimum and maximum of the colored range, click and drag the sliders below the frame display to adjust the color of the brightest and darkest pixels.

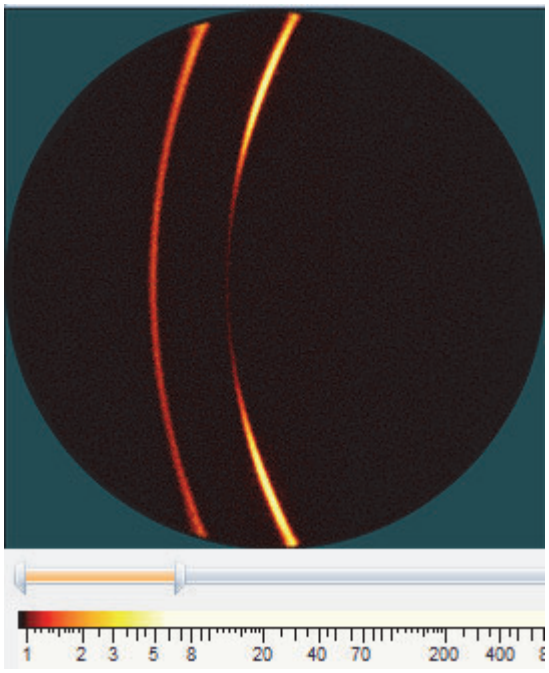


Fig.9: Normal frame image after loading (0-6 counts)

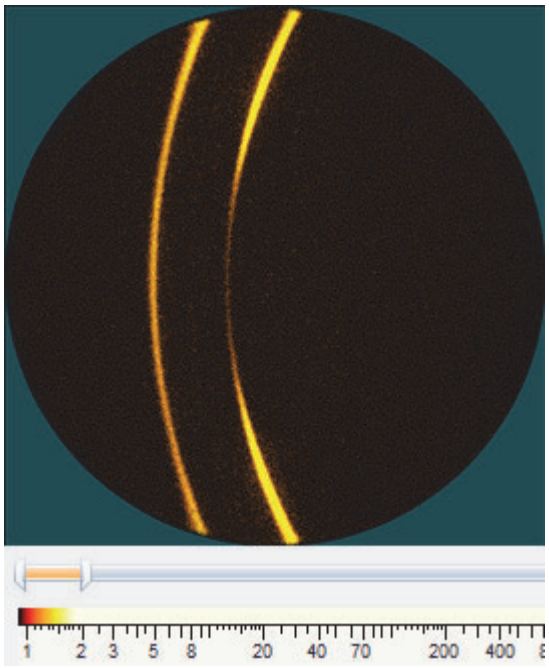


Fig.10: Image with reduced maximum pixel color (i.e., white pixel slider dragged down to 2 counts)

Color Options

The color control on the right of the Frame View changes the color palette.

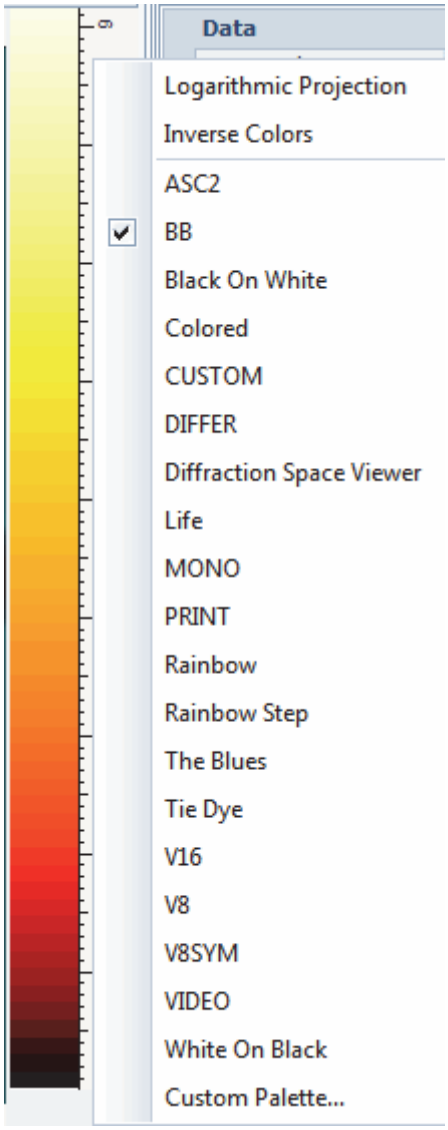


Fig.11: Color control with predefined palettes

A number of predefined palettes are available. The default, “BB”, approximates a black-body radiation curve.

Zooming in a Frame View

Zooming is performed by clicking and dragging the mouse from left to right.

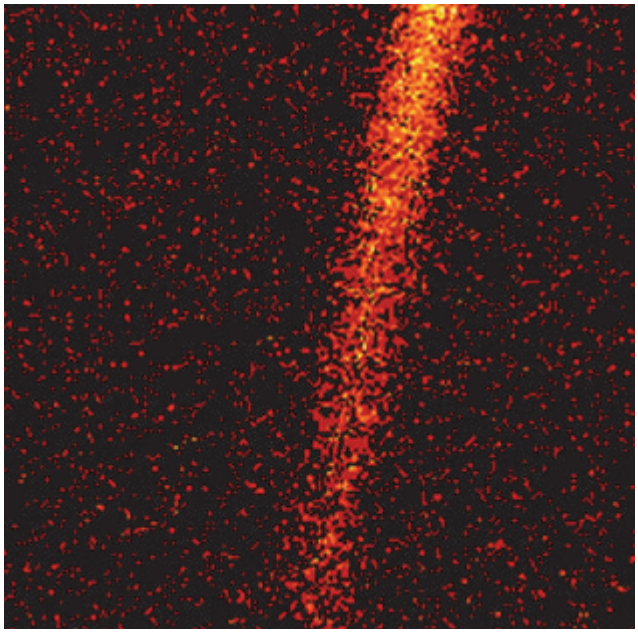


Fig.12: Mid-level zoomed area

When the zoom level leads to a considerable enlargement of the pixels, the count values are displayed in the Frame View.

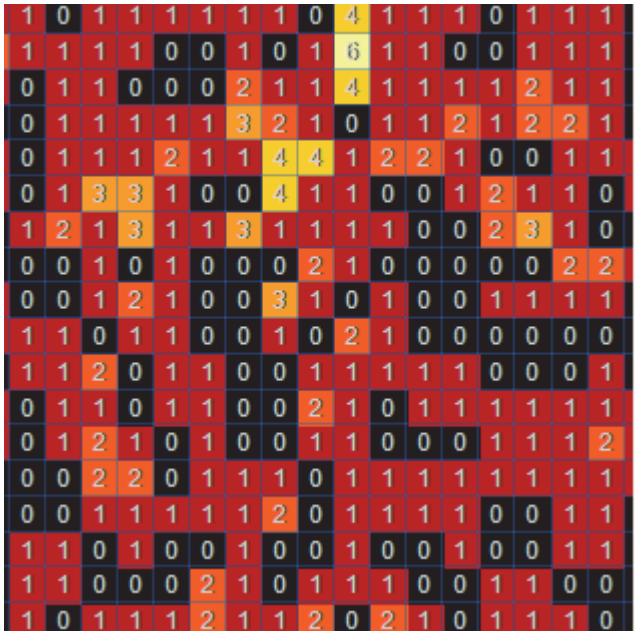


Fig.13: High zoom level with displayed counts

Zooming is undone by clicking and dragging from right to left.

Frame Thumbnail View
Frame thumbnail views are available by clicking the **Create Frame Thumbnail View** command.

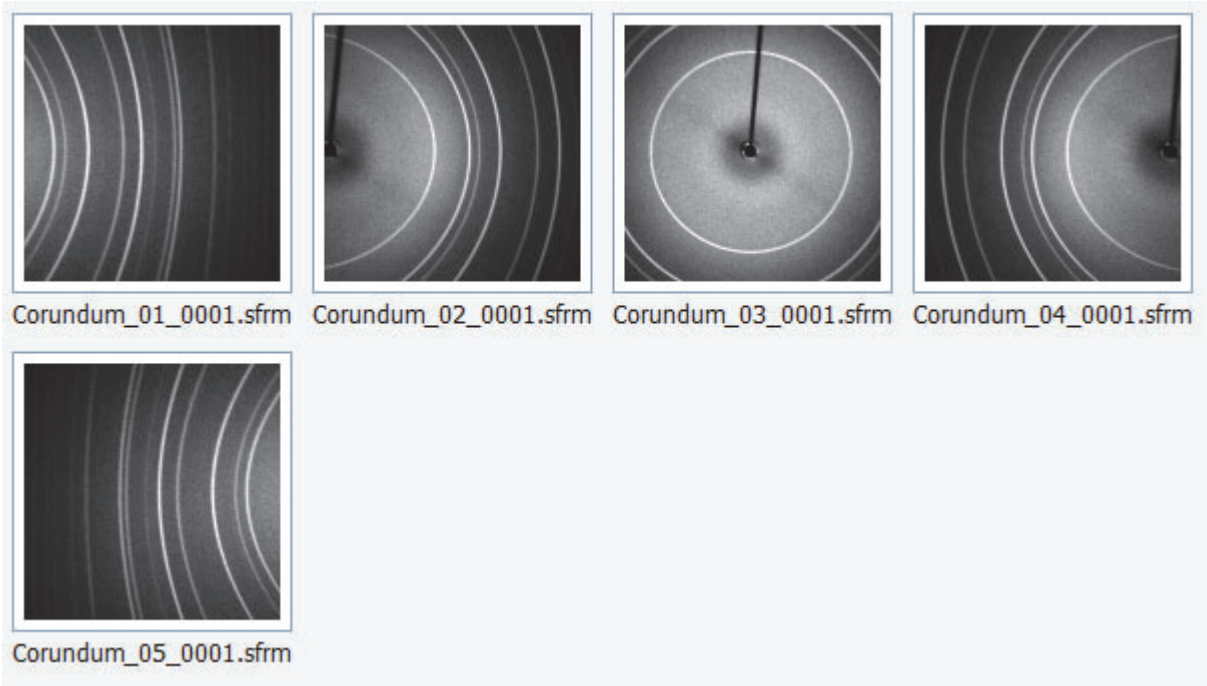


Fig.14: Example of a Frame Thumbnail View

A frame thumbnail view displays a small thumbnail picture of all of the frames in a frame list. Clicking on a thumbnail selects the associated frame in the list. Double-clicking the thumbnail opens a new Frame view if there is no Frame view already displayed.

Creating a View

Creating a Graphical View

A 1D view is automatically created when importing a scan.

The user can create a 1D view for a scan, a list of scans, a pattern (including DIF) or a list of patterns.

For this:

1. Select the object or object list of interest either in the data tree or on the graphical view.
2. Click **1D View** in the Create list of the Data Command panel
   — or —
   right-click and then click **Create.** Click **1D View** on the submenu.

For a list of scans a 2D view can be created. Proceed the same way but select **2D View** instead of 1D View.

Creating a Scan View

A scan view can be created to display the content of a scan.

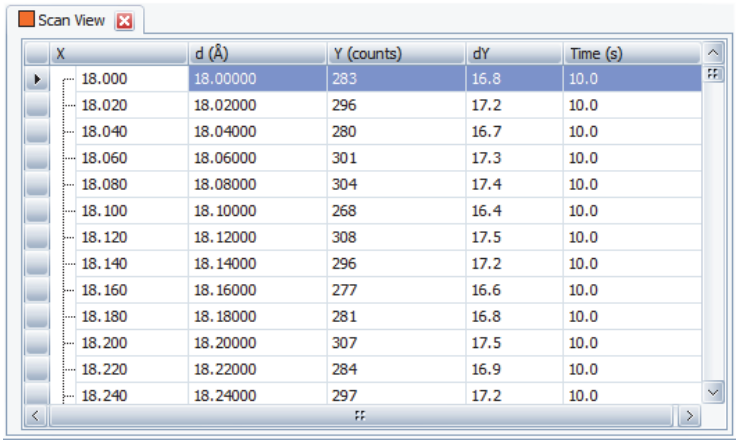
Four columns are displayed for all axes besides the 2-theta axis: X – the x-axis value; Y – the y-axis value in counts; dY – the counting statistics error in square root of counts; Time – the measurement time in seconds.

If the axis is a 2-theta axis, the d-value in Å is displayed as second column.

This feature is available from software version 3 up.

For this:

1. Select the scan either in the data tree or on the graphical view.
2. Click **Scan View** in the Create list of the Data Command panel
   — or —
   right-click and then click **Create.** Click **Scan View** on the submenu.



X	d (Å)	Y (counts)	dY	Time (s)
18.000	18.00000	283	16.8	10.0
18.020	18.02000	296	17.2	10.0
18.040	18.04000	280	16.7	10.0
18.060	18.06000	301	17.3	10.0
18.080	18.08000	304	17.4	10.0
18.100	18.10000	268	16.4	10.0
18.120	18.12000	308	17.5	10.0
18.140	18.14000	296	17.2	10.0
18.160	18.16000	277	16.6	10.0
18.180	18.18000	281	16.8	10.0
18.200	18.20000	307	17.5	10.0
18.220	18.22000	284	16.9	10.0
18.240	18.24000	297	17.2	10.0

Fig.15: Example of a scan view

Creating a Column View

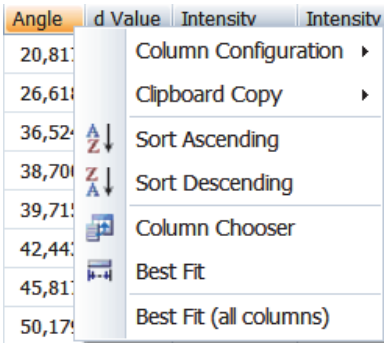
A column view can be created for a list of objects.
It is possible to create various types of Column List views from a Scan List or a Document data node. Lists will mix data from multiple child nodes of the same type. For example, an Area Column List view can be created from a Scan List data node. It will display all the areas existing in all its scans below in its table.

To create a column view:

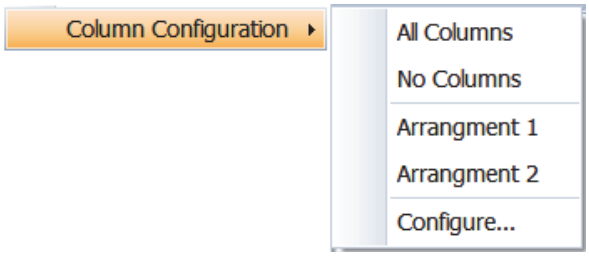
1. Select the object list of interest in the data tree.
2. Click **Column View** or ***Object* Column View** (depending on the data selected) in the Create list of the Data Command panel
   — or —
   right-click and then click **Create** in the menu displayed**.** Click **Column View** or ***Object* Column View** on the submenu.
   Objects include Scans, Patterns, Peaks, Areas and Levels.

Customizing and copying columns:

The columns of the table in the column view can be customized.
Right-click the column header to display the contextual menu.



To configure the columns, click the **Column Configuration** command: the corresponding menu will be displayed.



The commands of the Column Configuration menu are described in the following table:

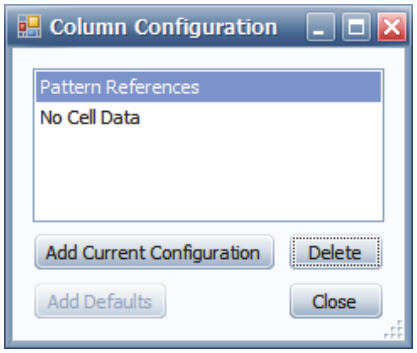
Command	Description
All columns	Click to display all the possible columns.
No columns	Click to remove all the columns from the display.
List of arrangements	List of the arrangements configured by the user. Click the desired arrangement.
Configure…	You can add or delete column configurations (arrangements). Click **Configure…** to display the Column Configuration dialog box. See section “Managing the column configurations” below for details.

Managing the column configurations

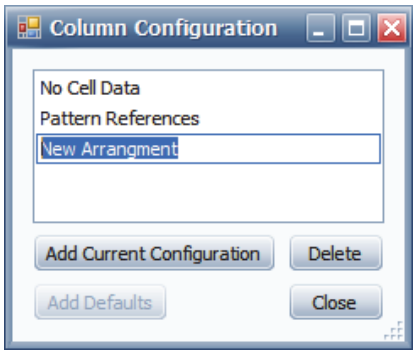
⇒ Adding a column configuration

Once the columns are configured as desired, it is possible to save the corresponding column configuration. To do so:

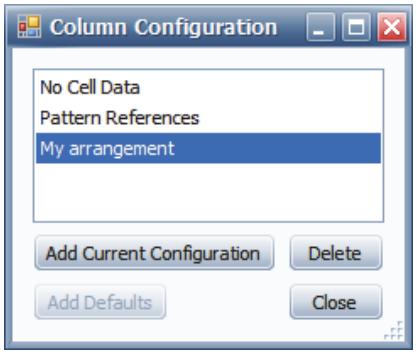
1. Display the Column Configuration dialog box as explained in the table above.



2. Click the **Add Current Configuration** button: a *New Arrangement* will be added to the list.

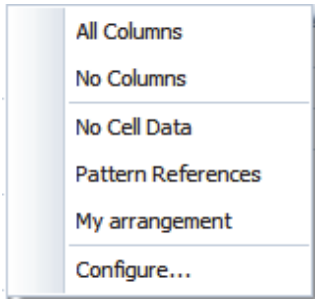


3. Enter the name for the *New Arrangement*.



4. Click the **Close** button.

5. The newly created column configuration is added to the arrangement list.



⇒ Deleting a column configuration

To delete a column configuration:

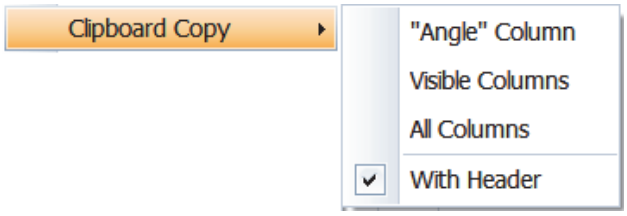
1. Select the column configuration in the list of the Column Configuration dialog box.
2. Click the **Delete** button.
3. Click the **Close** button.

⇒ Adding the default column configurations

Some default column configurations are proposed for each type of column view. To add them to the arrangement list:

1. Click the **Add Defaults** button (if the default column configurations are already in the list, the **Add Defaults** button is deactivated).
2. Click the **Close** button.

To copy the columns to the clipboard, click the **Clipboard Copy** command. The corresponding menu will be displayed:



The commands of the Clipboard Copy menu are described in the following table:

Command	Description
"*Column name*" Column	Click to copy the selected column to the clipboard
Visible Columns	Click to copy all the visible columns to the clipboard (all the rows are copied)
All Columns	Click to copy all the columns to the clipboard (all the rows are copied)
With Header	Select the **With Header** option to copy the columns with their header

The other commands available to customize the columns are described in the following table:

Command	Description
Sort Ascending	Self-explanatory
Sort Descending	Self-explanatory
Column Chooser	To choose the columns displayed in the column view. See below for details
Best Fit	Click to make the selected column fit the text
Best Fit (all columns)	Click to make all the columns fit the text

Using the Column Chooser

Click the **Column Chooser** command to display the Column Chooser box.

To remove a column from the table, click the column header and drag it to the **Column Chooser** box;
— or —
to add a column to the table, drag it from the **Column Chooser** box to the column header where it is to be inserted.

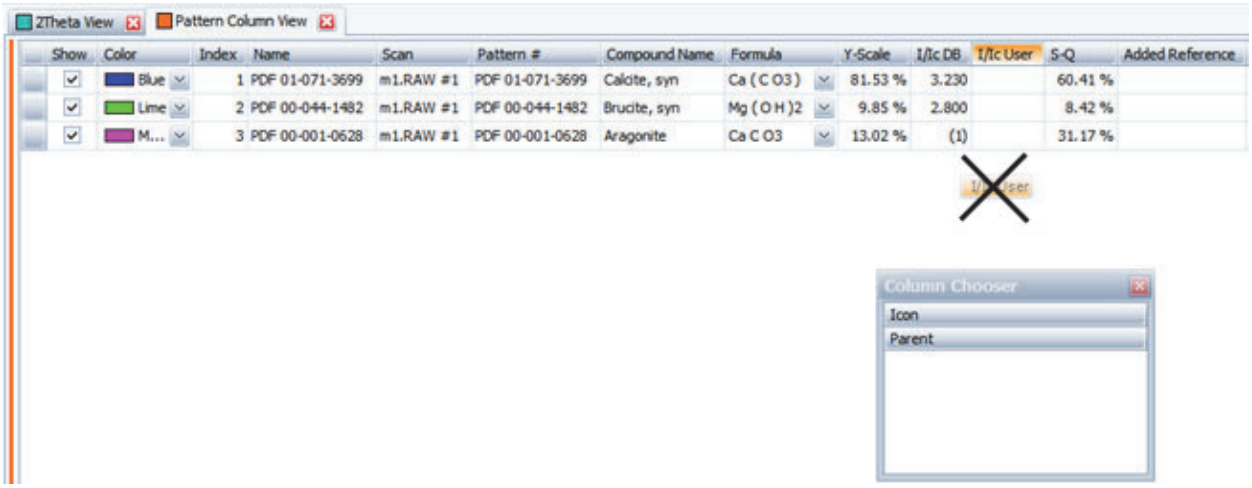


Fig.16: Removing the “I/Ic User” column from the Pattern Column View using the Column Chooser

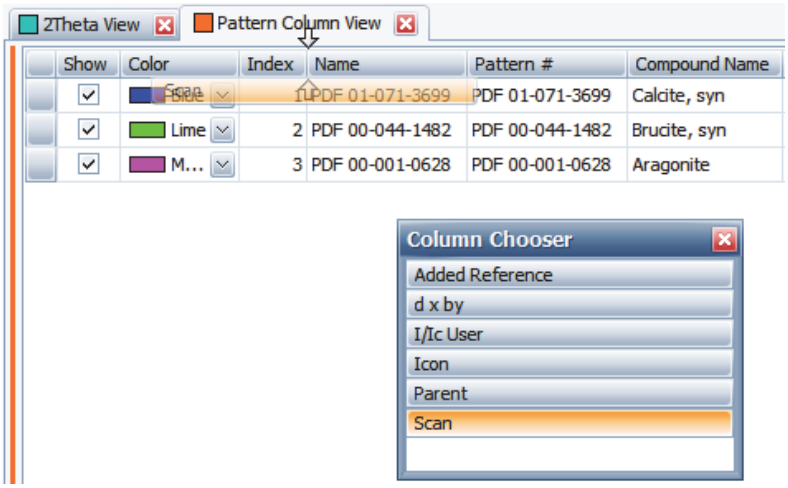


Fig.17: Adding the “Scan” column to the Pattern Column View using the Column Chooser

NOTE

Selected rows can be copied to the clipboard: right-click the corresponding empty column on the left to display the Copy Clipboard contextual menu. Then proceed as described for columns in the table above.
A manual multi-selection can be used for rows but not for columns.

Creating a DB View

A DB view or database view gives detailed information about a selected pattern.

To create a DB view:

1. Select the pattern of interest either in the data tree or on the graphical view.
2. Click **DB View** in the Create list of the Data Command panel
   — or —
   right-click and then click **Create** on the menu displayed**.** Click **DB View** on the submenu.

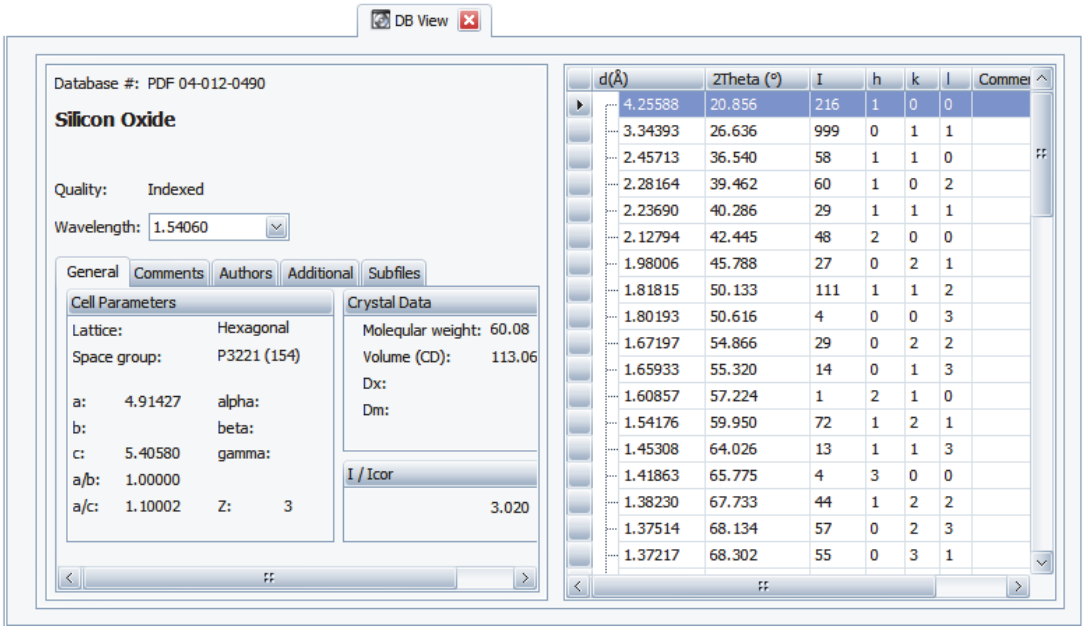


Fig.18: Example of a DB View

Creating a Chart View

A Chart view can be created from all possible data list nodes: Scan list, Pattern list, Element list…

1. Select the data list of interest in the data tree;
2. Click ***Data* Chart View** in the Create list of the Data Command panel
   — or —
   right-click and then click **Create.** Click ***Data* Chart View** on the submenu.

Creating a Document Log View

A scan view can be created to display the audit trail of the document. It gives a list of all actions performed in the current document as well as the user who performed these actions and when they were performed.

This feature is available from software version 3.1 up.

For this:

1. Select the document node in the data tree.
2. Click **Document Log View** in the Create list of the Data Command panel
   — or —
   right-click and then click **Create** on the menu displayed**.** Click **Document Log View** on the submenu.

View Properties

Graphical View Properties

1D View

The “Scans order” feature is available from software version 2.0 up.

Property	Description
Scale	
X-scale	Choose a unit for the X-scale
Y-scale	Choose a unit for the Y-scale
Y-scale projection	Select a Y scale projection
Wavelength	Wavelength forced for all the scans in the view. You can choose one in the predefined list. Enter a blank value to return to the default value
Zoom	
Left	Left position of the zoom area in X unit
Right	Right position of the zoom area in X unit
Top	Top position of the zoom area in Y unit
Bottom	Bottom position of the zoom area in Y unit
Zoom Add to Top (in %)	To set Y to the highest measured point available plus a given percentage
Zoom Add to Bottom (in %)	To set Y to the lowest measured point available plus a given percentage
Zoom Base Always Zero	To set the bottom of the working area to I = 0 (recommended). In case of a logarithmic Y-scale in counts, the base is not 0 but 1. In case of a logarithmic Y-scale in CPS, the base is 1 divided by the counting time per step
Zoom Always Fit Top	To adjust the top of the working area in order to fit the highest measured point available in the area
Zoom Always Fit Bottom	To adjust the bottom of the working area in order to fit the lowest measured point available in the area
Attributes	
Overview Auto-Hide	Select the check box to hide the Overview and only show it when the mouse is over its tab. (Selected by default)
Waterfall display	Select the check box to use the waterfall display
Waterfall Offset X	Enter the offset for the X axis in Waterfall mode in %.
Waterfall Offset X	Enter the offset for the Y axis in Waterfall mode in %.
Scans order	Select the data to use to sort the scans in the drop-down list
Reverse order	Select the **Reverse order** check box to reverse the scans order
Display Extended view	Select the check box to display the extended view
Display Stick View	Select the check box to display the stick view
Stick Length	Stick length in pixels (value from 4 to 30 pixels)
Stick Bold	Select the check box to display the stick in bold in the stick view
Grid Horizontal Lines	Select the check box to display a horizontal grid
Grid Vertical Lines	Select the check box to display a vertical grid
Grid Transparency (0-255)	Grid transparency value from 0 to 255

Property	Description
Attributes	
Toolbar Visible	Select the toolbar position in the drop-down list or **No** to hide it
Axis Visible	Clear the **Axis Visible** check box to remove the axis from the display
Match Coloration	Pattern coloration during a match, from gray to full color
Match Brightness	Pattern brightness during a match, from dark to light color
Scan Fill Color	Select the color used to fill each scan (from version 3.2 up) Choices are • Transparent • White • Scan color
Printing	
Printable	Select the check box to print the selected view
Paper orientation	Paper orientation: portrait, landscape or default. If the default option is selected, the paper orientation chosen in the print preview will be applied to the view.
Print size in x direction	Enter a print size for the X direction
Print size in y direction	Enter a print size for the Y direction
Stick view on top	Select the checkbox to add the stick view at the top of the view when printing
View	
Name	Name chosen for the view
Description	View description. Can be edited
Axis	
Left	Select the information to display for the left axis. See section “Creating Captions” on page 58 for more details
Left (display)	Display preview for the left axis
Bottom	Select the information to display for the bottom axis. See section “Creating Captions” on page 58 for more details
Bottom (display)	Display preview for the bottom axis
Legend	
Display Legend	Select the **Display Legend** check box to display the legend on the graphical view. (Selected by default)
Horz. Alignment	Select the type of horizontal alignment of the legend in the drop-down list
Vert. Alignment	Select the type of vertical alignment of the legend in the drop-down list
Background Color	Select a color for the background of the legend
Background Transparency	Enter the background transparency in %
Border Color	Select a color for the border of the legend box
Border Transparency	Enter the border transparency of the legend box in %
Text Color	Select the color of the text of the legend
Text Transparency	Enter the text transparency of the legend box in %

Property	Description
Font	Description of the font used for the legend. Click the + sign to access and define each font parameter
Name	Select the desired font in the drop-down list
Size	Enter the desired font size
Unit	Select the desired size unit
Bold	Select True in the drop-down list to set the text in bold
Italic	Select True in the drop-down list to set the text in italic
Strikeout	Select True in the drop-down list to strike out the text
Underline	Select True in the drop-down list to underline the text
Display Markers	Select the corresponding check box to display the objects markers in the legend box
Display Images	Select the corresponding check box to display the objects images in the legend box
Text Color as Object	Select the corresponding check box if the text should have the same color as the object it is related to
Border size in pixels	Size of the border of the legend box in pixels
All	Border size used for all the borders if the fields below are not modified afterwards. Enter the desired size in pixels

Left	Size of the left border
Top	Size of the top border
Right	Size of the right border
Bottom	Size of the bottom border
Max Lines	Enter the maximum of lines used for the legend

2D View

Property	Description
Attributes	
Scan Grid	Select the check box to display a scan grid
Grid Color	Select a color for the grid
Grid Transparency	Enter the desired value for the grid transparency
Intensity Map	Select the **Intensity Map** check box to display the intensity map
Levels	Select the **Levels** check box to display the levels
Smoothness	Select the type of smoothness in the drop-down list
Y-axis	Select the data to use to sort the scans on the Y-axis in the drop-down list
Reverse Y-axis	Select the corresponding check box to reverse the order of the scans on the Y-axis
Tooltip	Select the data to display for the Y-axis in the tooltip
Printing	
Printable	Select the check box if you want the selected view to be printed
Paper orientation	Paper orientation: portrait, landscape or default. If you select default, the paper orientation chosen in the print preview will be applied to the view
Property	**Description**
View	
Name	Name chosen for the view
Description	View description. Can be edited
Axis	
Left	Select the information to display for the left axis. See section “Creating Captions” on page 58 for more details
Left (display)	Display preview for the left axis
Bottom	Select the information to display for the bottom axis. See section “Creating Captions” on page 58 for more details
Bottom (display)	Display preview for the bottom axis

2D Frame View

Property	Description
Attributes	
Mirror Horizontal	If checked, the X-axis has reverse direction
Mirror Vertical	If checked, the Y-axis has reverse direction

Show Color Palette	Indicates whether the color palette should be displayed on the right side of the frame view (available from version 3.2 on)
Show Intensity Range	Indicates whether the intensity range should be displayed at the bottom of the frame view (available from version 3.2 on)
Printing	
Printable	Select the **Printable** check box to select the view to be printed
Paper Orientation	Paper orientation: either portrait or landscape
View	
Name	Name chosen for the view
Description	View description. Can be edited

Scan View

Property	**Description**
Printing	
Printable	Select the **Printable** check box to select the view to be printed
Paper Orientation	Paper orientation: either portrait or landscape
Font Header	To customize the font header displayed in the **Font** dialog box click the **Browse** button
Font Row	The font header in the **Font** dialog box can be displayed by clicking the **Browse** button
View	
Name	Name chosen for the view
Description	View description. Can be edited

Column view

Property	Description
Printing	
Printable	Select the **Printable** check box if the selected view should be printed
Paper Orientation	Paper orientation: portrait, landscape or default. If the default option is selected, the paper orientation chosen in the print preview will be applied to the view
Paper Full Width	Select the **Paper Full Width** check box to force the use of the paper full width when printing
Font Header	The font header in the **Font** dialog box displayed by clicking the **Browse** button can be customized. This can also be done using the fields described below
Vertical Table	Select the check box to permute columns and rows. The properties of the object list are then listed vertically and the objects horizontally. The resulting table can be viewed in the print preview
Vertical/Horizontal Drawing Style	Define which lines will be drawn when printing the table
Shaded headers	Select the check box so the headers will be shaded when printing the table
Font Header	To customize the font for headers, click the **Browse** button or use the fields described above
Name	Select the desired font in the drop-down list
Size	Enter the desired font size
Unit	Select the desired size unit
Bold	Select **True** in the drop-down list to set the text in bold
Italic	Select **True** in the drop-down list to set the text in italic
Strikeout	Select **True** in the drop-down list to strike out the text
Underline	Select **True** in the drop-down list to underline the text
Font Row	To customize the font for rows, click the **Browse** button or use the fields described above
Word wrapping	Select the type of word wrapping for the table text when printing
Column Layout	Select how the columns will be arranged when printing
Rightbound Table	Choose whether the table will be right bound for printing
Autosize Columns	Choose whether the columns size will be automatically adjusted for printing
Column Layout Vertical	Define the sizing of the columns in vertical tables when printing
First Column Width	Column width for the first column in a vertical table when printing
Next Columns Width	Column width for the other columns in a vertical table when printing
View	
Name	Name chosen for the view
Description	View description. Can be edited

DB view

Property	Description
Attributes	
Original	Clear the **Original PDF card** check box to display the user modified card
Printing	
Printable	Select the **Printable** check box to select the view to be printed
Paper Orientation	Paper orientation: either portrait or landscape
Paper Full Width	Select the **Paper Full Width** check box to force the use of the paper full width when printing
Font Header	To customize the font header displayed in the **Font** dialog box click the **Browse** button
Font Row	The font header in the **Font** dialog box can be displayed by clicking the **Browse** button
View	
Name	Name chosen for the view
Description	View description. Can be edited

Chart view

Property	Description
Attributes	
Type	Select the type of chart: either pie chart, bar chart or stack chart
Use as Legend	Select the data used as Legend: the horizontal axis for a bar chart, the sector legend for a pie chart
Use as Value	Select the data used as Value: the y axis or the sector size for a pie chart
Printing	
Printable	Select the **Printable** check box to print the selected view
Paper Orientation	Paper orientation: portrait, landscape or default. If the default option is selected, the paper orientation chosen in the print preview will be applied to the view
View	
Name	Name chosen for the view
Description	View description. Can be edited
Legend	
Font	Description of the font used for the legend. Click the + sign to access and define each font parameter

Grouping Views...

It is possible to group several views in a single tab. The views can be grouped vertically or horizontally. If there exist more than two views, they can also be grouped in an array or a grid.

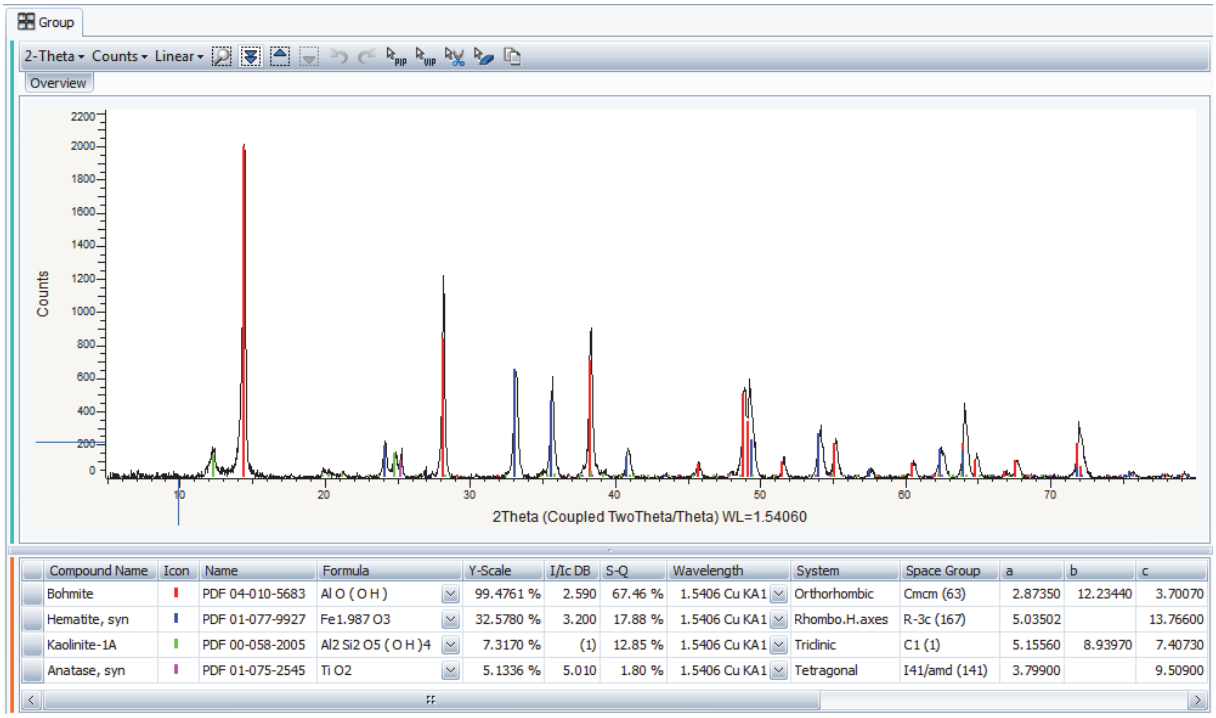
To group views:

1. Multi-select the views of interest in the Data Tree.
2. Click the **Vertical**, **Horizontal**, **Array** or **Grid** command in the Data Command Panel to group the views respectively vertically, horizontally, in an array or a grid
   — or —
   right-click the multi-selection and then click **Group** on the contextual menu**.** Click **Vertical**, **Horizontal**, **Array** or **Grid** on the submenu to group the views respectively vertically, horizontally, as an array or as a grid.

The grouped views become the children of a parent group in the Data Tree. The user can give this group a name by clicking it and entering a name in the **Name** field of the Group Property table.

To ungroup a group of views:

1. Select the group in the Data tree.
2. Click the **Ungroup** command in the Data Command Panel
   — or —
   right-click the multi-selection and then click **Ungroup** on the contextual menu.



Compound Name	Icon	Name	Formula	Y-Scale	I/Ic DB	S-Q	Wavelength	System	Space Group	a	b	c
Bohmite		PDF 04-010-5683	Al O (O H)	99.4761 %	2.590	67.46 %	1.5406 Cu KA1	Orthorhombic	Cmcm (63)	2.87350	12.23440	3.70070
Hematite, syn		PDF 01-077-9927	Fe1.987 O3	32.5780 %	3.200	17.88 %	1.5406 Cu KA1	Rhombo.H.axes	R-3c (167)	5.03502		13.76600
Kaolinite-1A		PDF 00-058-2005	Al2 Si2 O5 (O H)4	7.3170 %	(1)	12.85 %	1.5406 Cu KA1	Triclinic	C1 (1)	5.15560	8.93970	7.40730
Anatase, syn		PDF 01-075-2545	Ti O2	5.1336 %	5.010	1.80 %	1.5406 Cu KA1	Tetragonal	I41/amd (141)	3.79900		9.50900

Fig.19: Grouping two views horizontally

Panels

A brief description of the different panels is the content of this chapter.

The panels can be arranged as desired: they can be hidden and moved. See Section “Organizing the Workspace” on page 36.

Data Command Panel

The data command panel groups all the commands available for the selected data or view.

It includes:

- basic commands such as the Delete command;
- commands to create different types of views such as a Column view;
- tools to perform operations on the data such as peak search.

This command panel is made of several “boxes”. Each “box” is composed of a title bar and a list of commands. You can hide the list of commands of a box by clicking the **Hide/Display** button ( ) below.

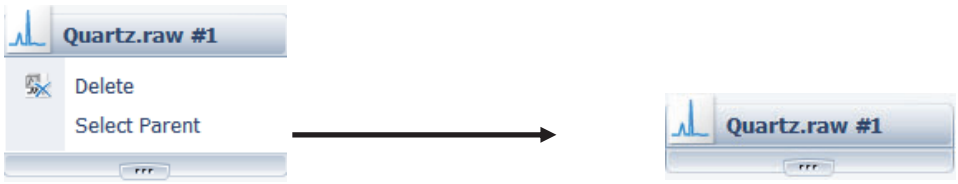
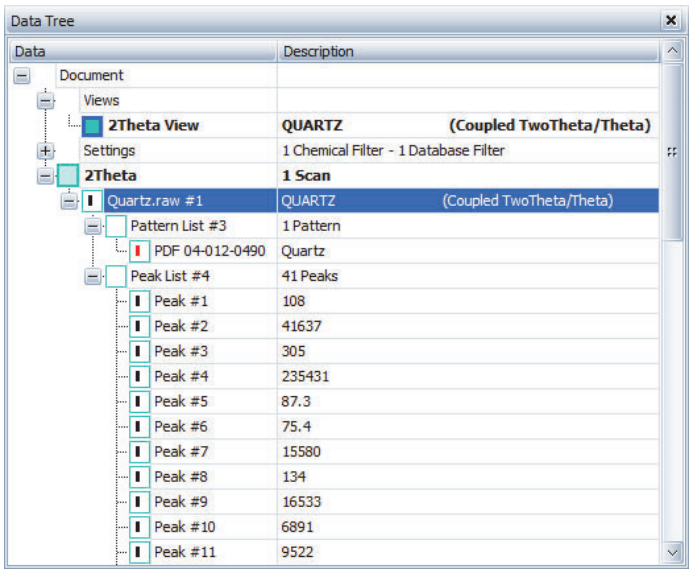


Fig.20: Hiding a list of commands

To show the commands, click the **Hide/Display** button again.

Data Tree Panel

The different types of data and views are listed in the same panel and organized in tree form as shown below:



The current document is the base of the tree. Then the tree is separated into three branches:

- The Views branch which lists the document views: graphical views, column views, DB views etc…
- The Parameters branch which lists the document chemical and database filters
- The Data branch which lists the document data: scans, patterns, peaks, levels etc…

The data are arranged according to their dependent data. The terms “Parent” and “Children” are used. For example, a peak list has a scan as parent and all the peaks as children.

To select the Parent or Children data of an item the user can either:
click **Select Parent**, and then **Select Children**, in the Data command panel
— or —
right-click the item to display the related menu and click **Select Parent**, and then **Select Children**.

A color coding shows the connection between data and views.
Each view (graphical view, column view or chart view) is given a color. A color dot is displayed before the view name in the view tab and data tree but also before the related data in the data tree. Additionally, a color line is displayed on the left of the general view.

Automatic Display of Views

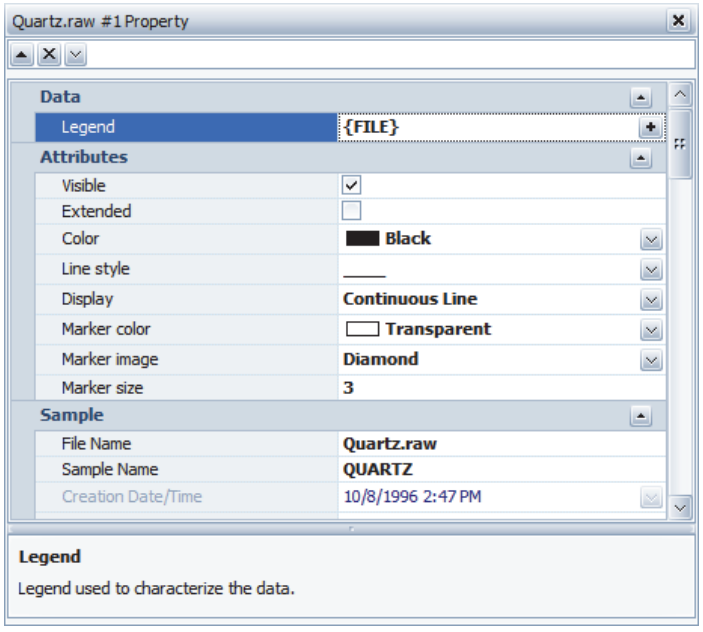
Managing a multitude of data and views can make the user interface complicated. Therefore an automatic display of views depending on the selection in the data tree is implemented.

When data are selected, all related views are automatically displayed and marked bold in the tree. Similarly, when a view is selected, the related data node is marked bold in the tree.

In contrast to the Windows tree view implementation the selection in DIFFRAC.EVA is not removed when clicked elsewhere.

Property Panel

The property panel displays the selected data or view properties in detail.



When selecting data, only the corresponding data properties are displayed in the Property panel. When selecting a view, only the corresponding view properties are displayed in the Property panel.

The properties can either be viewed or modified.

Editing Multiple Properties

It is possible to display and modify properties common to the same type of data. If a property is modified, the change will be applied to all the selected data. For this:

1. Select the desired data (they must be of the same type, for example, several scans). You can use the **Select Children** command to make sure that only data of the same type are selected.

2. Select the **Edit multiple properties** check box in the Property Panel. Properties common to the data will be displayed.

NOTE

If the selected data nodes are not all of the same type (for example, scans with peaks or patterns as children), the **Edit multiple properties** check box will be available but editing of multiple properties will not be possible. No property will be displayed.

Organizing the Workspace

All the panels are dockable and can be easily hidden, displayed and moved, which allows the organization of the workspace as desired.

NOTE

The Search/Match dialog box behaves the same way as the panels. It can be docked and use automatic hiding functionality as usual panels.
It can prove useful when the user often performs Search/Match operations.

Hiding Panels

Panels can be removed from the screen and then displayed again whenever required.
To remove a panel:
Click its close button ( )
— or —
click the corresponding **Show/Hide panel** button on the toolbar
— or —
Use the dedicated shortcut key. See “Shortcut Keys for Panels” on page 206.

To show a hidden panel, click again the corresponding **Show/Hide panel** button or use the dedicated shortcut key.

Managing the Dockable Windows

Docking operations use drag-and-drop. Dragging can be initiated in the caption area of a dock panel or in its corresponding tab.

The panels can be docked to the top left, bottom or right edge of a form.

When a panel is dragged, docking markers appear and indicate the sides of the targeted panel where it is allowed to be docked.

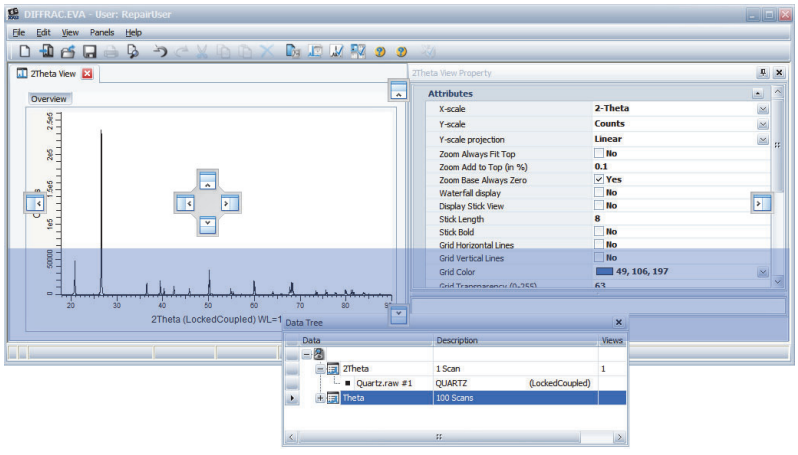


Fig.21: Docking a panel

Fig.22: Docking markers

If the panel is dropped on one of the outer markers, a split container will be created on the corresponding side of the targeted panel.

If the panel is dropped on the middle marker, a tab container will be created.

See the examples below.

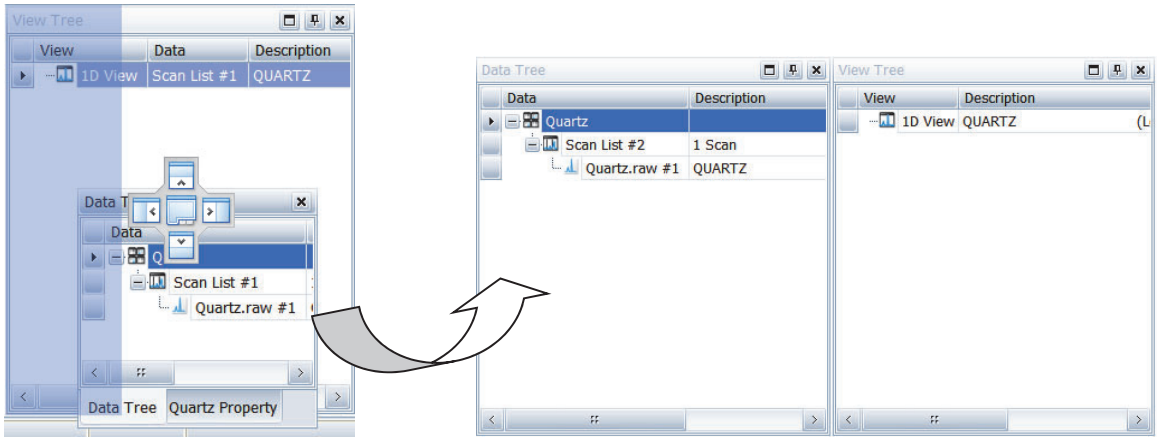


Fig.23: Creating a horizontal split container consisting of two dock panels.

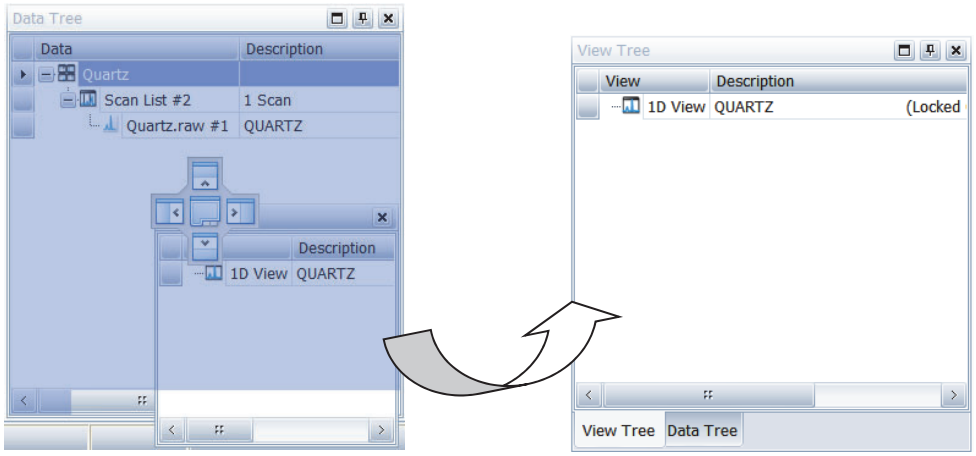


Fig.24: Creating a tab container.

Making a Panel Float

A dock panel is floated if it is not docked to a form or to another panel.

To make a panel float it can be either:
dragged from the control it was docked to
— or —
double-clicked on its caption. If it is double-clicked on the panel's caption a second time, the dock panel is restored to its previous position.

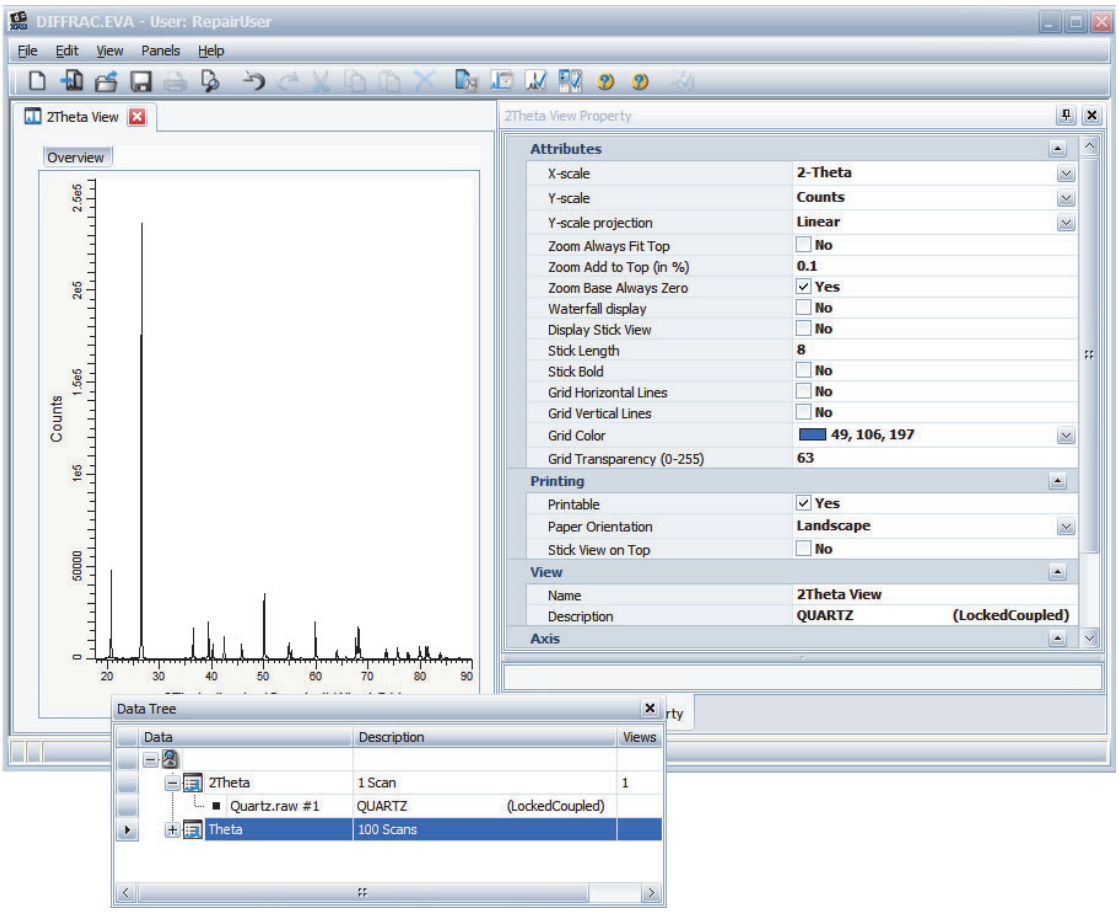


Fig.25: Making a panel float

NOTE

Floating panels can be used in multi-monitor setups to move parts of the user interface to other monitors.

Automatic Hiding Feature

With the automatic hiding feature, a panel can be automatically hidden when the mouse pointer leaves its area. Only the panel's label will be displayed at the form's corresponding edge.

To enable this feature, click the **Auto-hide** button ( ) displayed within the panel's caption.

To show the hidden dock panel, point to its label.

To deactivate the feature, click the **Auto-hide** button ( ) again.

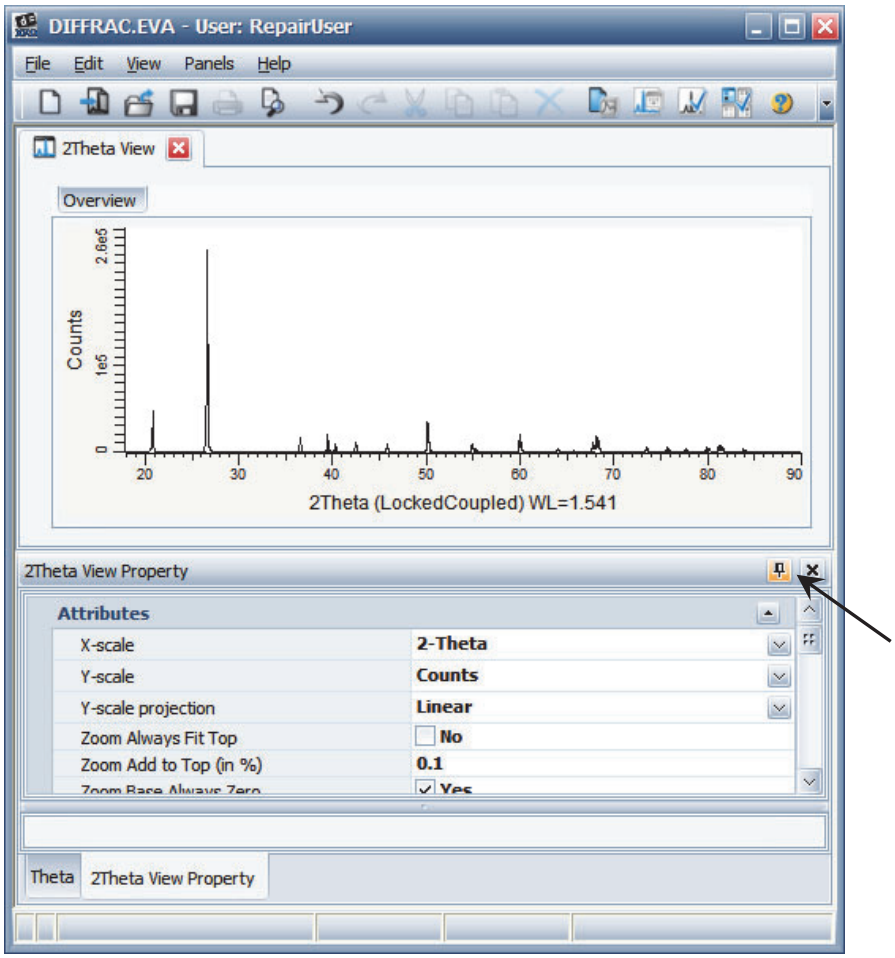


Fig.26: Clicking the Auto-hide button

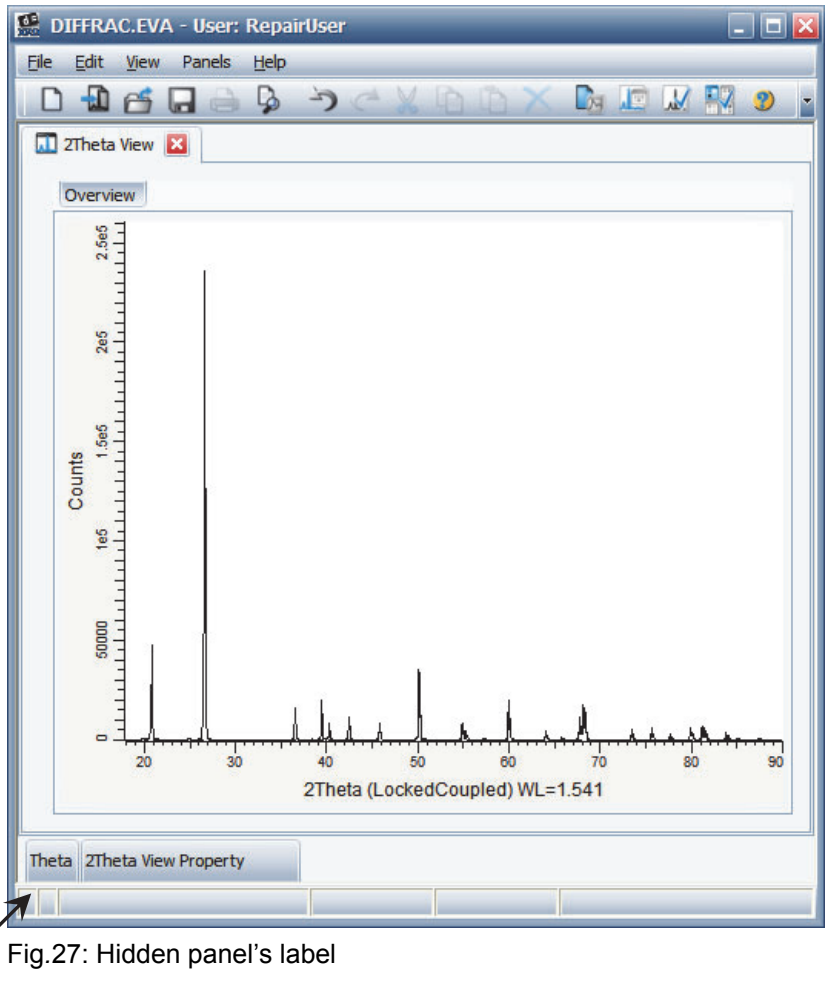


Fig.27: Hidden panel's label

Saving the Workspace Layout

This feature is available from software version 4.0 up

By default, the workspace layout is saved when closing EVA. When restarting EVA, the workspace layout will be the same as when it was closed.

NOTE

In case, the layout is not saved by default, the access permissions should be checked for the folder "C:\Documents and Settings\your_user_name\Application Data\BrukerAXS\" in Windows XP or the folder "C:\Users\ your_user_name\AppData\Roaming\Bruker AXS" in Windows 7. The user must write and modify permissions for this folder. As soon as these permissions have been acquired, the program's layout should be maintained between sessions. If the user still cannot access the folders, the hidden folders must be made visible.

To acquire the necessary permissions, open the folder's context menu and click **Properties** located on the **Security** tab of the Properties dialog. There should be a list of users and their corresponding permissions. Set check marks on **Full Control** or at least **Write** and **Modify**.

The workspace can also be saved. It can be, for example, used to transfer the layout between installations. To save the workspace layout:

1. Click **Save Layout…** on the **Tools** menu.
2. Browse the desired folder and enter a name for the Layout file (.EVAPlugin.V4.Layout_*.xml file).

3. Click **OK** to save the layout.

To load a previously saved layout:

1. Click **Load Layout…** on the **Tools** menu.
2. Browse for the EVA Layout File (.EVAPlugin.V4.Layout_*.xml file) and click **OK.** The layout will be applied.

Different Ways to Perform an Operation

There are different ways to perform an operation.

- Click the object of interest either in the Data tree or on the graphical view. Then click the desired command in the Data Command Panel.
- Right-click the object of interest either in the Data tree or on the graphical view and click the desired command on the contextual menu displayed.

The ways to proceed will be detailed again each time an operation will be described.

The user can work with a 1D view only, without any trees or panels. All commands can be accessed by right-clicking the object of interest.

NOTE

It is possible to perform an operation directly on a pattern selected in the candidate list.
To do so :
Right-click the row of the selected pattern to display the contextual menu and click the desired command.

Handling the ICDD Database Licenses

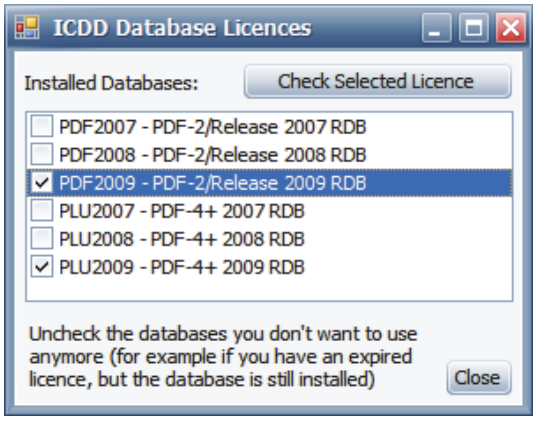


Fig.28: ICDD Databases Licences dialog box

The ICDD Databases Licenses dialog box gives the list of the installed databases and makes it possible to check the corresponding licenses.

To open it:

ICDD RDB Databases button

1. Click the **ICDD RDB Databases** button on the toolbar.
   —or—
   Click the **ICDD RBD Databases** command on the **Tools** menu.
2. Click the **Check Selected License** button to check the selected license information.
3. Clear the check boxes of the obsolete databases.

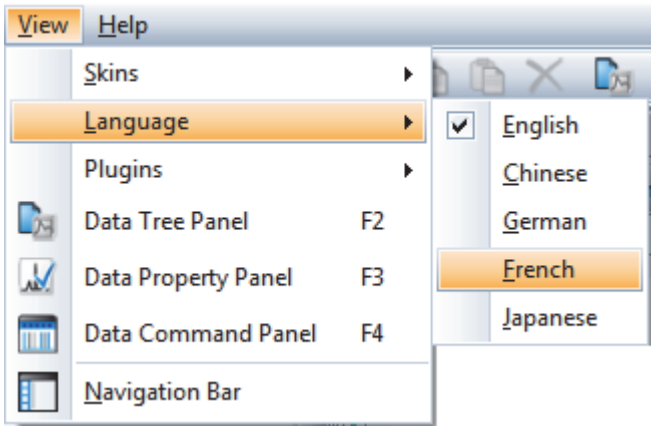
Setting the Language

DIFFRAC.EVA is available in different languages.

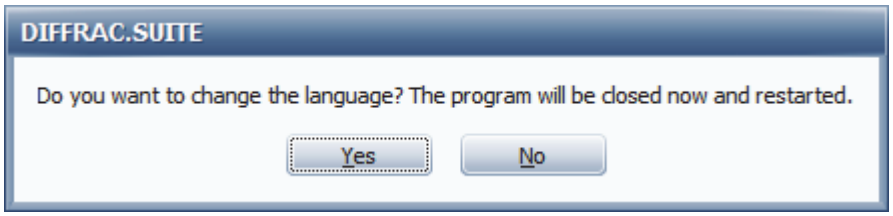
By default, DIFFRAC.EVA will open in the language which has been set by the operating system's used regional settings or in English if the language is not available.

To change the language used:

1. On the **View** menu, select **Language** and then the desired language among those available.



The program will ask you to confirm.



2. Click **Yes**. The program will be closed and restarted in the selected language.

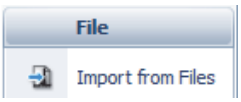
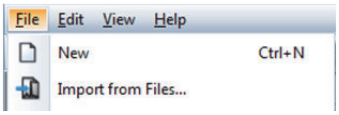
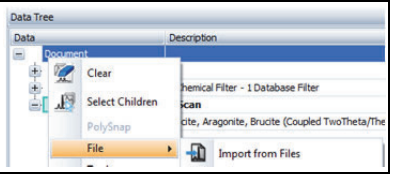
Working with EVA Documents

Creating EVA Documents and Importing Scans

To create a new EVA document, click **New** on the **File** menu or the **New** button on the toolbar. An empty EVA document will be displayed.

To import a scan file (either .BRML or .RAW file):

1. Choose one of the ways to proceed described in the table below:

Description	Illustration
Click the **Import from files…** button on the toolbar	
Click **Import from files…** in the Data command panel	
Click **Import from files…** on the **File** menu	
Right-click a Document or a Scan list in the data tree to display the related menu. Then in this menu, click **Import from files…**	

2. Locate the data .BRML or .RAW file to be imported in the directory containing the raw data files.

3. Click **Open**.

The selected scan is displayed in the graphical view and listed in the Data tree. If the raw data file is a multi-range, each range corresponds to 1 scan. All of the scans are displayed in the graphical view as well as in the Data tree.

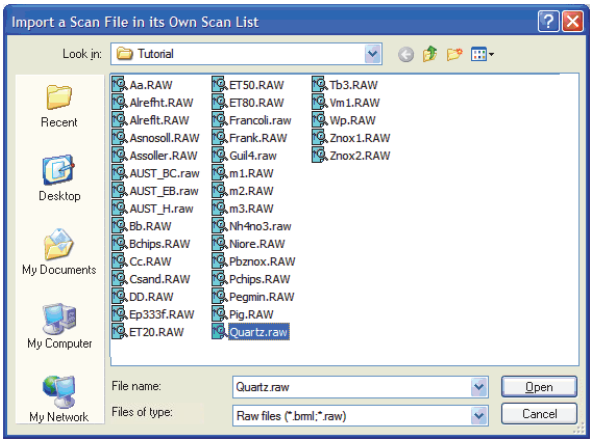


Fig.29: Import from files dialog box

Opening the BRML and RAW files by a double-click

This feature is available from software version 2.0 up

BRML and RAW files can be directly opened by a double-click in Windows Explorer.
It may be necessary to link the files with the program. For this:

1. Right-click the in Windows Explorer.
2. Click the **Open with | Choose default program…** command.
3. Browse for the program "EVALauncher.exe".
4. Click **OK.**

Importing Scans from the DIFFRAC.SUITE Database

Scans can be imported from the DIFFRAC.SUITE database. To do so, select use **the Import from database** button/command instead of the **Import from files** button/command.

Importing Several Scans at the Same Time

To import several scans at the same time, open the **Import a Scan File** dialog box and proceed as described:

1. Click the first scan to import.
2. Press **CTRL** while clicking on the other scans separately.
3. Click **Open**.

The imported scans are displayed in the graphical view and listed in the Data tree.
When the imported files contain only single scans which were measured with the same scan axis, one scan list containing all scans will be created. If they were measured with multiple scan axes, multiple scan lists will be created.
When at least one file among the imported files contains multiple scans, one scan list for all scans with the same scan axis will be created, regardless if the files contained single or multiple scans.

Once imported into the document, the scans become individual data objects.

NOTE

When importing 2θ scans measured with a wavelength different from that of the first scan in the scan list (in which the import is carried out), the newly imported scans are recalculated according to the wavelength of the first scan in the list. Two transformations are carried out: First in d and then in 2θ for the wavelength of the first scan in the list.

The wavelength which is used to display all scans is indicated in the view's property: "Wavelength".

Saving EVA Documents

To save the EVA document:


Save button

1. On the **File** menu, click **Save As**
   —or—
   click the **Save** button on the toolbar.
2. Specify a name for the active EVA document in the **File Name** field. The file name proposed by default is that of the first imported scan.
3. Click **Save**.

Opening EVA Documents

The best way to open an EVA document is to use the **Open** dialog box as follows:


Open button

1. On the **File** menu, click **Open**
   — or —
   click the **Open** button on the toolbar.
2. Click the desired file.
3. Click **Open**.

Opening the EVA files by a double-click

This feature is available from software version 2.0 up

EVA files can be directly opened by a double-click in Windows Explorer.
It may be necessary to link the files with the program. For this:

1. Right-click the in Windows Explorer.
2. Click the **Open with | Choose default program…** command.
3. Browse for the program "EVALauncher.exe".
4. Click **OK.**

Opening DIFFRAC^{plus} EVA Documents: Automatic Conversion of DIFFRAC^{plus} EVA Document Files (*.eva) into DIFFRAC.EVA Document Files

This feature is available from software version 2.1 up

DIFFRAC.EVA can read DIFFRAC^{plus} EVA files without a separate conversion step. If the software detects the old file format it converts the file content and creates a new document named similar as the old document with the addition “- converted” in the file name. This prevents an accidental overwrite with the File|Save command. The original EVA document will be preserved.

There is no one-to-one equivalency between data objects and their properties in DIFFRAC^{plus} EVA files and DIFFRAC.EVA files. The following objects will be converted:

- Scans
- Patterns
- DIFs
- Peaks
- Areas
- Labels

DIFFRAC.EVA tries to match the PDF information of imported patterns to the currently installed PDF database, if available. If a match could not be achieved, the pattern is imported as DIF with the PDF number in brackets.
In a first step the long PDF numbers XX-XXX-XXXX are matched exactly to all installed databases. If no match is found and if the number starts with 00-0 the three zeros are removed and a second match is attempted in case there is an older PDF database installed that could accept it. Finally, the first three digits XX-X are removed, and another match is attempted for older databases with short number schemes but only for strictly identical chemical formulas. This is to avoid potential conflicts with identical short numbers used for different cards.

The stick intensities are treated as in DIFFRAC^{plus} EVA. The background display for the converted scans is now always "Original" by default. This was implemented to have an identical display compared to a DIFFRAC^{plus} EVA document, but also to match exactly DIFs or patterns that could have been carefully scaled to match the scan. "Original" should reproduce exactly the display and the matching stick heights.

Labels are treated like peaks in DIFFRAC.EVA. To differentiate them from peaks they are imported into a separate peak list.

Palettes and automatic display of 2D views are not supported.

Zooming in the EVA Document

Move the cursor to one end of the targeted zoom area, press and hold the left mouse button while dragging the mouse until the cursor reaches the opposite end, then release the button.

The zoom area can be adjusted and moved easily in the overview.

NOTE

Move the cursor from the left to the right; otherwise a zoom reset will occur.

To return to the complete view:

Zoom reset button

Click the **Zoom reset** button on the view toolbar.
—or—
right-click anywhere on the graphical view and click the **Zoom Reset** command on the contextual menu.

To undo or redo a zoom:

Zoom Undo and **Redo** buttons

Click the **Zoom Undo** or **Zoom Redo** button on the view toolbar.
—or—
right-click anywhere on the graphical view and click the **Zoom Undo** or **Zoom Redo** command on the contextual menu.

Setting automatically Y when zooming

When zooming, Y will be set automatically in order to fit the highest or lowest measured point available. This mode can be selected as a default setting with the **Zoom Always Fit Top** or **Zoom Always Fit Bottom** check box in the View property table. Y can also be set to the highest or lowest measured point available in addition to a given percentage. The given percentage must be specified in the **Zoom Add to Top (in %)** or **Zoom Add to Bottom (in %)** text field in the View property table.

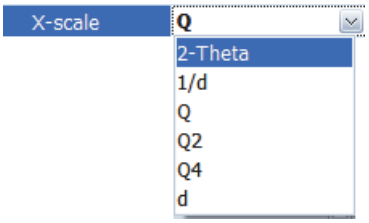
Changing Scales

Scales can be changed in the 1D view property table or in the view toolbar.

Changing the X and Y Scales

The X-scale is fixed according to the scanning drive of the scans in the 1D view (it is not possible to compare scans measured with different drives; they are listed in different scan lists).

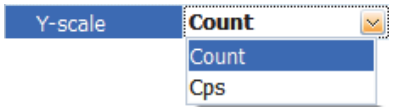
- Scans measured in 2θ can be displayed in 2θ, $1/d$, Q (with $Q=2\pi/d$)), $Q2$, $Q4$ and d
- Rocking curves (θ scan)
- Chi scan
- Phi scan
- X scan
- Y scan
- Z scan



The $1/d$ scale permits the user to compare 2θ scans measured with different wavelengths. The scans look very similar with the usual 2θ scale.

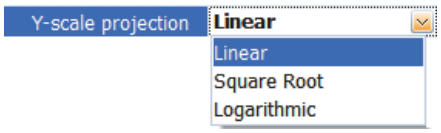
The d scale is linear in $1/d$, but labeled in d for convenience (a scale linear in d is not useful).

Two Y units are available: Counts and Counts per second (Cps). Selecting the X- and Y-coordinates affects the printout of the plot, but not the results of the Area computations (these are given in both 2θ and d units, and always in Cps).



Changing the Y Scale Projection

You can choose a linear, square root or logarithmic Y-scale.



Extending the X-scale

It is possible to extend the X-scale on the right or on the left of the graphical view.
To do so:

- Right-click the graphical view and drag the mouse pointer (the mouse pointer will become a hand) to extend the X-scale as much as desired on the left or on the right.

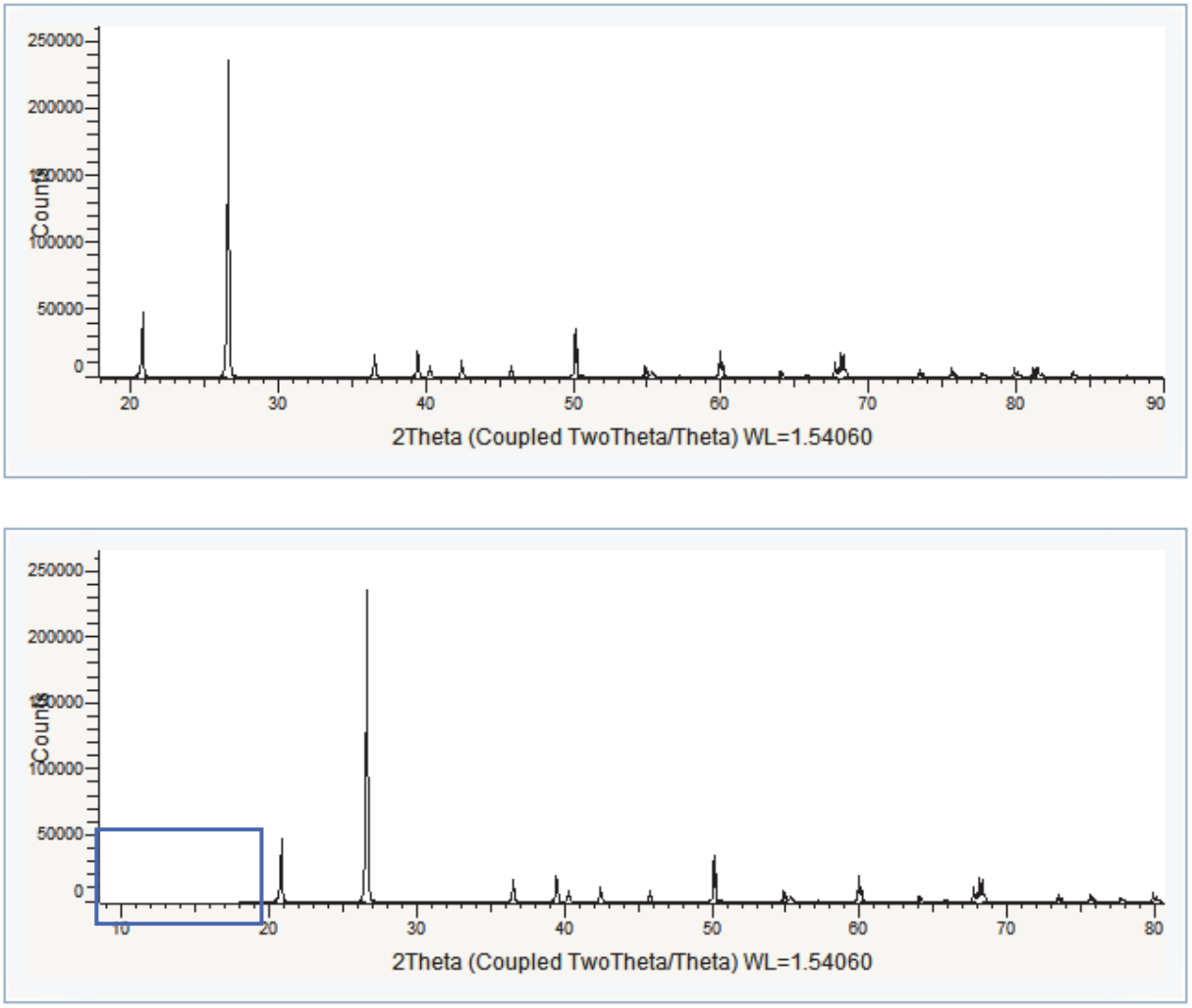
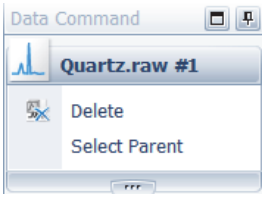
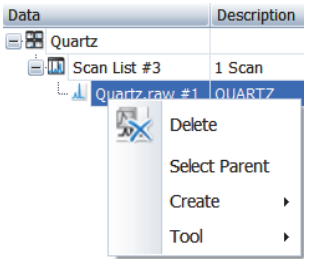


Fig.30: General view before and after extending the X-scale on the left

Deleting an Object

To delete an object in EVA: a scan, a pattern, a peak or a view, etc. Once the object has been selected either in the Data tree or on the graphical view, one method among those described below should be chosen.

Description	Illustration
Click **Delete** in the Data command panel	
Right-click to display the object related menu and then click **Delete**.	

Performing an Action on Several Objects at Once

It is possible to perform an action[2] on several objects at once. For example, Kα_2 Stripping can be computed on several scans at once.

If the action on multiple objects does not make sense it cannot be accessed. For example, a Search / Match operation cannot be performed on several scans at once. Such a command is deactivated if more than one scan is selected.

To perform an action on several objects at once, use the Windows multi-selection to select the objects of interest in the Data tree. Then proceed as for a unique object for the desired action.

Displaying the Legend

A legend can be displayed in the graphical view. It shows the scans and patterns displayed in the graphical view.

To display the legend, select the **Display Legend** box in the View Property table. The legend display can be modified in this same table. See "View Properties" on page 25.

[2] An action is a generalized command. It can be executing a command or invoking a tool on data or view objects.

Undoing an Action

To reverse actions performed during the current session, either:


Undo button

Click the **Undo** button on the toolbar
— or —
click **Undo** on the **Edit** menu.

An undone action can be redone. To do so:


Redo button

Click the **Redo** button on the toolbar
— or —
click **Redo** on the **Edit** menu.

Working with PIP and VIP views

Creating a PIP View

To create a PIP (picture in picture) view:

PIP mode button

1. Click the **PIP mode** button on the view toolbar
   — or —
   right-click anywhere on the graphical view to display the context menu. In the context menu, click the **PIP Mode** command.
2. A **PIP** text box will open.
3. Select the zone of interest: a window corresponding to the selected zone is created.

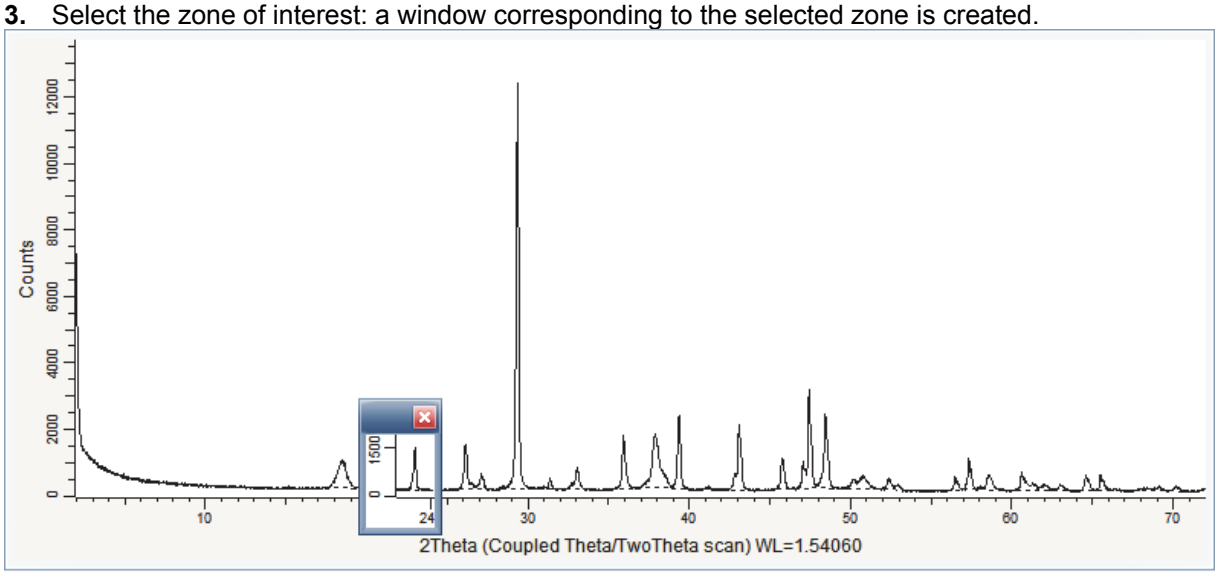


Fig.31: Creating a PIP view

4. Move and resize the window if necessary.
5. Once the PIP view is satisfactory, click anywhere on the graphical view. The PIP view is inserted into the graphical view and is by default linked to the corresponding zone in the scan.

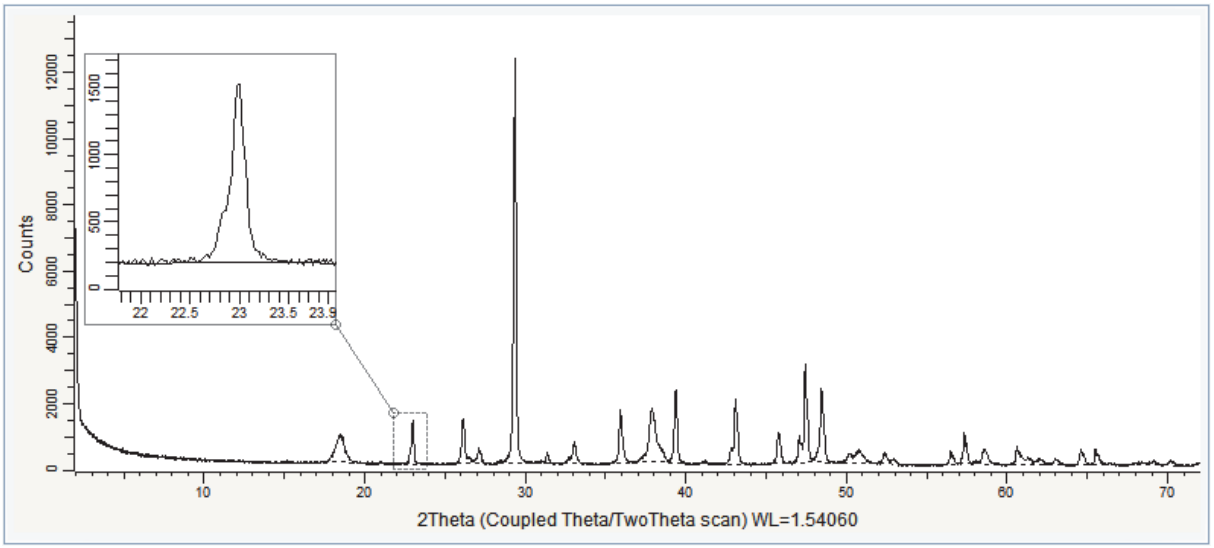


Fig.32: PIP view inserted and linked to the original zone

Creating a VIP View

To create a VIP (vertical in place) view:

VIP mode button

1. Click the **VIP mode** button on the view toolbar
— or —
right-click anywhere on the graphical view to display the context menu. In the context menu, click the **VIP Mode** command.

   A **VIP** text box will open.

2. Select the zone of interest: the VIP view editor is displayed.

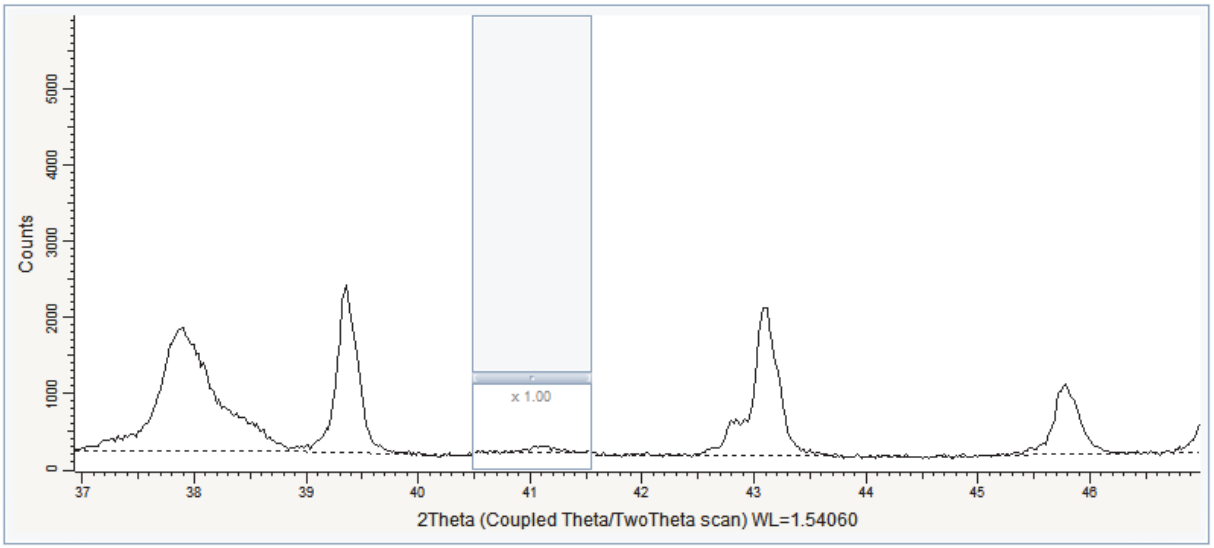


Fig.33: Creating a VIP view

3. Move the scale bar up or down to adjust the scale factor as you wish.

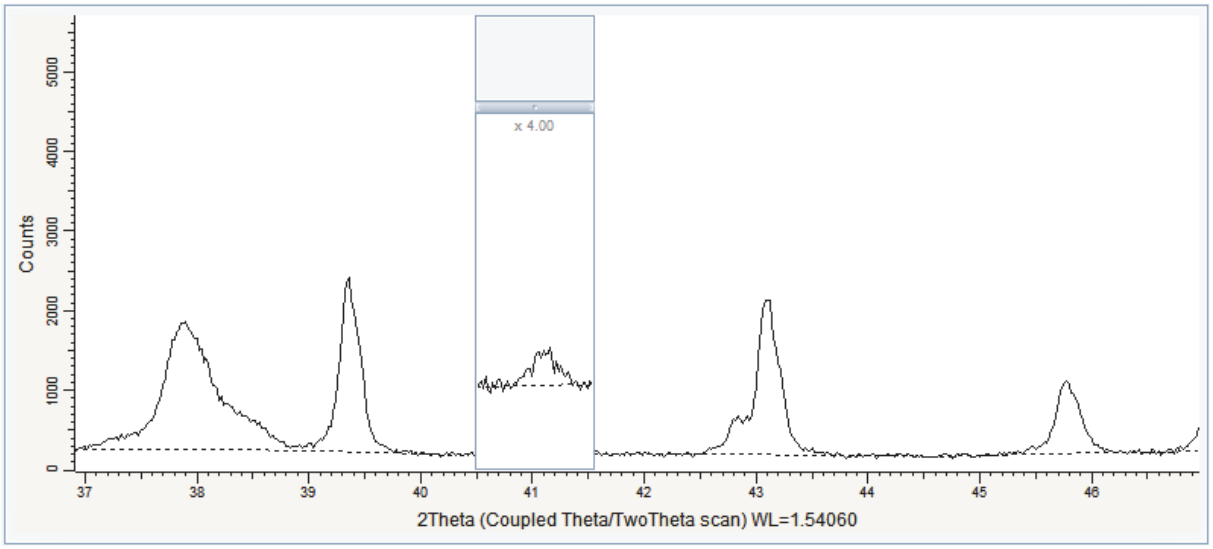


Fig.34: Changing the scale

4. To insert the VIP view in the document, click anywhere on the graphical view.

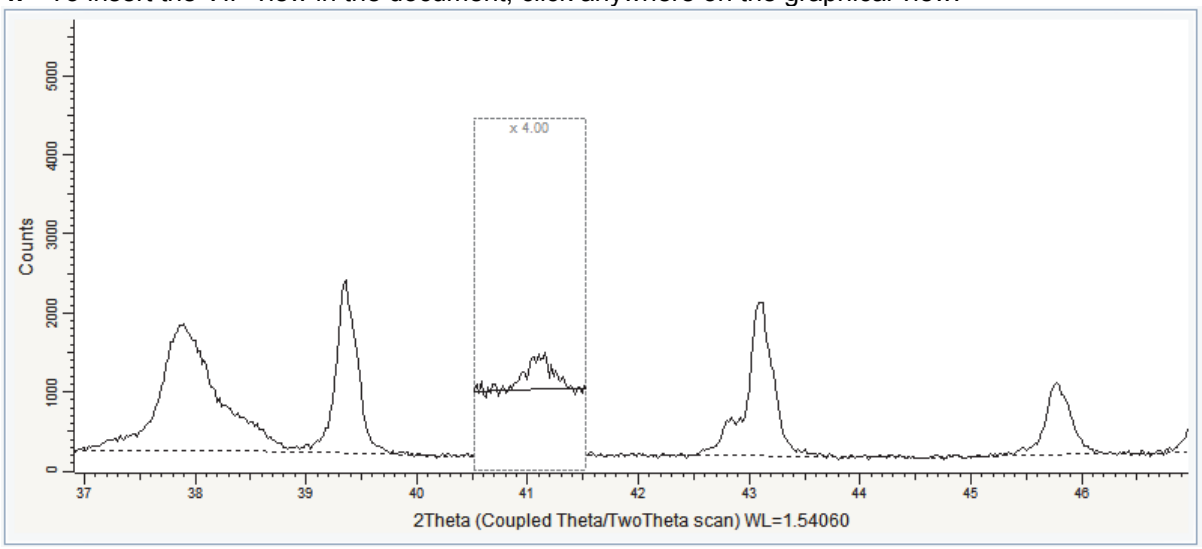


Fig.35: VIP view inserted into the graphical view

Deleting or editing a PIP or VIP View

To delete a PIP or VIP view:

1. Right-click the view of interest.

2. On the context menu, click **PIP** or **VIP** to display the relative sub-menu.

3. Click either **Edit** or **Delete** to edit or delete the view.

PIP/ VIP View Properties

You can view and/or modify the properties of the PIP and VIP views in the PIP or VIP property table. Click the PIP or VIP view to display the corresponding properties.

PIP properties

Property	Description
Attributes	
Borders and Link Color	Select a color for the borders and the link in the drop-down list
Borders and Link Transparency	Enter the desired transparency percentage for the borders and the link
Link	Select the **Link** check box to display the link between the PIP view and the original zone
Background Color	Select a color for the background in the drop-down list
Background Transparency	Enter the desired transparency percentage for the background
Position	
Left	Start value for the X-axis of the PIP view (X unit)
Right	End value for the X-axis of the PIP view (X unit)
Top	Start value for the Y-axis of the PIP view (Y unit)
Bottom	End value for the Y-axis of the PIP view (Y unit)

VIP properties

Property	Description
Attributes	
Borders Color	Select a color for the borders in the drop-down list
Scale Color	Select a color for the scale in the drop-down list
Borders Transparency	Enter the desired transparency percentage for the borders
Background Color	Select a color for the background in the drop-down list
Background Transparency	Enter the desired transparency percentage for the background
Position	
Left	Start value for the X-axis of the VIP view (X unit)
Right	End value for the X-axis of the VIP view (X unit)
Scale	Current scale factor: enter the desired value

NOTE

After clicking a PIP or VIP view its properties are automatically displayed. To come back to the object's properties which were shown before, click the object, for example a scan, in the data tree.

Minimizing a Tool Dialog Box

It is possible to minimize a tool in order to save space.

To do so:

- Double-click the title bar of the dialog box to be minimized.

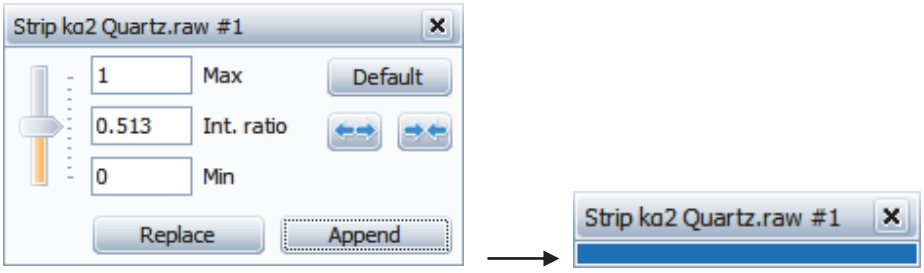
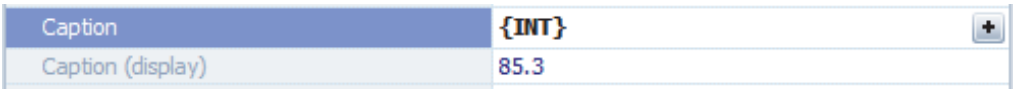


Fig.36: Minimizing a tool dialog box

To restore it, double-click the title bar again.

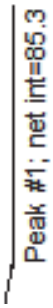
Creating Captions

It is possible to customize the information used to characterize some data. For example, the caption used by default for a peak is the net intensity of the peak. The parameter {INT} is selected for the property Caption in the Peak Property table as shown in the example below.

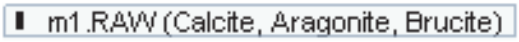


For each type of data, some parameters are defined by default. However, it is possible to set a user defined caption to characterize the data.
The parameters proposed for each type of data can be used.
For this, click the “+” button on the right of the field. A list with all the parameters available for the data will be displayed. Select a parameter in the list to add it to the caption.
Individual text can be combined with the predefined parameters.

Example #1:
To define a peak with its peak number and its net intensity separated by a semi-colon and using additional text, one possibility is: Peak #{NDX}; net int={INT}; where {NDX} gives the index and {INT} the net intensity.



Example #2:
To define the legend of a scan in the graphical view with the file name and the sample name between brackets, enter: {FILE} ({NAME}); where {FILE} gives the file name and {NAME} the sample name.
The resulting legend is



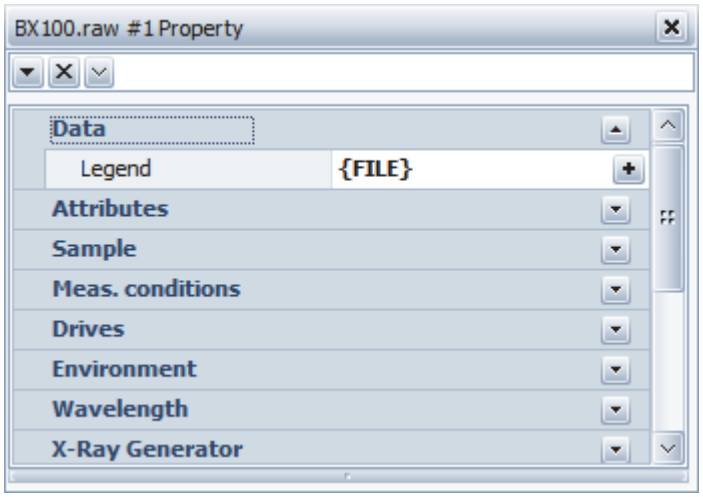
Filtering/Sorting Properties

The properties contained in the data property table or in the view property table can be filtered, grouped or ordered alphabetically.

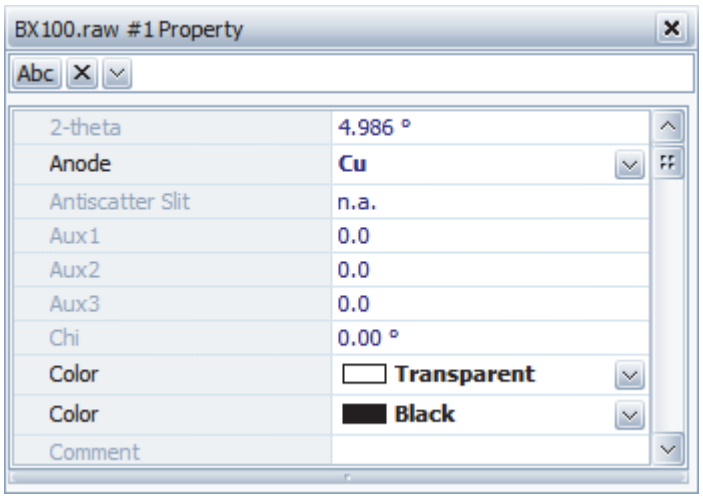
In the property table, the properties are sorted in several “groups”. For example for a scan, there are the “Data” group, the “Attributes” group, the “Sample” group, the “Measurement Conditions” group, etc.

It is possible to hide the properties and display only the group names or to order all the properties alphabetically.

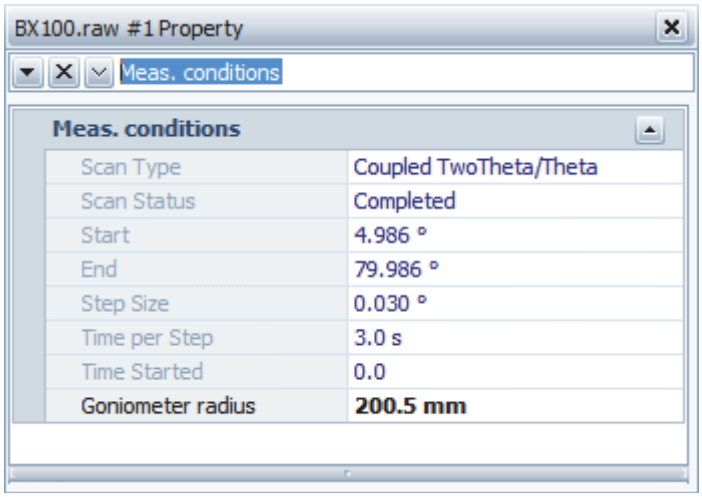
To display only the group names without the corresponding properties, click the arrow button at the top left of the property table.
Then each group’s properties can be displayed by clicking the drop-down button at the right of the group name.



To order all the table properties alphabetically, click again the arrow button until it is changed into the Abc button.



It is also possible to filter the properties by group name. To do so:
Click the drop-down button and select a property group name in the drop-down list. Only the corresponding properties will be displayed.



To cancel this filtering, click the cross button and all the property groups will be displayed again.

EVA Settings

Settings button

The Settings dialog box permits customizing the EVA working environment. Access the settings using the Menu **Panels | Settings...**, or the shortcut button.

This feature is available from software version 4.0 up

The settings can be saved into a XML file to be loaded later. It can be, for example, used to transfer the settings between installations. To save the settings:

1. Click **Save Settings…** on the **Tools** menu.
2. Browse the desired folder and enter a name for the EVA Settings file (.EVAPlugin.V4.Defaults.xml file).
3. Click **OK** to save.

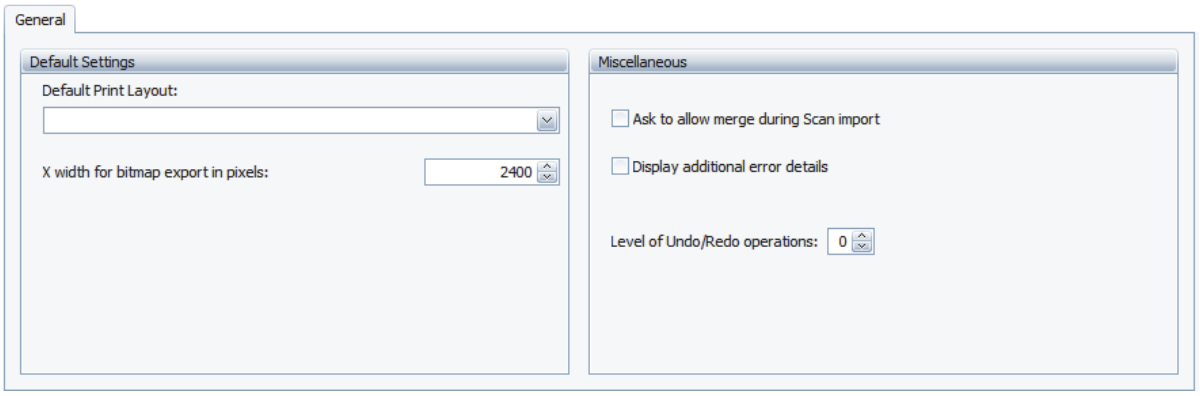
To load previously saved settings:

1. Click **Load Settings…** on the **Tools** menu.
2. Browse for the desired Eva Settings File (.EVAPlugin.V4.Defaults.xml file) and click **OK.** The settings will be applied to new documents.

General Tab

This tab is available from software version 3.2 up.

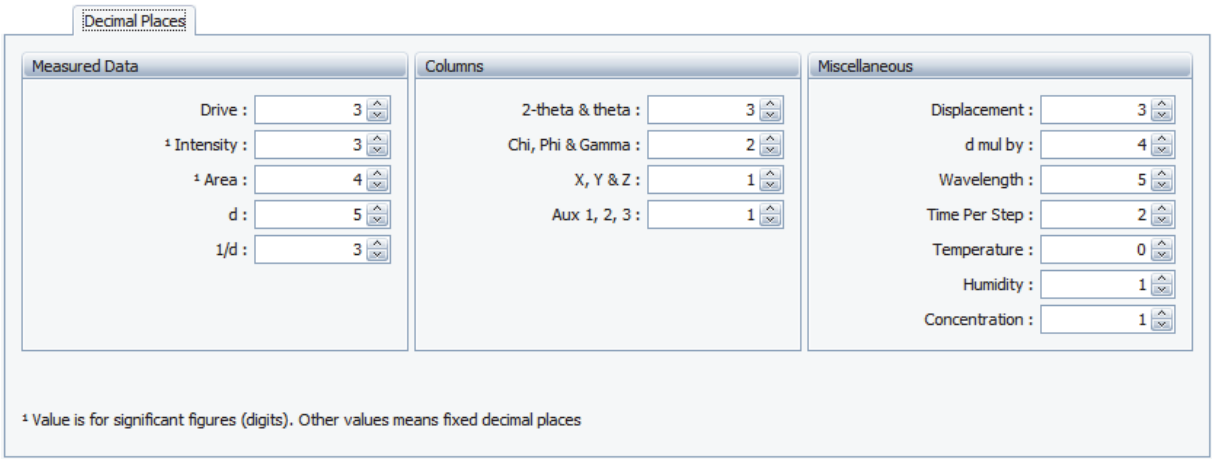
Use this tab to set general settings in EVA.



Option	Description
Default Settings	
Default Print Layout	Select the desired default print layout or leave the field empty
X width for bitmap export in pixels	Enter the width used by default for the export of the graphical view as bitmap
Miscellaneous	
Ask to allow merge during Scan import	Select the check box to be asked to allow merge during scan import
Display additional error details	Select the check box to display additional error details
Level of Undo/Redo operations	Enter the number of possible Undo/Redo operations. An undo level set to 0 switches the undo/redo mechanism off. This is advisable in low memory situations.

Decimal Places Tab

Use this tab to specify the number of decimals used for different values in EVA.

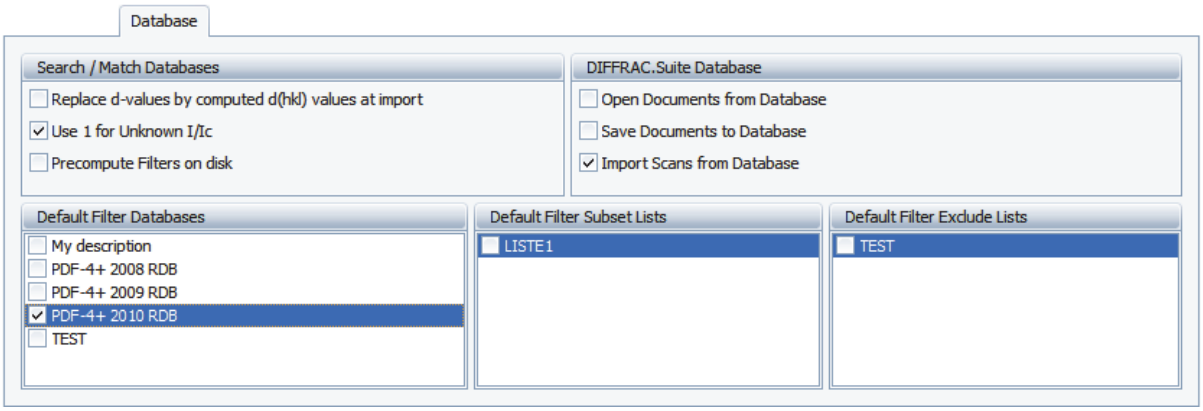


NOTE

Drive in the Measure box gives the decimal places for the **Start** and **End** points of measurement of the scans (listed in the Meas. Conditions of the scan property table).

Database Tab

The Database tab permits defining settings for the Search/Match databases, the DIFFRAC.SUITE database and the default databases and filter lists for use.



Option	Description
Search / Match Databases	
Replace d-values by computed d(hkl)-values at import.	This option permits recalculating the d values using the crystal system, the lattice parameters and the Miller indices. This option is more accurate than the rounded values used for the Search/Match
Use 1 for Unknown I/Ic	Select the **Use 1 for Unknown I/Ic** check box to calculate the concentrations even when the pattern has no I/I_{cor} coefficient, check the **Use 1 for the unknown I/Ic** option.
Precompute Filters on disk	This option saves time during Search/Match operations if multiple filters are used repeatedly
DIFFRAC.Suite Database	
Open Documents from Database	Select the **Open Documents from Database** check box to access the documents stored in the database when opening an EVA document
Save Documents to Database	Select the **Save Documents to Database** check box to save the EVA documents to the database when saving
Import Scans from Database	Select the **Import Scans from Database** check box to access the scans stored in the database when importing a scan.
Default Filter Databases	Select the desired database(s) to be used as default filter database(s). When opening the Search/Match dialog to perform a Search/Match operation or a search by name, the here selected databases will be selected in the database filter tab and used by default for the search. To know more about database filter see “Database Filter” on page 86.
Default Filter Subset Lists	Select the desired subset list(s) to be used as default filter subset list(s). When opening the Search/Match dialog to perform a Search/Match operation or a search by name, the here selected subset lists will be selected in the database filter tab and used by default for the search. To know more about Subset lists see “Creating a Filter List" on page 97.

Option	Description
Default Filter Exclude Lists	Select the desired exclude list(s) to be used as default filter exclude list(s). When opening the Search/Match dialog to perform a Search/Match operation or a search by name, the here selected exclude lists will be selected in the database filter tab and used by default for the search. To know more about Exclude lists see section “Creating a Filter List” on page 97.

Information about the databases

Search/Match Databases

Powder Diffraction File databases (PDF databases)

The usual powder diffraction file (PDF-2 and PDF-4/Full File) database contains more than 300,000 reference patterns which are used to recognize a chemical phase in a measured 2θ-scan. The database is delivered on a CD sold by the ICDD, in a format called PDF-2 or PDF-4+. Each record, also called “card” or “pattern” contains data that allows phase identification:

- the list of characteristic peaks which is the “fingerprint” of the phase with the corresponding Miller indices when available
- the I/I_{cor} values for the semi-quantitative evaluation, when available, several data for reference purpose, such as the name(s) of the phase, the chemical composition and the cell parameters

EVA uses its own version of the database (for speed). Therefore the PDF databases must be compiled using the DRSD Compiler to use them in EVA. See chapter “Compiling the Reference Database using the DSRD Compiler” on page 187 to learn how to perform the compilation.

Crystallography Open Database (COD)

DIFFRAC.EVA now supports a reference pattern database derived from the free-of-charge Crystallography Open Database (COD) for phase identification.
This reference pattern database contains d/I-patterns calculated from crystal structure data taken from the Crystallography Open Database, which integrates crystal structure data published by the IUCr journals, the American Mineralogist Crystal Structure Database (AMCSD), and other sources.
The COD is distributed with DIFFRAC EVA. To use it as reference database, install it and select the Crystallography Open Database box in the Default Filter databases list.

User Databases

If the user has a set of reference patterns, obtained from his own acquisitions, he can create a database, called “User Database” (see “Creating a User Database” on page 138). The User databases will also be listed in the Default Filter databases.

NOTE

DIFFRAC.EVA generally supports phase identification using several databases simultaneously. However, the current license policy of ICDD does not permit its databases (PDF) and results generated from its databases to be combined with other non-ICDD databases. Accordingly, DIFFRAC.EVA allows simultaneous searches on:

- the COD reference databases and any user reference databases
- all PDF2 and PDF 4 databases and any user reference databases.

Simultaneous search on any PDF reference databases and the COD reference database is NOT supported; attempts to do so will result in an error message.

DIFFRAC.SUITE Database

DIFFRAC.SUITE Database is the database used to store measurements. It is used and controlled by the measurement software and maintained with the Database plugin. It is filled with Job measurements. The data can be visualized with the Results Manager plugin.
In DIFFRAC.EVA it can be used to store EVA documents as well.

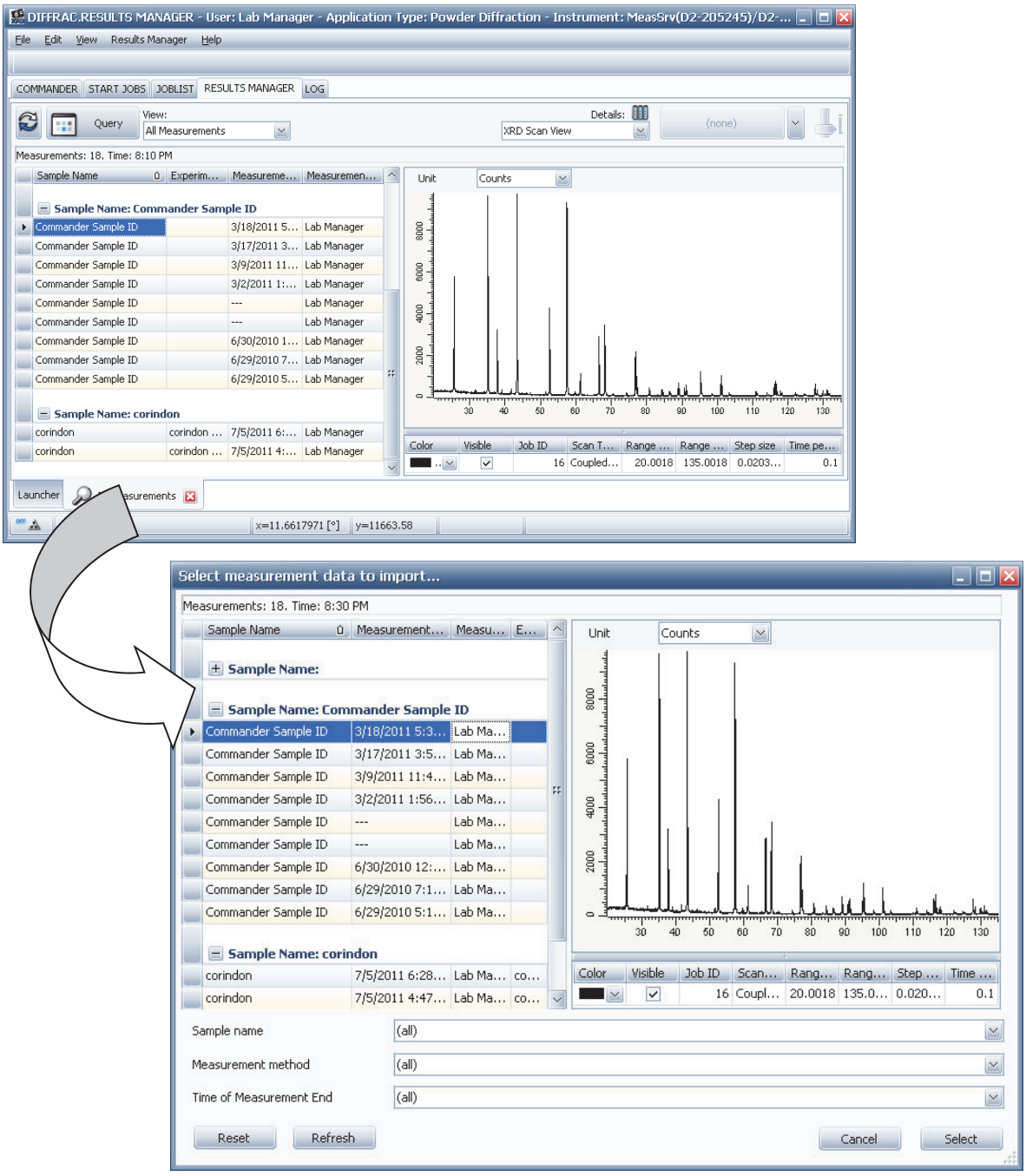


Fig.37: The measurement data stored in the DIFFRAC.SUITE Database are visible within the Results Manager and can be imported into DIFFRAC.EVA

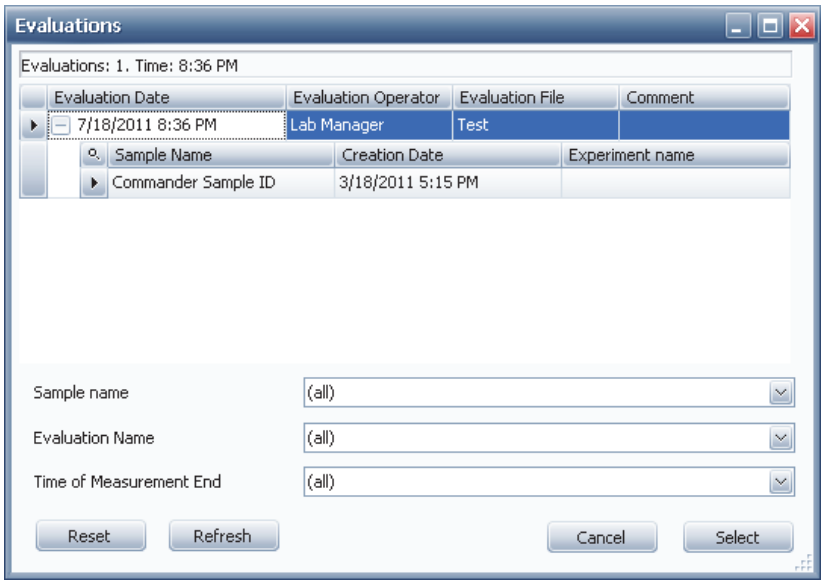
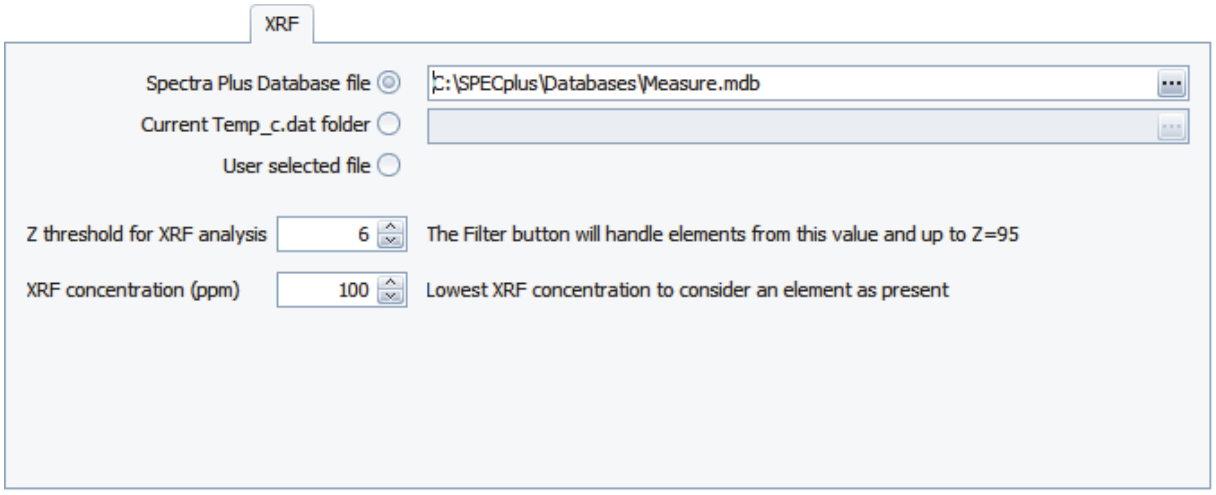


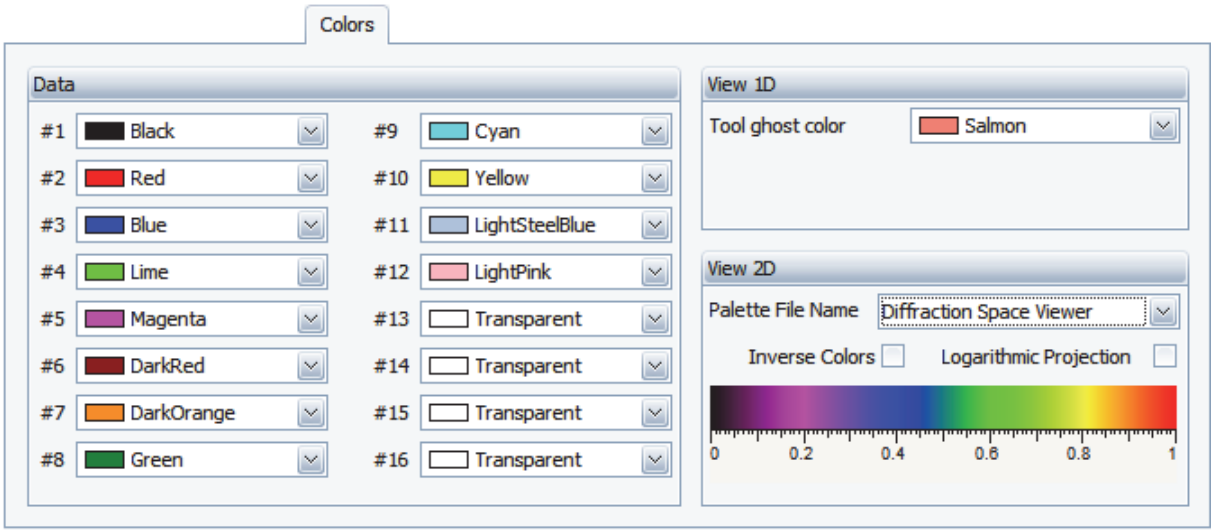
Fig.38: Opening an EVA document stored in the DIFFRAC.SUITE Database

XRF Tab



This tab contains the settings for the import of chemical analysis results for comparison with the semi-quantitative analysis made from the diffraction measurement (SQD). See section “Chemical balance: comparison with a chemical analysis” on page 143 for a complete description of this tab.

Colors Tab



Use this tab to set the default colors for all the EVA items. The newly defined colors will be applied when creating a new item. No change will occur to existing items.

Data

To assign a color to an index choose a color in the corresponding drop-down list.
The palette contains seventeen colors to choose from. Twelve colors are defined by default.

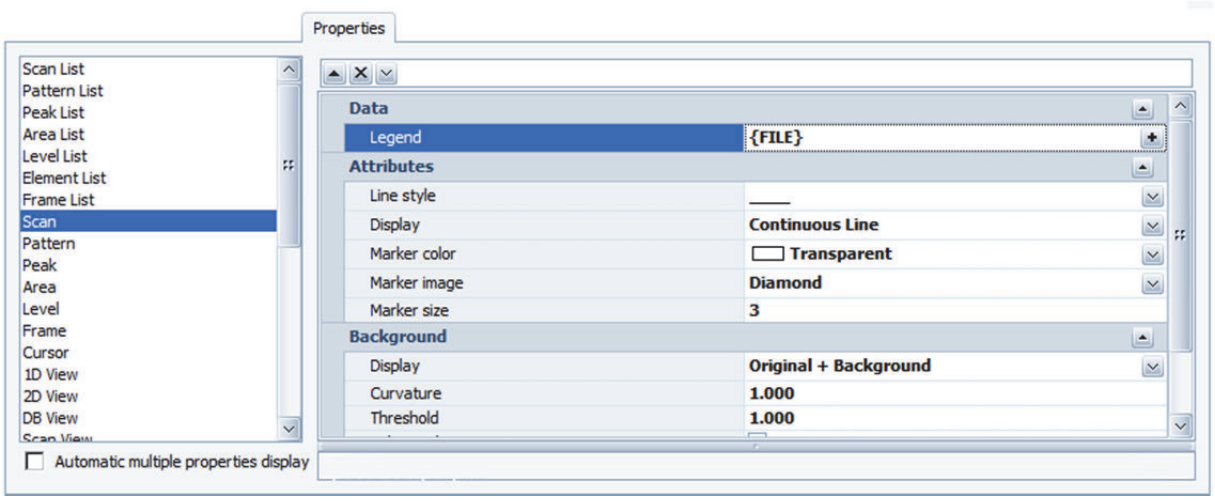
View 1D

The ghost curve shows the results that are not yet part of the document. Select the desired ghost line color in the drop-down list.

View 2D

Choose a color palette for the 2D view in the drop-down list.
Selecting the **Inverse Colors** check box will inverse the colors used for the 2D View display.
Selecting the **Logarithmic Projection** check box will apply a logarithmic projection to the color palette.

Properties Tab



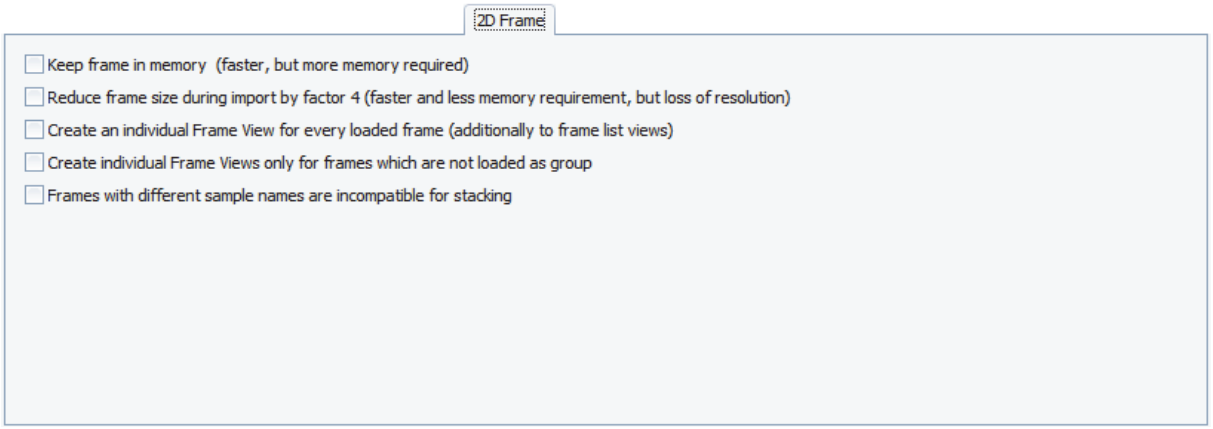
Use this tab to set the default properties for all EVA items:

1. Select an item in the list.
2. Set the corresponding properties in the property table on the right. View the item properties section for a detailed description.
3. Click **OK**.

The newly defined parameters will be applied when creating a new item. No change will occur to existing items.

At the bottom left of the tab, selecting the **Automatic multiple properties display** check box allows an automatic merge of properties, which is useful if there are only a few elements selected simultaneously. Properties are automatically merged for up to hundred items.
By default, the check box is not selected.

2D Frame Tab



Option	Description
Keep frame in memory (faster, but more memory required)	Select this check box to keep frame in memory. It will be loaded faster but more memory will be required
Reduce frame size during import by factor 4 (faster and less memory requirement, but loss of resolution)	Select this check box to reduce the frame size during import by cutting the pixel number in both directions in half. This allows loading up to four times more frames compared to frames with original size. Frames consume a lot of memory and are therefore limited in number depending on the free memory. Out of memories situations will be signalled.
Create an individual Frame View for every loaded frame (additionally to frame list views)	Select this check box to create an individual Frame View for every loaded frame in addition to the frame list views at import
Create individual Frame Views only for frames which are not loaded as group	Select this check box to create an individual Frame Views for frames which are not loaded as group at import
Frames with different sample names are incompatible for stacking	Select this check box for the frames with different sample names not to be stacked

Saving EVA Settings

This feature is available from software version 4.0 up

The settings can be saved into a XML file to be loaded later. It can be, for example, used to transfer the settings between installations. To save the settings:

1. Click **Save Settings…** on the **Tools** menu.
2. Browse the desired folder and enter a name for the EVA Settings file (.EVAPlugin.V4.Defaults.xml file).
3. Click **OK** to save.

To load previously saved settings:

1. Click **Load Settings…** on the **Tools** menu.
2. Browse for the desired Eva Settings File (.EVAPlugin.V4.Defaults.xml file) and click **OK.** The settings will be applied to new documents.

Resetting EVA Defaults

It is possible to reset EVA defaults: the default values, the default tool positions and the default column configurations. The program will have to be restarted for the changes to be applied.

Property	Description
Reset default values	To return to the default properties
Reset tool positions	To reset all the tool and panel positions to their default positions
Reset column configurations	To return to the default column configuration

Working with Scans

Scan Properties

The user can view and modify the scan properties in the Scan property table.
The properties are described in the tables below.

NOTE

Some scan properties are displayed only if they are applicable or only if they have a valid value.

Not all properties are provided for the legacy file format.

Property	Description
Data	
Legend	Legend used to characterize the data. See section “Creating Captions” on page 58 to customize the legend
Attributes	
Visible	Clear the **Visible** check box to remove the current scan from the graphical display. Select the check box to display the current scan
Extended	Select the **Extended** check box to display the scan in the extended view. The extended view will be displayed in case the Extended view check box is selected in the View properties. See section “View Properties” on page 25
Color	Choose a color for the display of the current scan
Line style	Choose a line style for the scan display
Display	Choose to display either the line, the markers or both
Marker color	Choose a marker color. Use the “transparent” color for the color of the scan
Marker image	Choose a marker image
Marker size	Choose a marker size
Sample	
File Name	Self-explanatory
Experiment File Name (from V3.2)	Name of the experiment file (*.bsml file)
Sample Name	Name given in the Wizard or in Start jobs
Scan’s Sample Name (from V3.2)	Name given for an individual scan
Creation Date/Time	Date and time of the scan file creation
Last Write Date/Time	Date and time of the last write of the scan file
Measurement Duration (from V3.2)	Time elapsed between the start and the end of the measurement
Company name	Name of the company as found in the configuration file
Operator Name	Operator name as found in the configuration file
Comment	Self-explanatory
User comment	User’s comment about the file entered when the measurement was started
Sample Position	Sample position in the sample changer

Property	Description
Meas. Conditions	
Scan Type	Type of scan
Scan Mode (from V3.2)	Scan mode used for the scan measurement
Scan Status	Indicates whether the scan is completed or not
Start	Start point in scan unit
End	End point in scan unit
Step Size	Step size in scan unit
Steps (from V3.2)	Number of measured data points
Time per Step	Step time in seconds
Time Started	Elapsed time in seconds since sample measurement started
Axis Offset (from V3.2)	Value of the offset for unlocked coupled scans in degrees.
Goniometer Radius	Goniometer radius with which the current scan has been measured. The goniometer radius is taken into account for the correction of the sample displacement error. This value can be changed interactively
Goniometer Radius Primary (from V3.2)	Goniometer radius of the primary track. This is only displayed if primary and secondary tracks have different radii
Goniometer Radius Secondary (from V3.2)	Goniometer radius of the secondary track. This is only displayed if primary and secondary tracks have different radii
Drives	
2-theta	2-theta angle at scan startup in degrees
Theta	Theta angle at scan startup in degrees
Detector (from V3.2)	Value of the detector angle at scan startup in degrees
Chi	Chi angle at scan startup in degrees
Phi	Phi angle at scan startup in degrees
X-Drive	X position at scan startup in mm
Y-Drive	Y position at scan startup in mm
Z-Drive	Z position at scan startup in mm
Aux1	Location of auxiliary drive 1 at scan startup (unit not specified)
Aux2	Location of auxiliary drive 2 at scan startup (unit not specified)
Aux3	Location of auxiliary drive 3 at scan startup (unit not specified)
Sample rotation speed	Sample rotation speed in degrees/min

Property	Description
Environment	
Humidity	Relative humidity when using the HUMID-CONTROL humidity controller with an environmental chamber
Temperature	Temperature in °C (or “Room” when temperature is not controlled)
Temp. Diff.	Temperature difference in °C for DTA measurements
Heating Rate (from V3.2)	Value of the non-ambient chamber’s heating rate in degrees per minute
Wavelength	
Anode	Anode material of the X-ray tube.
$K\alpha_1$	Usually, $K\alpha_1$ value for the radiation used, as read from the scan header (d-values are always computed from this value)
$K\alpha_2$	Usually, $K\alpha_2$ value for the radiation used, as read from the scan header (used for $K\alpha_2$ stripping)
$K\alpha_2$ Ratio	Intensity ratio between $K\alpha_2$ and $K\alpha_1$ lines as stored in scan header (used as the default for $K\alpha_2$ stripping)
Kβ	Usually, Kβ value for the radiation used, as read from the scan header
Wavelength for display	Wavelength used for the scan display
X-Ray Generator	
Generator kV	High voltage of the X-ray generator used for the measurement
Generator mA	Intensity in the X-ray tube used for the measurement
Detector	
Detector Name	Detector used for the measurement
Calcium Channel	Calcium channel value given in Cps for raw files which contain Ca channel information
Calcium Channel Time	Calcium channel measurement time given in s
LynxEye 0D	LynxEye detector used in 0D mode or not
PSD Opening	PSD opening in degrees or mm
PSD Opening Initial (from V3.2)	Initial detector opening angle in degrees for VDO scans
PSD Opening Final (from V3.2)	Final detector opening angle in degrees for VDO scans
2Theta for Final PSD Opening (from V3.2)	2Theta angle at which the full detector opening is reached for VDO scans
Detector opening angle	Detector opening angle in degrees
Detector slit opening	Detector slit opening angle in mm
Lower discriminator	Lower discriminator voltage of the detector electronics
Upper discriminator	Upper discriminator voltage of the detector electronics
Discriminator Width	Width of the discriminator voltage of the detector electronics. Only for V4 scintillation detector measurements.
Detector Counts 0D	Detector counts for LynxEye 0D mode still measurements

Property	Description
Slits	
Primary Soller slit	Primary Soller slit opening angle in degrees
Secondary Soller slit	Secondary Soller slit opening angle in degrees
Antiscatter Slit	Opening of the antiscatter slit in °.
Divergence Slit	Opening of the divergence slit in °. If the slit mode is variable, the value this value is always the sample illumination length in mm.
Slit Mode	Type of slit (fixed or variable) used for scan measurement
Simul. Slit Mode	Type of slit (fixed or variable) used to display the scan. Default means the same as used for the scan measurement
Corrections	
Displacement	Applied displacement value (in mm)
X-Offset	Applied X-Offset value (in degrees)
Y-Scale Factor	Applied scale factor value
Y-Offset	Applied Y-Offset value (in counts)
Background	
Display	The background is automatically displayed in addition to the original scan. The original measurement or the background subtracted scan can be displayed alone
Curvature	The background curvature can be adjusted.
Threshold	The threshold can be adjusted
Enhanced	Select the **Enhanced** check box to use the enhanced background method (see Section “Performing a Background Subtraction” on page 102 for more details)
Color	Color used for the display of the background
Crystallinity	
Compute Crystallinity	Select the corresponding check box to compute automatically the crystallinity
%-Crystallinity	Computed crystallinity in %
%-Amorphous	Computed amorphousness in %
Global area	Global area including the peak and the amorphous hump
Reduced area	Area of the whole scan subtracted by the background adjusted by the user

Many scan properties are displayed only if they have a valid value. Not all properties are provided for the legacy RAW file format.

Scans and wavelength

- When importing 2θ scans measured with a wavelength different from that of the first scan in the scan list (in which the import is done), the newly imported scans are recalculated according to the wavelength of the first scan in the list. Two transformations are carried out: first in d and then in 2θ for the wavelength of the first scan in the list.
  The wavelength forced for all scans is indicated in the view's property: Wavelength.
  If a view is created from one of the scans in the list, it will be displayed with its original wavelength.
- The same data, e.g. a scan with areas and peaks, can be displayed in several views at different wavelengths. Please note, that the angular limits of an area or a peak location can still be edited. However, if the angular limits of an area or peak location are changed directly in the properties table it is necessary to use the view which displays the original wavelength of the data.
  There is no similar problem with graphical input since the software performs the angle projections and stores the values for the original wavelength. There is also no problem in case of peak search or graphical insertion of peaks.
  In practice, it is better to refrain from using views made with modified wavelengths for purposes other than comparing data measured at different wavelengths.

List of Scan Operations

Here is the list of operations that can be performed on scans:

To	See
Perform a Search/Match operation	Section “Performing a Search/Match Operation” on page 80
Perform an Automatic Search/Match operation	Section “Performing an Automatic Search/Match Operation” on page 92
Perform a Search by Name operation	Section “Performing a Search by Name” on page 94
Perform a Search by Number operation	Section “Performing a Search by Number” on page 101
Perform a Background Subtraction	Section “Performing a Background Subtraction” on page 102
Perform a Peak Search operation	Section “Performing a Peak Search” on page 103
Compute $K\alpha_2$ Stripping	Section “Computing Kα2 Stripping” on page 104
Use Fourier Smoothing	Section “Fourier Smoothing and Expansion” on page 105
Smooth	Section “Smoothing Scans” on page 107
Correct the X-Offset	Section “Correcting the X-Offset” on page 108
Correct the Sample Displacement Error	Section “Correcting the Sample Displacement Error” on page 109
Remove Aberrant Points	Section “Suppressing Aberrant Points” on page 110
Compute Areas	Section “Computing Areas” on page 111
Duplicate Scans	Section “Duplicating Scans” on page 113
Accumulate Scans	Section “Accumulating Scans” on page 113
Add and Subtract Scans	Section “Adding and Subtracting Scans” on page 114
Merge Scans	Section “Merging Scans” on page 101
Re-Scale a Scan	Section “Re-Scaling the Current Scan” on page 119
Normalize Scans	Section “Normalizing Scans” on page 120
Compute the Crystallinity	Section “Computing the Crystallinity” on page 121
Simulate a Slit Mode	Section “Simulating a Slit Mode” on page 122
Export a Scan	Section “Exporting Scans” on page 123
Replace/Clone a Scan	Section “Replacing and Cloning Scans” on page 125

Performing a Search on a Scan

Performing a Search/Match Operation

Description

The search is performed on the background subtracted scan. It is not necessary to perform the subtraction as it is done automatically at scan import. Select “Original+ Background” in the properties of the scan (it is the default) to see the background as a dash line and to correct it with the “Scan Background” tool, if necessary. Furthermore, the selected patterns will be displayed as sticks based on this background in this display mode. This is usually more convenient than that which is based on the horizontal axis, as done when the background-subtracted scan is displayed.

To perform a Search/Match operation on a scan:

1. Select the scan of interest either in the data tree or in the 1D view.
2. Click **Search / Match (scan)** in the Data command panel
   — or —
   right-click the current scan, click **Tool** on the menu which appears and then **Search / Match (scan)** on the related submenu.

The Search/Match (scan) dialog box is displayed as follows:

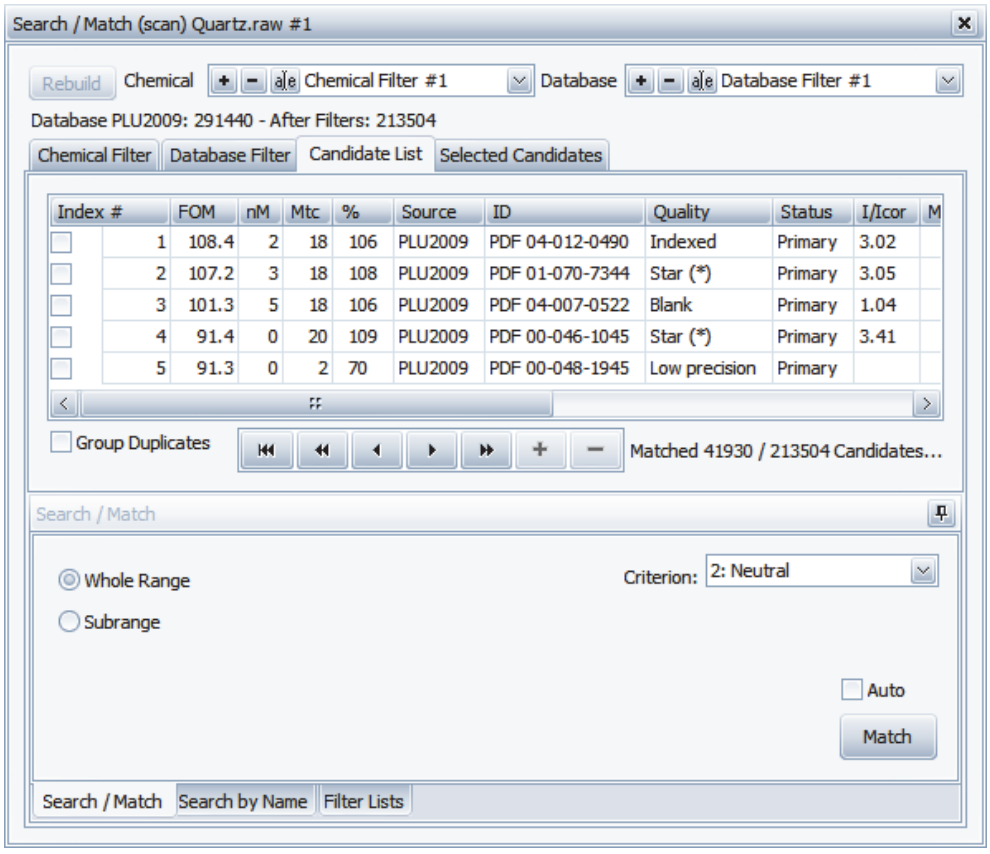


Fig.39: Search / Match (scan) dialog box filled with results

NOTE

The Search/Match dialog box can be docked or use the automatic hiding functionality as panels. It can prove useful when the user often performs Search/Match operations.
See section “Organizing the Workspace” on page 36 for more details about the docking system.

3. Select the scan range for the search to be performed:
   - Click **Whole Range** to perform the search on the whole scan;
   - Click **Subrange** to perform the search on a defined scan range. Enter either the desired start and end values of the scan range in the **From** and **To** fields, or click the **Get Range from Current View** button to use the part of the scan currently displayed.
4. Set the other Search/Match parameters described in the following sections.

Search/Match Parameters

Selecting the Search/Match Main Parameter: Criterion

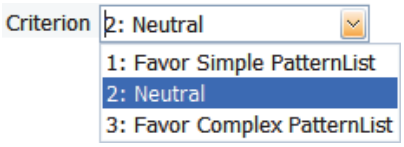


Fig.40: Criteria list

The criterion “1” favors simple reference patterns. Candidates which share only one or a few lines with the unknown scan may rank before patterns sharing many lines with the scan.
To analyze an unknown scan, start with the criterion “2” (selected by default) and then use the criterion “1”.
This criterion is not used when searching on a pattern.

The criterion “2” can be considered as a “neutral" criterion. Prepare a synthetic sample and test it - a 50/50 mixture of Silicon and Feldspar. This criterion was devised to give an equal chance to both phases. Always start with this criterion when analyzing an unknown scan.

The criterion “3” favors patterns sharing many lines with the unknown scan. Therefore, it favors complex reference patterns and is disfavors reference patterns with only a few lines.
Use this value when searching on a reference pattern.

NOTE

The auto-hide feature can be used for the lower part of the dialog box. To display the lower part again, click the tab label and click the **Auto-hide** button.
See section “Automatic Hiding Feature” on page 34 to learn how to use this feature.

Chemical and Database Filters

The chemical and the database filters can be used to limit the search domain for the Search/Match and Search by Name tools.
Both types of filters are parts of the document. They are added to the Settings list at the top of the Data Tree when creating a document.
The filters are initially filled with the default parameters and subsequently with the user parameters.

Creating a Chemical or Database Filter

To create a new chemical filter or a database filter:

1. Click the button next to the **Chemical** or **Database** text field at the top of the Search/Match (scan) dialog box;
2. **Chemical Filter #...** or **Database Filter #...**, is displayed in the Chemical field or in the Database field. The filter can be renamed by clicking the **Rename** button .
3. Click the **Chemical Filter** or **Database Filter** to set the desired filter. See sections “Chemical Filter” on page 84 and “Database Filter” on page 86 below for a complete description.

Deleting a Chemical or Database Filter

To delete a chemical or database filter, click the button next to the corresponding text field. It can also be deleted from the data tree by right-clicking the desired filter and then clicking **Delete** in the related context menu.

NOTE

Once the filters set, click the **Rebuild** button to rebuild the search database and be given the number of remaining patterns.
This is done automatically when starting the search run.

Setting a Chemical or Database Filter as Default Filter

This feature is available from software version 2.0 up

Once a chemical/database filter created, it is possible to define it as the chemical/database default filter.
The filter will not be taken as default filter for the current document. It will be taken as default filter when creating a new document.

To set a chemical or database filter as default filter:

1. Select the chemical or database filter in the data tree.
2. Click **Use as default Chemical/Database Filter** in the Data command panel
   — or —
   right-click the filter, click **Use as default Chemical/Database Filter** on the related submenu.

In a new document, this filter will be used by default when performing a Search/Match or a Search by Name.

NOTE

The default filters will not be saved when closing DIFFRAC.EVA. You will not be able to use them later expect if they are part of an EVA document which has been saved.
To be able to reuse a filter, it is possible to export the filter in file. The filter can then be imported when needed.

Exporting and Importing a Chemical or Database Filter

This feature is available from software version 2.0 up

It can prove useful to export chemical or database filters into files to be able to retrieve them whenever needed.

To export a chemical or database filter into a file:

1. Select the chemical or database filter in the data tree.
2. Click **Export Chemical/Database filter** in the Data command panel
   — or —
   right-click the filter, click **Export Chemical/Database filter** on the related submenu.
   The Export a Chemical/Database Filter File dialog box will be displayed.
3. Enter a name for the filter file and click the **Save** button.

To import a filter file:

1. Select the settings node in the data tree.
2. Click **Import Chemical/Database filter** in the Data command panel
   — or —
   right-click the settings node, click **File** and then the **Import Chemical/Database filter** command on the related submenu.
   The Import Chemical/Database Filter dialog box will be displayed.
3. Select the desired filter and click the **Open** button.

The filter will be added to the data tree and to the Chemical/Database drop-down list of the Search/Match dialog box.

Chemical Filter

Click the **Chemical filter** tab to access it.

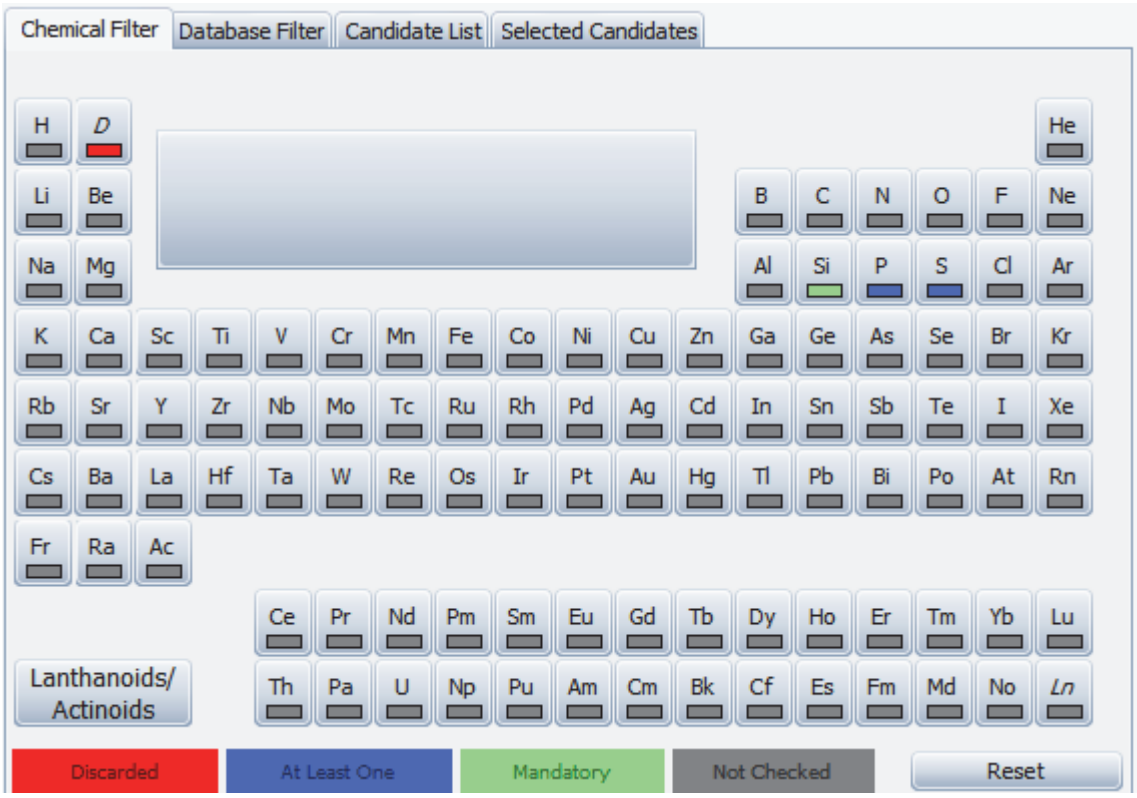


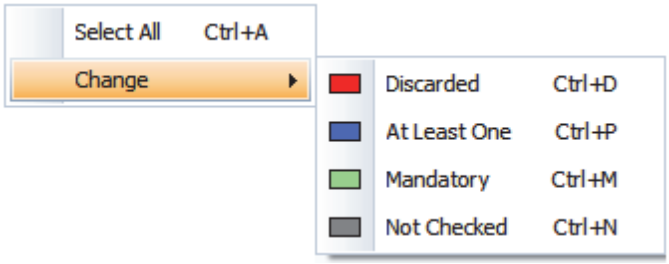
Fig.41: Chemical Filter tab

The chemical filter is set by selecting elements in the periodic table. A color code is used to define the "status" of each element:

- Blue indicates at least one element among all the elements in blue must be present in the search result
- Green indicates that the element is mandatory
- Red indicates that the elements are discarded (must be absent)
- Gray indicates that the element is not checked (present or absent)

  To change an element color:

  Click on the element until the right color appears
  — or —
  right-click the element to open the selection menu:



To return to the default chemical filter, click the Reset button.

It is possible to select a group of elements to be discarded. To do so:

1. Click one of the corners of the group of elements to be selected.
2. While holding down the left button, drag the mouse to select the chosen elements.
3. Release the button when the selection is complete.

To use the Windows multi-selection: keep the **Control** key pressed when clicking the elements.

NOTE

A group of elements can only be discarded or set to “At Least One”. Making a group of elements mandatory does not make sense in most of the cases.

Two uncommon symbols are available in the table used for the search by chemistry: **D** for Deuterium, and **Ln** for undetermined lanthanides and actinides. As a consequence, the table is no longer a genuine periodic table. The table takes into account all the chemical symbols to be found in the PDF.

D is forbidden (in red) by default, since it is likely to be the wish of most users to eliminate phases that include deuterium.

Ln stands for one or more unspecified lanthanides or actinides in the corresponding phases.

Click the **Lanthanoids/Actinoids** button to exclude all the lanthanides and actinides (including the patterns containing Ln).

NOTE

Some database patterns have no chemical formula. Therefore, they appear only when all elements have not been tested, i.e. all boxes are gray. When only one box is red or green, these patterns do not appear, except in one case: when **D** is red.

Database Filter

Click the **Database Filter** tab to access it.

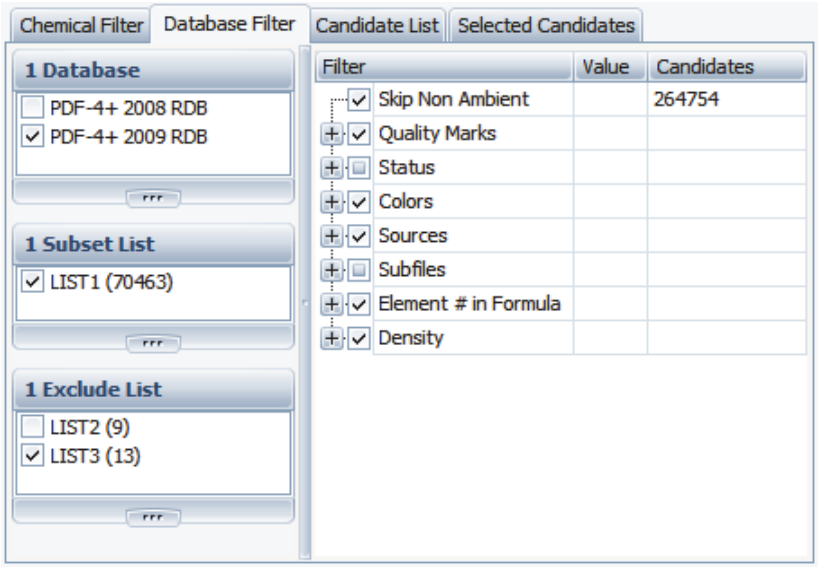


Fig.42: Database Filter tab

The available databases are listed on the left. The Subset and Exclude lists, when available, are also listed (see section “Creating a Filter List” on page 97). The number between the parentheses indicates the number of patterns in the corresponding list and belongs to the currently selected database(s).

Select the desired database by selecting the corresponding check box.

Select the desired Subset and/or Exclude list(s).

When rebuilding the search database, the remaining patterns will be the result of the sum of all the subset lists checked minus the sum of all the exclude lists checked.

NOTE

It is not recommended to select several PDF databases simultaneously since they share a lot of common candidates.

On the right, patterns with defined parameters can be excluded from the search by clearing the corresponding check boxes. Enter a value in the column “Value” for the criteria which require one, for example Element # in Formula or Density. The column “Candidates” of the table indicates the number of candidates complying with each filter.

Filter	Description
Skip Non Ambient	Reject the patterns measured at a non-ambient temperature
Quality marks	Reject patterns with a defined quality mark
Status	Reject patterns with a defined status from the search
Colors	Limit the possible color(s) of the compound searched for
Sources	Select the sources to use for the search
Subfiles	Limit the subfiles of the database to search in
Element # in formula	Define a minimum and/or maximum number of elements in the compound formula
Density	Define a minimum and/or maximum density for the compound formula

Quality Marks

The quality marks in the PDF databases are described in the following table (they have been assigned by the PDF editorial board).

Mark	Description
Low precision	Low precision pattern
Indexed	Good quality pattern with indexed lines
Blank	Pattern not meeting the Star, Indexed, or Low-Precision criteria
Star (*)	High quality pattern
Calculated	Pattern computed from single-crystal structural parameters
Rietveld	Pattern resulting from a Rietveld refinement
Hypothetical	Pattern calculated theoretically from an isostructural compound
Prototyping	Quality given to patterns which structural data was assigned by an editorial action of this Linus Pauling File (not recovered from the primary literature). This quality mark is specific to PDF-4

Rejecting low quality patterns can reduce the number of duplicate patterns in the list allowing a better diversity in the products listed. A good quality pattern is obtained from a refined or theoretical product. Therefore, a low quality pattern may be closer to the user's own product and therefore, be listed at a better place.

Status

The pattern statuses in the PDF databases are described in the following table. They have been assigned by the PDF editorial board:

Status	Description
Primary	Pattern recommended by the PDF editorial board
Alternate	Pattern of reasonable quality which has been flagged as a duplicate of a primary pattern
Deleted	Pattern which has an improved replacement (a primary pattern). Its use is not recommended by the PDF editorial committee

Starting a Search Run

Click **Match** to start. The duration of the search depends on the number of patterns to scan (usually a few seconds). At completion, the results are listed in the **Candidate list** tab.

The Group duplicates option

The integration of the Structure patterns to the PDF database introduces many duplicates. These are different patterns corresponding to the same phase.

To group patterns in the search results, select the **Group duplicates** check box. To display the grouped duplicates click on the plus sign preceding the first candidate.

EVA checks the patterns that have:

- very similar powder patterns,
- and the same chemical composition or the same mineral name

and marks them as Duplicate.

Only the first part of the name is checked, up to a comma, a dash or a space.

Search Results

The results of the search are displayed in a table in the Candidate List tab.

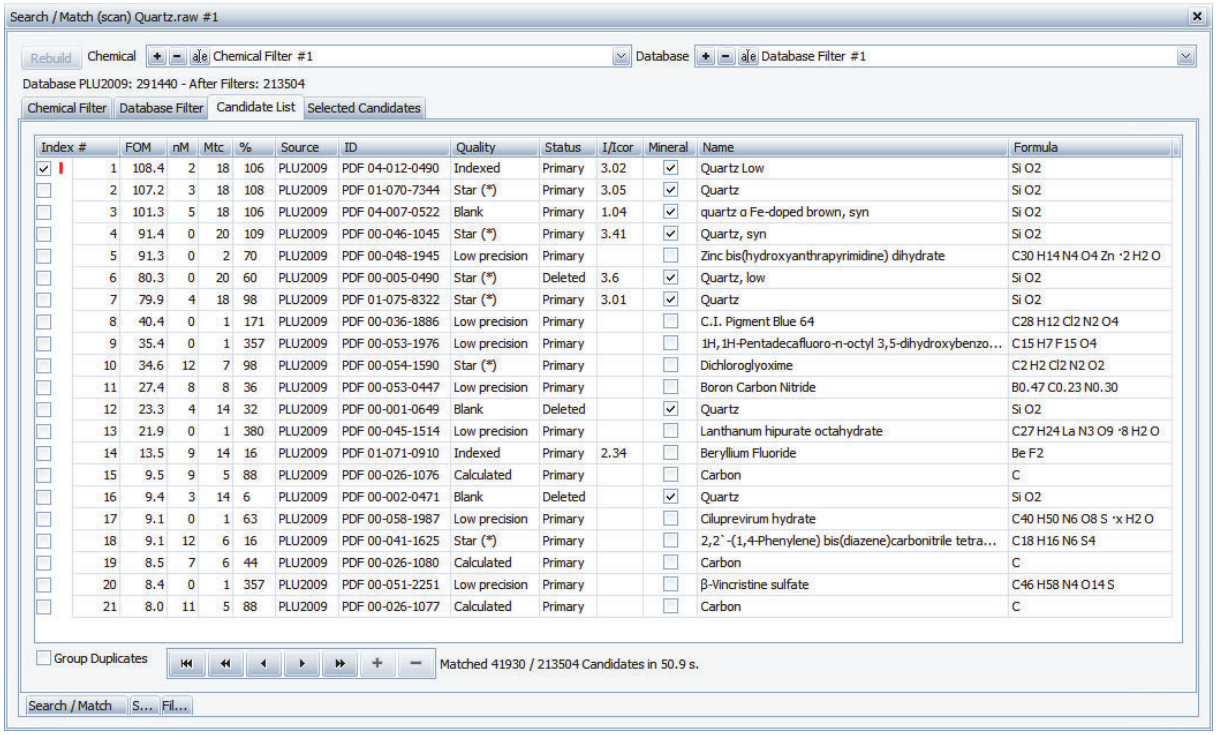


Fig.43: Search / Match (scan) dialog box shown with results. The bottom user interface elements are hidden.

All items are described below.

Column	Description
Index #	Rank number of the given pattern during the search run
FOM	Figure Of Merit: the higher this number, the better the match. Patterns are sorted by decreasing figures of merit (FOM)
Mtc	Number of reference pattern lines matching the unknown in the displayed range
nM	Number of reference pattern lines not matching the unknown in the displayed range
%	Actual Y-Scale percentage
Source	Name of the original database
ID	Pattern number in the database
Q	Quality mark
S	Pattern status
I/Icor	I/Icor is the ratio I/I_{cor} between the intensities of the strongest line of the compound of interest and the strongest line of corundum, both measured from a scan made of a 50-50 mixture, as stored in the PDF database
Mineral	Mineral compound or not
Name	Compound name as written in the database
Formula	Chemical formula

Button	Description
	To go back to the top of the list
	To display the N previous patterns; N is the number of patterns currently displayed
	To go back to the previous pattern in the list
	To go to the following pattern in the list
	To display the N following patterns; N is the number of patterns currently displayed
	To select a pattern in the list
	To remove a pattern from the selection

The number of matched candidates compared to the total number of candidates, and the elapsed time for the search in seconds, are indicated next to the buttons.

When a candidate in the list is clicked on, its ghost pattern is displayed in the graphical view. See below for more details.
To select a candidate, select the corresponding check box or click the **Check** button. The candidate is then associated to a color. This color is used to display the corresponding pattern in the graphical view.

Search/Match and Graphical Display

This feature is available from software version 2.0 up

While a new phase (candidate) is inspected the sticks of the other phases in the document are toned down and become pale. The candidate is clearly distinguished from previously added phases by its intense color. The view properties “Match Coloration” and “Match Brightness” allow customizing these features. Additionally, the phase being inspected is displayed in the color of the next potential candidate.
A dotted line is displayed below the background and through the ruler. This helps to maintain the current pattern which is visible when there is no background height or when the scan is displayed without a background.
When the selected line in the list is a candidate, three dots are displayed on the side of the dot color. If the line already exists as a pattern in the document no dots will appear.
When the selected line depicts an existing pattern, the dotted line below the background is displayed in the color of the pattern itself and the line drawn through the ruler is a plain line. This minimizes confusion between a candidate and an existing pattern.

NOTE

To increase the length of the visible list, use the auto-hide feature to hide the bottom part of the dialog box. To display the bottom part again, click the tab label and then the **Auto-hide** button.
See section “Automatic Hiding Feature” on page 39 to use this feature.

NOTE

It is possible to perform an operation directly on a pattern selected in the candidate list.
To do so :
Right-click the line of the selected pattern to display the contextual menu and click the desired command.

The selected candidates have a dedicated tab.

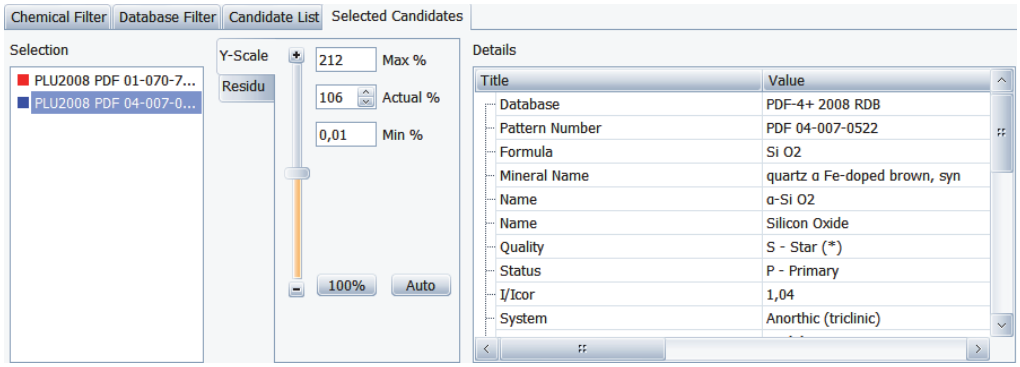


Fig.44: Selected Candidates tab

The candidates are listed in the **Selection** list.
The data corresponding to the selected candidate are detailed in the Details table.

Scale of the pattern

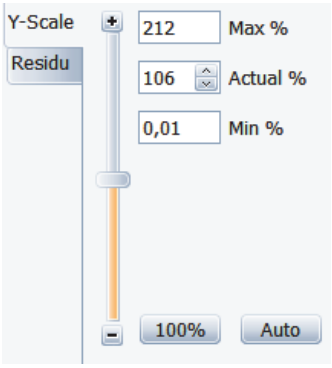


Fig.45: Adjusting the Y-Scale

Adjust the scale of a pattern with the **Y-Scale** slider manually, when necessary.

The **Auto** button makes it possible to reverse to the automatic scaling after an unsuccessful manual adjustment.
The auto-scaling algorithm is based on all the lines with more than 10% relative intensity. Please note that a manual adjustment will still be required in most cases, but should prove faster when starting from auto-scaled patterns.

Clicking the **100%** button scales the pattern to give the highest height of the scan to the 100% line of the pattern.

Residue

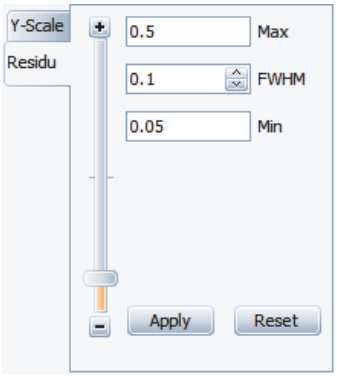


Fig.46: Preparing a residual scan

Minor phases are often difficult to identify because the patterns corresponding to the major peaks have a better position in the list. It is possible to exclude previously explained regions in order to increase the weight of the unexplained regions. The minor phases are then more likely to be identified.

When some phases have been identified, it is possible to use the patterns to exclude the regions around the peak positions. This is much faster but less accurate than the manual procedure.

To do this:

1. In the Search/Match (scan) dialog box, choose the **Selected Candidates** tab.
2. In the list, select the pattern of interest.
3. Select the **Residu** tool.
4. Adjust the width of the zone to exclude around the pattern sticks with the slider. It is also possible to enter a value manually in the **FWHM** text zone; the width of the excluded region is derived from each peak height and the FWHM.
5. Click the **Apply** button.

To restore the cancelled part, click **Reset**.

Performing an Automatic Search/Match Operation

This feature is available from license level and software version 2.0 up

EVA provides an option to perform an automatic Search/Match.

An Automatic Search is likely to deliver accurate results if the three following conditions are fulfilled:

- low overlap between phases
- every phase in the unknown sample shall have relative intensities matching the phases of its reference pattern in the database
- no phase showing a significant line broadening

The interactive Search/Match is quite insensitive to line overlaps, to relative intensity mismatches, whereas line broadening is not a major issue, which makes the identification of phases possible in complex scans, even with relatively strong preferred orientations.
The user must be very careful when using the automatic search. It is a versatile tool when the three conditions are fulfilled. However, the successfulness of the search cannot be known beforehand. In practice, it will be necessary to continue the search with the interactive Search/Match after a trial with the Automatic Search.

To perform an automatic Search/Match operation on a scan:

1. Select the scan of interest either in the data tree or in the 1D view.
2. Click **Search / Match (scan)** in the Data command panel
   — or —
   right-click the current scan, click **Tool** on the menu which appears and then **Search / Match (scan)** on the related submenu.

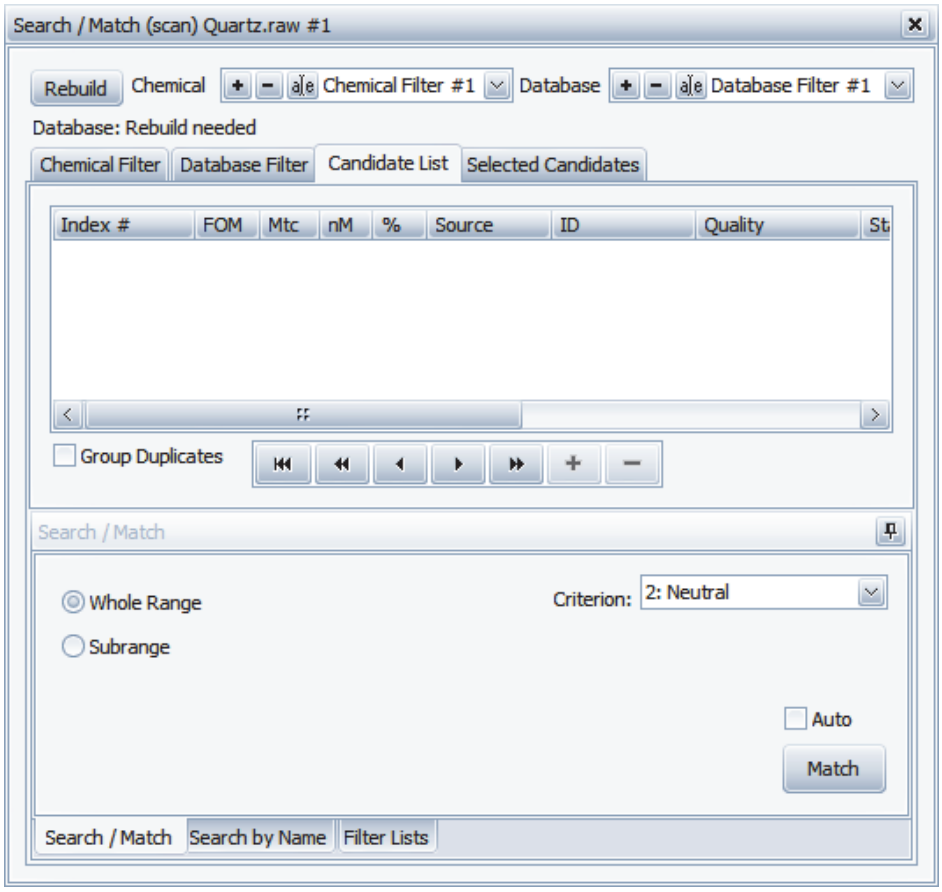


Fig.47: Search / Match (scan) dialog box

3. Set the Search/Match parameters.

4. Select the **Auto** check box.
5. Click the **Match** button: the results will be displayed in the candidate list and the corresponding pattern(s) added to the graphical display and to the data tree.

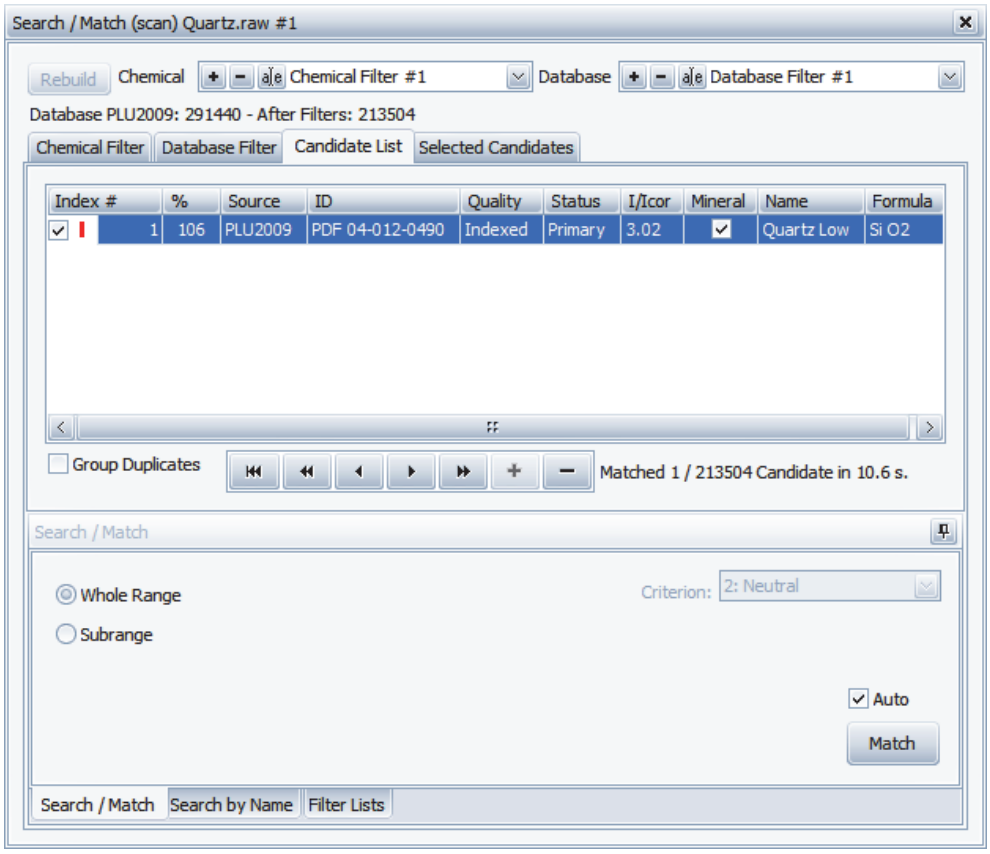


Fig.48: Result pattern of the automatic Search/Match

Performing a Search by Name

To perform a scan search by name:

1. Select a scan either in the data tree or in the 1D view to be able to access the scan tools.
2. Click **Search/Match (scan)** in the Data command panel
   — or —
   right-click the current scan, click **Tool** on the context menu and then **Search/Match (scan) i**n the related submenu.

The **Search/Match (scan)** dialog box will be displayed as follows:

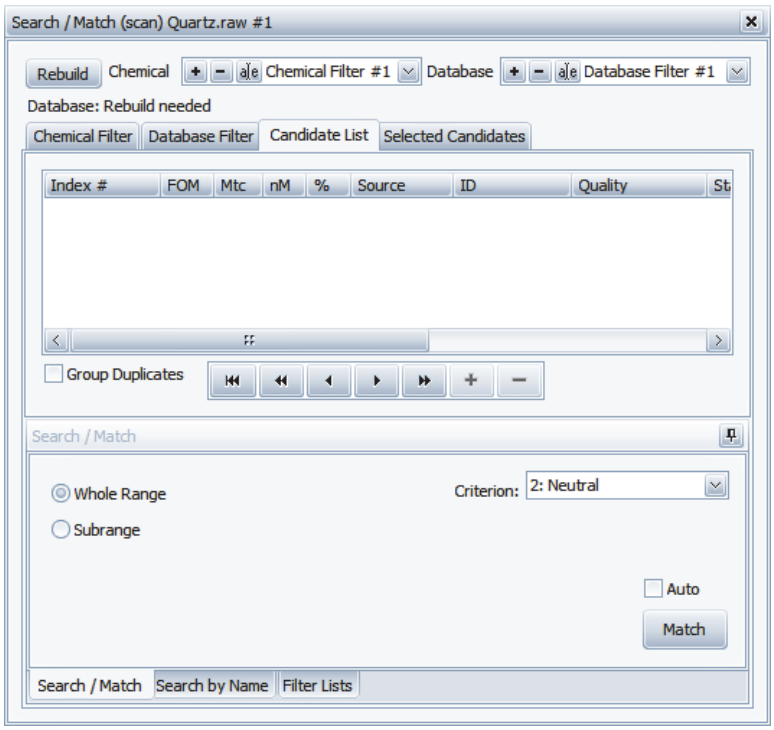


Fig.49: Search/Match (scan) dialog box

3. Click the **Search by Name** tab to access the Search by Name.

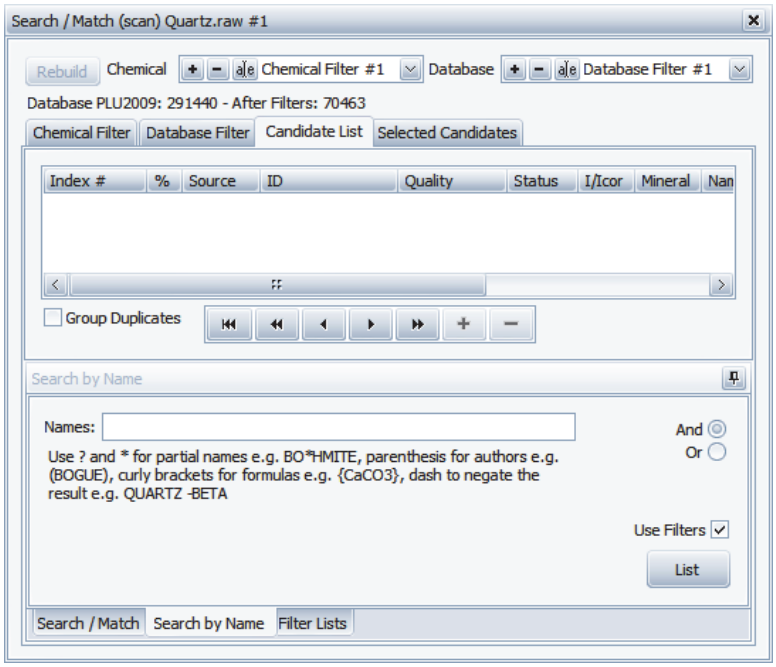


Fig.50: Search by Name tab

Search Parameters

The search can be performed either by:
- Compound name, for example: quartz
- Author name, for example: Lauer
- Chemical formula, for example: {Fe3O4}

Several strings can be used at the same time. In this case, spaces must be inserted as separators. The strings are interpreted according to the And/Or operators. The And operator gives the intersection of all results sets for each string. The Or operator gives the union of all result sets.

Examples with the And operator:
Corundum
The results include the compounds with impurities in Al2O3.
Corunduml {Al2O3}
Results are limited to Corundum whose formula is Al2O3 or equivalent.

Examples with the Or operator:
{PbO} {PbO2}
Results include all the files corresponding to each formula.

The choice of the operator is always applied to all the strings defined.

Rules for all the strings:
Forbidden characters are removed automatically.

Syntax for the compound names:
All strings not included in brackets are treated as compound names.
Upper case and lower letters are not differentiated. There exist wildcards: an asterisk (*) represents any string, a question mark represents for one character.
Numbers are filtered out. For example, to find Kaolinite-1A, search for the string kaolinite.

Syntax for author names:
Strings in brackets are treated as author names.
The wildcards asterisk (*) and question mark (?) are not allowed in author names. Upper and lower case letters are not differentiated.

Syntax for formulas:
Strings in curly brackets are treated as formulas.
The wildcards asterisk (*) and question mark (?) are forbidden in chemical formulas.
Authorized characters in chemical formulas:

- All the chemical element names: an upper case letter must be used for the first character of the element name and a lower case letter for the second character.
- Square brackets and standard brackets can be used. They are synonymous.
- Numbers with or without decimals as well as the variables x, z and n. These variables are replaced by numerical values for the search: x and z by 0.01 and n, by 5 if there is a centered dot, by 10 else (the centered dot separates molecules, for example {Al2(OH)6·H2O}).
- The characters centered dot (·), comma (,), dash (-), space ( ) and slash (/). The centered dot separates 2 molecules. It must be replaced by a common dot when typing. The slash indicates the end of a formula. However, it is not mandatory.
- The plus sign (+) and the minus sign (-). For example: {Fe1-xS}.
- Spaces between element names possibly followed by their stoichiometry are optional. For example: {Fe2O3} and {Fe2 O3} are equivalent.
- The chemical formulas are tested with regards to the concentration equality in mass percentage within 4/10000. For example, the formulas {Al2O3.H2O}, {AlO2H} and {AlO(OH)} are equivalent; Al2O3 and Al2.667O4 too.

Excluding results
It is possible to use a minus sign (-) before a string to negate the corresponding results. The results obtained this way are all the patterns which do not comply with the search criterion on this string.
Please note that the And operator is forced in case a string preceded by a minus sign is used.
Example: Quartz -beta
The search results will give all the quartz except those named β-quartz.

Other database filters

Select the **Use other filters** check box to display the other database filters and define those of choice. See Section “Database Filter” on page 86 for their description.

Starting a Search Run

Click **List** to start the search. The duration of the search depends on the number of patterns to scan. At completion, the results are displayed in the **Candidate List** tab.

Search Results

The results of the search are displayed in a table in the **Candidate List** tab.

See Section “Search Results” on page 88 for a detailed description of the Candidate List and Selected Candidates tabs.

Creating Filter Lists

A list of patterns can be created from search results or document patterns and can be used as a database filter.

NOTE

Filter lists can prove useful to create sub-databases from the PDF database.
Indeed, due to restrictions enforced by the ICDD it is no longer possible to create subsets of the PDF database.
If the filter lists are not sufficient, it is possible to create user databases from individual patterns. Note only PDF patterns with “Tune Cell” or “d x by” commands applied can be added to a user database.

Creating a Filter List

Filter lists are created from the Candidate List tab of the Search/Match dialog box.

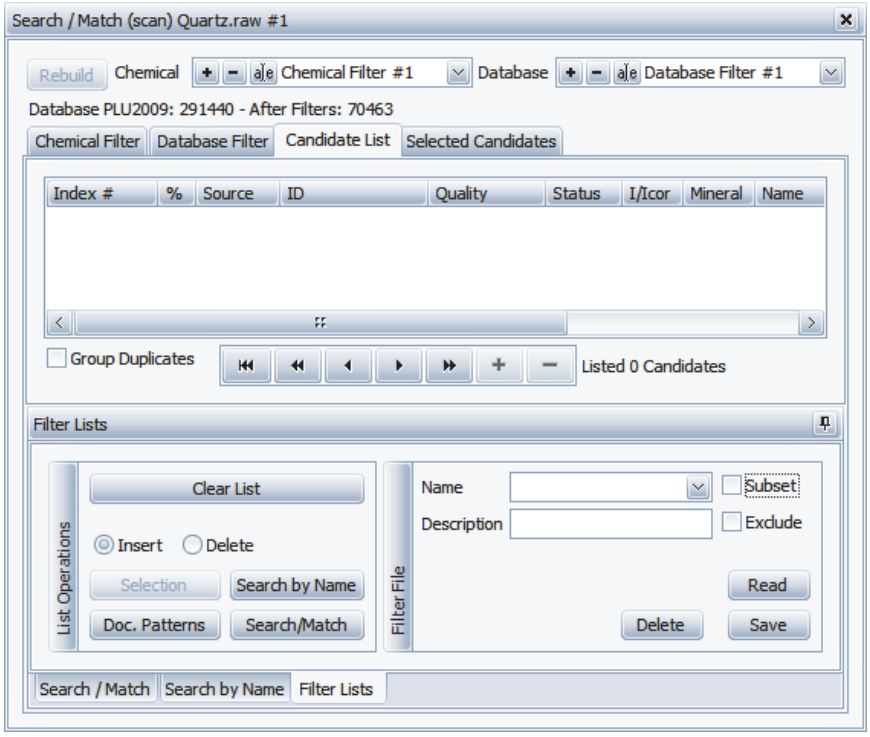


Fig.51: Filter Lists tab

To create a filter list:

1. Click the **Filter Lists** tab at the bottom at the bottom of the context menu. An empty candidate list is displayed at the top of the Filter Lists tab. At the bottom of the context menu there are tools to create and save lists.
2. Create a pattern list using the List Operations (on the left) :
   - To add patterns to the current filter list, select **Insert** and then click the button corresponding to the patterns to be inserted (see table below for the buttons description).
   - To remove patterns from the current filter list, select **Delete** and then click the button corresponding to the patterns to be removed (see table below for the buttons description).

   The entire list of patterns can be cleared by clicking the **Clear List** button.

Button	Description
Selection	Patterns selected in the candidate list. Only the Delete operation can be applied to this selection
Doc. Patterns	All the patterns of the current document
Search by Name	All the patterns from the current Search by Name results
Search/Match	All the patterns from the Search/Match results

3. Save the Filter List as a filter file (on the right) :
   - Enter a name for the list (limited to 13 characters, spaces are replaced by "_").
   - Enter a description for the list (optional).
   - Select the list type on the Filter file in the Database Filter tab, **Subset** and/or **Exclude**, by selecting the corresponding check box. If none are selected, the list will not appear in the database filter. The list can be used as a memory list. Selecting both options is recommended.
   - Click the **Save** button to save the Filter List.
4. Rebuild the search database by clicking the **Rebuild** button. Two groups will be added below the PDF databases group in the Database Filter tab: one for all the subset lists available and one for all the exclude lists.

NOTE

If no description is entered, the name will be used as the list name. If a description is entered, the description will be used as the list name in DIFFRAC.EVA.

Selecting the Patterns to Add to or Delete from a Filter List

There are four buttons corresponding to the different ways of selecting the patterns for a filter list:

- Selection: click the **Selection** button to select the patterns currently selected in the candidate list. Only the **Delete** operation can be applied to this selection.
- Doc. Patterns: click the **Doc. Patterns** button to select all the patterns from the current document.

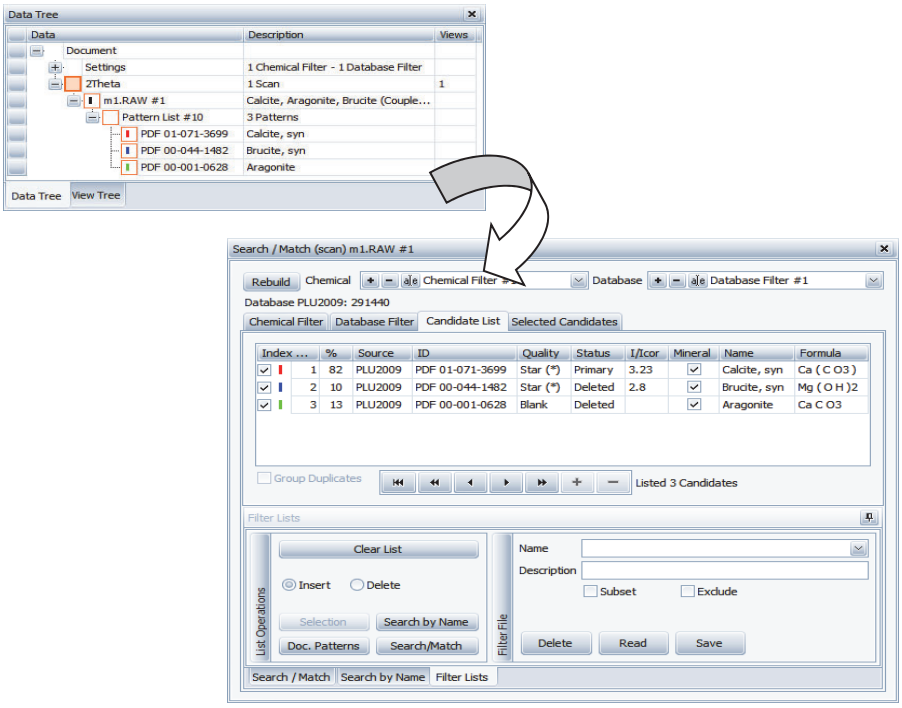


Fig.52: The patterns from the document are inserted into the filter list.

- Search by Name: click the **Search by Name** button to select all the patterns from the current Search by Name results.

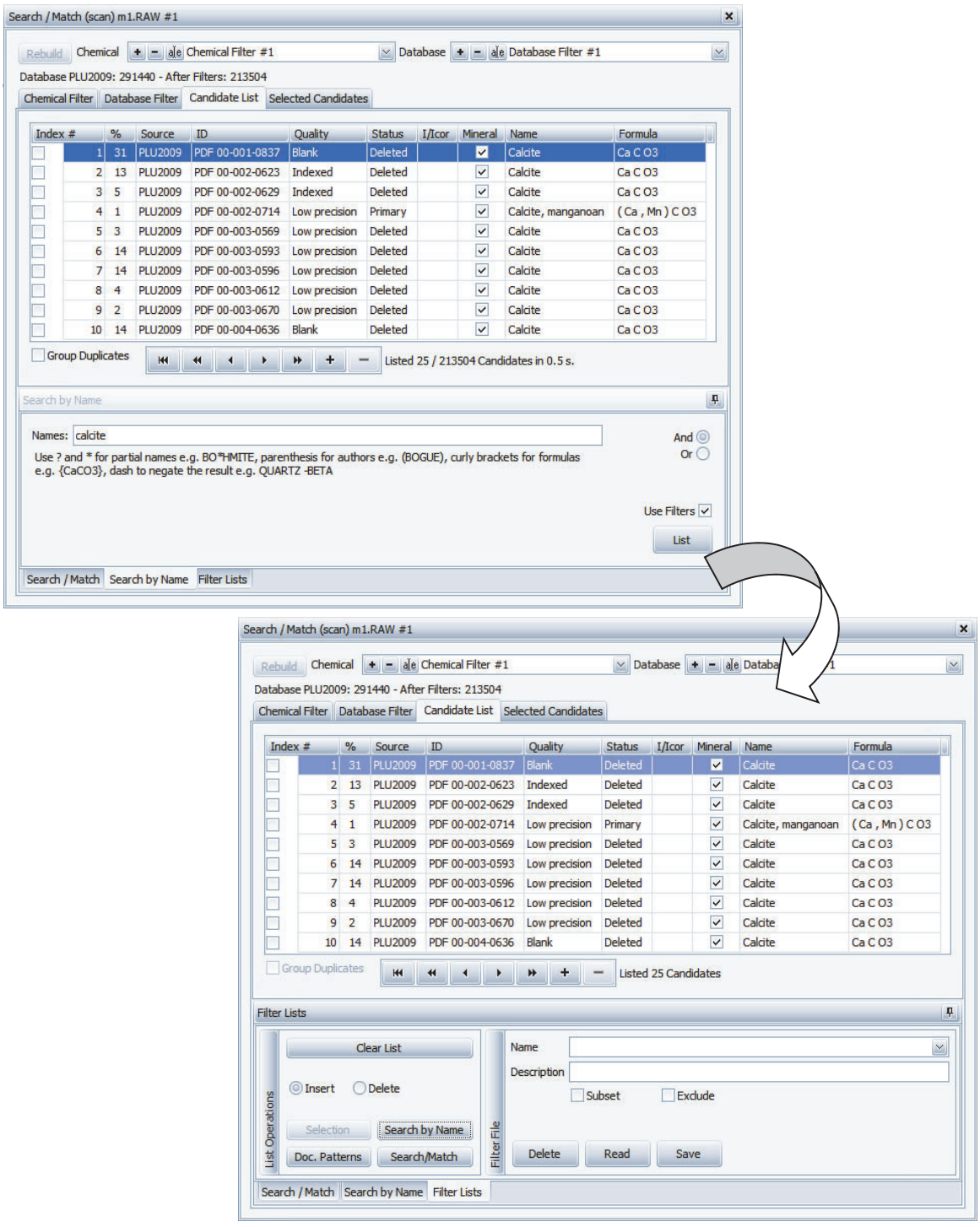


Fig.53: The patterns resulting from the Search by Name are inserted into the filter list.

- Search/Match: click the **Search/Match** button to select all the patterns from the current Search/Match results. This operation is versatile, since the chemical and database filters are comprehensive. Please see section “Performing a Search/Match Operation” on page 80 for more details.

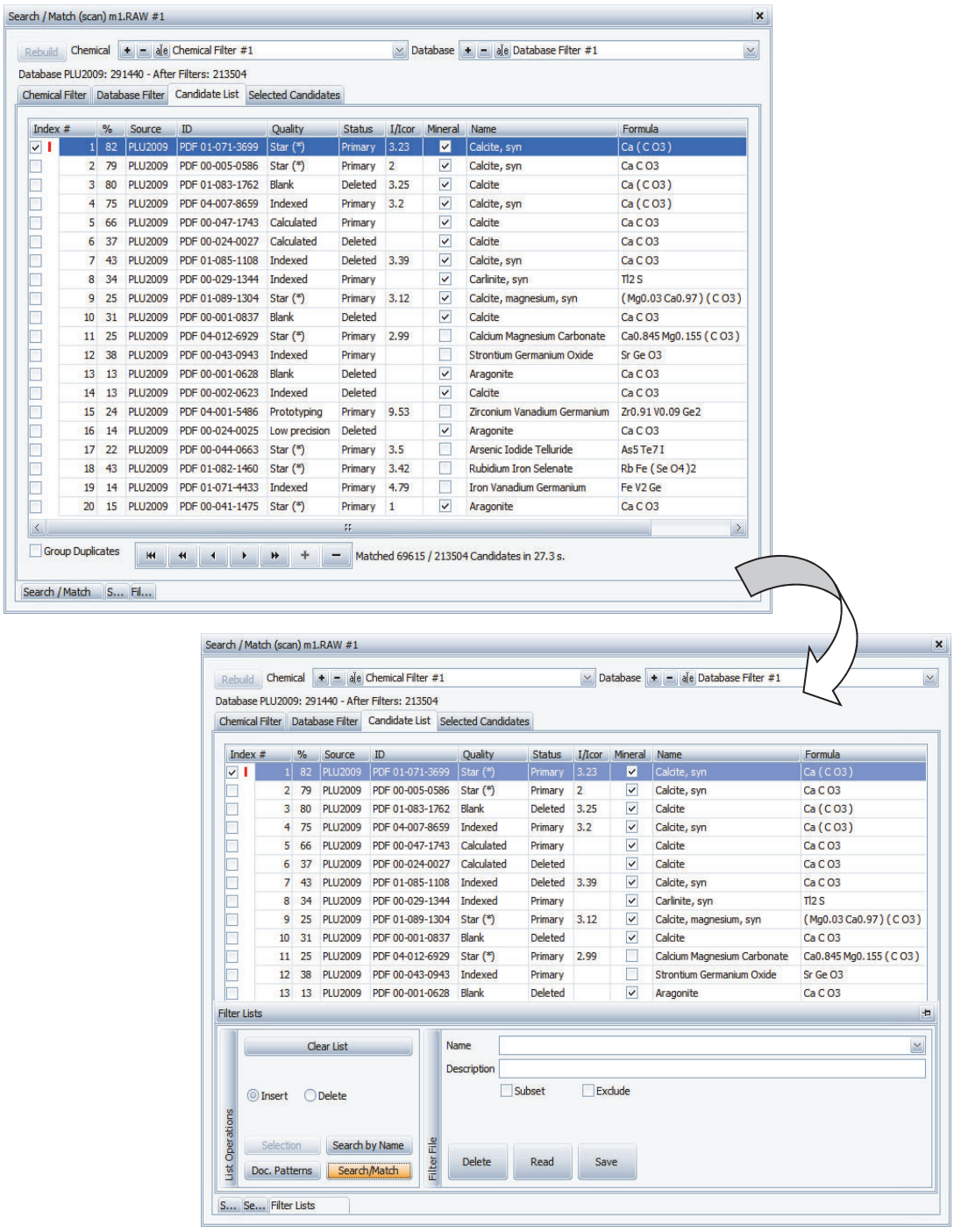


Fig.54: The patterns resulting from the Search/Match are inserted in the filter list.

Reading a Filter List

To read a Filter List, select the list in the **Name** drop-down list and click the **Read** button. The list of patterns belonging to the filter list will be displayed.

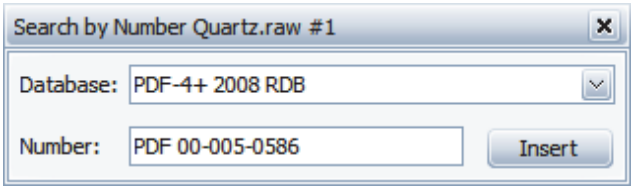
Deleting a Filter List

To delete a Filter List, select the list in the **Name** drop-down list and click the **Delete** button.

Performing a Search by Number

To perform a scan search by number:

1. Select a scan either in the data tree or in the 1D view to access the scan tools.
2. Click **Search by Number** in the Data command panel
   — or —
   right-click to display the scan related menu. Then click **Tool.** Click **Search by Number** on the submenu: the **Scan Search by Number** dialog box will be displayed.



3. Select the desired database in the **Database** drop-down list, if necessary.
4. Enter the pattern number.

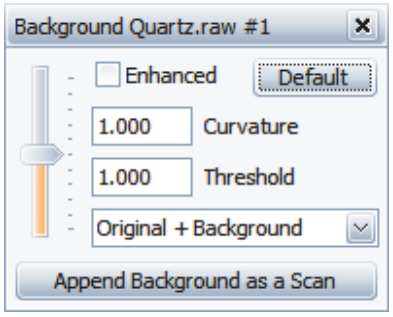
   The numbering scheme to enter the pattern number is the scheme of the corresponding database. For example, it is VV-XXXX for PDF-2 databases until release 2004 and SS-VVV-XXXX for PDF-2 starting with release 2005 and for all PDF-4.
5. Click the **Insert** button to insert the corresponding pattern on the graphical view and in the data tree.

Performing a Background Subtraction

When a scan is imported, the original scan and background are displayed by default. The background is displayed as a dashed line. The initial background is calculated with the default parameters.

To subtract the background from a scan with the DIFFRAC or the enhanced method:

1. Select the scan of interest either in the data tree or in the 1D view.
2. Click **Background** in the Data command panel
   — or —
   right-click the scan and then click **Tool** on the contextual menu.
3. Click **Background** on the Tool submenu. The **Background** dialog box will be displayed.



4. To display only the subtracted background select **Background subtracted** in the drop-down list.
5. Select the **Enhanced** check box if the corresponding method is preferred. This check box should be cleared to prepare Search/Match data and selected for other purposes.
6. Use the slider to adjust the curvature if there are background humps.
7. To make a scan from the background line, click the **Append Background as a Scan** button. The new scan will be added to the scan list in the data tree.

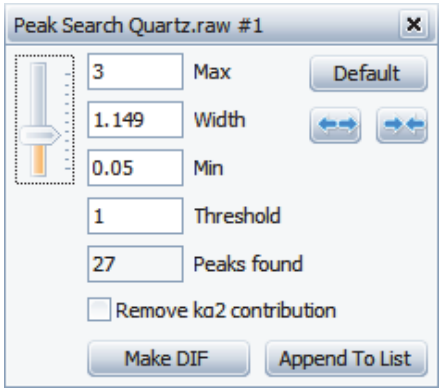
The DIFFRAC and Enhanced methods are described in the “Appendix” on page 209.

Performing a Peak Search

To perform a peak search on a scan:

1. Select the scan of interest either in the data tree or in the 1D view.
2. Click **Peak Search** in the Tool list of the Data Command panel
   — or —
   right-click the scan and then click **Tool i**n the context menu. Click **Scan Peak Search** in the Tool submenu.

The **Peak Search** dialog box will be displayed.



Expand and Reduce Interval buttons

3. Move the slider to see ghost peaks. If the amplitude of the slider is too small, use the **Expand Interval** button; if the precision of the slider is too low, use the **Reduce Interval** button. Click the **Default** button to return to the default parameters.
4. Remove the $K\alpha_2$ contribution by selecting the **Remove ka2 contribution** check box if necessary. It is not necessary to use the $K\alpha_2$ stripping which creates numerous artefacts. Please note that the peak intensities are the intensities resulting only from the $K\alpha_1$ contributions.
5. When the peak search is finished, continue with either of the following steps:
   - If manual editing is not required, click **Make DIF** to create a DIF pattern. A pattern list will be created in the Data tree and can be edited as well as the sticks which compose it.
   - When manual editing is required, click **Append To List**. Edit the list using the **Edition** tool for the Peaks from the control panel. A peak list will be created in the Data Tree. Each peak in the property table can be edited.

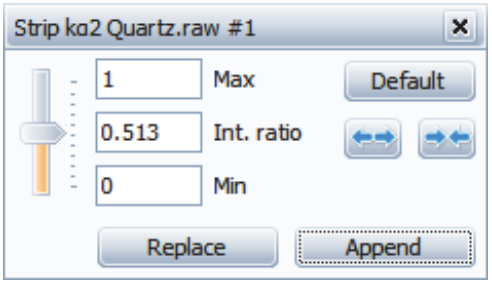
EVA's default width is 0.3 degrees or the equivalent in degrees of 15 steps, depending on the scan range.
If the value of 0.3 degrees falls within the range of 1 to 30 steps (if the step size is between 0.01 and 0.3 °), 0.3 ° is kept as the default value. If the width is larger, the default Width value will be set to 15 steps.

See section "Properties" on page 127 for the description of the pattern properties and section "Changing the Properties of a Peak" on page 152 for a description of the peak properties.

Computing Kα2 Stripping

To compute the $K\alpha_2$ stripping on a scan:

1. Select the scan of interest either in the data tree or in the 1D view.
2. Right-click the scan, and then click **Tool** on the context menu. Click **Strip Kα2** on the submenu: the **Strip Kα2** dialog box is displayed.



The ghost line shows the $K\alpha_2$-stripped line.

The default Intensity Ratio is read from the scan data and should be correct (if it is 0, the scan was measured with monochromatic radiation and does not require this treatment).

Expand and Reduce Interval buttons

3. Use the slider to adjust the ratio. If the amplitude of the slider is too small, use the **Expand** Interval button; if the precision of the slider is too low, use the **Reduce Interval** button. Click the **Default** button to return to the default parameters.
4. Once the result is satisfactory:
   - Click **Append** to append the $K\alpha_2$ subtracted scan to the document. The scan will be added to the scan list and its properties will be editable in the property table.
   - Click **Replace** to replace the original scan with the $K\alpha_2$ subtracted scan.

NOTE

The tool is of limited use for scans with a measurable amount of Kβ and W Lα lines because it cannot differentiate between these lines and Kα1/2.

Fourier Smoothing and Expansion

Smoothing with Fourier gives results similar to polynomial smoothing. The combination of smoothing and interpolation with a Fourier transformation is quite beneficial for a better-looking continuous curve when plotting the data and for data improvement.

The Fourier control panel displays a curve to adjust the Fourier filter. This curve is called the power spectrum, where:

- X is the bandwidth in degree^{-1} (maximum setting: 1 / Step_size)
- Y is the power density per bin, relative to the maximum in dB

The cutoff (threshold) for frequencies to attenuate can be adjusted. The other adjustment is for the expansion (x1 for no expansion; or x2, x4, x8, and x16).

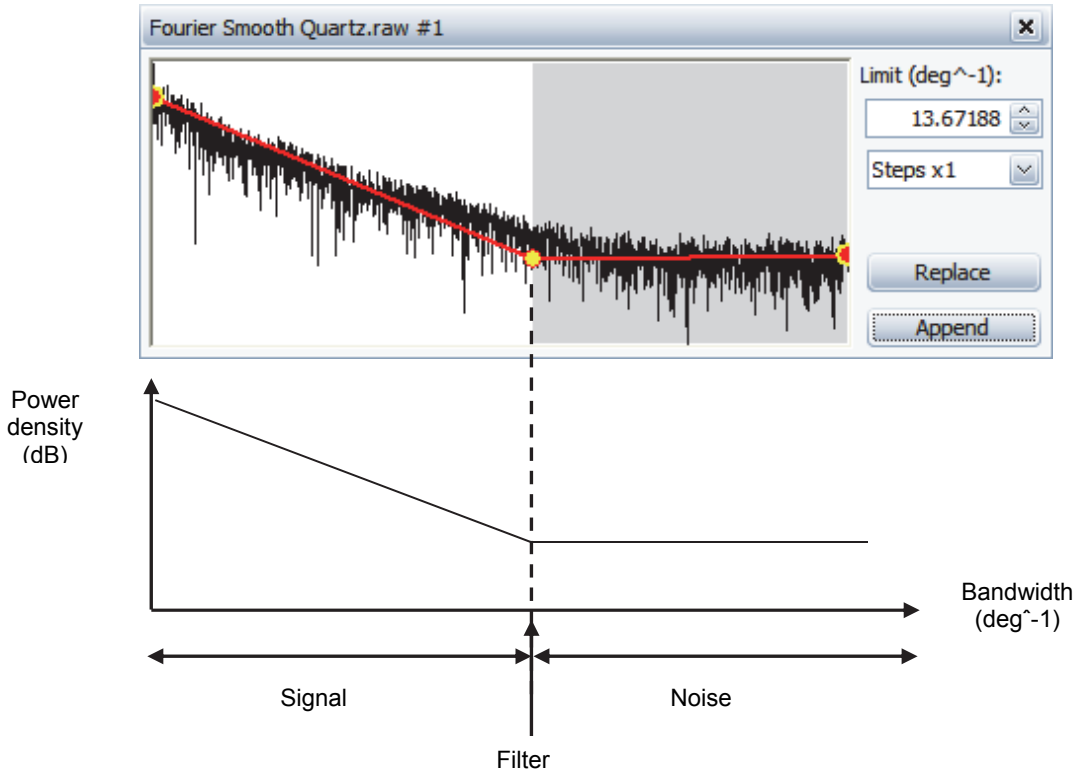


Fig.55: Schematic representation of the Fourier smoothing

The estimated power spectrum of the raw data usually exhibits a bend like an elbow. On the left, data are representative of the significant part of the signal (low frequency range); the flat tail in the upper frequency range represents high frequency noise (usually not desired). The frequency of the breakpoint (expressed in number of data points per degree) is directly related to the width of the narrowest peaks in the scan. This depends on the sample and has an absolute limit for a given instrument configuration.

In some cases, the scan appears to be distorted due to an oversized step, even though the frequency cutoff is clearly lower than 1/step size. In this case, data expansion allows interpolation between steps and facilitates a smoother scan. These points are computed to yield the only frequency-limited curve through the original set of points. Experience and theory suggest that the diffraction measurements are frequency limited. Therefore, the extra points can be considered reliable.

Using Fourier Smoothing

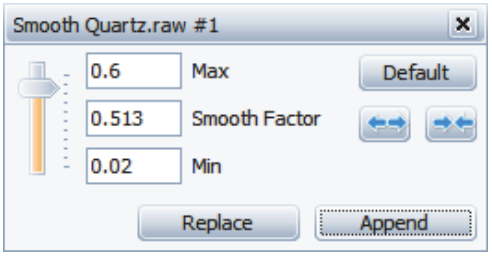
To use Fourier:

1. Select the desired scan either in the data tree or in the graphical view.
2. Click **Fourier Smooth** in the Tool list of the Data Command panel
   — or —
   right-click the scan, and then click **Tool** on the context menu. Click **Fourier Smooth** on the Tool submenu;
3. In the drop-down list, select the expansion (stepsx1, x2, x4, x8, and x16).
4. If necessary, adjust the cutoff by changing its value in the Limit (deg^-1) field or by moving the red and yellow circles. To move a circle, point to it and when the pointer becomes a hand, drag it to the desired position. A ghost of the enhanced scan is displayed in the 1D view.
5. Finally:
   - Click **Append** to append the smoothed scan to the document. The scan is added to the scan list and its properties can be edited in the property table.
   - Click **Replace** to replace the original scan with the smoothed scan.

Smoothing Scans

To smooth a scan:

1. Select the scan of interest either in the data tree or in the 1D view.
2. Right-click to display the related menu and then click **Tool.** Click **Smooth** on the submenu: the **Smooth** dialog box will be displayed.



Expand and Reduce Interval buttons

3. Use the slider to adjust the Smooth factor: the ghost line shows the smoothed line. If the amplitude of the slider is too small, use the **Expand Interval** button. If the precision of the slider is too low, use the **Reduce Interval** button. Click the **Default** button to return to the default parameters.
4. Once the result is satisfactory:
   - Append the smoothed scan to the document: click **Append**.
   - Replace the original scan with the smoothed scan: click **Replace**.

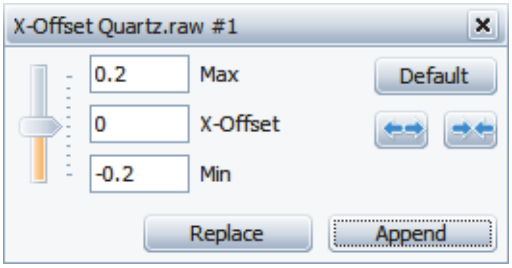
Correcting the X-Offset

Use this function to correct a scan for a systematic zero shift. For instance, a systematic 2θ shift in a 2θ scan can be corrected with a reference pattern known to be present in the sample.

EVA default adjustment range for X-Offset is the equivalent of ± 10 steps in degrees.

To correct the X-Offset:

1. Select the scan of interest either in the data tree or in the 1D view.
2. Right-click to display the related menu and then click **Tool.** Click **X-Offset** on the submenu: the **X-Offset** dialog box will be displayed.



Expand and Reduce Interval buttons

3. Use the slider to adjust the X-Offset: the ghost line shows the resulting line. If the amplitude of the slider is too small, use the **Expand Interval** button. If the precision of the slider is too low, use the **Reduce Interval** button. Click the **Default** button to return to the default parameters.
4. Once the result is satisfactory:
   - Append the modified scan to the document: click **Append**.
   - Replace the original scan with the modified scan: click **Replace**.

NOTE

A systematic X shift is very unlikely with a modern diffractometer.

Correcting the Sample Displacement Error

Sample displacement error is difficult to avoid, especially with top-loading samples. For 2θ and θ scans, EVA can correct the displacement error based on the goniometer radius. The radius can be changed directly in the Properties table of the scan.

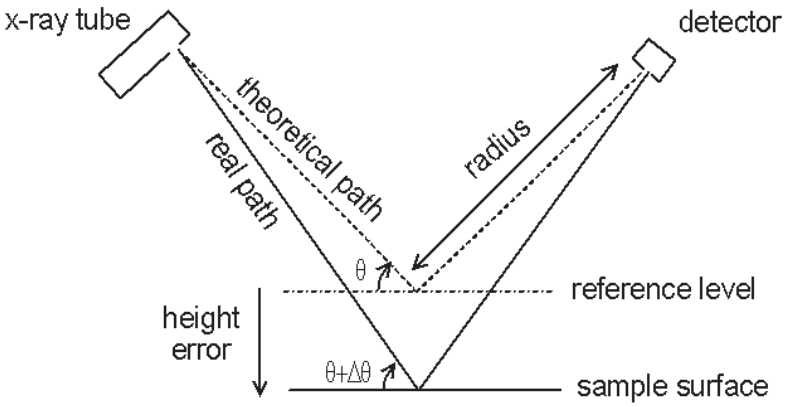
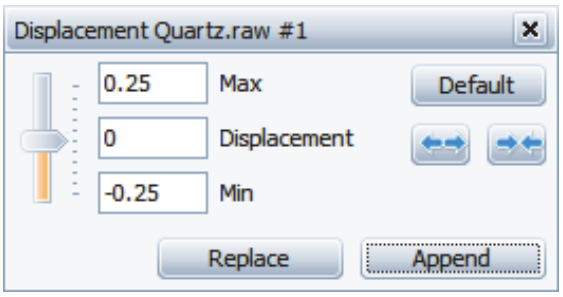


Fig.56: Sample displacement error

1. Select the scan of interest either in the data tree or in the 1D view;
2. Right-click to display the related menu and then click **Tool.** Click **Displacement** on the submenu: the **Displacement** dialog box will be displayed.



Expand and Reduce Interval buttons

3. Use the slider to adjust the Displacement: the ghost line shows the resulting line. If the amplitude of the slider is too small, use the **Expand Interval** button. If the precision of the slider is too low, use the **Reduce Interval** button. Click the **Default** button to return to the default parameters.
4. Once the result satisfactory:
   - Append the modified scan to the document: click **Append**.
   - Replace the original scan with the modified scan: click **Replace**.

NOTE

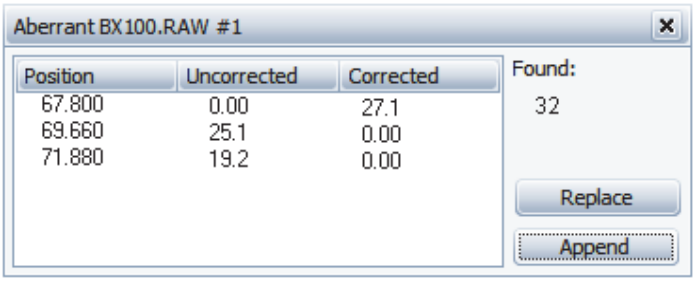
X offset and displacement errors are difficult to distinguish from one another, especially for scans measured below 90° 2θ. There is no disadvantage for phase analysis using the X offset treatment to correct an error caused by a sample displacement. However, it is unsuitable for crystallography — in fact, none of these corrections should be used for crystallography, because most crystallography software can refine similar corrections.

Suppressing Aberrant Points

EVA performs a statistical test for every point by comparing it with its two neighbours. The point values that fail the test are usually aberrant (parasitic signal) and can be replaced by the mean value of the two neighbours.

To remove aberrant points from a scan:

1. Select the scan of interest either in the data tree or in the graphical view.
2. Click **Aberrant** in the Tool list of the Data Command panel
   — or —
   right-click the scan, and then click **Tool** on the contextual menu. Click **Aberrant** on the Tool submenu.



3. Then either:
   - Click **Replace** to replace the original scan with the corrected scan.
   - Click **Append** to append the corrected scan to the document. The scan is added to the scan list and its properties can be edited in the property table.

NOTE

This feature is normally unnecessary for modern diffractometers.

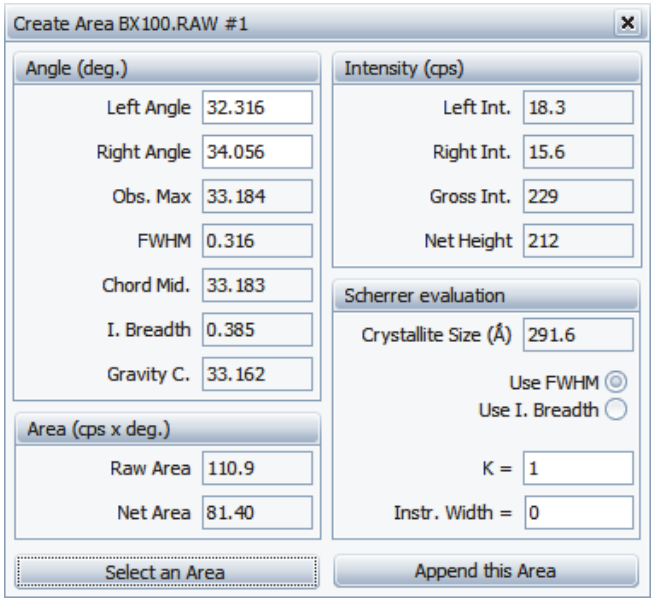
Computing Areas

The area computation is a statistical computation which assumes that there is a unique peak in the interval. The area computations are performed between two points, called "entry points" (usually entered with the mouse). The computation gives information such as the position of the peak maximum and the net area of the peak. This is *not* a profile fitting. For profile fitting, use dedicated software such as DIFFRAC.TOPAS for this purpose.

To compute an area:

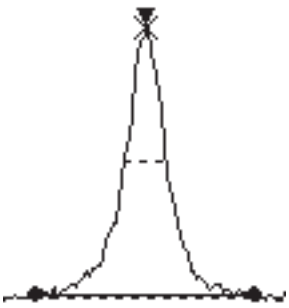
1. Select the scan of interest either in the data tree or in the 1D view.
2. Click **Create Area** in the Tool list of the Data Command panel
   — or —
   right-click the scan and then click **Tool.** Click **Create Area** in the Tool submenu;

The **Create Area** dialog box will be displayed.



3. Click **Select an Area** to select an area with the mouse (press and hold the left mouse button with the pointer on one end of the selection, then point to the opposite end and release the button). The results computed for the current scan will be displayed in the corresponding boxes.
4. Click **Append this Area** to add the area in the Data tree.

The areas are graphically displayed by:



- A base line at the area bottom
- A dashed line at the half maximum value (shows **FWHM** and the chord)
- A cross representing the gravity center position
- A vertical arrow representing the maximum position

To modify an area, drag any filled circle of the area bottom line.

NOTE

Area computations on multiple scans are allowed only when all scans have been measured with the same wavelength.

Item	Description
Angle	
Left/Right Angle	Ends of the computation: angles. The input is rounded to the closest data point in X while the input is retained in Y
Obs. Max	Angle corresponding to the maximum intensity
FWHM	Full Width at Half Maximum value
Chord Mid.	Middle of the chord drawn between the mean values of the crossing points used to determine **FWHM**
I. Breadth	Net area (in cps×scan units) divided by the net height (in cps). It is the breadth of a rectangle having the same net height and the same surface as the peak. Given in scan unit
Gravity C.	Third estimate for the peak location. It is the center of gravity of the net peak. It is the mean of each X position in the interval weighted by the net intensity. It is also given in d (Å) if the scan is 2θ
Area (cps×deg)	
Raw area	Computed with the trapeze method and given in cps×scan units (cps×degrees for angular scans)
Net area	
Intensity (cps)	
Left/Right Int.	Left/right height given in cps
Gross Int.	Gross intensity
Net Height	Self-explanatory
Scherrer evaluation	
Crystallite Size	Crystallite size in Angstroms (Á)
Use FWHM	Select this option if you want to use the FWHM for the calculation of the crystallite size
Use I. Breadth	Select this option if you want to use the Intensity Breadth for the calculation of the crystallite size
K =	Scherrer constant for the calculation of the crystallite size with the Scherrer formula usually taken as 1 or 0.89. The default value is 1
Instr. Width =	Instrumental FWHM (FWHM for a material that exhibits no broadening beyond the instrument contribution) used for the calculation of the crystallite size with the Scherrer formula. The default value is 0

Duplicating Scans

This feature is available from software version 3.2 up.

Duplicating a scan consists in creating a copy of the scan.

To duplicate a scan:

1. Select the scan to be copied in the data tree.
2. Click **Duplicate** in the Tool list of the Data Command panel
   — or —
   right-click the selection and then click **Tool** on the context menu. Click **Duplicate** on the Tool submenu.

The resulting scan is displayed in the graphical view and added to the scan list in the data tree. The resulting scan is given the name of the original scan plus the mention (Duplicate).
The properties of the resulting scan can be accessed in the same way as the properties of the original scans.

Accumulating Scans

This feature is available from software version 3.2 up.

Accumulating scans consists in adding their times and counts.

To accumulate scans:

3. Multi-select the scans of interest in the data tree.
4. Click **Accumulate** in the Tool list of the Data Command panel
   — or —
   right-click the multi-selection and then click **Tool** on the context menu. Click **Accumulate** on the Tool submenu.

The resulting scan is displayed in the graphical view and added to the scan list in the data tree. The resulting scan is given the name of the first selected scan plus the mention (Accumulate).
The properties of the resulting scan can be accessed in the same way as the properties of the original scans.

Adding and Subtracting Scans

To add scans:

5. Multi-select the scans of interest in the data tree.
6. Click **Add** in the Tool list of the Data Command panel
   — or —
   right-click the multi-selection and then click **Tool** on the context menu. Click **Add** on the Tool submenu.

The resulting scan is displayed in the graphical view and added to the scan list in the data tree. The resulting scan is given the name of the first selected scan.
The properties of the resulting scan can be accessed in the same way as the properties of the original scans.

To subtract two scans:

Using two scans as an example, scan A and scan B. If the user would like to subtract scan B from scan A, the following procedure should be used:

1. Select scan A first and then scan B, using a multi-selection tool in the data tree.
2. Click **Subtract** in the Tool list of the Data Command panel
   — or —
   right-click (the multi-selection) and then click **Tool** on the context menu. Click **Add** on the Tool submenu.

To subtract scan A from scan B:

1. Select scan B first and then scan A using a multi-selection tool in the data tree.
2. Click **Subtract** in the Tool list of the Data Command panel
   — or —
   right-click (the multi-selection), and then click **Tool** on the context menu. Click **Add** on the Tool submenu.

Each resulting scan is displayed in the graphical view and added to the scan list in the data tree. The resulting scan is given the name of the first selected scan.
The properties of the resulting scan can be accessed the same way as the properties of the original scans.

Merging Scans

Merging several scans to create a single one can be useful when performing a Search/match on data that have been measured and stored in separated scans.

Scans are merged in Cps even if the current Y-scale is in counts. As a result, the user can work with scans that have not been measured with the same measuring time per step.

The **Merge** function works as follows:

- The difference between the end angle of the scan at the lower angles and the start angle of the scan at the higher angles must be less or equal to 1.1 step of the scan with the bigger step. This condition is satisfied when the scans share one or more data points. It is recommended that the scans share at least one data point.
- The scan used as the reference is the first selected scan, the other scan is called "slave scan".
- The measuring conditions of the reference scan are retained for the merged scan.

To merge scans:

1. Multi-select the scans of interest in the data tree.
2. Click **Merge** in the Tool list of the Data Command panel
   — or —
   right-click the multi-selection and then click **Tool** on the context menu. Click **Merge** on the Tool submenu.

The resulting scan is displayed in the graphical view and added to the scan list in the data tree. The resulting scan is given the name of the first selected scan.
The properties of the resulting scan can be accessed the same way as the properties of the original scans.

Description of the Merge algorithm

- The slave scan is multiplied by a scaling factor. Therefore, the average intensity over the shared region is the same as in the reference scan.
- If the step size is different in both scans, the slave scan is resampled (interpolated) to have the same step size.
- In the shared region, there is a smooth transition between scans.

  $I = p.I_A+(1-p)I_B$

  where p is the proportion of scan A. The proportion varies from 1 to 0.

If the scans are displayed in counts, the Cps are converted using the step time of the reference scan.

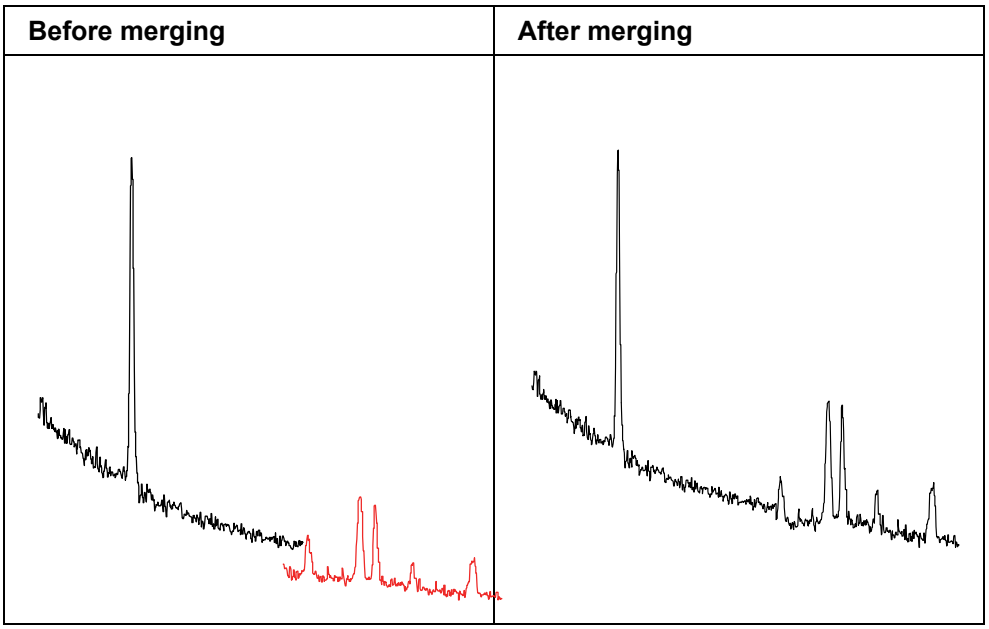


Fig.57: Merging algorithm, Y-scale in counts per second (Cps)

Creating a Pattern from the Lattice Parameters with the [hkl] Generator

This feature is available from software version 3.0 up.

The [hkl] Generator creates patterns from lattice parameters.

This tool can be applied from the scan node where it will start without parameters. A pattern with user-chosen lattice parameters will be created.

This tool can also be applied directly from an existing pattern which automatically enters the crystal system, space group information and lattice parameters. See section “Creating a Pattern from an Existing Pattern with the [hkl] Generator” on page 136.

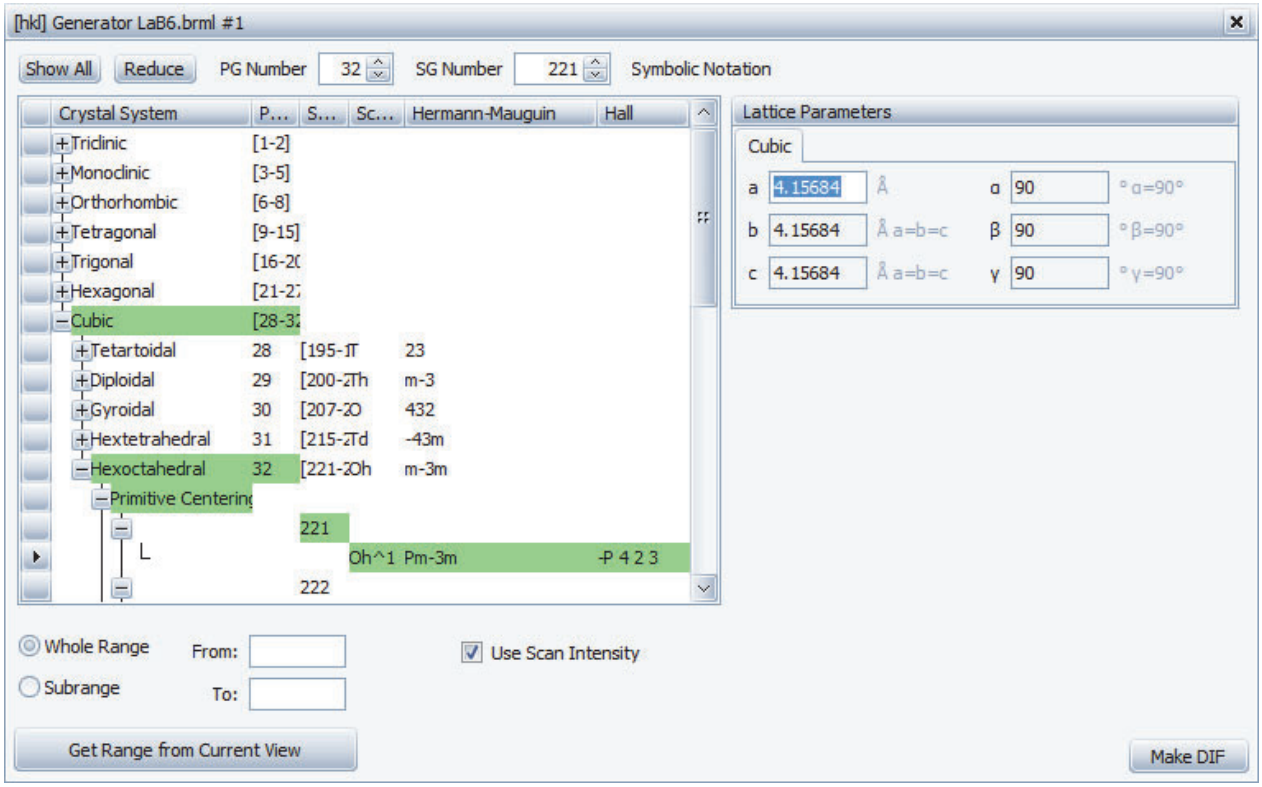


Fig.58: The [hkl] Generator tool applied from parameters entered by the user

The [hkl] Generator is useful in the following situations when:

- Observed lines are missing in a PDF pattern. This might be the case for low quality PDF patterns.
- A pattern is found that explains a significant part of the unknown scan, but its chemistry is not compatible with prior knowledge. As a result, both materials might have similar cells.
- The lines outside the pattern limits should be checked.

To create the hkl's for arbitrary cell parameters:

1. Select the scan for which the pattern should be created.
2. Click **[hkl] Generator** in the Data command panel
   — or —
   right-click the selection to display the scan related menu. Click Tool and then **[hkl] Generator**.
3. Choose the crystal system in the tree control
   — or —
   enter the space group number
   — or —
   enter the Herman-Maugin symbol in the respective controls.
   The required lattice parameters edit controls are enabled accordingly.
4. Enter the lattice parameters. When the last parameter has been entered, the **Make DIF** button becomes is activated.
5. Click the **Make DIF** button. The calculated pattern will be appended to the pattern list.

Additional controls

Control	Description
Whole Range	The angular range of the scan is used as a limit for calculating the line positions.
Subrange	The positions given in the From: and To: fields are used as calculation limits.
From:	Start limit for line position calculation
To:	End limit for line position calculation
Get Range From Current View	Fill the **From:** and **To:** controls with the (possibly zoomed) limits of the current view.
Use scan intensity	If activated, the line intensity is calculated from the scan's net intensity at the position of the line. Otherwise, all lines have the same intensity.

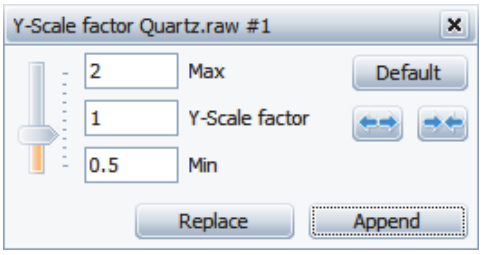
Re-Scaling the Current Scan

This feature is available from software version 2.0 up

To compare two scans it is useful to re-scale one of the scans. To do this, multiply the scan by a given factor or by adding an offset value to it.

To multiply the current scan by a given factor:

1. Select the scan of interest either in the data tree or in the 1D view.
2. Click **Y-Scale factor** in the Tool list of the Data Command panel
— or —
Right-click to display the related menu and then click **Tool.** Click **Y-Scale factor** on the submenu: the **Y-Scale factor** dialog box will be displayed.



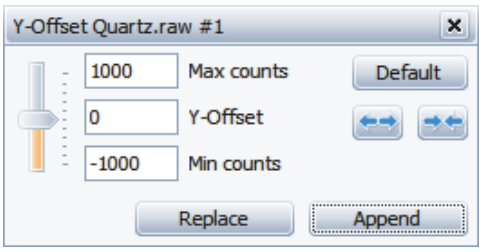
Expand and Reduce Interval buttons

3. Use the slider to adjust the Y-Scale factor: the ghost line shows the resulting line. If the amplitude of the slider is too small, use the **Expand Interval** button. If the precision of the slider is too low, use the **Reduce Interval** button. Click the **Default** button to return to the default parameters.
4. Once the result is satisfactory:
    - Append the modified scan to the document: click **Append**.
    - Replace the original scan with the modified scan: click **Replace**.

It is possible to enter a Y-Scale factor value directly in the **Y-Scale factor** field of the Scan Property table.

To add an offset value to the scan:

1. Select the scan of interest either in the data tree or in the 1D view.
2. Click **Y-Offset** in the Tool list of the Data Command panel
— or —
Right-click to display the related menu and then click **Tool.** Click **Y-Offset** on the submenu: the **Y-Offset** dialog box will be displayed.



Expand and Reduce Interval buttons

3. Use the slider to adjust the Y-Offset: the ghost line shows the resulting line. If the amplitude of the slider is too small, use the **Expand Interval** button. If the precision of the slider is too low, use the **Reduce Interval** button. Click the **Default** button to return to the default parameters.
4. Once the result is satisfactory:
    - Append the modified scan to the document: click **Append**.
    - Replace the original scan with the modified scan: click **Replace**.

It is possible to enter an offset value directly in the **Y-Offset** field of the Scan Property table.

Normalizing Scans

There are three different ways of normalizing scans using EVA. The scans can be normalized to share the same maximum intensity, to share a common point or to share all points of a scan. All the scans displayed in the graphical view will be normalized.

To normalize the scans at one position:

1. To normalize the scans, right-click at the chosen position in the graphical view. The context menu will be displayed.
2. Click **Normalize all visible scans…**
3. Click **Normalize at position 2Th=… CPS**… on the related sub-menu,

To normalize the scans at the maximum intensity:

1. Right-click at the position in the graphical view to be normalized. The context menu will be displayed.
2. Click **Normalize all visible scans…**
3. Click **Normalize at Max Intensity CPS=…** on the related sub-menu.

To normalize the scans on a scan:

1. Right-click the scan of interest. The context menu will be displayed in the graphical view.
2. Click **Normalize all visible scans…**
3. Click **Normalize on Scan** on the related sub-menu.

Computing the Crystallinity

It is possible to compute the crystallinity of a sample from its scan.

The formulas used to compute the amorphousness and crystallinity percentages are as follows:

$$\%\text{Amorphous} = \frac{\text{Global area - Reduced area}}{\text{Global area}} \times 100$$

$$\%\text{Crystallinity} = 100 - \%\text{Amorphous}$$

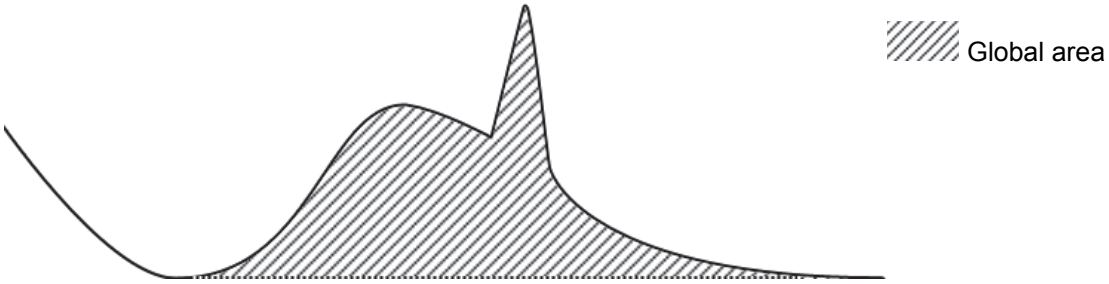


Fig.59: Global area: background with a 0.01 curvature taken automatically

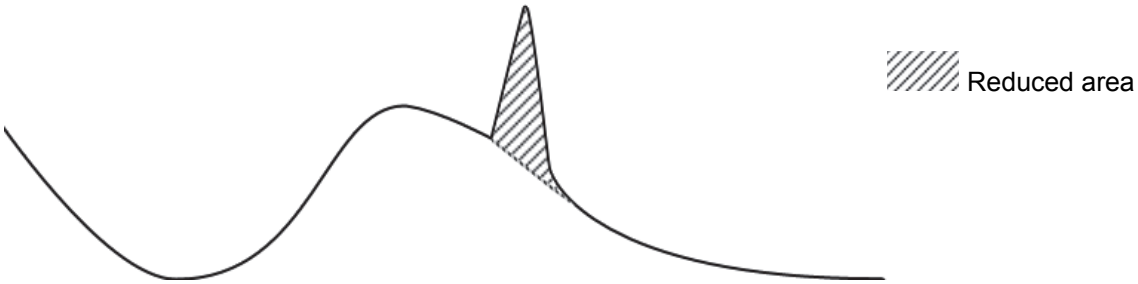


Fig.60: Reduced area: background adjusted by the user

To compute the crystallinity:

1. Select the scan of interest either in the data tree or in the graphical view.
2. In the scan property table, select the **Compute Crystallinity** check box.

The crystallinity percentage is given at the table row below: **%-Crystallinity**.

Simulating a Slit Mode

Measurements can be performed using either fixed or variable slits. A measurement carried out using a certain type of slit can be simulated with the other type of slit, as well.

Slit simulation is a special projection of the y-values of the original data, which depends on the slit type used. The other scan related data (peaks, areas, sticks, background) will be projected as well if they are displayed with the simulated scan.

To simulate a slit mode:

1. Make certain that the scan of interest is selected in the data tree.
2. Change the **Simul. Slit Mode** property in the Scan Property Table.

Exporting Scans

Exporting a Complete Scan

It is possible to export a scan in a file. To do so:

1. Select the scan in the data tree or in the graphical view.
2. Click **Export Scan…** in the File list of the Data Command panel
   — or —
   Right-click to display the related menu and then click **File.** Click **Export Scan…** on the submenu: the Export a Scan File dialog box will be displayed.
3. Enter a name for the RAW file and click the **Save** button.

The following features are available from software version 3.0 up.

If a multi-range scan should be exported, proceed the same but select the scan list and use the **Export Multi-Range Scan…** command.

It is also possible to export all the scans from a list of scans at once. To do so:

1. Select the scan list in the data tree or in the graphical view.
2. Click **Export All Scans…** in the File list of the Data Command panel
   — or —
   Right-click to display the related menu and then click **File.** Click **Export All Scans…** on the submenu: the Export a Scan File dialog box will be displayed.
3. Enter a name for the RAW file and click the **Save** button. All the exported scans will have this name plus a number as follows: name_0.raw for the first scan, name_1.raw for the second scan etc.

Exporting a Background Subtracted Scan

This feature is available from software version 3.2 up.

When using this command, the background subtraction is automatically applied to the scan before exporting.

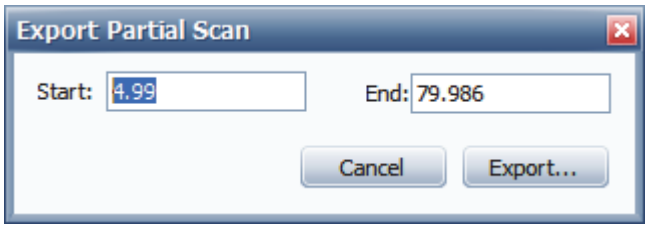
1. Select the scan in the data tree or in the graphical view.
2. Click **Export Bg Subtracted Scan…** in the File list of the Data Command panel
   — or —
   Right-click to display the related menu and then click **File.** Click **Export Bg Subtracted Scan…** on the submenu: the Export a Scan File dialog box will be displayed.
3. Enter a name for the RAW file and click the **Save** button.

Exporting a Partial Scan

This feature is available from software version 2.0 up

It is possible to export a part of a selected scan into a raw file. To do so:

1. Select the scan in the data tree or in the graphical view.
2. Click **Export Partial Scan…** in the File list of the Data Command panel
   — or —
   Right-click to display the related menu and then click **File.** Click **Export Partial Scan…** on the submenu: the Export Partial Scan dialog box will be displayed.



3. The initial values are taken from the current zoom range. Enter the **Start** and **End** values of the desired export range.
4. Click the **Export…** button: the Export Partial Scan dialog box will be displayed.
5. Enter a name for the RAW destination file and click the **Save** button.

Exporting a Background

This feature is available from software version 2.0 up

It is possible to export the calculated background of a scan into a raw file. To do so:

1. Select the scan in the data tree or in the graphical view.
2. Click **Export Background…** in the File list of the Data Command panel
   — or —
   Right-click to display the related menu and then click **File.** Click **Export Background…** on the submenu: the Export a Scan File dialog box will be displayed.
3. Enter a name for the RAW destination file and click the **Save** button.

Replacing and Cloning Scans

These features are available from software version 2.0 up

Replacing a Scan

It is possible to replace a scan in the EVA document with another scan read from a different file. While the scan data are replaced all children data of the scan such as peaks, areas and patterns are retained.
There is one condition which must be fulfilled for a successful scan replacement: the scan axes must be similar. All children of the original scan which are outside of the new scan's domain will be hidden.
It is not possible to replace a scan with a multi-range scan.

To replace a scan with another scan:

1. Select the scan to be replaced in the data tree or in the graphical view.
2. Click **Replace Scan…** in the Tool list of the Data Command panel
   — or —
   Right-click to display the related menu and then click **Tool.** Click **Replace Scan…** on the submenu: the Import a Scan File dialog box will be displayed.
3. Select the desired scan file RAW file and click the **Open** button.

Cloning a Scan

Cloning a scan consists in copying the children data of a selected scan to an imported scan (cloned scan). The original scan and corresponding data will be retained.

Several assumptions are made to predict how the cloned scan will be displayed:

- If a 1D View exists on the scan list, both scans will be displayed in the same view.
- If a 1D View exists specific only to that particular scan, a second view will be created.
- If there is no 1D View either for that scan or its list, no 1D View will be created.

To clone a scan:

1. Select the scan to be replaced in the data tree or in the graphical view.
2. Click **Clone Scan…** in the Tool list of the Data Command panel
   — or —
   Right-click to display the related menu and then click **Tool.** Click **Clone Scan…** on the submenu: the Import a Scan File dialog box will be displayed.
3. Select the desired scan file RAW file and click the **Open** button.

Working with Patterns

Importing a Pattern

To import a pattern into an empty document, use either the Search by Name or the Search by Number tool. To do so:

1. Click the **New** button to create a new document (if necessary).
2. Select the document node in the Data Tree.
3. Click **Search by Name** or **Search by Number** on the Tool list of the Data Command panel
   — or —
   right-click the document node and then click **Tool** on the context menu. Click **Search by Name** or **Search by Number** on the Tool submenu.
4. Proceed as described in sections “Performing a Search by Name” on page 75 and “Performing a Search by Number” on page 82.

Properties

Pattern properties

Property	Description
Data	
Legend	Legend used to characterize the data. See section “Creating Captions” on page 53 to customize the legend
Attributes	
Visible	Clear the **Visible** check box to remove the selected pattern from the graphical display. Select the check box to display the current pattern
Color	Choose a color for the display of the current pattern
Display	Choose the information to display for the pattern
Line thickness	Choose a line thickness
Marker image	Choose a marker image
Marker size	Choose a marker size
Stick visibility	Choose the view(s) in which the sticks should be visible
Material	
Compound name	Compound name(s) as stored in the database
Formula	Chemical formula
SS-VVV-PPPP	Reference pattern number (SS=source number, VVV=volume number, NNNN=pattern number)
Scalings	
Y-Scale	Scaling factor used for this pattern in % (height of strongest line divided by the highest point of the parent scan multiplied by 100)
d x by	Factor used to multiply the d values to simulate isotropic dilatation or compression of the unit cell (e.g. solid solution effects)
Scan WL	Wavelength for the pattern is the same as for its parent scan by default. Clear the check box to enter another wavelength for the pattern
Wavelength	Wavelength value used for the display. Choose a value in the predefined list if the **Scan WL** check box is cleared. Enter a blank value to return to the default value
Quantification	
I/Ic DB	I/c PDF is the ratio I/I_{cor} between the intensities of the strongest line of the compound of interest and the strongest line of corundum, both measured from a scan made of a 50-50 mixture, as stored in the PDF database
I/Ic User	I/Ic User: same as above, but the value is determined by the user
S-Q	Semi-quantitative (S-Q) weight percentage of the phase corresponding to the selected pattern. This value is computed from the I/Icor value as stored in the PDF database or specified by the user. When both ratios I/Ic PDF and I/Ic User exist, the latter is used for computing the **S-Q** value
Added Reference	Select the corresponding check box to enter a value for the added reference in the pattern column view when a semi-quantitative phase analysis is carried out

Property	Description
Cell	
System	Crystal system
Space Group	The three dimensional space group symbol (Hermann-Mauguin notation) and, in parentheses, the number of the space group (from 1 to 230) as given in the **International Tables for X-ray Crystallography**
a, b and c	Unit cell parameters in angstroms
alpha, beta and gamma	Interaxial angles in degrees
Z	Number of molecules per unit cell
Volume	Cell volume in Å
Density	Type of Bravais lattice
Cell tuned	Indicates if the cell has been tuned or not
Figure of Merit	
F(N)	Figure of Merit of the pattern
Children Columns	
Data	Choose the way the sticks are characterized in the stick list. See section “Creating Captions” on page 53 to customize the data
Description	Choose a description for the sticks in the list. See section “Creating Captions” on page 53 to customize the description

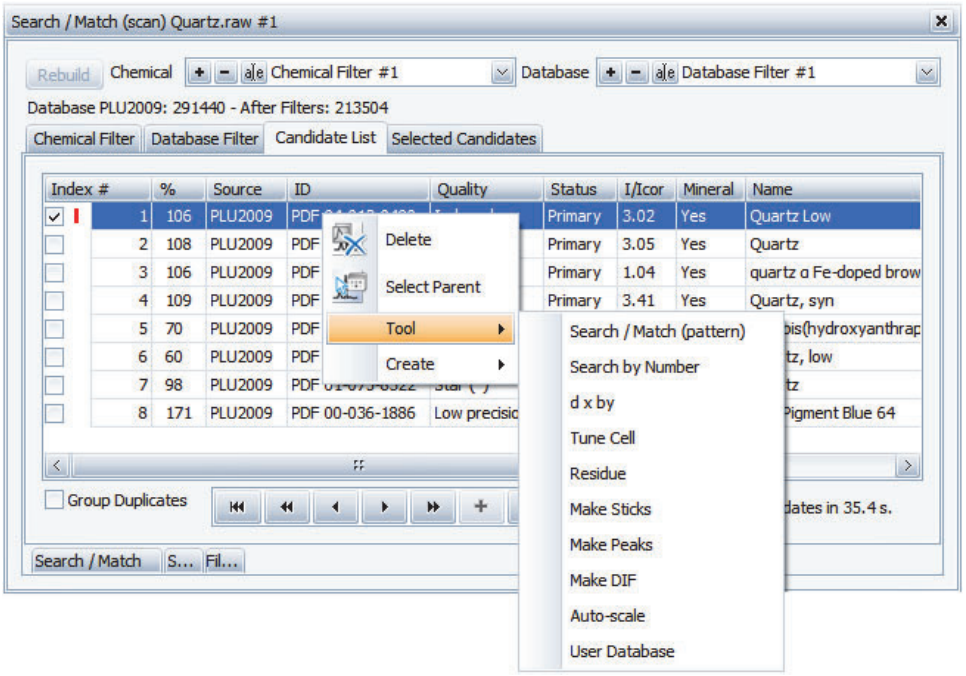
Sticks Properties

Property	Description
Attributes	
Caption	Choose the information to display for the stick. See section “Creating Captions” on page 53 to customize the caption
Caption (display)	Display preview
Stick	
Angle	Stick position in 2θ°
d Value	d value of the selected stick
Intensity	Intensity of the stick (Counts)
Rel. intensity	Relative intensity
h, k, l	hkl indices corresponding to the stick; Click + to view the indices separately
Remark	Self-explanatory

Different Ways to Perform an Operation on a Pattern

There are different ways to perform an operation on a Pattern.

- Click the pattern of interest either in the Data tree or in the graphical view. Click the desired command in the Data Command Panel.
- Right-click the pattern of interest either in the Data tree or in the graphical view and click the desired command on the context menu displayed.
- Perform an operation directly on a pattern selected in the candidate list after a Search/Match or a search by Name operation:
  Right-click the line of the selected pattern and click the desired command on the context menu.



Performing a Search/Match Operation on a Pattern

To perform a Search/Match operation on a pattern:

1. Select the pattern of interest either in the data tree or in the 1D view.
2. Click **Search / Match (pattern)** in the Data command panel
   — or —
   right-click, click **Tool** in the menu which appears and then **Search / Match (pattern)** on the related submenu.

The **Search/Match (pattern)** dialog box is displayed as follows:

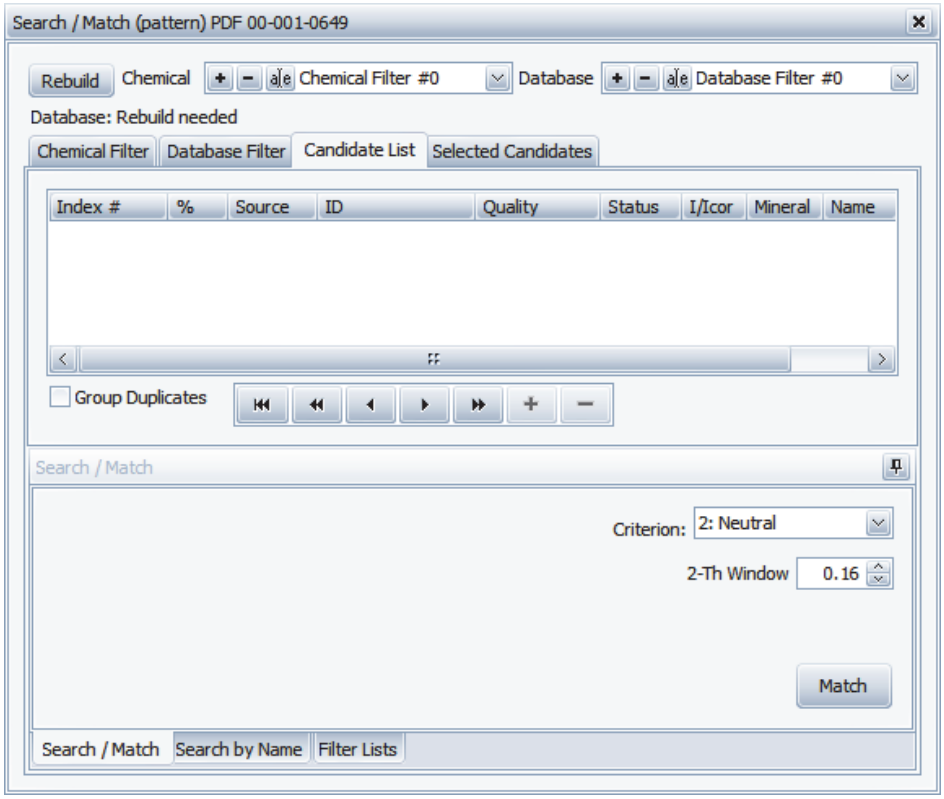


Fig.61: Search/Match (pattern) dialog box, Candidate List tab

When searching for a pattern on a pattern, there is no natural error window (as in the case of a scan). The **2-Th Window** field is the error window. The default error window is 0.16 (± 0.16°).

See “Performing a Search on a Scan” on page 80 for a detailed description of the tab and its usage.

NOTE

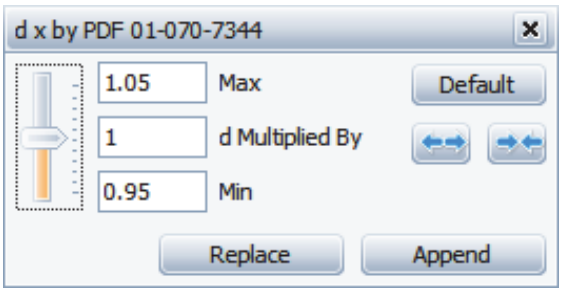
The Search/Match (scan) tool is available for a list of patterns: the search will be performed on the parent scan.

Performing a d x By (d multiplied by) Operation on a Pattern

This option permits simulation of a pattern with an increase or decrease of the lattice parameters due to a solid solution formation. The d-values are multiplied by the same factor, simulating an isotropic dilatation (factor >1) or contraction (factor<1).

To multiply d-values by a factor:

1. Select the scan of interest either in the data tree or in the 1D view.
2. Click **d x by** in the Data command panel
   — or —
   right-click the selection to display the context menu and then click **Tool.** Click **d x by** on the submenu: the **d x by** dialog box is displayed.



3. Use the slider to adjust the “d Multiplied By” factor: The ghost provides a graphical representation of the modified pattern. If the amplitude of the slider is too small, use the **Expand Interval** button. If the precision of the slider is too low, use the **Reduce Interval** button. Click the **Default** button to return to the default parameters.

Expand and Reduce Interval buttons

5. When the result is satisfactory:
   - Append the modified pattern to the document: click **Append**.
   - Replace the original pattern with the modified pattern: click **Replace**.

NOTE

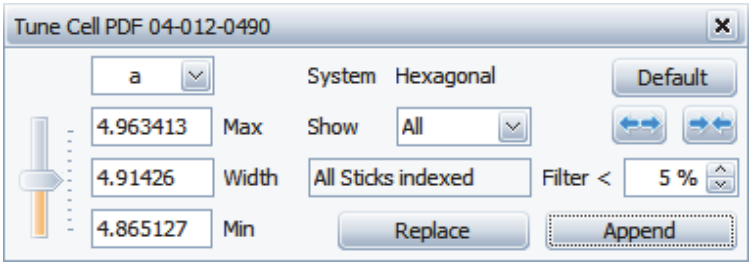
A factor of 1.005 is significant; 1.05 is very large.

Anisotropic Deformation of a Pattern by using the Tune Cell Operation

The goal is to match a scan that shows solid-solution effects with a pattern that represents the same phase without the solid-solution effect (or with a different effect). The less symmetric the crystal is, the more parameters are to be adjusted. If the effect of the solid solution on the parameters is known, the operation can be simplified. For example, a user may know that there is compression on direction a, and an expansion on direction b and c for a given orthorhombic phase.

To change a cell parameter:

1. Select the scan of interest either in the data tree or in the 1D view.
2. Right-click the selection to display the context menu and then click **Tool.** Click **Tune Cell** on the submenu: the **Tune Cell** dialog box will be displayed.



3. Select the parameter of interest in the drop-down list.
4. Move the slider up or down to adjust the cell parameter. The ghost provides a graphical representation of the modified pattern. If the amplitude of the slider is too small, use the **Expand Interval** button. If the precision of the slider is too low, use the **Reduce Interval** button. Click the **Default** button to return to the default parameters. A filter can be set to remove small lines.

Expand and Reduce Interval buttons

5. Once the result is satisfactory, the following options can be carried out:
   - Append the modified pattern to the document: click **Append**.
   - Replace the original pattern with the modified pattern: click **Replace**.

To make the graphical adjustment easier:

- Remove the Kα_2-lines, which may facilitate the adjustment. It ensures that the Kα_2 lines will not be accidentally used (see section “Computing Kα2 Stripping” on page 104).
- The **Show** drop-down list allows display of the ghosts of a subset of lines instead of all lines. The subset is made of lines corresponding to the h00, 0l0, 00l and, only for tetragonal and hexagonal crystal systems, the hk0 Miller indices. When adjusting a parameter, it is possible to display only a subset of lines influenced by this parameter (e.g. h00 for a). This can minimize a trial and error process.

NOTE

If a pattern line is not indexed (e.g. pattern #00-010-0100), then the line will not be modified by the tune cell. Non-indexed lines indicate that the quality of the pattern is doubtful.

Displaying the Current Pattern with Another Wavelength

The patterns are usually displayed for the $K\alpha_1$ radiation. To display the pattern that would be obtained with another wavelength:

1. Clear the **Scan WL** check box in the Pattern Property table.
2. Choose a wavelength in the predefined list or enter the chosen value in the Wavelength field below.

Enter a blank value to return to the default value.

Generally, this option is used to display patterns that would be obtained with:

- The $K\alpha_1$+$K\alpha_2$ gravity center, for example, for broad lines.
- The $K\alpha_2$ radiation - to check whether a peak is the $K\alpha_2$ peak of the phase or if it belongs to another phase.
- The $K\beta$ radiation - to check how well $K\beta$ is attenuated if a $K\beta$ filter is used (at least for the strongest line).
- The $WL\alpha_1$ radiation, which is the most frequently encountered spurious X-ray line in sealed X-ray tubes. These lines are a result of spectral impurities caused by the X-ray tube filament.

NOTE

This option is to be used when the **X-Unit** is **2-Theta**.

Creating Sticks from a Pattern

To convert a pattern into a list of Sticks:

1. Select the pattern of interest.
2. Click **Make Sticks** in the Data command panel
   — or—
   right-click to display the pattern related menu and click the **Make Sticks** command.

The stick list is added to the Data tree.

Creating Peaks from a Pattern

You can convert a pattern into a list of Peaks:

1. Select the pattern of interest.
2. Click **Make Peaks** in the Data command panel
   — or—
   right-click to display the pattern related menu and click the **Make Peaks** command.

The peaks are displayed in the graphical view and the corresponding peak list is added to the Data tree.

Creating a DIF from a Pattern

To create a DIF pattern from a pattern:

1. Select the desired pattern.
2. Click **Make DIF** in the Data command panel
   — or —
   right-click the selection to display the pattern related menu. Click Tool and then **Make DIF**.

After it is created, the DIF is appended to the pattern list.

Exporting and Importing a DIF

It is possible to export a DIF as a DIF file. To do so:

1. Select the DIF of interest.
2. Click **Export DIF…** in the Data command panel
   — or —
   right-click the selection to display the DIF related menu. Click File and then **Export DIF…**.

   The Export file dialog box will be displayed.
3. Enter a name for the .DIF file and click **Save**.

To import a DIF file:

1. Select a scan in the data tree.
2. Click **Import a DIF File** in the Data command panel
   — or —
   right-click the selection to display the DIF related menu. Click File and then **Import a DIF File.**

   The Import a DIF File dialog box will be displayed.
3. Select a DIF file and click **Open**.

Re-Scaling the Current Pattern

Re-scaling a pattern can prove useful in the case of a semi-quantitative analysis.

To do so:

1. Make sure the pattern of interest is selected.
2. Press the **Control** key and point to the scan to change the pointer into a hand. Move the hand up or down to adjust the scale,
   — or —
   enter a scale factor in % directly in the **Y-Scale** field of the Pattern Property table.

To return to automatic scaling:

1. Select the pattern of interest.
2. Click **Auto-scale** in the Data command panel
   — or —
   right-click the selection to display the peak list related menu. Click Tool and then **Auto-scale**.

Creating a Pattern from an Existing Pattern with the [hkl] Generator

This feature is available from software version 3.0 up.

The [hkl] Generator creates patterns from lattice parameters.

This tool can be applied from the scan node where it will start without parameters. A pattern with user-chosen lattice parameters will be created. See section “Creating a Pattern from the Lattice Parameters with the [hkl] Generator” on page 117.

This tool can also be applied directly from an existing pattern which automatically enters the crystal system, space group information and lattice parameters.

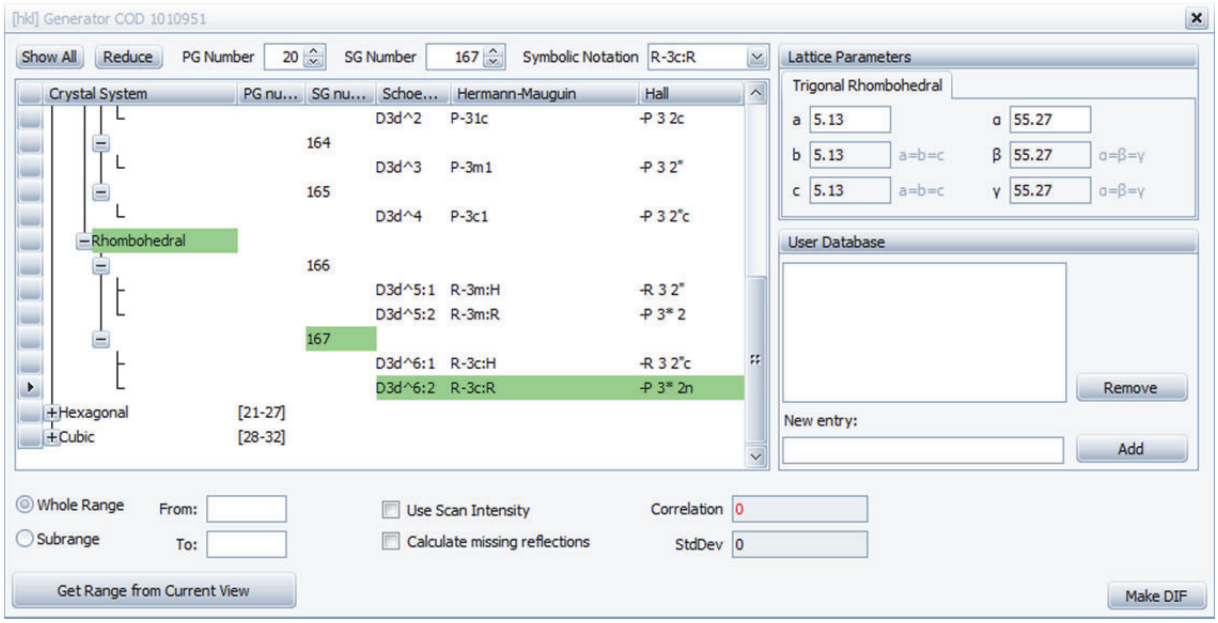


Fig.62: The [hkl] Generator tool applied from the pattern COD1010951 (Corundum)

The [hkl] Generator is useful in the following situations when:

- Observed lines are missing in a PDF pattern. This might be the case for low quality PDF patterns.
- A pattern is found that explains a significant part of the unknown scan, but its chemistry is not compatible with prior knowledge. As a result, both materials might have similar cells.
- The lines outside the pattern limits should be checked.

To create the hkl's from the current pattern (i.e. using the cell parameters described in a pattern):

1. Select the pattern of interest.
2. Click **[hkl] Generator** in the Data command panel
   — or —
   right-click the selection to display the pattern related menu. Click Tool and then **[hkl] Generator**.
3. Click the **Make DIF** button. The calculated pattern will be appended to the current pattern list.

Additional controls

Control	Description
Whole Range	The angular range of the scan is used as a limit for calculating the line positions.
Subrange	The positions given in the From: and To: fields are used as calculation limits.
From:	Start limit for line position calculation
To:	End limit for line position calculation
Get Range From Current View	Fill the **From:** and **To:** controls with the (possibly zoomed) limits of the current view.
Use scan intensity	If activated, the line intensity is calculated from the scan's net intensity at the position of the line. Otherwise, all lines have the same intensity.
Calculate missing reflections	If activated and the [hkl] Generator was applied from a pattern, any missing reflections will be calculated. Otherwise, only the positions for the lines in the parent pattern will be calculated.

Creating a User Database

It is possible to create and maintain a separate database containing the user's own patterns. This database is called a user database. During a search/match process in EVA, the user can add the user database to the database on which the search/match is performed.

A user database can be created from a tuned PDF pattern or a DIF.

NOTE

The tool is not allowed for original ICDD patterns. If attempted, an error message will be displayed. Use the **Tune cell** tool and replace this pattern by one using computed d(hkl) values.

NOTE

Former DIFFRACplus user databases (*.UCA) can be compiled into DIFFRAC.EVA's user database format. See section "Compiling DIFFRAC^{plus} User Databases" on page 189 for more details.

To create a user database:

1. Select a pattern or DIF in the data tree.
2. Click **User Database** in the data command panel
   — or —
   right-click the pattern or DIF of interest and click **User Database** on the pop-up menu.

   The User Database dialog box will be displayed.

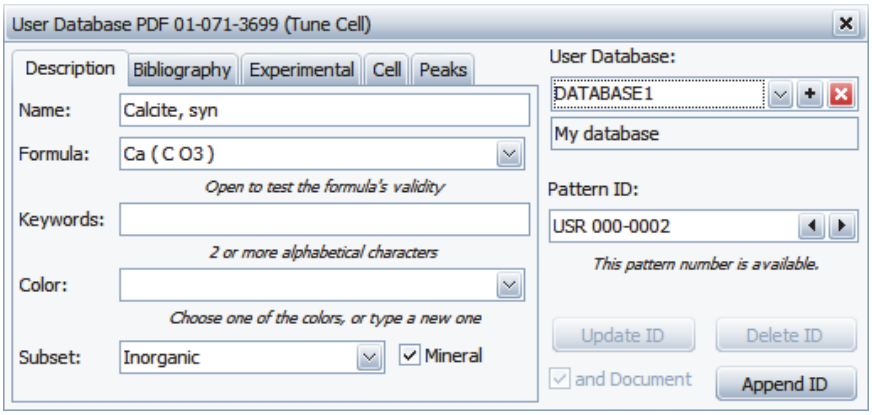


Fig.63: User Database dialog box

3. Click the button next to the **User database** field. The User Database Creation dialog box will be displayed.

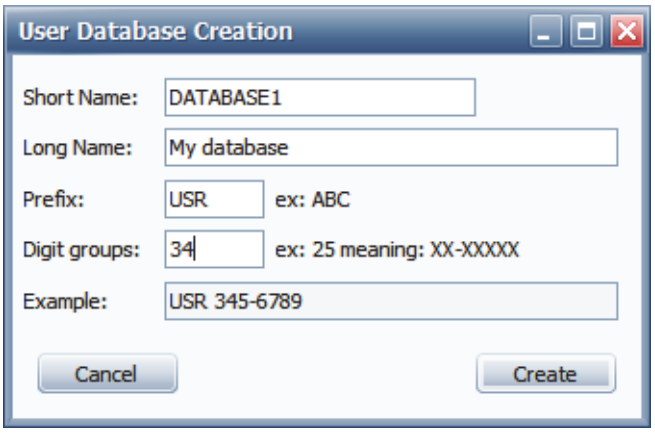


Fig.64: User database creation dialog boxFill in the fields described in the table below:

Property	Description
Short Name	Enter a name for the new user database
Long Name	Enter a description for the new user database
Prefix	Enter a prefix for the user patterns' name
Digits groups	Define the way the user database patterns are numbered. To do so enter two digits: the first digit gives the number of digits in the first digits group; the second digit gives the number of digits in the second digits group. For example, if 34 is entered, the name given to the patterns will have the form XXX-XXXX
Example	Preview of the name given to the user database patterns

4. Click the **Create** button.

The database will be added to the database list of the Database Filter tab in the Search/Match dialog box.

Deleting a User Database

To delete a user database:

1. Select a user pattern or DIF in the data tree.
2. Click **User Database** in the data command panel
   — or —
   right-click the pattern or DIF of interest and click **User Database** on the pop-up menu.

   The User Database dialog box will be displayed.
3. Select the desired user database in the **User database** drop-down list.
4. Click the button next to the User database field. A user database creation dialog box will be displayed.

Managing the User Patterns

Adding a pattern to a user database

To add a new pattern to a user database:

1. Select the desired pattern or DIF in the data tree.
2. Click **User Database** in the data command panel
   — or —
   right-click the pattern or DIF of interest and click **User Database** on the pop-up menu.

   The User Database dialog box will be displayed.
3. Select the desired database in the **User database** drop-down list.
4. The pattern is given the first available pattern ID by default. The user can enter another pattern ID in the **Pattern ID** field or use the arrow buttons search for another available pattern ID.
5. Modify the pattern settings in the tabs on the left, if necessary. See their description in the following table.
6. Click the **Append ID** button to add the new pattern to the selected user database.

Property	Description
Description tab	
Name	Phase name
Formula	Compound formula. Open to test the formula's validity
Keywords	Type 2 or more alphabetical characters
Color	Select the compound color in the drop-down list or enter a new one
Subset	The user can define the user database as a subset of the main databases. Select the chosen database in the drop-down list
Mineral	Select the **Mineral** check box to define the user database as a subset of the Mineral database
Bibliography tab	
Author	Self-explanatory
Comment	Self-explanatory
Experimental tab	
Wavelength	Measurement wavelength
I/Icor	Ratio I/I_{cor} between the intensities of the strongest line of the compound of interest and the strongest line of corundum, both measured from a scan made of a 50-50 mixture
Temperature	Measurement temperature. Room temperature if left blank. Default unit is Kelvin but you can specify Celsius or Fahrenheit
Pressure	Measurement pressure. Normal pressure if left blank. Default unit is kPa but you can specify Bar, atm or psi

Property	Description
Cell tab	
Lattice	Crystal system
Space Group	Three dimensional space group symbol (Hermann-Mauguin notation)
SP # Int. tables	Number of the space group (from 1 to 230) as given in the **International Tables for X-ray Crystallography**
Z	Number of molecules per unit cell
Volume	Cell volume in Å
Density	Unit cell density in g/cm^3
Mol. Weight	Self-explanatory
a, b and c	Unit cell parameters in angstroms
alpha, beta and gamma	Interaxial angles in degrees
Peaks tab	List of the peaks

Updating a pattern from a user database

To update a user pattern:

1. Select the user pattern to be updated in the data tree.
2. Click **User Database** in the data command panel
   — or —
   right-click the user pattern of interest and click **User Database** on the pop-up menu.
3. The User Database dialog box will be displayed with the user pattern already selected in the Pattern ID field.
4. Modify the settings in the tabs on the left.
5. Click the **Update ID** button to apply the changes to the pattern. Select the **and Document** check box to force the update of the pattern already present in the document.

Deleting a pattern from a user database

To delete a user pattern:

1. Select the user pattern to be deleted in the data tree.
2. Click **User Database** in the data command panel
   — or —
   right-click the user pattern of interest and click **User Database** in the pop-up menu.

   The User Database dialog box will be displayed with the user pattern already selected in the pattern ID field.
3. Click the **Delete ID** button.

Semi-Quantitative Phase-Analysis

Performing the Semi-Quantitative Analysis

The semi-quantitative analysis is meaningful only if all the phases have been identified. The semi-quantitative analysis is performed based on the pattern's relative heights and I/I_{cor} values. The latter are read when importing the patterns, provided that the values are available from the PDF. The user can enter his own I/I_{cor} values.

Please note that all the patterns from structure databases have I/I_{cor} values, which are generally more reliable than the measured ones. Therefore, using these patterns for a semi-quantitative analysis is recommended. They can be identified by the source number of their reference pattern number which is 01, 02, 03 or 04.

The semi-quantitative analysis is based on one of the following hypothesis:

- All the phases are crystalline and detected, which means that the software assumes that their sum is 100% $\left(\sum c_i = 100\%\right)$.
- The concentration of one phase is known: this concentration is set in the pattern column view, in the **S-Q** text field which becomes editable when the phase is defined as an added reference. By definition, only one phase can be used as an added reference.

To exploit a semi-quantitative phase analysis:

1. Select the first pattern of interest either in the data tree or in the graphical view. Point to the pattern and press the **Control** key to change the pointer into a hand. Move the hand up or down to adjust the Y-Scale.
2. Proceed in the same way for the other phases.
3. The phase concentrations are automatically computed. The results are given in the **S-Q** field of the Pattern Property table of each pattern. Creating a Pattern Column view in which they will all be listed is recommended.

NOTE

The user can define an added reference. Select the **Added reference** check box in the Property table of the pattern of interest. Enter a value for the added reference in the Pattern Column view.

Estimating the precision

The quality of the results of the semi-quantitative analysis relies on three main factors:

- The accuracy of the I/I_{cor} values: the value for a phase can vary between two patterns. Please note that some patterns correspond to specific conditions. Read the **Comments** in the data sheet of the Selected Candidates tab carefully.
- The visual adjustment of the Y-scale values of each pattern: the relative height of a pattern may not match the measured scan (e.g. in case of peaks overlapping or orientation effect).
- The peak height is proportional to the net area, which is true only if the peak broadening is similar for all the compounds of interest.

Performing an Elemental Analysis

Once:
- the qualitative analysis on the sample has been carried out,
- the I/I_{cor} coefficient is known for every pattern (or estimated by 1),
- the heights of the patterns (Y-scale) have been adjusted to the scan,

an elemental analysis can be performed.

To do so:

1. Select the scan of interest either in the data tree or in the graphical view.
2. Click **Element Analysis** in the data command panel
   — or —
   right-click the scan, then click **Create** on the context menu. Click **Elemental Analysis** on the related submenu.
3. The results of the elemental analysis are listed in the element list below the parent scan in the data tree. An Element Column view can be created.

Chemical balance: comparison with a chemical analysis

Laboratories often perform an elemental analysis on the samples before analysis with X-ray diffraction. In such a case, it is possible to compare this elemental analysis with the results given by EVA semi-quantitative analysis: EVA calculates the concentrations for every element from the concentrations of the compounds.

Additionally, it is possible to use the chemical analysis to automatically define the chemical filter for the Search/Match.

NOTE

XRF is the most common elemental analysis associated to XRD. For simplicity, the software interface and the present document use the term "XRF". However, any other elemental analysis method can be used.

Prerequisites

Access to the Settings dialog box

The patterns used may not have a I/I_{cor} coefficient. However, the qualitative information can be useful. To force the calculation of the concentrations even when the pattern has no I/I_{cor} coefficient, check the **Use 1 for the unknown I/Ic** option in the Settings dialog box, **Database** tab (see section “Database Tab” on page 63).

A user I/I_{cor} value that will be used by EVA for this pattern (see section “Properties” on page 127) can also be entered.

If the result of the elemental analysis is the SPECTRA*plus* Results database, make sure that the following preconditions are fulfilled:

- The EVA user must have the Read, Write, Create and Delete permissions on the directory where the Measure.MDB is placed (usually `C:\SPECPlus\Databases\` on the computer connected to the spectrometer). This is mandatory because the Microsoft Jet database engine that is used creates a temporary .LDB file. The database itself can be read only for the EVA user.

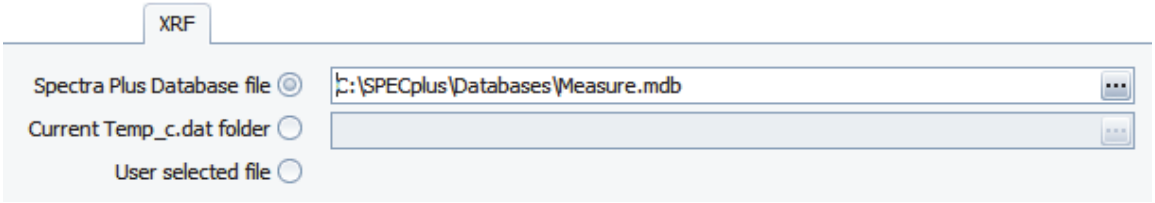
Access to the Settings dialog box

To set the location of the Results database to EVA:

1. In the Settings dialog box, go to the **XRF** tab.
2. Choose the **SpectraPlus database** option.
3. Use the **Browse** button to locate the database. It may be located on a remote computer through the local network (LAN).

Browse button

If same computer is used for both XRF and XRD evaluation, EVA automatically retrieves the position of the Results database from the registry.



If the elemental analysis is performed with a Bruker AXS XRF spectrometer running SPECTRA*plus*, EVA can read the temporary file Temp_C.DAT directly to establish the concentrations. This feature can be also used with Temp_C.DAT files generated by other software.

Browse button

Choose the **Current Temp_c.dat folder** option, and use the **Browse** button to locate the file.

Please note that this file is temporary. Its content is replaced with every new evaluation and in the event of a new measurement. If the user intends to rename the Temp_C.DAT file each time (for example to keep track of different measurements or to avoid accidental replacement), then choose the **Use selected file** option. In this case, the user will be asked for the DAT file for each evaluation.

If the elemental analysis is performed by another system than those described above, then a text (ASCII) file containing the results must be created. The format of this file is described in the “Appendix” on page 214. Select the **User selected file** option. EVA will ask for the text file to be used for each evaluation.

Importing the Results of the Chemical Analysis

Once:
- the qualitative analysis on the sample has been carried out,
- the I/I_{cor} coefficient is known for every pattern (or estimated by 1),
- the heights of the patterns (Y-scale) have been adjusted to the scan,

the semi-quantitative results are displayed in the **S-Q** column of the Pattern Column view.

To retrieve the results of a chemical analysis:

1. Click **Import XRF Results** in the data command panel
   — or —
   right-click the scan of interest and click **Import XRF Results** in the pop-up menu.

The dialog box that is displayed depends on the source of the chemical analysis result:

- **User selected file**: EVA displays the Open an XRF results filename dialog box. Select the file that contains the results and click the Open button.
- **Current Temp_c.dat**: The dialog box is not displayed. The results are automatically retrieved.
- **SpectraPlus database**: EVA displays the Select measurement data to import dialog box.

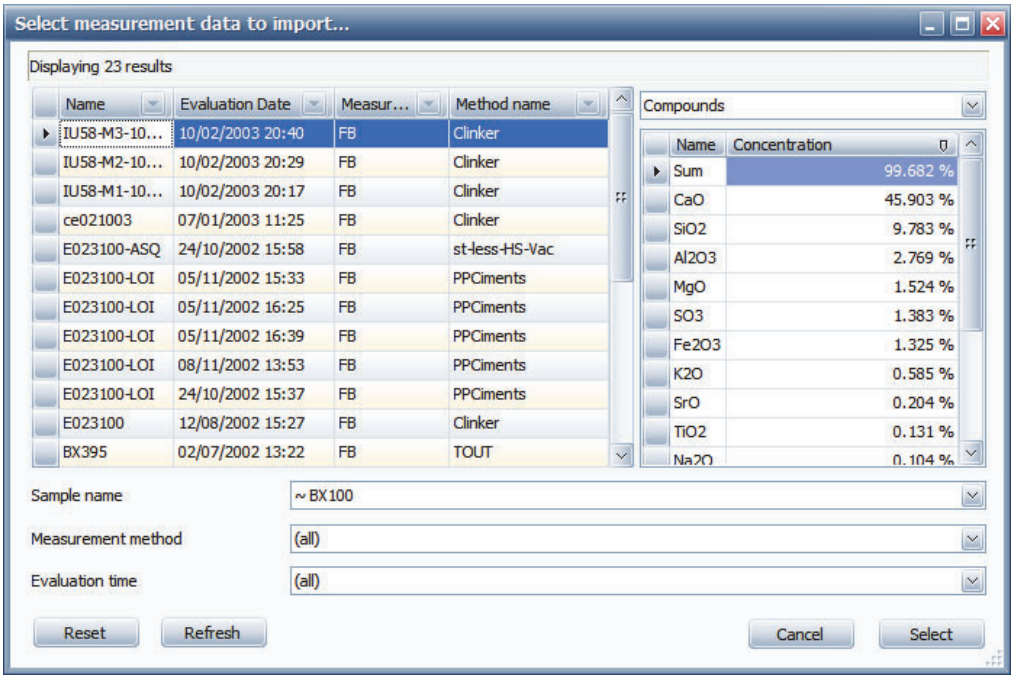
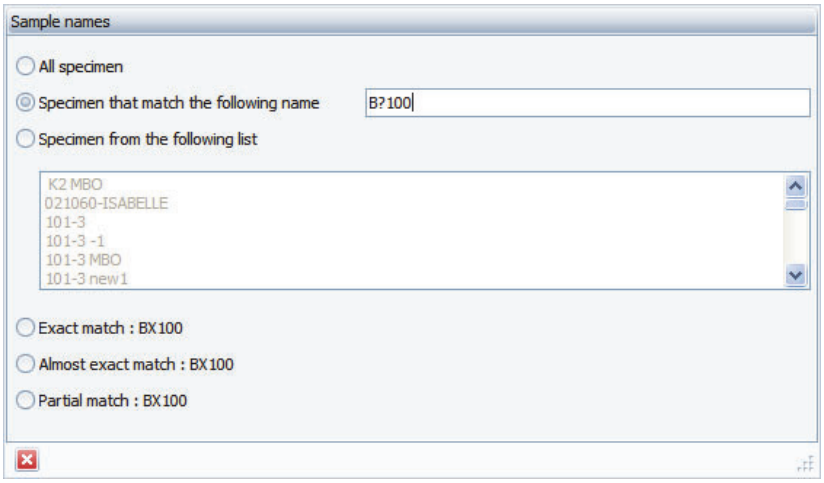


Fig.65: Selecting measurement data to import in the SpectraPlus database

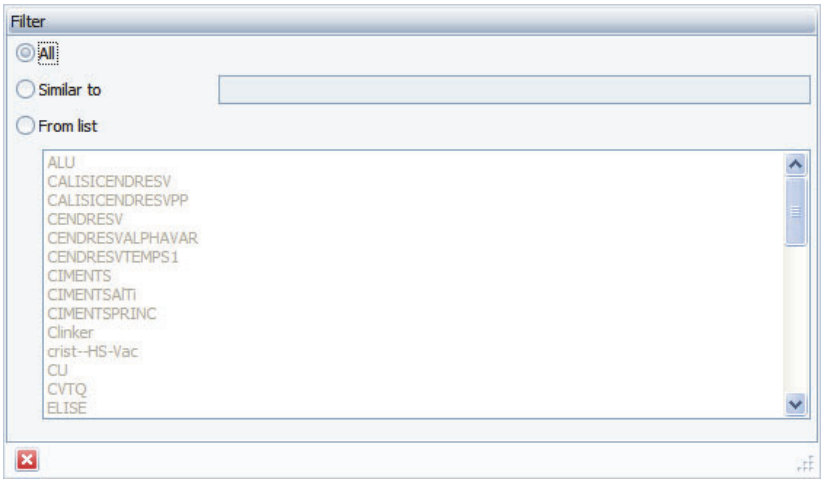
The measurements can be filtered three different ways. The user can access the filter settings by clicking on the corresponding fields.

Sample name:



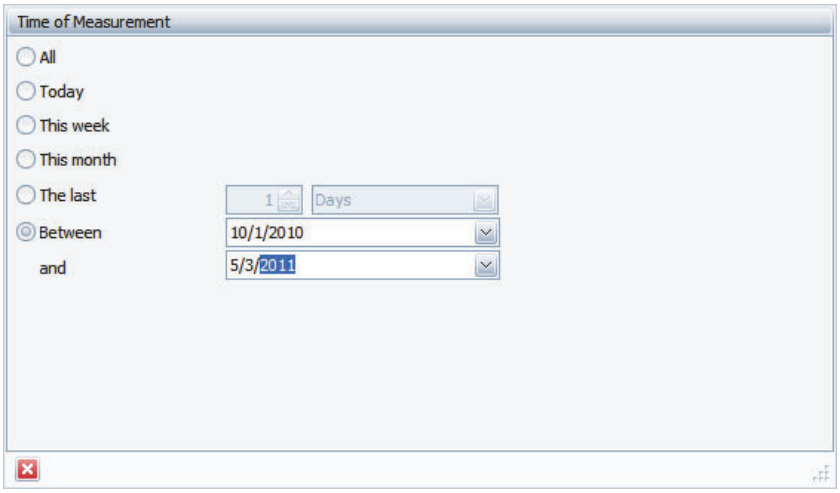
Filter	Description
All specimen	No sample name filtering. Selected by default
Specimen that match the following name	Type in the name of the sample which is being sought. The wildcards * (stands for any character string included the empty string) and ? (stands for any single character) can be used
Specimen from the following list	Select a sample in the list
Exact match: "*scan name*"	EVA displays the measurement whose sample name is the same as the current Scan name
Almost exact match: "*scan name*"	Same as above, but spaces, commas, dashes... are ignored
Partial match: "*scan name*"	Same as above but less restrictive

Measurement method:



Filter	Description
All	No measurement method filtering. Selected by default
Similar to	Type in the name of the measurement method. The wildcards * (stands for any character string included in the empty string) and ? (stands for any single character)
From list	Select a measurement method in the list

- **Time of Measurement End:**



Filter	Description
All	No time of measurement filtering. Selected by default
Today	Samples measured today
This week	Samples measured this week
This month	Samples measured this month
The last	Samples measured in a given period defined by a number of minutes, hours, days or years
Between … and …	Samples measured in a given period defined by a start and end time

The filtered results are listed in the table on the left. The table on the right shows the concentrations of the elements or of the compounds (according to the options) to assist in choosing the right sample.

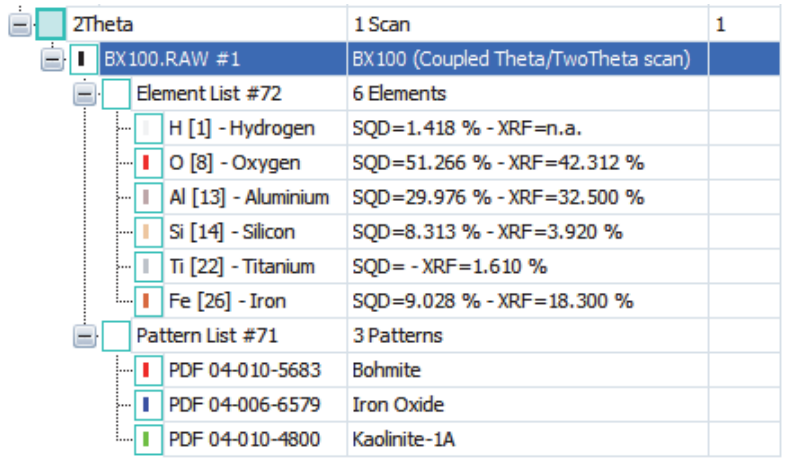
If the filter is changed, click **Refresh** to refresh the display.

To reset the filters, click the **Reset** button.

To import the XRF results of interest, select the corresponding sample in the list and click the **Select** button.

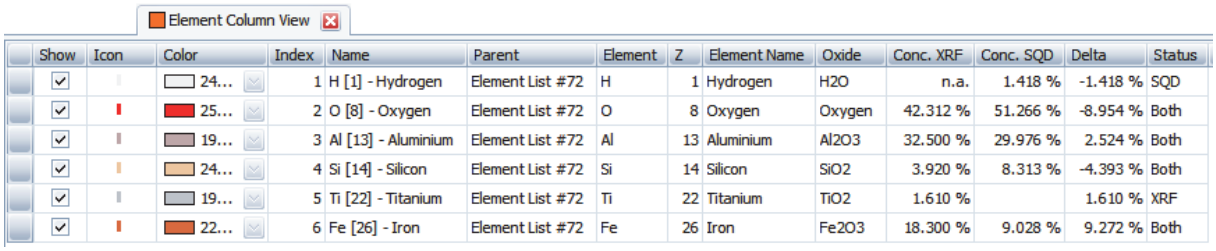
Performing the comparison

You can compare the results in the data tree and the Element properties are listed in the Element Property table.



2Theta	1 Scan	1
BX100.RAW #1	BX100 (Coupled Theta/TwoTheta scan)	
Element List #72	6 Elements	
H [1] - Hydrogen	SQD=1.418 % - XRF=n.a.	
O [8] - Oxygen	SQD=51.266 % - XRF=42.312 %	
Al [13] - Aluminium	SQD=29.976 % - XRF=32.500 %	
Si [14] - Silicon	SQD=8.313 % - XRF=3.920 %	
Ti [22] - Titanium	SQD= - XRF=1.610 %	
Fe [26] - Iron	SQD=9.028 % - XRF=18.300 %	
Pattern List #71	3 Patterns	
PDF 04-010-5683	Bohmite	
PDF 04-006-6579	Iron Oxide	
PDF 04-010-4800	Kaolinite-1A	

The creation of an Element Column view is recommended. The user can copy results to the clipboard in an Element Column view.



Element Column View

Show	Icon	Color	Index	Name	Parent	Element	Z	Element Name	Oxide	Conc. XRF	Conc. SQD	Delta	Status
☑		24...	1	H [1] - Hydrogen	Element List #72	H	1	Hydrogen	H2O	n.a.	1.418 %	-1.418 %	SQD
☑		25...	2	O [8] - Oxygen	Element List #72	O	8	Oxygen	Oxygen	42.312 %	51.266 %	-8.954 %	Both
☑		19...	3	Al [13] - Aluminium	Element List #72	Al	13	Aluminium	Al2O3	32.500 %	29.976 %	2.524 %	Both
☑		24...	4	Si [14] - Silicon	Element List #72	Si	14	Silicon	SiO2	3.920 %	8.313 %	-4.393 %	Both
☑		19...	5	Ti [22] - Titanium	Element List #72	Ti	22	Titanium	TiO2	1.610 %		1.610 %	XRF
☑		22...	6	Fe [26] - Iron	Element List #72	Fe	26	Iron	Fe2O3	18.300 %	9.028 %	9.272 %	Both

Property	**Description**
Name of the column	**Content**
Atomic Number	Self-explanatory
Concentration SQD	Concentration calculated from the Semi-Quantitative analysis of the Diffraction data
Concentration XRF	Atomic number of the element
Delta	Difference between the XRF and the SQD values
Element name	Self-explanatory
Element symbol	Self-explanatory
Oxide name	Chemical formula of the oxide
Status	Whether the element is found in the external chemical analysis alone (XRF), in the XRD analysis alone (SQD), or in both analyses (both)

Click a column header to sort the elements according to the value in this column, click again to sort them in the reverse order.

Information for the element list is also available. Select the Element List of interest and look at the Element List Property table.

Property	Description
Data	
Name	Name of the element list. Can be edited
Legend	Legend used to characterize the data
Elemental Analysis Results	
Oxide	When the **Oxide** option is checked, then: • The oxygen is ignored in the patterns formulas. • The other elements are considered to be present and linked to oxygen, as in the most common oxides found in geology (for example Fe_2O_3 for the iron). The elements that never (or rarely) form oxides (such as the halides or the rare gases) are left in the elemental form. • The concentrations of these oxides are displayed.
Oxygen Imbalance SQD	When the **Oxide** option is checked, then: The concentration in oxygen can be calculated in two ways: from the formulas of the patterns or from the formulas of the oxides. The difference between these two values is called "oxygen imbalance". Here, the value is calculated from the SQD results
Oxygen Imbalance XRF	When the **Oxide** option is checked, then: The concentration in oxygen can be calculated in two ways: from the formulas of the patterns or from the formulas of the oxides. The difference between these two values is called "oxygen imbalance". Here, the value is calculated from the XRF results
Sum Concentration SQD	Sum of all concentrations given in the SQD column
Sum Concentration XRF	Sum of all concentrations given in the XRF column
Children Columns	
Data	Choose the way the elements are characterized in the Element List. See section “Creating Captions” on page 58 to learn how to customize the data
Description	Choose a description for the peaks in the list. See section “Creating Captions” on page 58 to learn how to customize the caption

NOTE

If the oxygen imbalance is significantly different from 0, then the use of the **Oxide** option is not recommended. The **Oxide** option will only give acceptable results when either:

- the compounds are the most common form of oxides found in geology
- or the compounds can be decomposed into such common oxides (for example $CaCO_3$ = CaO + CO_2, $CuSO_4$ = CuO + SO_3). It is the responsibility of the user to check that the oxide forms correspond to what is expected.

Additional Options


Access to the Settings dialog box

Two options are available in the Settings dialog box of the **XRF** tab, as described below.

- **Z threshold for XRF analysis**: The light (low-Z) elements cannot be measured in XRF. When setting the filter for the Search/Match, these light elements should not be discarded. Type the lowest Z that is to be used for the chemical filter (6 by default) in the text field. The presence or absence of an element in the chemical analysis result will not be taken into account if it is below this Z value.
- **XRF Concentration (ppm):** This is the lowest XRF concentration, in which an element is considered to be present. When the concentration of an element is below this value as the result of the chemical analysis, the element will be marked as **discarded** (red).

Defining a Chemical Filter from the Results

The user can define a chemical filter directly from an element or the element list.

To set an element as mandatory (green):

1. Select the element of interest.
2. Click **Green Filter data** in the data command panel
   — or —
   right-click the element of interest, click **Create** and then **Green Filter data** in the context menu.
3. A new chemical filter is created and will be listed in the Settings in the data tree. It is described by the parent scan name.

To set an element list as “at least one” or as discarded:

1. Select the element list of interest
2. Click either **Blue Filter data** or **Red Filter data** in the data command panel
   — or —
   right-click the element of interest, click **Create** and then **Blue Filter data** or **Red Filter Data** on the context menu.
3. A new chemical filter will be created and listed in the Settings in the data tree. It is described by the parent scan name.

Preparing a Residual Scan

Minor phases are sometimes difficult to identify because the patterns corresponding to the major peaks have a better position in the list. It is possible to exclude previously explained regions in order to increase the weight of the unexplained regions. The minor phases are then more likely to be identified.

To do this:

Residual scan:apply to…button

1. Click the **Residual scan: Apply to all visible scans** button on the view toolbar
   — or —
   right-click anywhere on the graphical view. Click **Residual scan|Apply to all visible scans** on the context menu.
   Scissors will be displayed with the pointer.
2. Select the zones to be removed. They will be displayed using the ghost color.

To restore the excluded part:

Residual scan:restore… button

Click the **Residual scan: Restore all visible scans** button in the view toolbar
— or —
right-click anywhere on the graphical view. Click **Residual scan|Apply to all visible scans** on the context menu.

NOTE

Please note, that it is possible to apply the residual scan to a given scan. To do so, right-click on the chosen scan. Then click **Residual scan|Apply to scan…*(name of the selected scan)*** in the context menu. Do the same to restore the scan.

When certain phases have been previously identified, it is possible to use the patterns to exclude the regions around the peak positions. This is much faster but less accurate than the manual procedure.

To do this:

1. Choose the **Selected Candidates** tab in the Search/Match (scan) dialog box.
2. Select the pattern of interest in the list.
3. Select the **Residu** tool.
4. Adjust the width of the zone to exclude the area around the pattern sticks with the slider. It is possible to enter a value manually in the **FWHM** text zone.
   The width of the excluded region is derived from each peak height and the FWHM.
5. Click the **Apply** button.

Click **Reset** to restore the cancelled part.

This operation can also be performed from the data tree or the graphical view:

1. Select the pattern of interest either in the data tree or in the 1D view.
2. Click the **Residue** tool in the Data command panel
   — or —
   right-click the selection to display the context menu and then click **Tool.** Click **Residue** on the submenu. The **Residue** dialog box will be displayed.

Expand and Reduce Interval buttons

3. Adjust the width of the zone to exclude around the pattern sticks with the slider. It is possible to enter a value manually in the **FWHM** text zone. If the amplitude of the slider is too small, use the **Expand Interval** button. If the precision of the slider is too low, use the **Reduce Interval** button. Click the **Default** button to return to the default parameters. A filter to remove small lines can be set.
4. Click the **Apply** button.

   To restore the cancelled part, click **Reset**.

Working with Peaks

Changing the Properties of a Peak

To view or modify properties for a peak in particular, it is possible to do so in the Peak property table once the peak has been selected. The peak properties are described below.
You can also modify the Peak List properties.

Peak list properties

Property	Description
Data	
Name	Enter the name for the peak list
Legend	Legend used to characterize the data
Attributes	
Peak visibility	Choose in which view(s) the peaks are visible
Children columns	
Data	Choose the way the peaks are characterized in the peak list. See section “Creating Captions” on page 58 to learn how to customize the data
Description	Choose a description for the peaks in the list. See section “Creating Captions” on page 58 to learn how to customize the caption

Peak properties

Property	Description
Attributes	
Visible	To remove the current peak from the graphical display, click the **Visible** check box. Select the check box to display the current peak
Color	Choose a color for the display of the current peak
Caption	Choose the parameter(s) to be displayed. See section “Creating Captions” on page 58 to learn how to customize the caption
Caption (display)	Cannot be edited. View of display for the caption chosen
Background Color	Choose a background color for the text (Transparent stands for the line color)
Text Color	Choose a text color (Transparent stands for the line color)
Font Size	The caption’s font size in points
Caption rotation	Enter the chosen angle for the caption display
Caption margin	Enter the chosen margin between the anchor and the caption in pixels
Caption Offset	Fixed distance between the anchor’s tip and the caption in pixels, value can be negative
X	X distance
Y	Y distance
Anchor Style	Choose the chosen anchor style to display the peak position and the caption
Anchor/Caption lock	Select “Yes” to move the caption and anchor as a whole. Select “No” to move the caption or the anchor’s tip separately
Peak	
Angle	Angle value
d value	d value
Gross Intensity	Gross intensity of the selected peak
Net Intensity	Net intensity of the selected peak
h,k,l values	hlk values. Click the “plus” sign to edit values separately

Adding Peaks Manually

In some cases, the user may choose to input a few peaks directly instead of (or in addition to) performing an automatic peak search.

To do so:

1. Right-click the chosen scan at the position peak input: the context menu will be displayed.
2. Click **Create Peak at 2Th=…**;
3. The peak will be displayed in the graphical view and added to the peak list in the data tree. The peak stays at the same X position, but its ordinate is adjusted to the actual intensity of the scan at this abscise.

Performing a Search/Match Operation on a Peak List

To perform a Search/Match operation on a peak list:

1. Select the peak list in the data tree.
2. Click **Search / Match (peak list)** in the Data command panel
   — or —
   right-click, click **Tool** on the menu which appears and then **Search / Match (peak list)** in the related submenu.

The **Search/Match (peak list)** dialog box is displayed as follows:

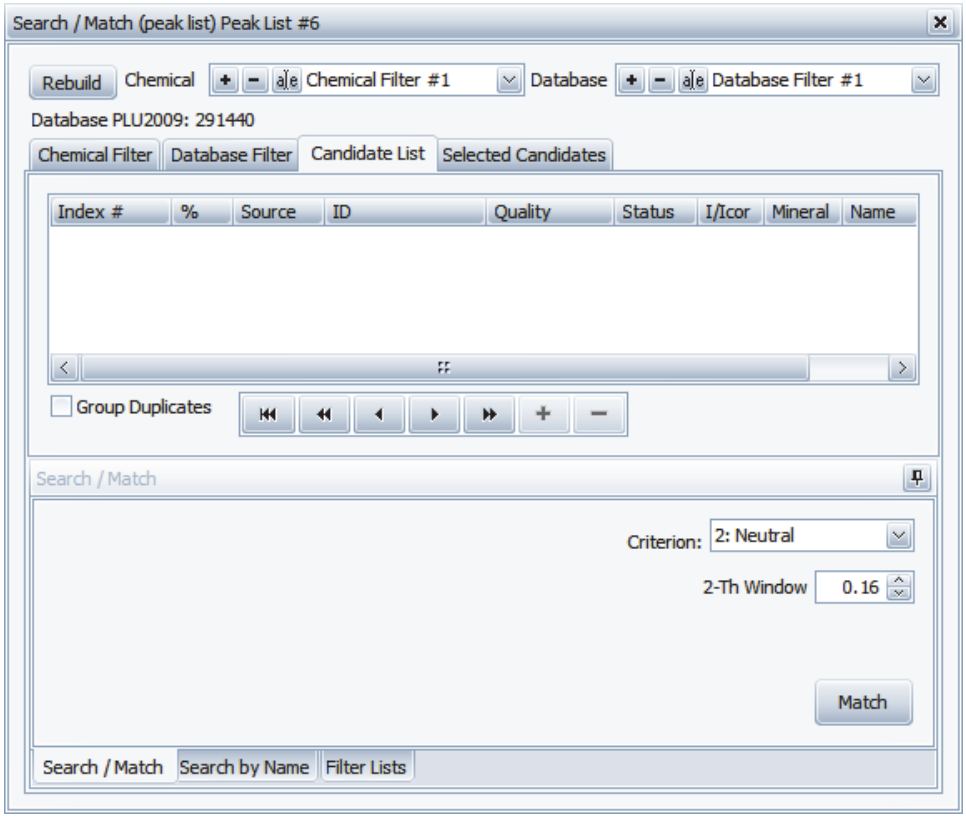


Fig.66: Candidate List tab

When searching on peaks, there is no natural error window (as with a scan). The **2-Th Window** field is the error window. The default is 0.16 (± 0.16°).

See “Performing a Search on a Scan” on page 68 for a detailed description of the tab and procedure.

Creating a DIF Pattern from a Peak List

The user can create a DIF pattern immediately after the peak search or from a list of selected peaks.

To create a DIF pattern immediately after the peak search, see section “Performing a Peak Search” on page 103.

To create a pattern from a list of selected peaks:

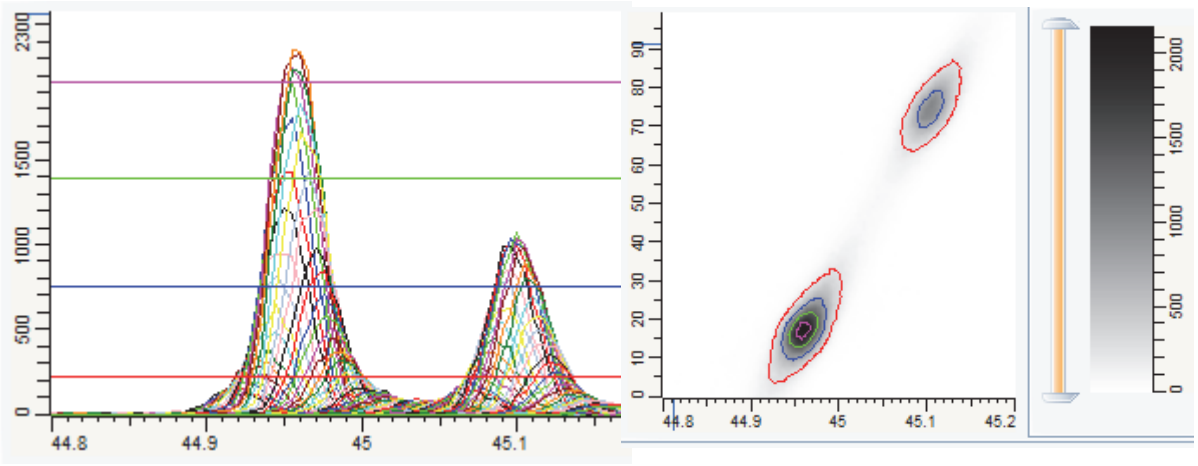
1. Select the peaks or the list of peaks.
2. Click **Make DIF** in the Data command panel
   — or —
   right-click the selection to display the peak list related menu. Click Tool and then **Make DIF**.

After it has been created, the DIF pattern is appended to the pattern list.

Working with Levels

Levels pertain to a scan list, since they can be useful only on multiple scans while displaying a 2D view: the iso-intensity curves (or contours) corresponding to the intersections of the levels with the scans are drawn in a view where X is the scans' axis and Y the scan number in the set of multiple scans.

It can prove convenient to create the levels on the 1D view so as to see the intersections of these levels with the scan.



1D view with levels Corresponding 2D view

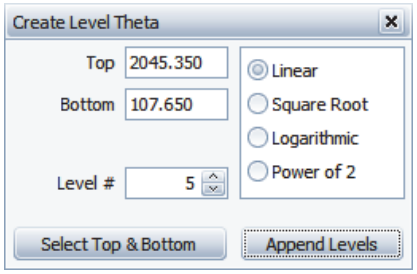
Fig.67: Levels in a 1D view and a 2D view

Creating Levels

To create levels:

1. Select the desired scan list in the data tree.
2. Click **Create Level** in the Create box of the Data command panel
   — or —
   right-click to display the related menu, click **Tool** and then **Create Level** on the submenu.

The **Create Level** dialog box will be displayed and will suggest the automatic levels.



Automatic levels

5 equidistant levels are proposed by default. The Top and Bottom values are calculated with regards to the highest peak maximum. They are the maximum and minimum values of the interval used for creating the equidistant levels. The levels are displayed as ghost lines on the graphical view.

1. The number of levels in the **Level #** field and the **Top** and **Bottom** level values can be modified.
2. The scale can be selected: Linear, Square Root, Logarithmic or Power of 2. To do so, click the corresponding option.
3. Once the levels are suitable, they can be added by clicking the **Append Levels** button.

The newly created levels are displayed on the graphical view and a Level list is added to the data tree.

To define the level range in the graphical view:

1. Click the **Select Top&Bottom** button.
   The ghost lines of the automatic level are removed from the display and a circle is added around the arrow of the mouse pointer.
2. Move the cursor to one end of the targeted level range, press and hold the left mouse button while dragging the mouse until the cursor reaches the opposite end, then release the button. The levels will be displayed as ghost lines.
3. If the level positions are suitable, click the **Append Levels** button. The newly created level is displayed on the graphical view and added to the data tree.

Manual levels

You can create levels directly in the graphical view:

1. Right-click where you want to create the level in the graphical view to display the context menu.
2. Click **Create Level at…**: the level is displayed in the graphical view and added to the level list in the data tree.

NOTE

A level can be modified at any time. To do so, select the level either in the data tree or in the graphical view. Modify the level position in the Level Property table.

Levels Properties

Level list properties

Property	Description
Data	
Name	Enter the name for the level list.
Children columns	
Data	Choose the way the levels are characterized in the level list. See section “Creating Captions” on page 58 to learn how to customize the data
Description	Choose a description for the levels in the list. See section “Creating Captions” on page 58 to learn how to customize the description

Level properties

Property	Description
Data	
Legend	Legend used to characterize the data. See section “Creating Captions” on page 58 to learn how to customize the legend
Attributes	
Visible	Clear the **Visible** check box to remove the current level from the graphical display. Select the check box to make it visible
Color	Choose a color for the level display
Level	
Intensity	Intensity value at the level position

Working with 2D Frames

This feature is available from license level 3 and software version 3.

2D frames are X-ray data measured in two dimensions. Compared to a scan which shows a relationship between an axis (e.g., 2theta) and the signal, a frame shows a relationship between two axes (e.g., 2theta and gamma) and the signal.

The fundamentals of working with 2D detectors are explained in “Introduction to 2-Dimensional X-ray Diffraction”, part number DOC-M86-EXX055.

Opening 2D Frames

2D frames are loaded in the same way as other measurement data:

1. Choose **File > Import…** from the Menu Bar or the Toolbar.
2. In the “File Open” window, select the .brml file(s) of the measurement(s) of interest and click **OK**.
   The frames are loaded into EVA.

   Alternatively, frames with the file extension “.gfrm” or “.sfrm” can be selected directly in the “File Open” window’s file list.

After loading, the frames will be displayed in the tree and a view will be created. The resulting frame view depends on the axis properties of the loaded frames.

Stackable Frames

If the frames have the same 2-theta axis position, they will be loaded into a “Stackable Frame List” and will be displayed in a thumbnail and summary view:

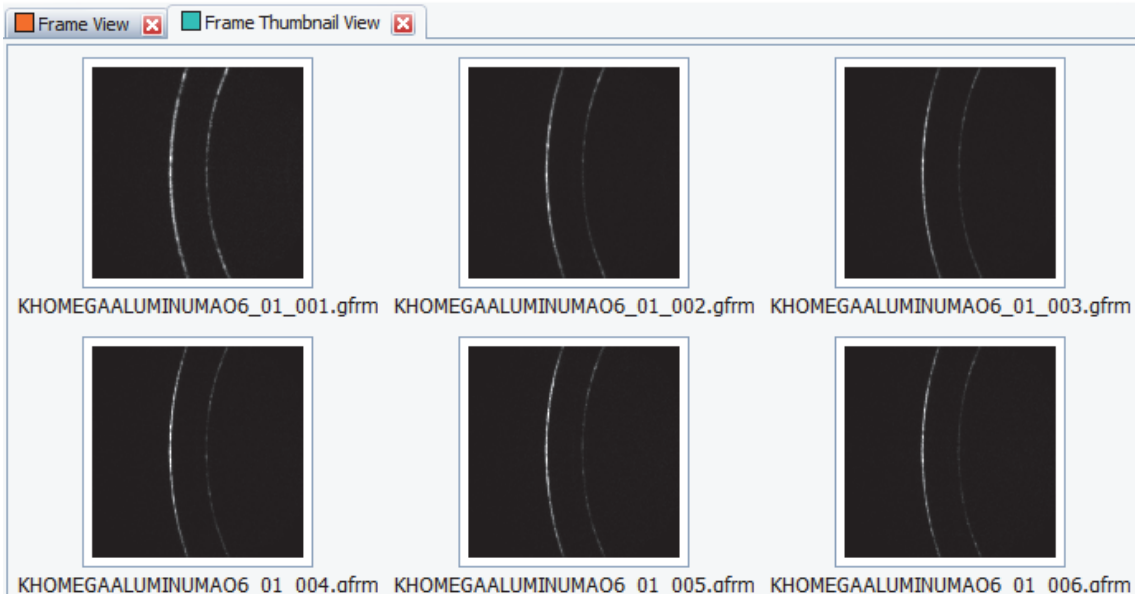


Fig.68: Thumbnail view of stackable frames

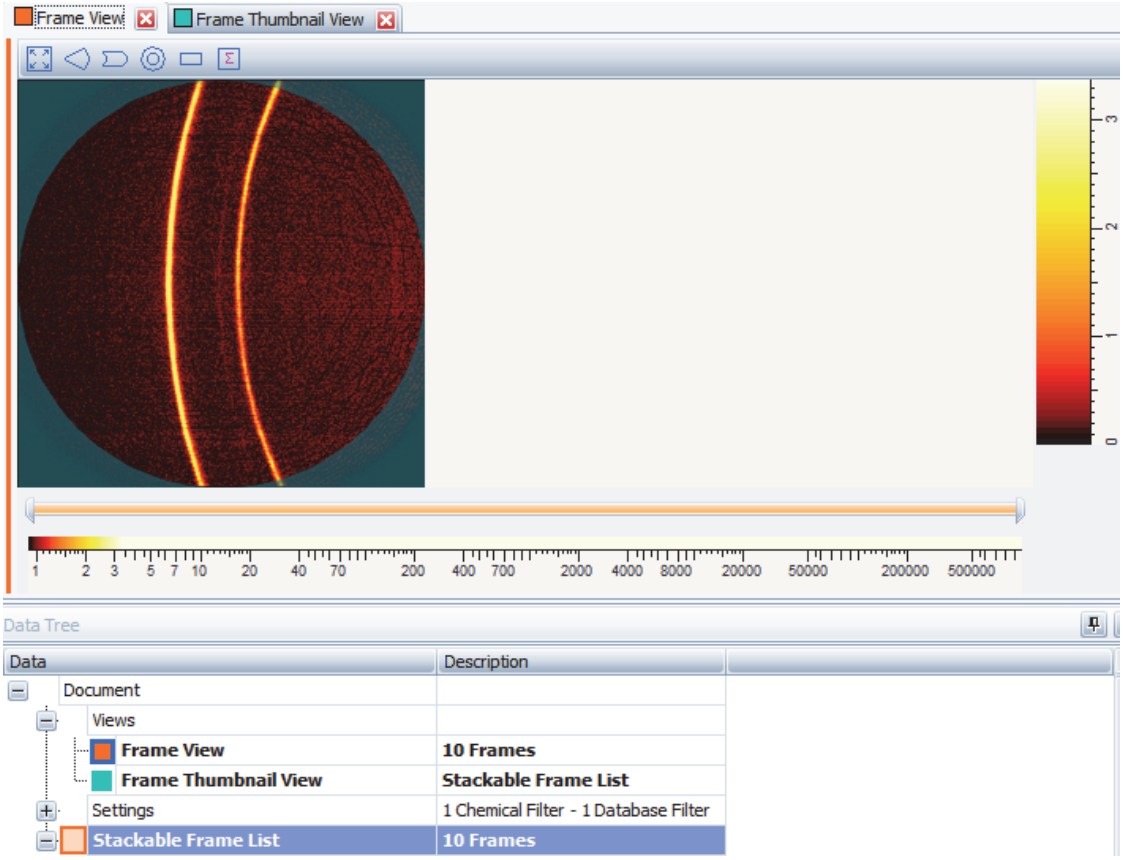


Fig.69: Default summary view after loading a stackable frame list

The summary view can display the mean value of all frames’ pixels (default), the minimum or the maximum.

Mergeable Frames

If the frames' 2-theta axis has different values while the other frame parameters are the same, the frames will be loaded into a "Mergeable Frame List". A frame view with the merged frames and a thumbnail view will be created.

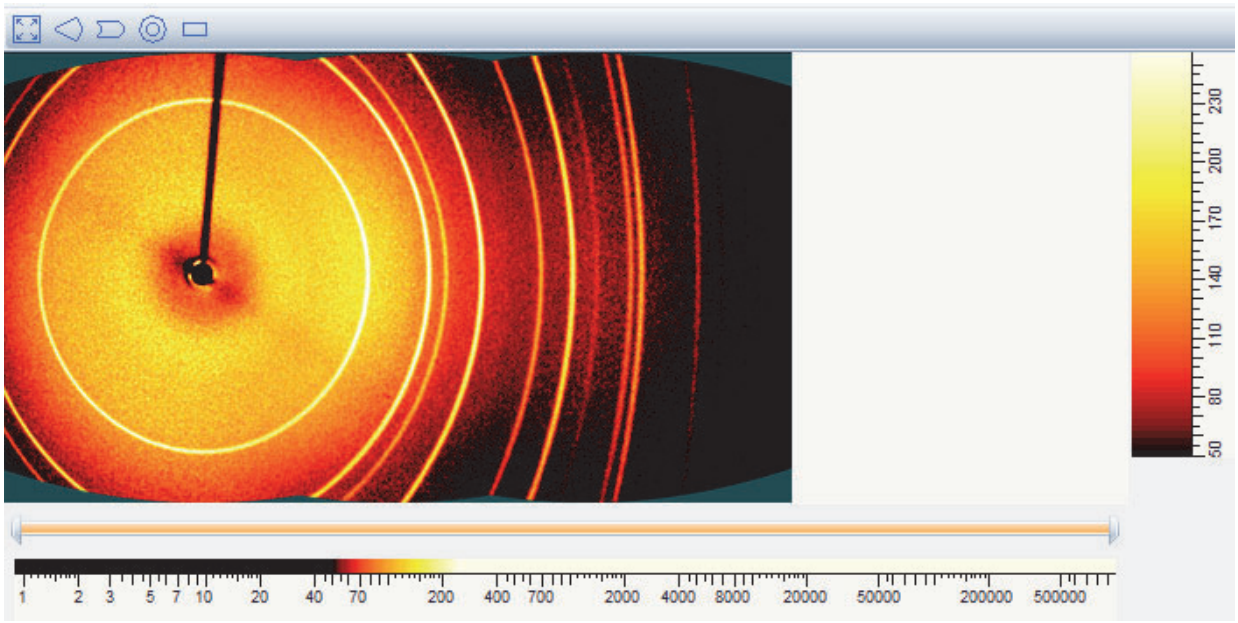


Fig.70: Frame view of mergeable frames

Single Frames

If a single frame is loaded, it will be placed in a "Single Frame List" which contains only one frame.

If several imported frames are neither mergeable nor stackable, they will be placed in "Single Frame List(s)".

Frame Integration and Mask Cursors

The frame cursors are tools to create integration areas or masks on 2D frames. The cursors are selected from the Frame View's toolbar.

Toolbar for a single Frame View:

Toolbar for a Mergeable Frame View:

Toolbar for a Stackable Frame View:

The **Refresh Mask** button appears in the frame view after inserting or changing cursors and masks.

This allows updating the mask visually. Note the correct frame integration does **not** require a visual mask update. The masks are automatically taken into account during integration regardless of their visual appearance but the display update is a time consuming process.

All cursors except the Full Frame Cursor can be created and modified (resized/moved) with the mouse.

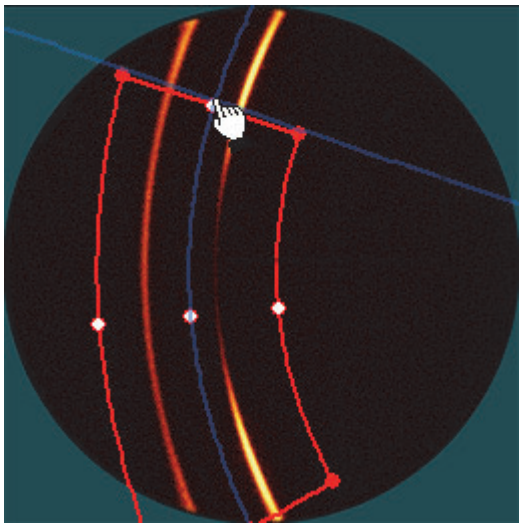


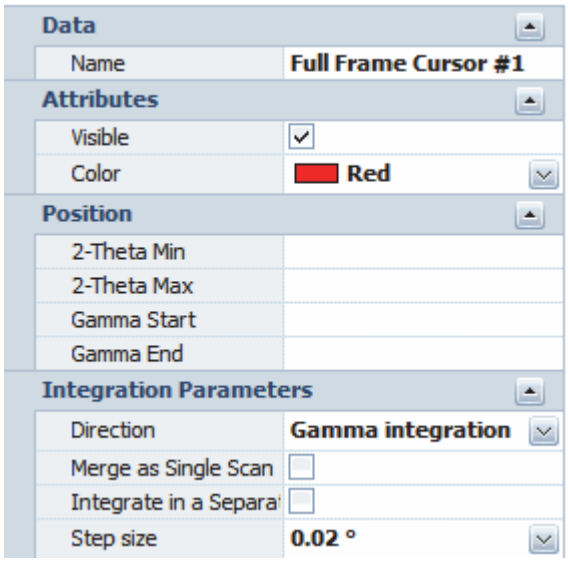
Fig.71: Wedge Cursor with mouse handles and a hand mouse pointer ready for resizing

The cursors are displayed as regions of the frame, bounded by round points. These points can be dragged with the mouse to resize the cursor, or—in the case of the center point—move the entire cursor.

The various cursor types are described in the following Sections.

Full Frame Cursor

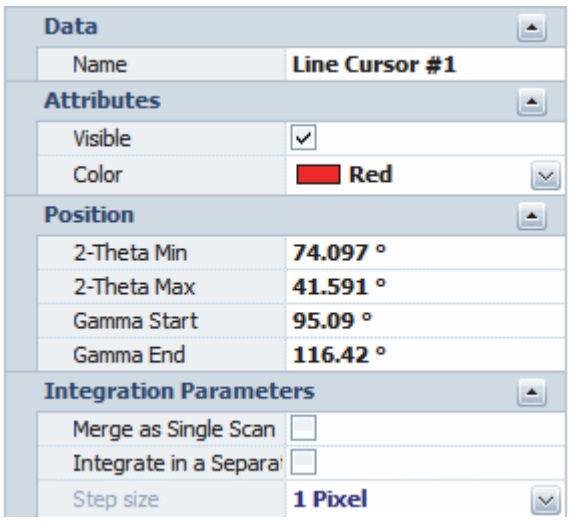
The Full Frame Cursor is an integration cursor which is applied to the entire frame. It can be applied to single frames, and all types of frame lists.



Property	Description
Name	A name which can be changed by the user.
Visible	If activated, the cursor shape is displayed.
Color	Cursor color, user-adjustable
2-Theta Min	<Not used>
2-Theta Max	<Not used>
Gamma Start	<Not used>
Gamma End	<Not used>
Direction	Integration direction: A gamma integration results in a 2-theta scan and a 2-theta integration results in a gamma scan.
Merge as Single Scan	The scans resulting from the integration are merged into a single scan.
Integrate in a Separate Scan List	The resulting scan(s) are stored in a new scan list.
Step size	Step size in degrees, user-adjustable

Line Cursor

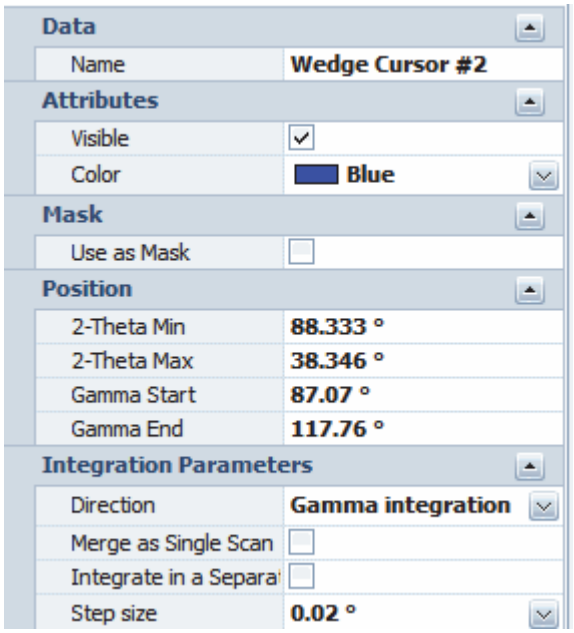
The Line Cursor is an integration cursor over a thin straight line in a single frame. It can be applied to single frames only.



Property	Description
Name	A name which can be changed by the user.
Visible	If activated, the cursor shape is displayed.
Color	Cursor color, user-adjustable
2-Theta Min	The start angle for the 2-theta integration. It is either selected with the mouse while drawing the cursor or entered here.
2-Theta Max	The end angle for the 2-theta integration. It is either selected with the mouse while drawing the cursor or entered here.
Gamma Start	The start angle for the gamma integration. It is either selected with the mouse while drawing the cursor or entered here.
Gamma End	The end angle for the gamma integration. It is either selected with the mouse while drawing the cursor or entered here.
Merge as Single Scan	The scans resulting from the integration are merged into a single scan.
Integrate in a Separate Scan List	The resulting scan(s) are stored in a new scan list.
Step size	1 Pixel, not user changeable

Wedge Cursor

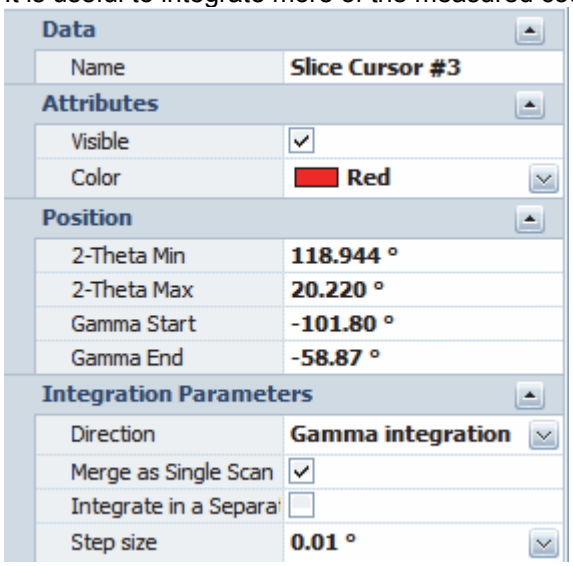
The Wedge Cursor is an integration cursor with constant 2-theta and gamma limits. It can be applied to single frames, and to all types of frame lists.



Property	Description
Name	A name which can be changed by the user.
Visible	If activated, the cursor shape is displayed.
Color	Cursor color, user-adjustable
2-Theta Min	The start angle for the 2-theta integration. It is either selected with the mouse while drawing the cursor or entered here.
2-Theta Max	The end angle for the 2-theta integration. It is either selected with the mouse while drawing the cursor or entered here.
Gamma Start	The start angle for the gamma integration. It is either selected with the mouse while drawing the cursor or entered here.
Gamma End	The end angle for the gamma integration. It is either selected with the mouse while drawing the cursor or entered here.
Direction	Integration direction: A gamma integration results in a 2-theta scan. A 2-theta integration results in a gamma scan.
Merge as Single Scan	The scans resulting from the integration are merged into a single scan.
Integrate in a Separate Scan List	The resulting scan(s) are stored in a new scan list.
Step size	Step size in degrees, user-adjustable

Slice Cursor

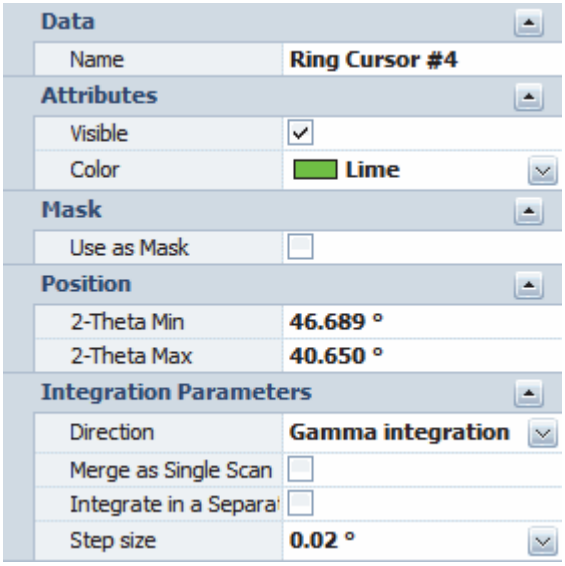
The Slice Cursor is an integration cursor which is applied to a merge frame list. It can also be applied to stacked frame lists. The Slice Cursor applies constant gamma end values but a variable 2-theta range. It is useful to integrate more of the measured counts from the frame compared to a wedge cursor.



Property	Description
Name	A name which can be changed by the user.
Visible	If activated, the cursor shape is displayed.
Color	Cursor color, user-adjustable
2-Theta Min	The start angle for the 2-theta integration. It is either selected with the mouse while drawing the cursor or entered here.
2-Theta Max	The end angle for the 2-theta integration. It is either selected with the mouse while drawing the cursor or entered here.
Gamma Start	The start angle for the gamma integration. It is either selected with the mouse while drawing the cursor or entered here.
Gamma End	The end angle for the gamma integration. It is either selected with the mouse while drawing the cursor or entered here.
Direction	Integration direction: A gamma integration results in a 2-theta scan. A 2-theta integration results in a gamma scan.
Merge as Single Scan	The scans resulting from the integration are merged into a single scan.
Integrate in a Separate Scan List	The resulting scan(s) are stored in a new scan list.
Step size	Step size in degrees, user-adjustable

Ring Cursor

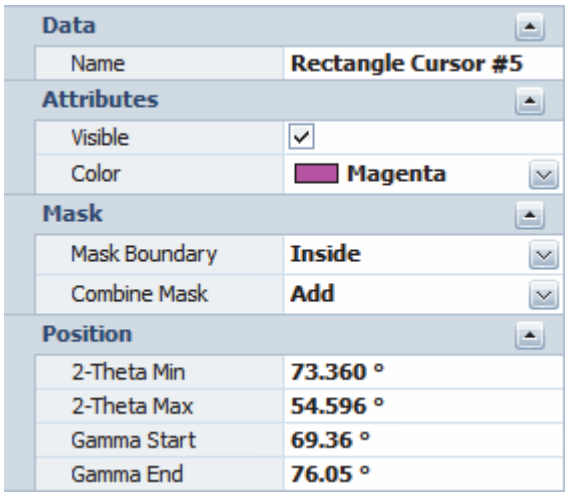
The Ring Cursor is an integration cursor which represents a closed Wedge Cursor with only 2-theta as the integration range. It can be applied to both single frames and all types of frame lists.



Property	Description
Name	A name which can be changed by the user.
Visible	If activated, the cursor shape is displayed.
Color	Cursor color, user-adjustable
Use as Mask	Cursor is used as mask if checked.
2-Theta Min	The start angle for the 2-theta integration. It is either selected with the mouse while drawing the cursor or entered here.
2-Theta Max	The end angle for the 2-theta integration. It is either selected with the mouse while drawing the cursor or entered here.
Direction	Integration direction: A gamma integration results in a 2-theta scan. A 2-theta integration results in a gamma scan.
Merge as Single Scan	The scans resulting from the integration are merged into a single scan.
Integrate in a Separate Scan List	The resulting scan(s) are stored in a new scan list.
Step size	Step size in degrees, user-adjustable

Rectangle Cursor

The Rectangle Cursor is a mask cursor which is applied to a rectangular part of the frame. It can be applied to both single frames and all types of frame lists. Its purpose is to provide differently shaped integration masks to mark areas which are to be excluded from the integration process.

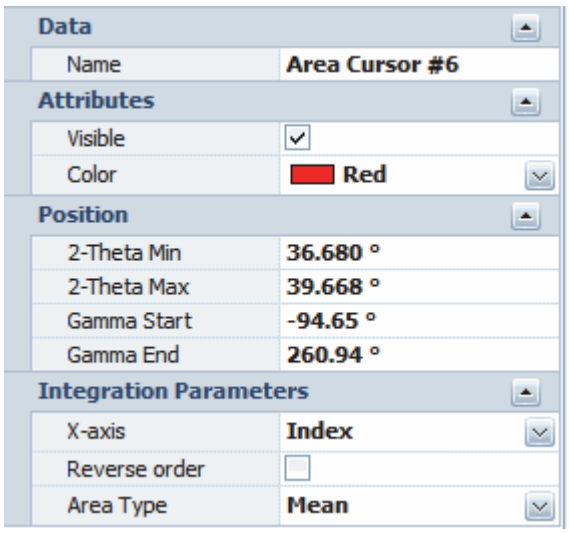


Property	Description
Name	A name which can be changed by the user.
Visible	If activated, the cursor shape is displayed.
Color	Cursor color, user-adjustable
Mask Boundary	Inside: The inner area of the cursor is the mask. Outside: The inner area of the cursor is kept for integration; the outer area is the mask.
Combine Mask	Several masks can be combined according to the following rules: Add: The masks are added and form a greater mask. Remove: The mask with the “Remove” property is used to cut out an area from another mask. Inverse: The common area of both masks is not masked anymore.
2-Theta Min	The start angle for the 2-theta integration. It is either selected with the mouse while drawing the cursor or entered here.
2-Theta Max	The end angle for the 2-theta integration. It is either selected with the mouse while drawing the cursor or entered here.
Gamma Start	The start angle for the gamma integration. It is either selected with the mouse while drawing the cursor or entered here.
Gamma End	The end angle for the gamma integration. It is either selected with the mouse while drawing the cursor or entered here.

Area Cursor

The Area Cursor is an integration cursor which is applied only to stackable frame lists. It can be applied to either the sum view of the frame list or on a single frame if it is part of a stackable frame list.

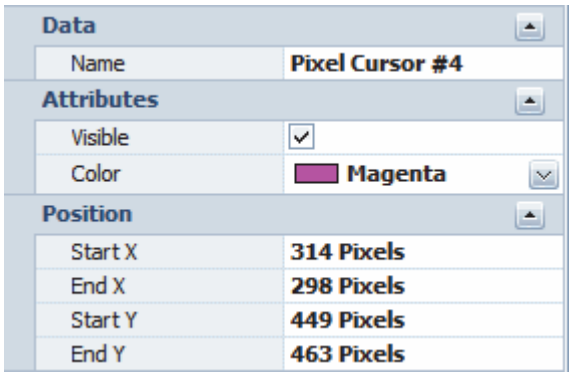
All counts from the pixels inside the cursor are added and displayed as a graph with the X-axis property as X axis.



Property	Description
Name	A name which can be changed by the user.
Visible	If activated, the cursor shape is displayed.
Color	Cursor color, user-adjustable
2-Theta Min	The start angle for the 2-theta integration. It is either selected with the mouse while drawing the cursor or entered here.
2-Theta Max	The end angle for the 2-theta integration. It is either selected with the mouse while drawing the cursor or entered here.
Gamma Start	The start angle for the gamma integration. It is either selected with the mouse while drawing the cursor or entered here.
Gamma End	The end angle for the gamma integration. It is either selected with the mouse while drawing the cursor or entered here.
X-axis	X-axis which is used for the integration result. Beside the Index and the Starting time of the measurement all other axes can be selected.
Reverse order	The X-axis is drawn inversely.
Area Type	Mean: average count value of all pixels (sum divided by number of pixels) Min: minimum count value of all pixels Max: maximum count value of all pixels Sum: sum count of all pixels

Pixel Cursor

The Pixel Cursor is a special mask cursor. Contrary to all other cursors, it works in pixel coordinates and is applied to every affected frame at the same pixel position. It can be applied only to single frames but will affect all frames in the frame's parent frame list.



Property	Description
Name	A name which can be changed by the user.
Visible	If activated, the cursor shape is displayed.
Color	Cursor color, user-adjustable
Start X	The start x position in pixels
End X	The end x position in pixels
Start Y	The start y position in pixels
End Y	The end y position in pixels

Exporting/Importing Integration Cursors

This feature is available from software version 3.1 up.

It is possible to save an integration cursor to a file and then, to import it when needed.

To export the integration cursor:

1. Select the cursor of interest in the data tree.
2. Click **Export Integration Cursor** in the File list of the Data Command panel
   — or —
   Right-click to display the related menu and then click **File.** Click **Export Integration Cursor** on the submenu: the Export an Integration Cursor File dialog box will be displayed.
3. Enter a name for the Integration Cursor File (*.evaic) and click the **Save** button.

To import a previously saved integration cursor:

1. Select the frame or frame list of interest in the data tree.
2. Click **Import Integration Cursor** in the File list of the Data Command panel
   — or —
   Right-click to display the related menu and then click **File.** Click **Import Integration Cursor** on the submenu: the Import Integration Cursor dialog box will be displayed.
3. Select the desired Integration Cursor file Enter a name for the Integration Cursor File (*.evaic) and click the **Open** button: the cursor will be added to the data tree and displayed in the graphical view.

Masks

2D Frames may have areas at the border which should not be included in subsequent integrations. Therefore, the detector area is masked. There are different types of masks which are explained in the following paragraphs.

Masked areas are displayed in green in the Frame View.

Default Mask

The default mask is pre-defined during detector calibration and a property of the 2D frame.

It is automatically displayed after frame loading:

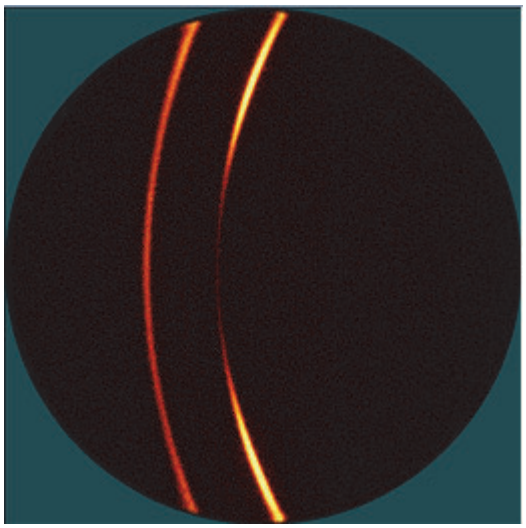


Fig.72: 2D frame with default mask after loading

There are two types of masks possible, circular and octagonal masks. All coordinates are given in pixels.

The properties for the **Circular Mask** are as follows:

Property	Description
X Center	The x value of the mask center.
Y Center	The y value of the mask center.
Radius	The mask radius.

The properties for the **Octagonal Mask** are as follows:

Property	Description
Use as circle	If selected, a circular mask calculated from the octagon's properties will be used.
Center X	The X value of the mask center.
Center Y	The Y value of the mask center.
Width	The mask radius.
Heigth	The mask height.
Symmetrical offset	If selected, all corners are treated symmetrical.
Corner offset	Corner offset in case of symmetrical offset.
Top-left corner offset	Corner offset for the top left corner.
Top-right corner offset	Corner offset for the top right corner.
Bottom-left corner offset	Corner offset for the bottom left corner.
Bottom-right corner offset	Corner offset for the bottom right corner.

The mask size and position can be modified using these properties. Corner offsets are measured on the connecting line from the center to the corner as distance from the corner. Corner angles are 45°.

User Defined Masks in Angular Coordinates

User defined masks are applied if parts of the frame should be excluded during integration. Their coordinates are measured in angular units. Therefore, masks which are rectangular on a single frame become bended on a merged frame due to the differences in the coordinate system.

The following cursors can be used as user defined masks:

- Rectangle Cursor (always a mask)
- Wedge Cursor (activate the **Use as Mask** checkbox)
- Ring Cursor (activate the **Use as Mask** checkbox)

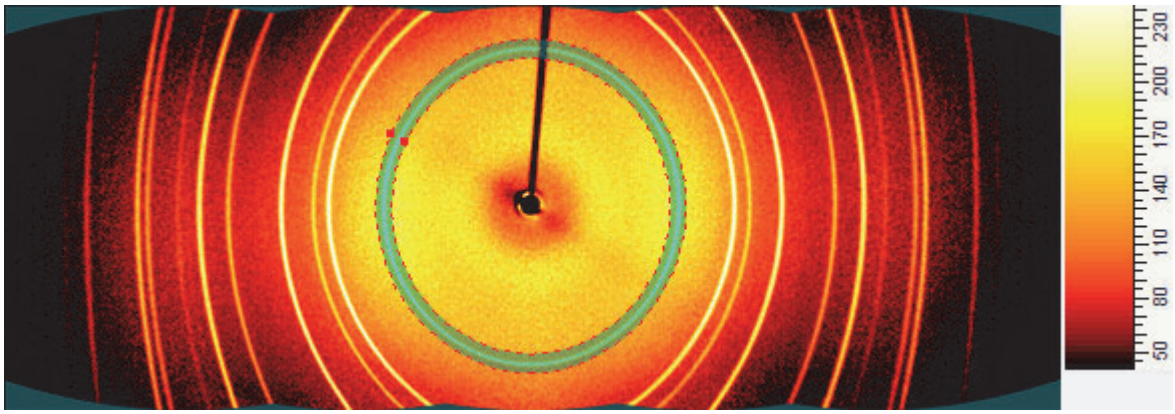


Fig.73: Ring mask applied to exclude an unwanted peak

User Defined Masks in Pixel Coordinates

A pixel mask is a mask which is applied at pixel level regardless of the angular coordinates of the 2D frame. It is created using the Pixel Cursor which is available in the single Frame View's Toolbar. A pixel mask that has been defined in one of a frame list's frames is automatically propagated to all other frames of the frame list.

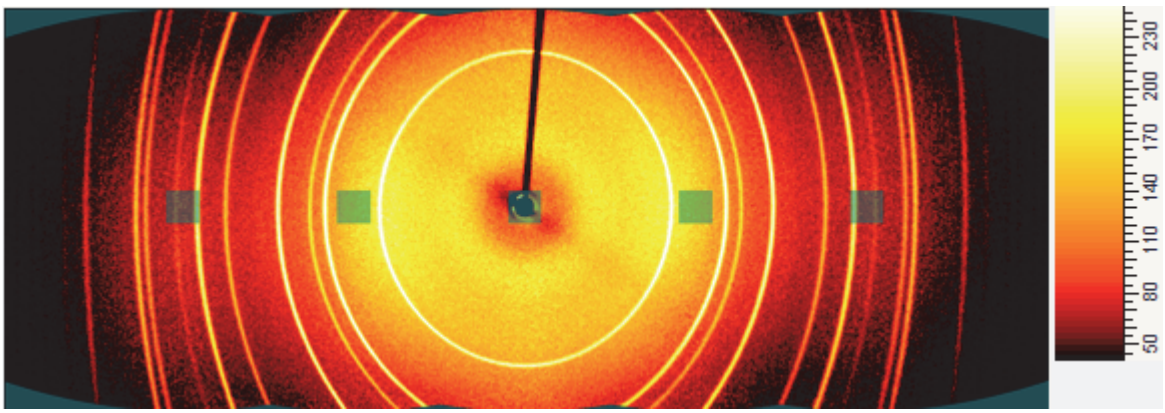


Fig.74: Pixel mask applied to the centre of the middle frame, propagated to the other frames in the list

The Integration Commands

Any cursor except the mask and the area cursor allow integrating the frames along either gamma or 2-theta. A **Cursors Preview** tool is available for the time consuming process of integration.

The integration of a single frame is a one-step process. The integration cursor is applied and the resulting scan is added in a scan list. The same procedure applies for all cursors except the area cursor on stackable frame lists.

The integration for mergeable and stackable frame lists is a two-step process. Each individual frame is integrated in the first step. The resulting scans are merged in the second step if the cursor's property **Merge as Single Scan** is checked.

Cursors Preview Tool

Integration cursors have a **Cursors Preview** tool which displays a minimized version of the integrated scan. If multiple cursors are defined, the Cursors Preview displays each cursor on a separate tab:

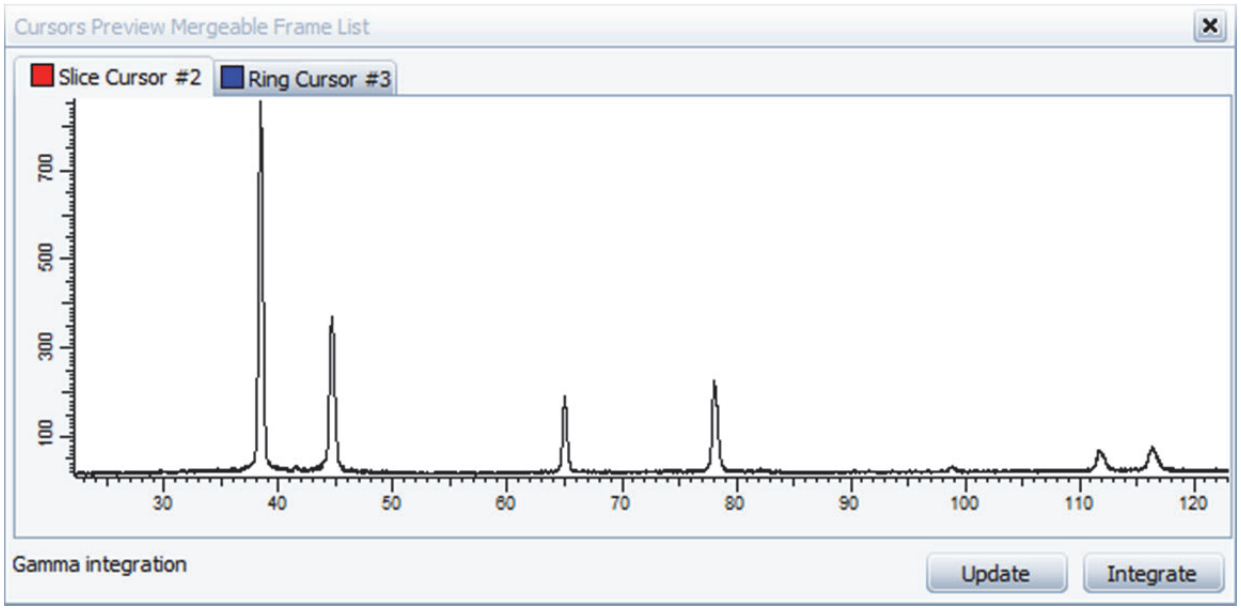


Fig.75: Cursors Preview tool with tabs for two integration cursors

If the mouse is located over the preview graphics or over the Frame View a cursor line is displayed in the tool window as well as in the Frame View at synchronized positions.

When a cursor's position or size has been changed interactively for a frame list, the Cursors Preview graph is deleted. It is necessary to click the Update button to refresh the display. Single frame cursor previews are refreshed automatically.

The **Integrate** button is a shortcut to the **Integrate Cursor** command.

Integrate Cursor Command

Integration cursors have an **Integrate Cursor** command which employs the integration immediately, regardless of whether the Cursors Preview tool is open or not.

The integration process is controlled by the cursors dimensions and its other properties. The results are added to the tree as scan(s). If several scans are created they may be placed in individual scan lists if the cursor property **Integrate in a Separate Scan List** is activated.

The Frame Header View

EVA's frame data display the most important frame properties, which are similar to the scan properties. It is sometimes desirable to have access to more frame properties. The Frame Header View serves this purpose. It can be created with the "Create Frame Header View" command of the frame.

⊞ Corrections	
⊞ Detector	
⊞ Experiment	
⊞ File	
⊞ Frame & Image(s)	
⊞ General	
⊞ Generator	
⊞ Goniometer	
⊞ Library / Plate Information	
⊞ Sample / Well	
⊟ Summary	
Beam Center	**Unwarped: 1009.69, 1005.34 Pixel; Raw: 1023.10, 1019.23 Pixel**
Ending Location	**X: -0.60 mm, Y: 0.55 mm, Z: 4.61 mm, Aux: 0.00**
Ending Position	**Distance: 221.94 mm, 2theta: 38.00°, Omega: 19.00°, Phi: 0.00°, Chi: 9...**
Frame Size	**2048 * 2048 Pixel**
Generator Settings	**40.00 kV, 40.00 mA**
Requested Exposure Time	**120.00 s**
Sample Temperature	**0.00 °C**
Scan Type	**ADD FRAME, UNWARPED**
Starting Location	**X: -0.60 mm, Y: 0.55 mm, Z: 4.61 mm, Aux: 0.00**
Starting Position	**Distance: 221.94 mm, 2theta: 38.00°, Omega: 19.00°, Phi: 0.00°, Chi: 9...**
Wavelength	**1.54180 Å (Cu)**

Fig.76: A Frame Header View with the default summary display of the extended frame properties

EVA Documents Containing 2D Frame Data

This section is relevant for software versions 3.0 and 3.1 only.
Starting with EVA 3.2 the binary file became part of the EVA file.

EVA documents containing frame data consist of two files. The first file with the extension ".eva" is the equivalent of the normal EVA document which has been saved in xml format.

The second file with the extension ".eva.bin" contains the compressed frame data in binary format. The choice of the binary format has been dictated by the size of the frame data files which has prevented them from being stored in the original xml file.

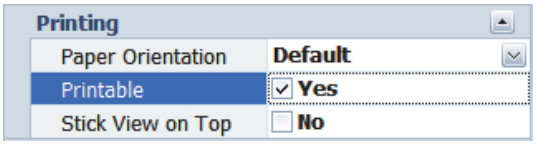
If an EVA document containing frame data should be transferred to another computer it is sufficient to transfer the ".eva" and the ".eva.bin" file. It is not necessary to transfer the individual frame files.

Printing in EVA

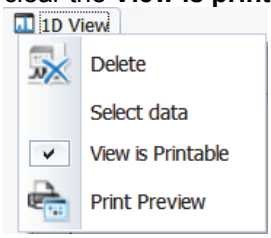
Selecting the Views to Print

To decide whether a view is printable or not:

1. Select the desired view in the Data tree or the corresponding view tab.
2. Select or clear the **Printable** check box in the View Property table to make the view printable or not



— or —
right-click the desired view in the Data tree or the corresponding view tab header. Then select or clear the **View is printable** check box to make the view printable or not.



Previewing the Printout

Opening the Print Preview

To open the print preview, either:

Click the **Print Preview** button on the toolbar 
— or —
click **Print preview** on the **File** menu
— or —
right-click the desired view in the Data tree or the corresponding view tab header and then click **Print preview** on the context menu displayed.

Overview

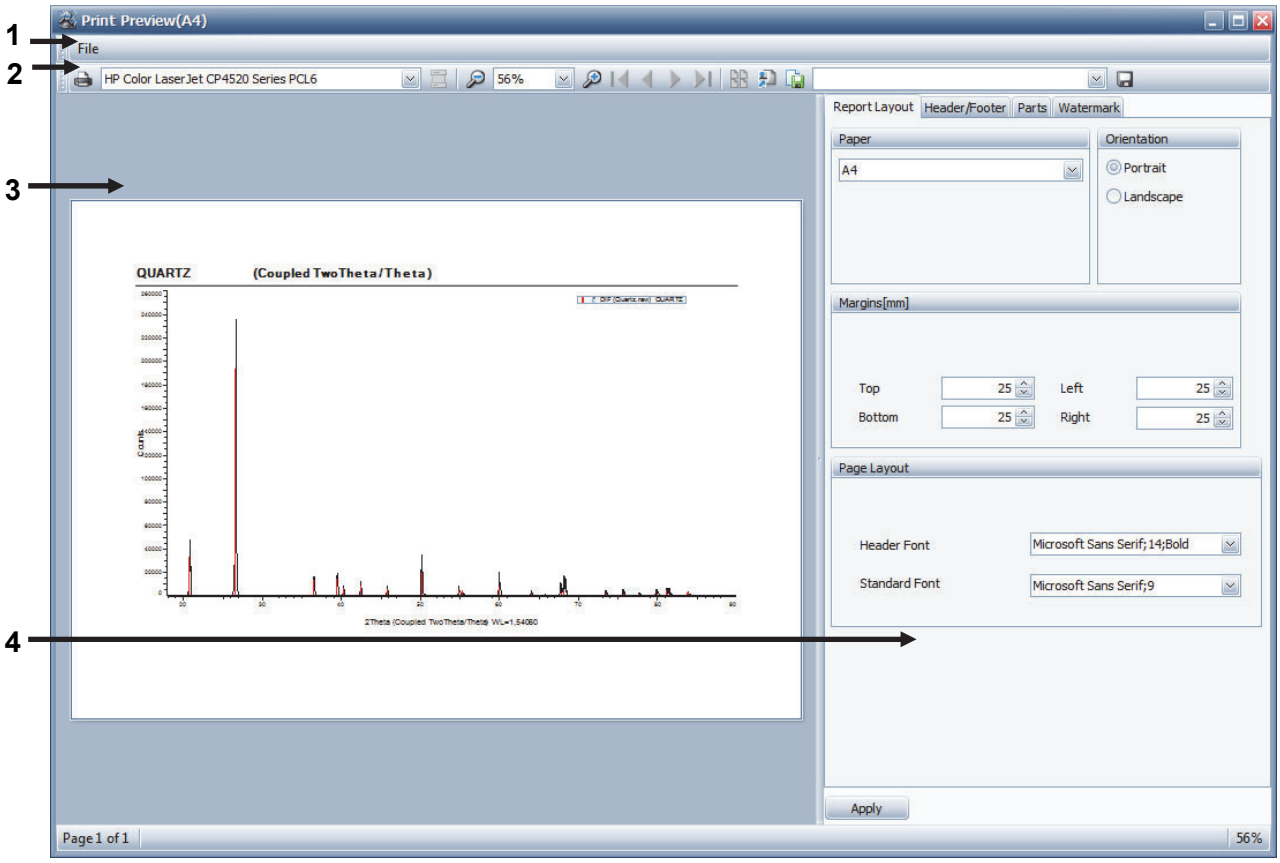


Fig.77: Exploring the Print preview

1	Menu bar	**3**	Preview
2	Toolbar	**4**	Printing settings

Menu Bar

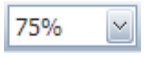
The menu bar gives access to commands. Point a menu name to display the corresponding commands and click the desired command.

File Menu

Command	Function
Print	For a quick print
Exit	To close the print preview

Toolbar

The toolbar gives easy access to commonly used tools.

Symbol	Description
	For a quick print
	Choose a printer in the drop-down list
	To zoom out
	Zoom factor
	To zoom in
	To display the first page
	To display the previous page
	To display the following page
	To display the last page
	To display multiple pages at once
	To export the view as an image
	Select a report layout in the drop-down list
	To save a new report layout: click the **Save** button, enter a name for the new report layout and click **OK**.

Printing settings

The printing settings are divided into four tabs: Report Layout, Header/footer, Parts and Watermark.

Select the desired settings and click the **Apply** button to apply them to the current document.

A report layout corresponding to the selected settings can be saved and be applied to another document:

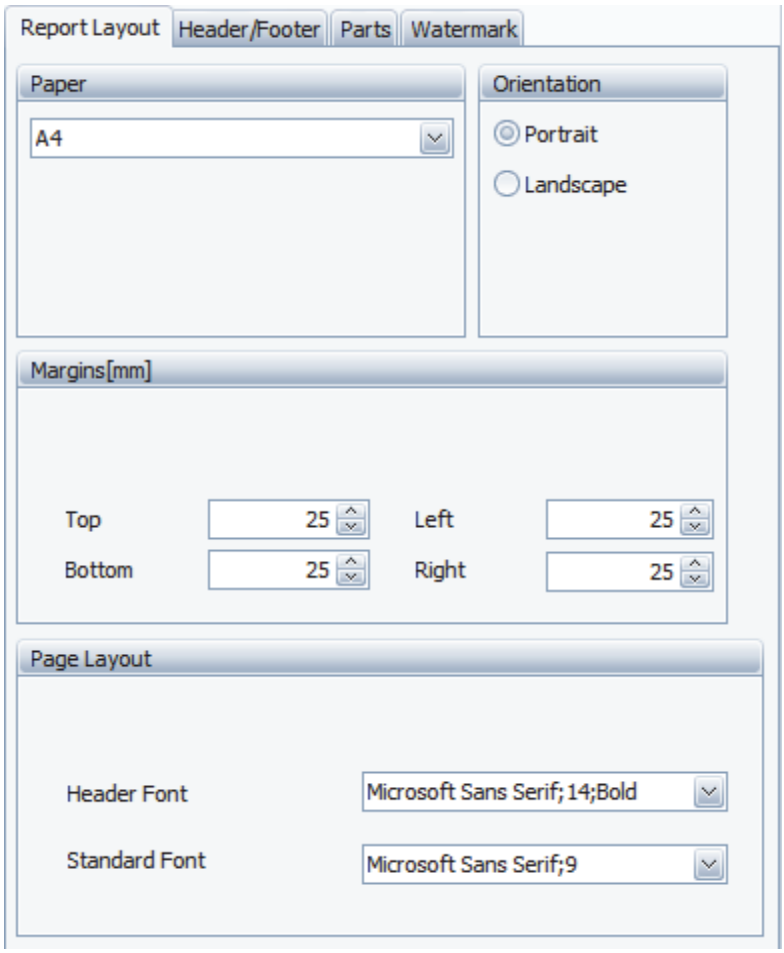
1. Click the **Save** button to display the New Report Layout dialog box.
2. Enter a name for the New Report layout.
3. Click **OK**.

To apply a layout which was previously saved, select it in the **Report Layouts Templates** drop-down box.

NOTE

The report layout template contains only the global print settings of the “Report Layout”, “Header/footer” and “Watermark” tabs. Settings defined in the “Parts” tabs are not saved into the report layout template. They are saved into the document. To apply the settings to newly created documents, the settings must be defined as defaults in the EVA settings. See section “Properties Tab" on page 70.

Report Layout tab



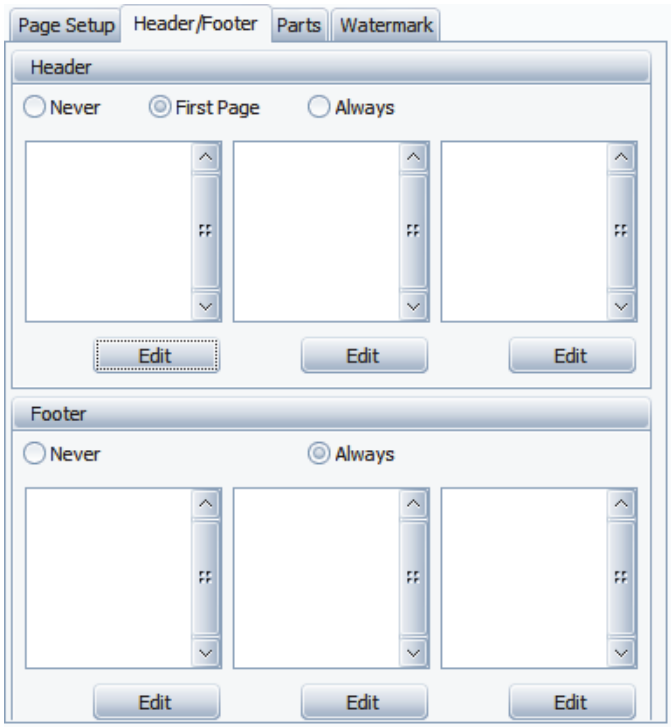
Setting	Description
Paper	Select the paper size in the drop-down list
Orientation	Select the paper orientation either Portrait or Landscape. This will be applied to the view only if default is selected for the paper orientation in the View Property table
Margins	Choose the margins' values in mm
Page Layout	Define the font use for headers and standard text

NOTE

A report is composed of one or several report parts. Each part corresponds to a view in EVA. The orientation of each part can be configured individually in the View Property table, so that the graphics are in landscape mode while the tables are in portrait mode.

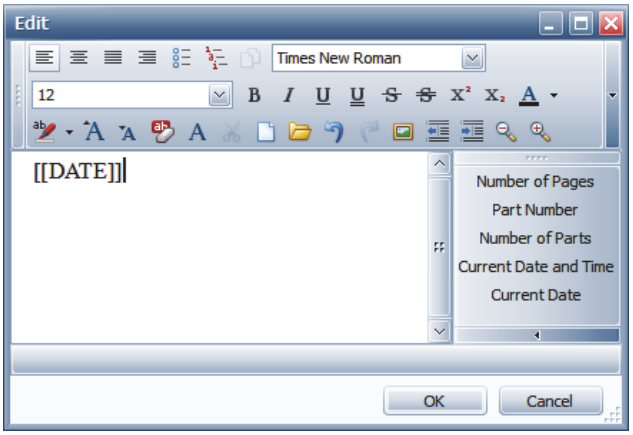
Additionally, a part of the report can be set to default. In this case, when the paper orientation in the Parts tab is changed all report parts that have been set to default will be changed. However, the parts that have been explicitly set to landscape or portrait will not be changed.

Header/Footer tab



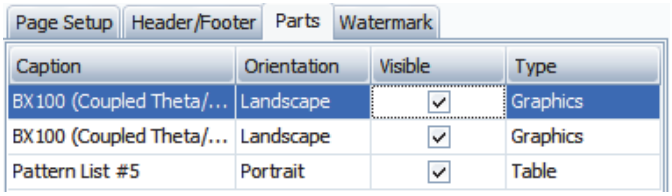
To define a header and/or footer for a document:

1. Select one the following options:
   - **Never**: No header or footer will be printed in the document.
   - **First Page**: The header will be added only to the first page of the document.
   - **Always**: The header or footer will be added to all the pages of the document.
2. Three list boxes appear below these options. Each list box is associated with a part of the page header. For example, the list box on the left corresponds to the left part of the page header. Click the **Edit** button to create or modify items in the lists. The Edit dialog box will be displayed.



3. Select information to add to the header by clicking the corresponding button(s) in the list on the right or enter the desired text using the text processor. Click **OK**.

Parts tab



At the top of the Parts tab the views (parts) initially included in the print preview are listed.
It is useful to select the parts to be printed directly.

Setting	Description
Caption	Name given to the view. Can be edited
Orientation	Paper orientation. Can be modified
Visible	Click to clear the **Visible** check box to remove the corresponding view from the print preview
Type	Type of the view: either graphics or table

Below are additional settings to customize views.

NOTE

Settings defined in the “Parts” tabs are not saved into the report layout template. They are saved into the document. To apply the settings to newly created documents, the settings must be defined as defaults in the EVA settings. See section “Properties Tab" on page 70.

- Print preview of a 1D or 2D view

To customize the axis as described in the table below, choose any of the following options. If the view (1D) includes a stick view, it can be displayed on top by selecting the **Stick View on Top** check box.

Setting	Description
Axis	
Title Color	Select the desired color for the title text.
Title Font	Select the desired font for the title text.
Numbers Color	Select the desired color for the axis numbers.
Numbers Font	Select the font for the axis numbers.
Numbers vertical	Numbers can be written either horizontally or vertically. They are written horizontally by default. To have numbers written vertically select the **Top & Bottom Axis** and/or **Left & Right Axis** check box.
Ticks color	Select the desired color for the ticks in the drop-down list.

Setting	Description
Left, Right, Top, Bottom, Palette	Customize settings for each possible axis.
Ruler visible	Select the check box to display the ruler.
Ruler size	Select the desired size for the ruler.
Title visible	Select the check box to display a title for the corresponding axis.
Title text	A title text is given by default. To use the desired title text, select the **View** check box and enter the desired text below.
Ticks display	Select the desired size for the ticks in the drop-down list or **None** to not display ticks.
Numbers display	Select the type of display used for the numbers or **None** to not display any numbers.
Ticks Orientation	Select the check box to give the sticks an internal orientation.
Min. Ticks Spacing	Adjust the minimum ticks spacing using the slider.

- Print preview of a column view

NOTE

Settings were modified from version 3.2.

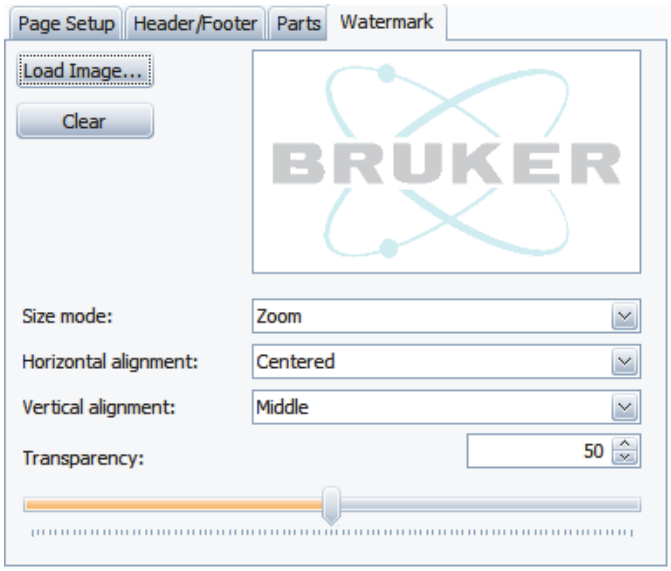
Settings up to version 3.1

Setting	Description
Appearance	
Vertical/Horizontal Lines	Define which lines will be drawn when printing the table
Shaded headers	Select the check box so the headers will be shaded when printing the table
Header Font	Click the **Browse** button to customize the font for headers
Cell Font	Click the **Browse** button to customize the font for cells
Word wrapping	Select the type of word wrapping for the table text when printing
Layout	
Fit columns in one row	Select this option so all columns will be fitted in one row
Distribute columns on several rows	Select this option so columns will be distributed on several rows and choose when the header will be displayed
Distribute columns on several tables	Select this option so columns will be distributed on several tables
Autosize Columns	Choose whether the columns size will be automatically adjusted for printing

Settings from version 3.2

Setting	Description
Paper Full Width	Select the **Paper Full Width** check box to force the use of the paper full width when printing.
Font Header	Click the **Browse** button or select a font in the drop-down list to customize the font for headers
Font Row	Click the **Browse** button or select a font in the drop-down list to customize the font for rows
Vertical Table	Select the check box to rearrange columns and rows. The properties of the object list will be listed vertically and the objects horizontally
Repeat Column	To repeat the N first columns in each row

Watermark tab



A watermark can be added to the document.

To do so:

1. Click the **Load Image** button to load the image to be used as a watermark.
2. Select the Size mode in the drop-down list.
3. Select the Horizontal and Vertical alignment.
4. Adjust the transparency by entering the desired value or by using the slider below.

To remove the watermark, click the **Clear** button.

Compiling the Reference Database using the DSRD Compiler

The DIFFRAC.SUITE Reference Database (DSRD) compiler is used for creating DIFFRAC.EVA compatible search databases from ICDD PDF databases.
It supports the PDF-2 release from 1988 to 2014 and the PDF-4 release to 2014 (to release 2015 for PDF-4 Organics only).
There are two main generations of PDF databases: non RDB databases for PDF-2 up to the release in 2004 and RDB databases beginning in 2004 to the present. All PDF-4 are RDB. RDB databases have to be installed and are copy protected by the ICDD: only duly licensed RDB databases can be used.

The DSRD Compiler also allows compiling DIFFRAC^{plus} user databases (*.UCA) into DIFFRAC.EVA's user database format.

Compiling Reference Databases

All RDB databases must be installed. The non RDB PDF-2 release from 2003 and 2004 must be installed because their CD's do not include a useable version rather only a Setup program. The PDF-2 from 1988 to 2002 can be compiled from their CD-ROM.

1. Start the DSRD compiler from the DIFFRAC.EVA start menu folder.

Administrative privileges are required for starting the DSRD compiler. If the user is not logged-in as an administrator, use the "Run as…" command with an administrative account. If the user is not logged-in as an administrator in Windows 7, use "Run as administrator" from the context menu.

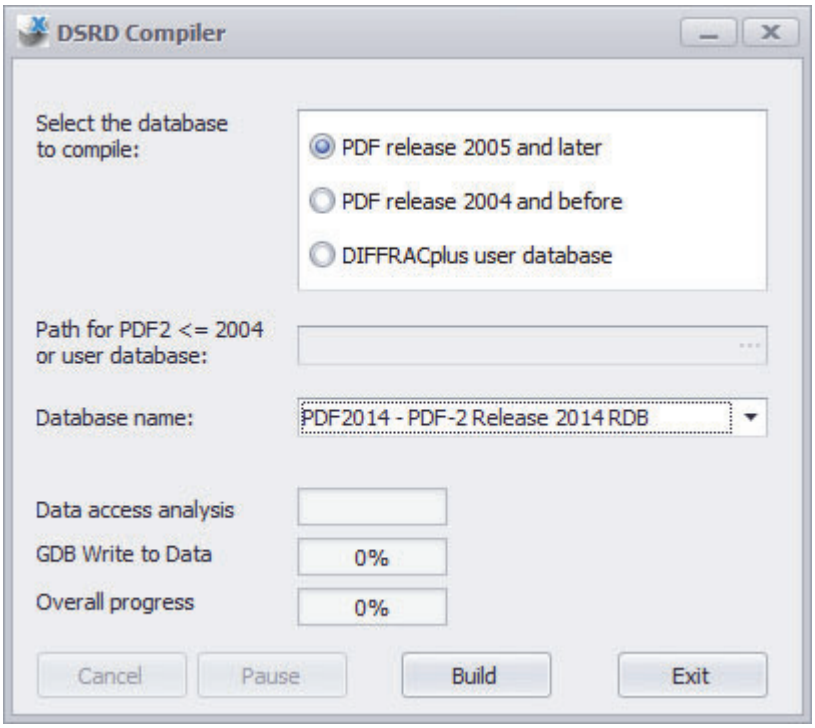


Fig.78: DSRD Compiler window

2. Select the type of database to compile:

2005 and newer

ICDD Databases with a date beginning in 2005 require the first selection “PDF release 2005 and later”. The drop down list field “ICDD Database >= 2005” will be filled with the available databases.

- Select the database to compile in the **Database name** drop-down list and click the **Build** button.
- The compilation progress will be displayed.
- The compilation is finished when the **Build** and the **Exit** buttons become active.

2004 and older

ICDD databases with dates up to 2004 require the second selection “PDF release 2004 and before”. In this case, the file search field will become activated.

- Click the **Browse** button (...) to select the CD where the database is located. This is the installation folder for PDF-2 2003 and 2004, or the CD-ROM for PDF-2 1988 to 2002.
- Click **Build** to compile the database.
- The compilation progress will be displayed.
- The compilation is finished when the **Build** and the **Exit** buttons become active again.

3. Repeat the compilation step for every database which should be used in DIFFRAC.EVA.

4. Leave the program by clicking **Exit**.

NOTE

The user may uninstall PDF-2 2003 or 2004 after compilation. On the contrary, the user is not allowed to uninstall a PDF RDB (2005 and newer) as long as the corresponding DSRD database with DIFFRAC.EVA is being used. This is required because the ICDD license scheme will no longer allow accessing the DSRD database if its corresponding PDF RDB is missing.

Compiling DIFFRAC^{plus} User Databases

The Save/Load Settings and Save/Load Layout commands are available from software version 4 up.

1. Start the DSRD compiler from the DIFFRAC.EVA start menu folder.

Administrative privileges are required for starting the DSRD compiler. If the user is not logged-in as an administrator, use the “Run as…” command with an administrative account. If the user is not logged-in as an administrator in Windows 7, use “Run as administrator” from the context menu.

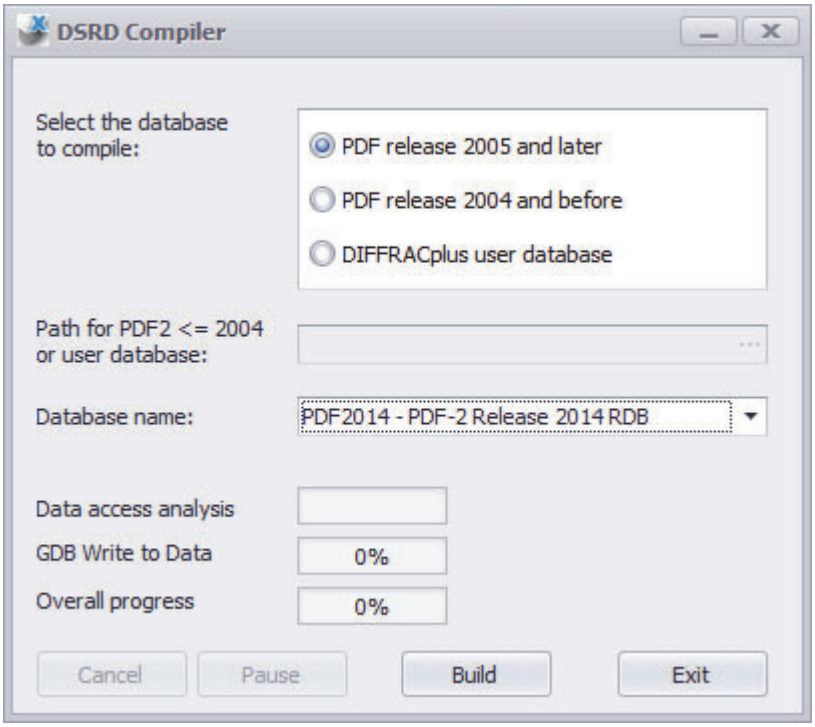
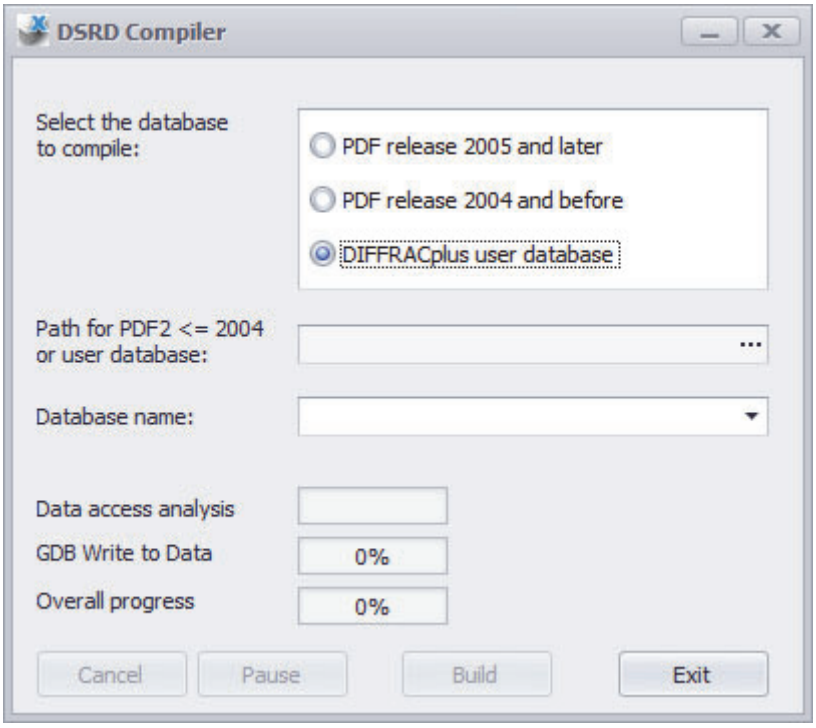
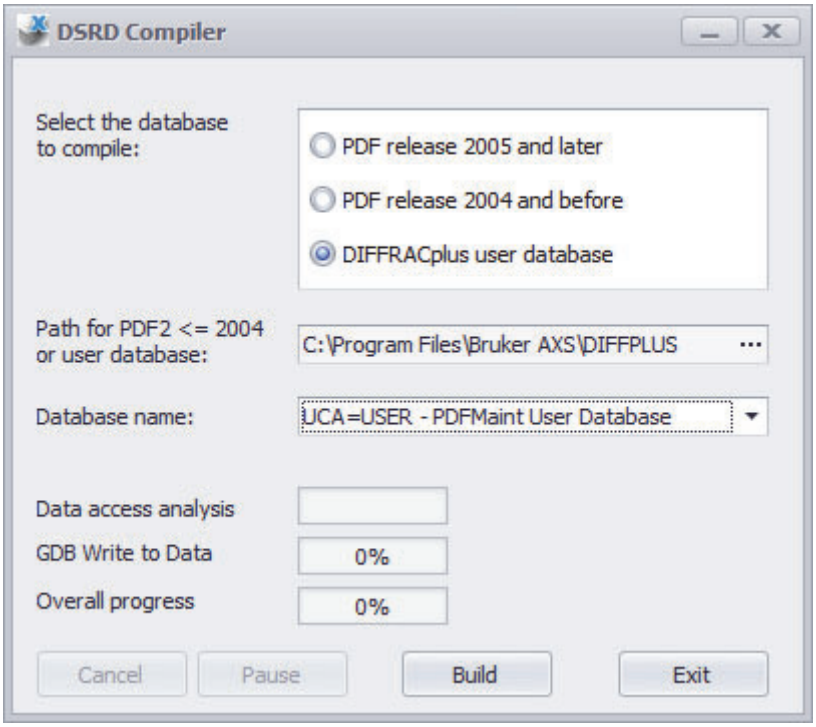


Fig.79: DSRD Compiler window

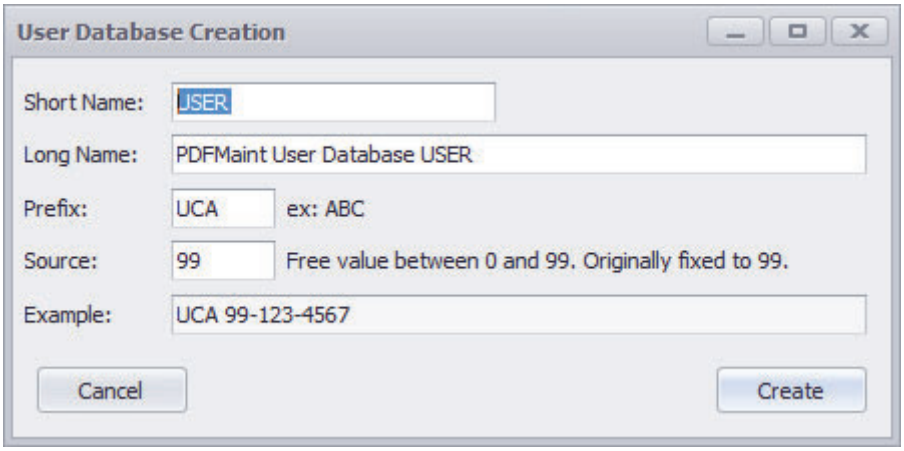
2. Select the type of database to compile: **DIFFRACplus user database**.
   In this case, the file search field will become activated.



3. Click the **Browse** button (...) to select the folder where the DIFFRACplus user database is located.
4. Select the user database to convert in the **Database name** drop-down list.



5. Click the **Build** button. The User Database Creation dialog will be opened.



6. Edit the fields as desired:

   - The **Short Name** is used for creating the files and is part of their file name.
   - The **Long Name** is the name displayed in EVA.
   - The **Prefix** and the **Source** are used to identify the user database. Originally all the sources were 99. Now it is possible to change this value to differentiate cards with same number but different sources.
   - The **Example** field gives an overview of the cards numbering.

7. Click the **Create** button. The new user database will be built.

8. Close the DSRD Compiler and start EVA. The newly built user database will be available for searches.

NOTE

If the destination is an existing user database the data from the DIFFRACplus user database are merged into this user database. It is important to keep the same information Short Name, Long Name, Prefix, but the source can be different to differentiate between cards with the same original number.

Calculating the Penetration Depth of the X-Rays in a Given Material using AbsorbDX

AbsorbDX is a program belonging to the software suite DIFFRAC.EVA. Its aim is to calculate the depth of the layer that is analyzed by X-ray diffraction, in given conditions, i.e. the depth of penetration of the X-rays in a given material. In standard powder diffraction, this feature allows, for instance, to check whether a sample has an "infinite thickness" or not.

When performing powder diffraction in grazing incidence conditions, the lower the incidence angle, the lower the depth of the analyzed layer. AbsorbDX is then especially useful because it gives the depth of the analyzed layer for the entered incidence angle.

In order to get the depth of the analyzed layer of a given sample, all you need is to enter its global chemical composition (i.e. the proportion of the different atoms), its density (specific mass), the X-ray radiation in-use (e.g. Cu Ka1), and the diffraction angles of the two-circle goniometer. AbsorbDX uses the classical absorption model described in the next section.

Theoretical Approach

Attenuation Formula

The X-rays are absorbed mainly by photo-electric effect, but also scattered by elastic diffusion (or Rayleigh diffusion) and inelastic diffusion (or Compton diffusion); the total attenuation follows the Beer-Lambert[1] law for a given wavelength λ:

$$I(d) = I_0 \cdot e^{-\mu \cdot \rho \cdot d}$$

where d is the length of the path of the X-rays into the material ("distance"), μ is the mass attenuation coefficient (usually in $cm^2.g^{-1}$), which depends on λ, and ρ is the specific mass of the material.

NOTE

As the main attenuation is due to the photoelectric effect, the attenuation coefficient is often referred as the absorption coefficient.

The mass absorption coefficient is computed from the composition of the material:

$$\mu = \sum_i c_i \cdot \mu_i$$

where i is a chemical element, c_i is its mass proportion, and μ_i its absorption coefficient for the element. The μ_i depend on the wavelength. Some authors use the linear absorption coefficient $\mu_L = \mu.\rho$, but this coefficient is structure-dependent, whereas μ only depends on the composition.

Considering the specific geometry of a diffractometer, and assuming a homogeneous sample, the path of the X-rays analyzing the depth x of the sample is:

$$d = x \cdot \left(\frac{1}{\sin\gamma} + \frac{1}{\sin(2\theta - \gamma)} \right)$$

with γ the angle between the incident beam and the surface of the sample and 2θ is the deviation of the beam. In the case of BRAGG-BRENTANO geometry, $\gamma = \theta$ so $d = 2x/\sin\theta$.

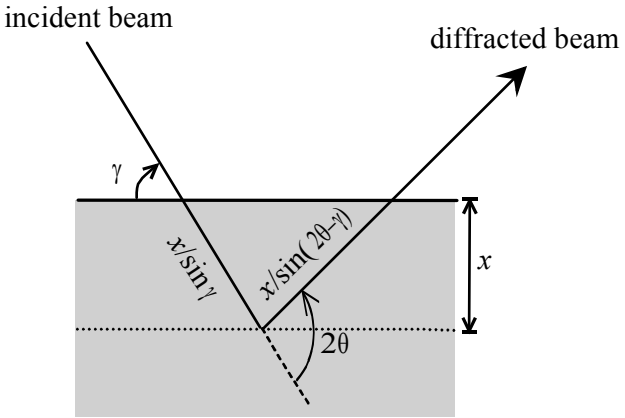


Fig.80: X-ray path and absorption in a sample

Thus, the intensity of the X-rays diffracted by the surface layer which thickness is x is equal to:

1 Wilhelm BEER (1797-1850), Johann Heinrich LAMBERT (1728-1777), Pierre BOUGUER (1698-1758)

$$I(x) = I_1 \cdot \left[1 - \exp\left(-\mu \cdot \rho \cdot x \cdot \left(\frac{1}{\sin\gamma} + \frac{1}{\sin(2\theta - \gamma)} \right) \right) \right]$$

with I_1 the total intensity collected by the detector (see the Appendix, chapter “Attenuation Calculation” on page 220).

This is an exponential law, which means that theoretically, the analyzed thickness is infinite; but we can consider that the analyzed thickness corresponds to the layer which gives a fraction p of the signal ($I(x)/I_1 = p$). p is usually taken equal to 0.9 ($90\,\%$ of the signal), this of course may depend on the measuring conditions. The analyzed depth is then estimated by:

$$x = -\ln(1-p) \times \left(\mu(\lambda) \cdot \rho \cdot \left(\frac{1}{\sin\gamma} + \frac{1}{\sin(2\theta - \gamma)} \right) \right)^{-1}$$

Bibliography

The $\mu_i(\lambda)$ values used for AbsorbDX are the values tabulated in the following publications:

- for the mass absorption coefficients due to photoelectric effect, the elastic (Rayleigh) and inelastic (Compton) scattering:
  Ebel H., Svagera R., Ebel M.F., Shaltout A. and Hubbell J.H., *Numerical description of photoelectric absorption coefficients for fundamental parameter programs*, X-ray Spectrometry, Issue 32, pages 442-451 (2003)
- for the absorption jump values:
  Elam W.T., Ravel B.D. and Sieber J.R., "A new atomic database for X-ray spectroscopic calculations", Radiation Physics and Chemistry, Issue 63, pages 121-128 (2002)

Using AbsorbDX

AbsorbDX can be opened from the Tools menu from software version 4 up.

1. Start AbsorbDX from the Tools menu or DIFFRAC.EVA start menu folder.

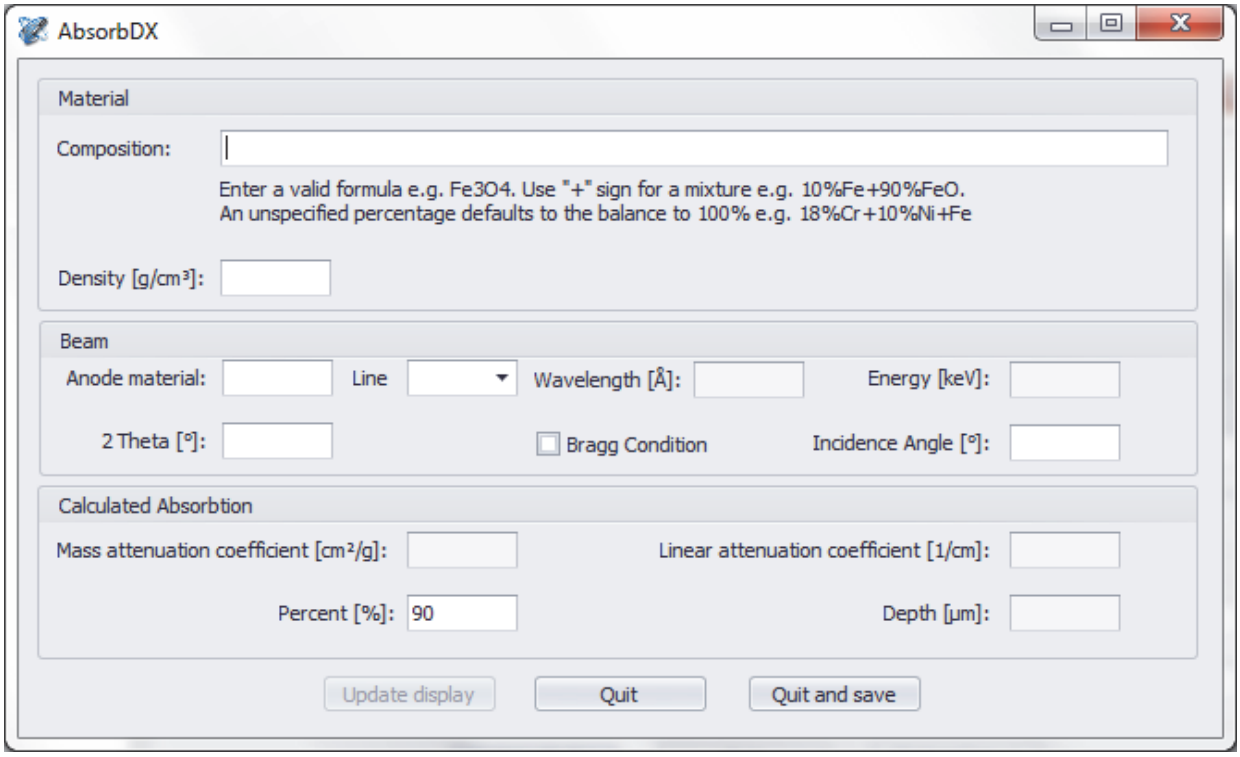


Fig.81: AbsorbDX window

In the area Material

2. In the field **Composition**, type in the elementary composition of the product. There are three ways to write the composition:

- if your product is a stoichiometric compound, directly write the chemical formula, i.e. the coefficient follows the element; e.g. for the magnetite, type `Fe3O4`;
- you can use the mass percentage of the elements; in this case, the coefficient stands before the element and the elements are separated by plus signs; e.g. for $FeAl_{40}$, type `60%Fe+40%Al`; you can also use percentages of compounds, e.g. `20%SiO2+80%CaCO3`;

In the preceding mode, you can define an element as a balance to 100 %; for this, do not write its concentration; e.g. for a 316L stainless steel, write:

`2%Mn+1%Si+17%Cr+12%Ni+2.5%Mo+`**`Fe`**

(We neglected the very low concentrations like C, P and S).

3. In the field **Density [g/cm^3]**, type in the specific mass of the sample, in g.cm^{-3} (i.e. kg.L^{-1} or ton.m^{-3});

In the area Beam

4. In the field **Anode material**, type in the nature of the anti-cathode of the tube. For example, for a tube with a copper anti-cathode, type in `Cu`.

5. In the Line drop-down list, select the reference of the line in the Siegebahn[2] notation; for example `KA1`.

The fields **Wavelength [Å]** and **Energy [keV]** are set automatically.

6. In the field **2 Theta [°]**, type in the total deviation 2θ (i.e. the angle between the incident and the diffracted beam) in degrees;

- if you work in Bragg conditions (i.e. the incidence angle is θ), let the **Bragg condition** box checked; if the incidence angle γ is different from θ (e.g. for grazing incidence measurements), clear this box and type in the incidence angle in degrees in the field **Incidence angle [°]**;

In the area Calculated Absorption

7. In the field next to **Percent [%]**, type in the proportion of signal p in % you want to use to estimate the analyzed depth d (i.e. the first d µm of the sample give p % of the signal); the default value is 90 %;

8. Click the **Update display** button to perform the calculations.

Display of the Results

ABSORBDX then calculates the attenuation coefficients and the depth d:

- the mass attenuation coefficient μ is displayed in cm^2.g^{-1} in the corresponding field;
- the linear attenuation coefficient μ_L is displayed in cm^{-1} in the corresponding field;
- the depth d is displayed in µm in the corresponding field

Exiting ABSORBDX

You can then quit ABSORBDX in two manners:

- using the **Quit and save** button: the next time you will use ABSORBDX, the current parameters will be used as default;
- using the **Quit** button: the parameters will not be saved for the next use.

2 Manne SIEGBAHN (1886-1978), Nobel prize in 1924

Examples

Thin Nitrided Layer on Iron

Let us suppose an iron sample that was nitrided, forming a γ-Fe_4N layer ($\rho = 7.212\ g.cm^{-3}$). It is analyzed in grazing incidence conditions, with a cobalt X-ray tube. The iron (111) peak (strongest peak, $2\theta = 48.2\ °$) appears at $\gamma = 1\ °$; the depth for 90 % contribution of the measured intensity for these angles is 1.0 μm.

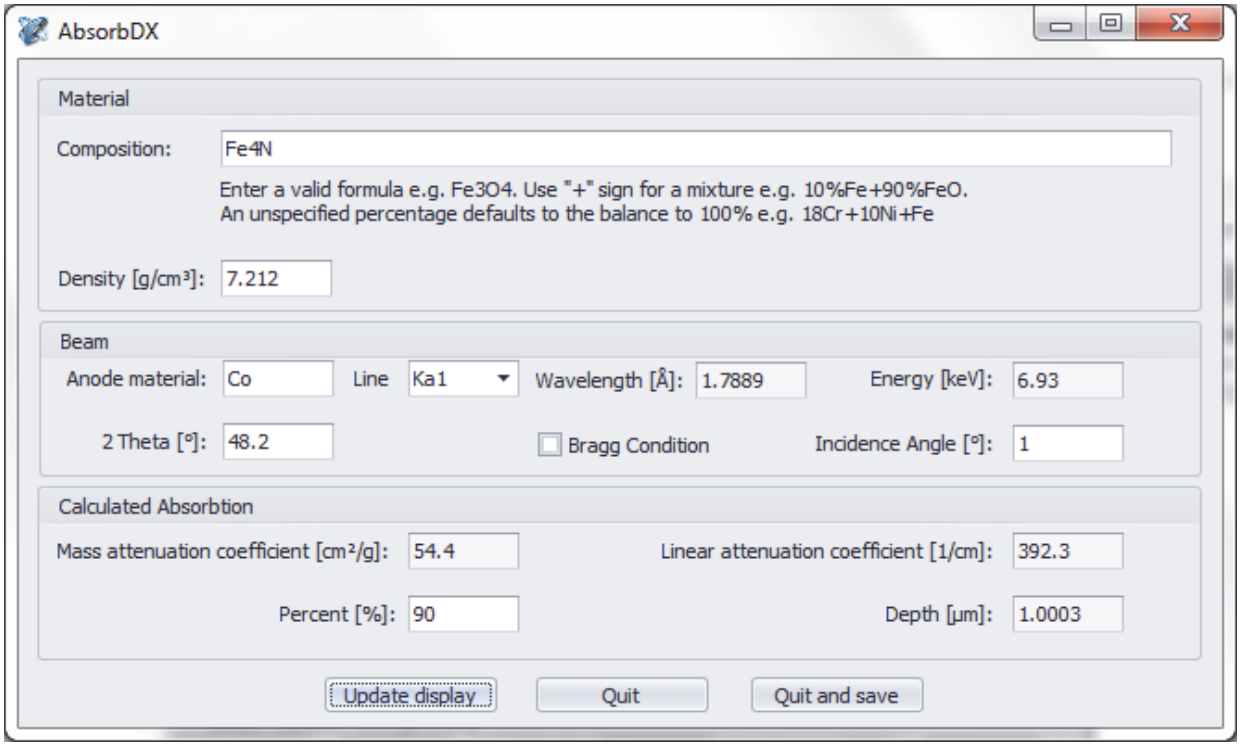


Fig.82: Absorption of an iron nitride layer

Mix of Corundum and Boehmite

Let us consider a powder mix of 20 mass % of corundum (α-Al_2O_3, ρ = 3.987 g.cm^{-3}) and 80 mass % of boehmite (AlOOH, ρ = 3.071 g.cm^{-3}) is analyzed in Bragg conditions with a copper X-ray tube. For the (020) peak of the boehmite (2θ = 14.5 °), the depth for 90 % contribution of the measured intensity is 15.6 μm.

$$\rho = \frac{100}{\frac{20}{\rho_{Al_2O_3}} + \frac{80}{\rho_{AlOOH}}} = 3.219\,\mathrm{g.cm^{-3}}$$

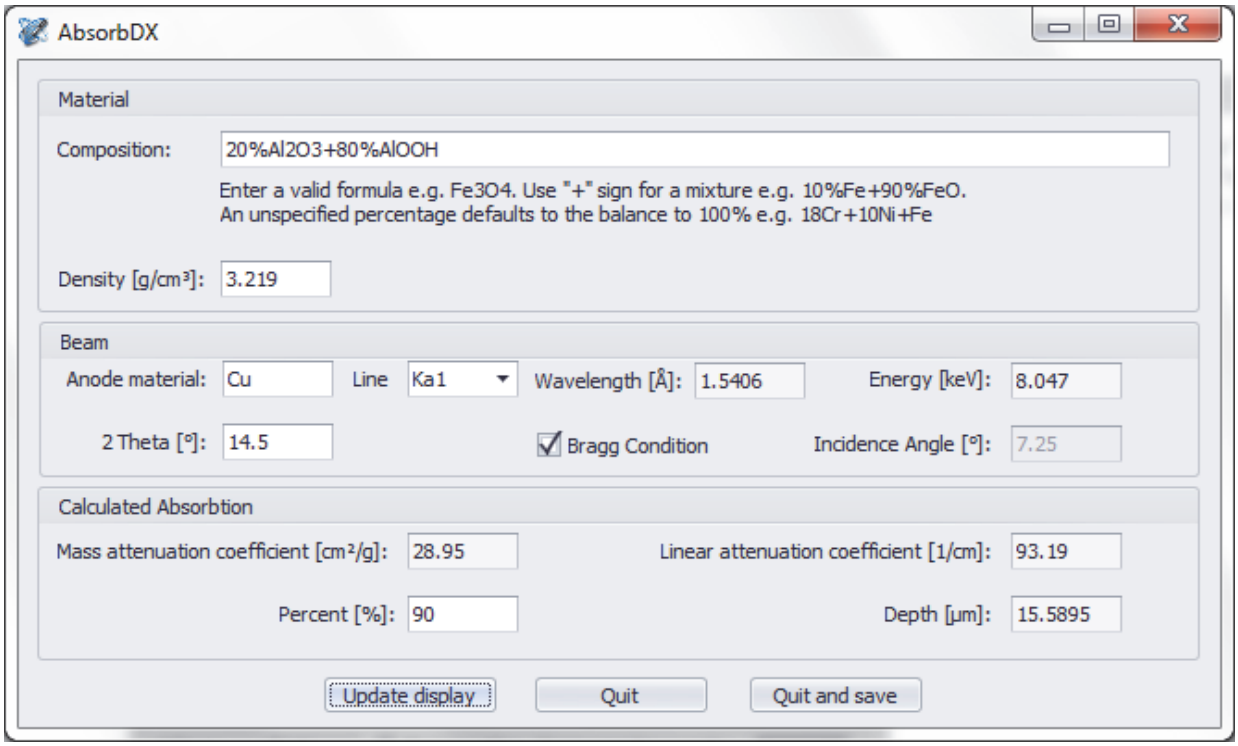


Fig.83: Mix of Corundum and Boehmite

Appendix

DIFFRAC.EVA V4 and License Level

Feature	Required version (license level)
Cluster Analysis	V4 (V4)
Saving the workspace layout	V4 (V1)
Saving the EVA settings	V4 (V1)
Support of DIFFRAC^{Plus} user databases	V3.2 (V1)
Duplicate scan	V3.2 (V1)
Accumulate	V3.2 (V1)
Export bg subtracted scan	V3.2 (V1)
Document log view	V3.1 (V1)
2D frame data loading and display in several view types	V3 (V3)
2D frame data integration	V3 (V3)
2D frame data masking	V3 (V3)
2D frame data rocking curve analysis	V3 (V3)
Property filtering and grouping	V3 (V1)
Scans in xy format	V3 (V1)
Scan View	V3 (V1)
AbsorbDX program	V3 (V1)
Automatic Search/Match	V2 (V2)
Export partial scan	V2 (V1)
Export background	V2 (V1)
Replace scan	V2 (V1)
Clone scan	V2 (V1)
Database and chemical filter commands	V2 (V1)
Scans order	V2 (V2)
Shortcut keys for panels	V2 (V1)
Automatic conversion of DIFFRAC^{plus} EVA document files (*.eva) into DIFFRAC.EVA document files	V2 (V1)

Supported Databases

COD Databases

DIFFRAC.EVA supports the COD database from version 2010 to 2013.

PDF Databases

DIFFRAC.EVA supports the PDF-2 release from 1988 to 2014 and the PDF-4 release to 2014 (to release 2015 for PDF-4 Organics only).

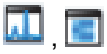
There are two main generations of PDF databases: non RDB databases for PDF-2 up to the release in 2004 and RDB databases beginning in 2004 to the present. All PDF-4 are RDB. RDB databases have to be installed and are copy protected by the ICDD: only duly licensed RDB databases can be used.

NOTE

Note that due to ICDD's license restrictions a search cannot be performed using the PDF and COD databases simultaneously.

Commands Accessible from the Command Panels

General Data Commands

Command	Icon	Description
Data		
Delete		To delete the selected data and their children data
Clear		To clear the children data of the selected data
Select Parent		To select the parent data
Select Children		To select the children data
Create		
Object Column View		To create a column view listing all the *objects* descending from the selected data and the corresponding information
1D or 2D View		To create a 1D or 2D View (available commands depending on the data selected)
Object Chart View		To create a chart view showing the *objects* descending from the selected node and corresponding information

Data Commands Specific to Documents

Command	Icon	Description
File		
Import from files…		To import a scan file

Data Commands Specific to Settings and Filters

These features are available from software version 2.0 up

Command	Icon	Description
Settings		
Clear default Filters	None	Previously defined default filers are removed
Create		
Chemical Filter data		To create a new chemical filter
Database Filter data		To create a new database filter
File		
Import Chemical Filter	None	To import a chemical filter
Import Database Filter	None	To import a database filter
Chemical/Database Filter		
Use as Default Chemical/Database Filter	None	The selected filter becomes the default filter for any new document. The current document is **not** affected
Export Chemical/Database Filter	None	To export a chemical/database filter

Data Commands Specific to Scan Lists

Command	Icon	Description
Tool		
Create Level	None	To create levels
File		
Export Multi-range scan	None	To export all the scans in the list to one file
Export all scans	None	To export all the scans in the list into individual files at once

Data Commands Specific to Scans

Command	Icon	Description
Create		
Scan View	None	To create a scan view
Elemental Analysis		To perform a semi-quantitative analysis
Tool		
Search/Match (scan)	None	To perform a Search/match operation or a Search by name
Search by Number	None	To perform a search by number
Background	None	To perform a background subtraction
Peak Search	None	To perform a peak search
Strip ka2	None	To compute the $K\alpha_2$ Stripping
Fourier Smooth	None	To smooth scans using Fourier
Smooth	None	To smooth scans
Displacement	None	To correct the sample displacement error
X-Offset	None	To correct the X-Offset
Y-Scale factor	None	To re-scale scans
Y-Offset	None	To re-scale scans
Aberrant	None	To remove aberrant points
Create Area	None	To compute areas
Duplicate	None	To create a copy of the scan
Accumulate	None	To add times and counts of scans
Add	None	To add scans
Subtract	None	To subtract scans
Merge	None	To merge scans
[hkl] Generator	None	To create a pattern from lattice parameters
File		
Import XRF Results		To import XRF results
Export/Import a DIF File		To export/import a DIF saved as a file
Export Scan…	None	To export a scan into a file
Export Bg Subtracted Scan…	None	To export a scan subtracted from its background
Export Partial Scan…	None	To export a part of a scan into a file
Export Background…	None	To export only the background defined for a scan into a file
Replace Scan…	None	To replace a scan with another scan
Clone Scan…	None	To copy the data of a scan to another scan

Data Commands Specific to Pattern Lists

Command	Description
Tool	
Search/Match (scan)	To perform a Search/Match operation on the parent scan
Search by Number	To perform a search by number

Data Commands Specific to Patterns

Command	Description
Tool	
Search/Match (pattern)	To perform a search/match operation on the parent scan
Search by Number	To perform a search by number
d x by	To multiply d-values by a factor
Tune Cell	To modify cell parameters
Residue	To prepare a residual scan
Make Sticks	To create the sticks corresponding to the pattern
Make Peaks	To create the peaks corresponding to the pattern
Make DIF	To create a DIF from the pattern
Auto-scale	To reset the scaling
User Database	To create and manage a user database
[hkl] Generator	To create a pattern from lattice parameters
Create	
DB View	To create a database view showing the pattern information

Data Commands Specific to Peak Lists

Command	Description
Tool	
Search/Match (peak list)	To perform a Search/Match operation on the peak list
Make DIF	To make a DIF from the peaks of the list
Normalize	Not yet available

Data Commands Specific to Peaks

Command	Description
Tool	
Search/Match (peak list)	To perform a Search/Match operation on the parent peak list
Make DIF	To make a DIF from the peak

Data Commands Specific to Views

Command	Icon	Description
1D, 2D, Column, Multiple views and Groups		
Delete		To delete the selected view
Select Data		To select the corresponding data
View is Printable		Select the check box to include the selected the view when printing
Print Preview		To have a print preview of the selected view
Select Group		To select the views belonging to the group
Ungroup		To ungroup the selected group of views
Group		
Vertical		To group the views vertically
Horizontal		To group the views horizontally
Array		To group the views in an array
Grid		To group the views in a grid

Data Commands Specific to Frames

Command	Description
Create	
Frame Thumbnail View	To create a thumbnail view for all the frames
Frame Merged View	To create a merged view of the frames
Tool	
Cursors preview	To preview the integration cursors
File	
Import Integration Cursor	To import a previously save integration cursor

Shortcut Keys for Panels

These features are available from software version 2.0 up

There are the shortcut keys available for panels. They prove useful when working on small screens.

Key combination	Function
F2	Show/hide the Data Tree panel.
F3	Show/hide the Data Property panel.
F4	Show/hide the Data Command panel.
F5	Show/hide all panels.
F6	Show/hide the Data Tree and Data Property panels.
Ctrl-F3	Delete current data.
Shift-F2	Show the Data Tree panel and hide all other panels.
Shift-F3	Show the Data Property panel and hide all other panels.
Shift-F4	Show the Data Command panel and hide all other panels.
Shift-F5	Show all panels.
Shift-F6	Show the Data Tree and the Data Property panels.

Search / Match

The Aim of EVA Search/Match

The purpose of EVA Search/Match is to search the current scan of an unknown material and then identify reference patterns that are likely to explain the unknown scan. A Search algorithm is applied, comparing the reference patterns of a database to the scan. The algorithm gives a rank to the Patterns and lists the "best candidates". The user must compare the pattern to the scan and accept or reject the found pattern. This is called the match procedure.

Algorithms

Pre-treatment of the Scan

The search is performed on the background subtracted scan. The subtraction is carried out automatically at scan import. This operation ensures that none of the lines, however weak, can be contained in the computed background. Thus, all relevant information is preserved.

Note that the background subtraction does not only "flatten" the scan, but it also defines the level of the noise and thus, allows the Search algorithm to determine which part of the scan contains a significant signal and which part of the scan contains only noise.

Please note that other pre-treatments, such as the Kα2 stripping or smoothing, are neither necessary nor desirable.

General Algorithm Implemented in EVA Search/Match

Instead of using a list of only d and I's, EVA Search/Match uses the entire scan after removal of the background. EVA Search/Match compares each reference pattern with regions of the unknown scan considered as null intensity when searching. Patterns whose lines fall in these regions tend to be rejected.

Computation of the Figure of Merit (FOM) of Each Potential Candidate

During the search, potential candidates are selected from the reference database in accordance with user-set parameters and the declared filters. These parameters and files are set in the EVA Search/Match tool box. A Figure Of Merit (FOM) is calculated for all potential candidates having at least one line falling in a region of non-zero intensity.
The traditional DIFFRAC^{plus} FOM, where the lowest value was the best value, has been replaced by a new value. The new value is 100% for a dummy stick pattern that explains perfectly the unknown scan. As a result, the new FOMs are more informative than the traditional FOMs. However, the searches deliver exactly the same results as in the previous algorithm. The difference is that the FOMs have changed. Please note that a FOM slightly over 100% can occur, especially for a scan of a pure phase.

User-Selected Criterion

Phases which are contained in geological samples can have 100 diffraction lines or more. Other phases have only a few lines in the same 2θ range. It is not possible to develop a search algorithm which treats all phases as equal regardless of their complexity.

Complex patterns are likely to be unique. Therefore, their identification is less ambiguous.

Simple patterns are likely to be more difficult to identify. The reasons are as follows:

- Phases giving simple patterns frequently have isostructural phases or phases giving highly similar patterns without being isostructural, which are called "Isotypes".

- Simple patterns might be randomly included in complex patterns. Thus, there is a clear danger in starting an identification process with Criterion **1: Favor Simple Patterns** as it may cause to find phases which are not present, but which powder patterns are included in the unknown scan. Additionally, starting identification with a wrong interpretation or result decreases dramatically the chance of finding other relevant answers, because the user focuses normally on unexplained lines.

The EVA Search/Match Criterion approach is based on these facts. Therefore:

- The Criterion **3: Favor Complex Patterns** deliberately increases the chances of complex patterns to rank best.
- The Criterion **1: Favor Simple Patterns** fully reverses this strategy by increasing the chances of simple patterns to rank best.
- The Criterion **2: Neutral** is an attempt to give equal chances to all kinds of candidates. It is selected by default and most search / match problems can be solved by using only this criterion.

There is no “minimum of line to match” criterion. Such a criterion does not reflect the unequal nature between a high symmetry (simple) pattern and a low symmetry (complex) pattern, and disqualifies those patterns having fewer lines than the minimum.

Background Subtraction

Traditional DIFFRAC Method

To understand how the traditional DIFFRAC method works, imagine an inflated elastic membrane in one dimension. Every time the membrane hits the scan curve in one point (contact point), the arc is divided in two arcs that subsequently grow separate. The arcs are parabolic in the DIFFRAC algorithm.

The shape of the parabola predicts the ″maximum concavity″ of the background curve. Once found, the contact points are corrected by adding n times the statistical error[5] of the corresponding intensity (where n is the Threshold; default = 1): the minimum intensity plus one time the statistical error is likely to fit the observed background. If a smoothing was performed before background subtraction or if the data are not obtained by powder X-ray diffraction (e.g. neutron diffraction or synchrotron radiation diffraction), then the statistical law is no longer valid and the Threshold (n) must be adjusted.

The Curvature is the main parameter of the background computation. It must be adjusted if there are background humps in the scan to fit the humps. There is no requirement to adjust the Curvature if there are no background humps.

The background curve must cross the background noise as close as possible to the middle. This is usually achieved without adjustment, as long as the data have not been treated (for example, for smoothed data, reduce the Threshold and find its optimal value with a few trials).

The major strength of the DIFFRAC method is to ensure that no peak of the scan, even if it is very weak, is below the background curve. The algorithm is therefore fully satisfactory for EVA search/match.

There are two drawbacks:

- Intensities of broad lines are often slightly reduced.
- The background curve is made of parabolic arcs; the nodes between 2 arcs are not a realistic description of the physical phenomena, which results in local inaccuracies.

Do not use the background subtraction to prepare profile fitting data, because profile fitting itself computes a more accurate local background. If a global background method is required because profile fitting cannot find a correct background, use the enhanced method described below.

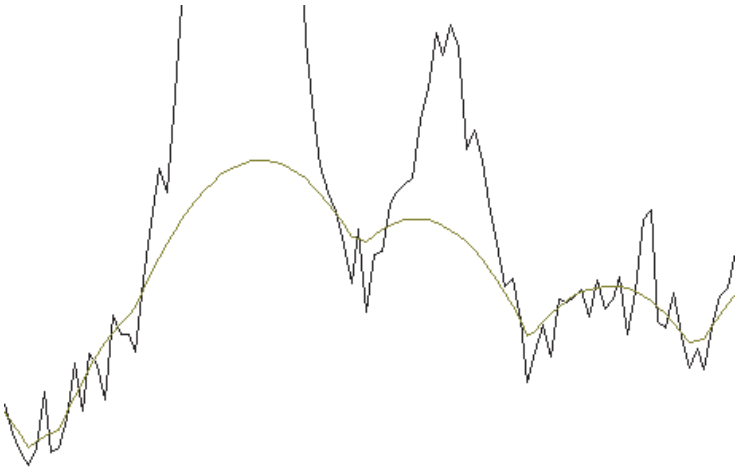


Fig.84: Parabolic arcs and "sharp turns" resulting from the DIFFRAC method

[5] the measured intensity for x-ray diffraction follows the statistical law of Poisson, so the standard deviation can be estimated by the square root of the intensity

Enhanced Method

The enhanced method was designed to draw a smooth background with the assumption that there is only one single "hump". This is a good hypothesis for the scattering by an amorphous phase in some cases.

This method uses the same contact points between the background curve and the scan as the DIFFRAC method, and the same curvature adjustment. However, some contact points can be eliminated by filtering. The Threshold is no longer used because the filtering method itself ensures that the background curve crosses every region recognized as a background region in the middle of its noise fluctuations.

Some peaks might be below the background curve in certain cases. This method is therefore not recommended to prepare Search/Match data. For other purposes, the enhanced background curve is usually more realistic than the traditional background curve.

Peak Search

The peak search is controlled by two parameters:

- The peak width
- The threshold

Peak Width

This is the width of the sliding interval on which the Savitzky-Golay filter is applied and on which the peaks are located by the second derivative method. The range is from four to 56 times the step size. The algorithm uses five to 57 data points centered on the desired point. Ideally, the peak width should be close to twice the peaks' full width at half maximum (FWHM) value. As a rule, the acceptable values for data of reasonable quality range from FWHM to FWHMx4. The actual range of acceptable peak width values depends on data quality.

The FWHM of a peak can be computed with the Area tool (see Section "Computing Areas" on page 111).

Threshold

This is the criterion which allows elimination of artificial peaks. This is based on the comparison of the computed maximum with the middle of the chord joining the two inflection points on both sides of the maximum. If I_P is the peak intensity at the computed maximum, I_M is the intensity at the chord center, and T is the threshold. Peaks are accepted if:

$$I_P > I_M + T \times \sqrt{I_M}$$

If no treatment has been applied to the data and if it is X-ray powder diffraction data, the natural value for the threshold T is 1. The range is from 0 to 5.

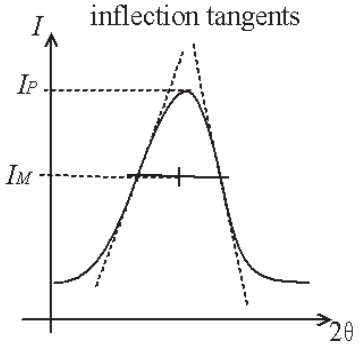


Fig.85: Definition of parameters used for the threshold filtering

Computing Areas

The area computations are performed on an interval between two points, called "entry points". These can be entered with the mouse. These are statistical computations assuming there is a unique peak in the interval. It supplies information about the position of the peak maximum and the net area of the peak. This is *not* a profile fitting. Dedicated software such as DIFFRAC.SUITE TOPAS should be used for this purpose.

Extremities of the Area computation: Left Angle and Right Angle

These are the angles (in °) of the scan point that are the closest from the entry points. The values typed in or determined by the mouse are rounded to match the recorded positions.

Intensities on Both Ends: Left Intensity and Right Intensity

The left and right background heights are given in cps. Each value is the average of the scan points around the entry points. The mean is computed on one to seven points. The number B of points involved in the average depends on the total number N data points included in the area selection:

N	B
$N < 10$	1
$10 \leq N < 20$	3
$20 \leq N < 30$	5
$N \geq 30$	7

The B values can be reduced if the selected interval is to be found on the left hand or right hand edge of the scan.

Peak Maximum: Obs. Max., Gross Int. and Net Height

The highest value in the interval may not be pertinent information due to the noise fluctuations. The position of the peak maximum is located by fitting a parabola through the points around the highest value, whose net heights are above 75% of the net observed maximum.

The position **Obs. Max.** of the peak maximum is given in scan unit (plus d in Å if the scan is a 2θ scan). The output gross height **Gross Int**. is the intensity of the summit of the fitting parabola, in cps. **Net Height** is the gross height minus the background intensity, which is determined by a linear background between the left and right extremities.

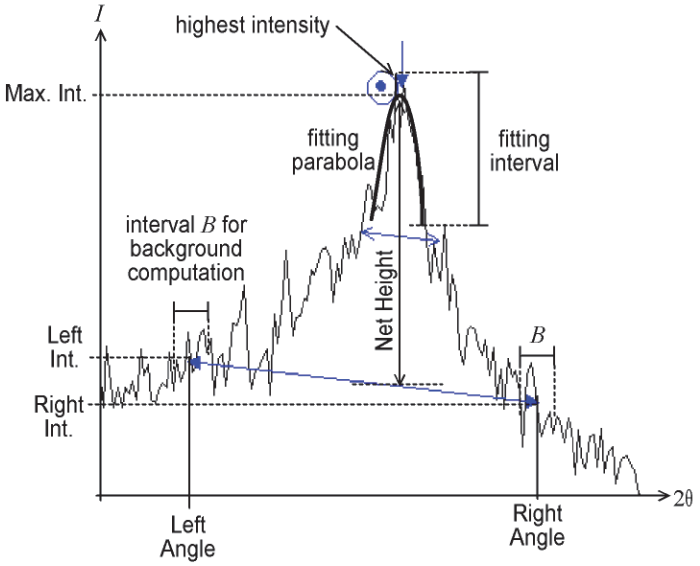


Fig.86: Determination of the background and maximum

Full Width at Half Maximum: FWHM

To compute the FWHM, EVA uses a line equidistant from the background line and the fitted maximum (peak maximum). This line is parallel to the computed background. The number of crossings between this line and the scan line is checked on both sides of the absolute maximum (highest intensity).
FWHM is output when the following conditions are filled:

- There are an odd number of crossings on the left- and right-hand sides of the observed maximum.
- The mean value of crossing points on the left- and right-hand sides must be at least one step away from the absolute maximum.

Chord Middle: Chord Mid.

This is the middle of the chord drawn between the mean values of the crossing points used to determine **FWHM** is another estimate for the peak location. It is given in scan unit and d (Å) if the scan is 2θ.

Integral Breadth (I. Breadth)

Given in scan unit. Integral breadth is, by definition, the net area (in cps×scan units) divided by the net height (in cps). It is the breadth of a rectangle having the same net height and the same surface as the peak.

Gravity Center (Gravity C.)

This is a third estimate for the peak location. It is the center of gravity of the net peak, i.e. the mean of each X position in the interval weighted by the net intensity. It is also given in d (Å) if the scan is 2θ.

Raw Area and Net Area

Computed with the trapeze method and given in cps×scan units (cps×degrees for angular scans).

EVA Stripping Method

The EVA stripping method assumes that the $K\alpha_1$ and $K\alpha_2$ line profiles are identical in shape and that both profiles are tied by a fixed intensity ratio r. If $\Delta\lambda$ is the wavelength difference between $K\alpha_1$ and $K\alpha_2$ radiations, the shift $\Delta 2\theta$ between the $K\alpha_1$ and $K\alpha_2$ profiles at the current 2θ angle can be computed with the Bragg's law (assuming $\Delta\lambda << \lambda$):

$$\Delta 2\theta = 2 \cdot \tan\theta \cdot \frac{\Delta\lambda}{\lambda}$$

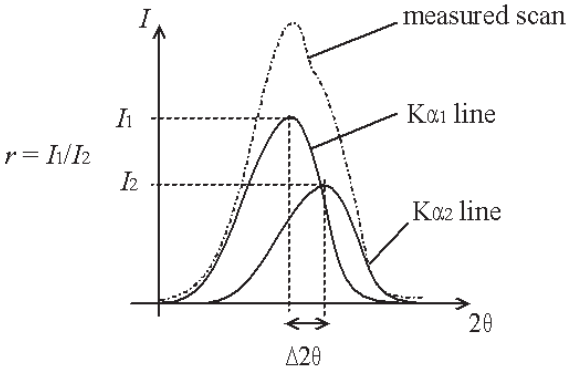


Fig.87: Superposition of the $K\alpha_1$ and $K\alpha_2$ diffracted intensities

As a result, the $K\alpha_1$ intensity can be computed from the measured intensity by subtracting the intensity of another point located at 2θ-$\Delta 2\theta$ and multiplied by r. The hypothesis is that the measurement is started in a background region in which the intensity is almost constant. Even when this hypothesis is false (the measurement was started on a peak), the errors are limited to the initial part of the diagram (about five times $\Delta 2\theta$).

This disadvantage is a result of the lack of a peak profile shape model. Due to statistical counting errors, subtracting a $K\alpha_2$ contribution which is too low or too high creates positive or negative artifacts. Using the Savitzky-Golay smoothing filter and Fourier expansion the creation of artifacts can be reduced dramatically.

Despite its disadvantages, the Rachinger method is very beneficial in performing a qualitative interpretation of a diagram. The quantitative interpretation examines whether a shoulder is a $K\alpha_2$ image or another peak. The implementation of this method may be beneficial before using profile fitting in order to find an initial solution for a complex problem (e.g. to detect the position of the peaks). Do not perform profile fitting on previously stripped data, because it may create artifacts.

To prepare data for crystallographic purposes (indexing, unit cell refinement, etc.) profile fitting is by far the most accurate method. If a profile-fitting program, such as TOPAS, is unavailable, $K\alpha 2$ stripping can be used prior to a peak search.

Do not use $K\alpha 2$ stripping to prepare search/match data. The $K\alpha_2$ shoulder could hide a small peak.

Chemical Balance

This appendix gives some additional details about the chemical balance (see section “Chemical balance: comparison with a chemical analysis” on page 143).

Format of the ASCII files

When the chemical analysis is not performed with a Bruker AXS XRF spectrometer under SPECTRA^{plus}, then the results must be stored in an ASCII file (text file). This text file can be typed by the user with a text editor (e.g. NOTEPAD.EXE) or a spreadsheet (e.g. EXCEL, but save the file in TXT format), or it can be created by the chemical analysis software and modified by the user if necessary.

The format must be the following:

- no header before the results list
- one element or compound per line
- on one line: element name or compound name + separator + concentration [+ separator + comments]

(The fields in bracket are optional.)

The valid format is described in the table below:

Field	Description
element name	Chemical symbol (e.g. C for carbon, Al for aluminum etc.)
compound name	In the simplest cases: write the compact formula (e.g. SiO2); more complex cases are described in appendix B.2 "Chemical formula translator"
separator	There are three valid separators: tabulation, equal sign '=', pipe (vertical bar) '|' It is possible to embed **all** the fields in double-quotes. In this case, any character (included a space) can be the separator.
concentration	There are three valid units (mass concentration only): • per one (i.e. write '0.5' for 50%): just write the value alone • percent: write the value and the percent sign ('%') • ppm: write the value and 'ppm' There can be a space but it is not mandatory between the value and the unit. The decimal separator can be a dot '.' or a comma ','.

Example of valid lines:

```
CaO | 0.40                (means "40% of calcium oxide")
"CaO" "0.40"
SiO2    60,0%             (the separator is a tabulation)
Ti=120ppm    comment      (the second separator is a tabulation)
```

Chemical formula translator

The compound formulas are used to translate the compound concentrations into elemental concentrations. This applies to the formula written in the PDF patterns and may apply to the compounds measured by chemical analysis.

In the simplest case, the compact formula is given: an element is present only once, and the number of atoms of its type in the molecule or cell is written after the chemical symbol (e.g. Al2O3 for alumina).

But the formula can also be given with more complex formulas, especially when it is made of several constituents. Here are some examples.

Pattern 00-041-1985

Formula: $C_7H_9CdN_5NiO \cdot 0.25(CH_3NHCH_2CH_2OH) \cdot 0.25[(CH_3)_3C_6H_3]$

$/Cd(CH_3NHCH_2CH_2OH)Ni(CN)_4 \cdot 0.25(CH_3NHCH_2CH_2OH) \cdot 0.25[(CH_3)_3C_6H_3]$

Translation:

Z	Element	Number of atoms in the molecule/cell	Weight % (to be multiplied by the concentration of the compound)
1	H	14.25	3.599
6	C	10	30.09
7	N	5.25	18.43
8	O	1.25	5.011
28	Ni	1	14.71
48	Cd	1	28.17

Comments:

- The alternate formula, given after the "/", is not taken into account. Alternate formulas may be available in PDF-2 but not in PDF-4.
- The centered points "·" are separators between individual constituents.

Pattern 00-043-0038

Formula: $[(C_3H_7)_4N]_{2x}Fe_{2-x}PO_4 \cdot zH_2O$

Translation:

Z	Element	Number of atoms in the molecule/cell	Weight % (to be multiplied by the concentration of the compound)
1	H	0.58 (56x+2z)	0.2784
6	C	0.24 (24x)	1.373
7	N	0.02 (2x)	0.1334
8	O	4.01 (4+z)	30.55
15	P	1	14.75
26	Fe	1.99 (2-x)	52.92

Comments:

x and z are arbitrarily replaced by 0.01.

Multiple levels of brackets are supported.

Pattern 00-052-1576

Formula: $(Ba,K,Pb,Na)_4(Y,Ca,Ln)_2[Si_8B_2(B,Si)_2O_{28}F]$

Translation:

Z	Element	Number of atoms in the molecule/cell	Weight % (to be multiplied by the concentration of the compound)
5	B	3	2.438
8	O	28	33.68
11	Na	1	1.728
14	Si	9	19
19	K	1	2.939
20	Ca	0.6667	2.009
39	Y	0.6667	4.456
56	Ba	1	10.32
57	La	0.04762	0.4973
58	Ce	0.04762	0.5016
59	Pr	0.04762	0.5044
60	Nd	0.04762	0.5163
62	Sm	0.04762	0.5382
63	Eu	0.04762	0.544
64	Gd	0.04762	0.5629
65	Tb	0.04762	0.5689
66	Dy	0.04762	0.5817
67	Ho	0.04762	0.5904
68	Er	0.04762	0.5987
69	Tm	0.04762	0.6047
70	Yb	0.04762	0.6194
71	Lu	0.04762	0.6263
82	Pb	1	15.57

Comments:

- When the elements are separated by commas, such as in `(Ba,K,Pb,Na)`, the translator gives the same atomic fraction to all of the elements. In this case, 0.25.
- Ln (undefined lanthanide or actinide) is distributed in equal fractions to the 14 lanthanides and actinides (Pm is not included in the list since it does not exist in nature), i.e. 0.07. In this case, there are 0.3333 atoms of lanthanides in the constituent and twice the constituent in the molecule/cell which equals 0.04762 atom of each lanthanide.

AbsorbDX

Mass Attenuation Coefficient

The mass attenuation coefficient for an element i depends on the wavelength λ of the X radiation. Let us consider the attenuation due to the photoelectric effect, the elastic scattering by Rayleigh effect and the inelastic scattering by Compton effect. The mass attenuation coefficient μ_i for the element i can thus be decomposed in three coefficients:

$$\mu_i = \mu_i^{pe} + \mu_i^R + \mu_i^C$$

where μ_i^{pe} is the absorption coefficient by photoelectric effect, μ_i^R the attenuation by Rayleigh dispersion and μ_i^C stands for the Compton effect.

Absorption by Photoelectric Effect

If the energy of a photon $E = h\nu$ is equal or higher to the ionization energy of a level of the atom. The photon can be absorbed, ejecting an electron of this level.

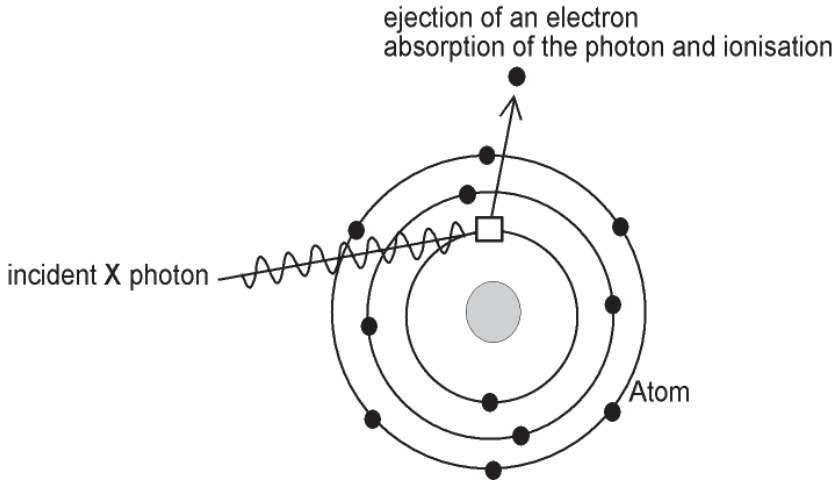


Fig.88: X-ray absorption by photoelectric effect

If the energy of a photon is lower than the energy of ionization of a given electronic level, then the photon is not affected by these electrons. Thus, there is a discontinuity of the absorption spectrum $\mu_i^{pe}(\lambda)$ for the wavelength corresponding to the ionization energy; the absorption is lower for the wavelength slightly higher than the one corresponding to the discontinuity. Between two discontinuities, the higher the wavelength (the lower the energy), the higher the absorption (the cross section of interaction of a photon grows the wavelength). Between two discontinuities, $\mu_i^{pe}(\lambda)$ follows the Bragg-Pierce empirical law:

$$\mu_i^{pe} = k \cdot Z^4 \cdot \lambda^3$$

where k is a constant which depends on the level of the ejected electron (K, $L1$, $L2$, $L3$...), and Z is the atomic number of the atom i.

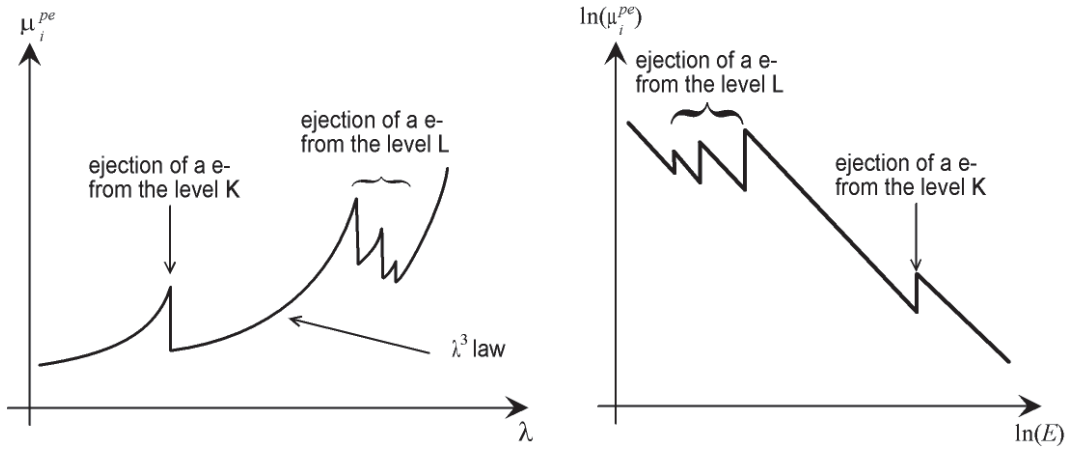


Fig.89: Bragg-Pierce empirical law

Attenuation by Elastic Scattering

The X-rays are scattered by single atoms; we consider here only the elastic scattering, i.e. the photon does not lose energy during the interaction, also called Rayleigh[6] diffusion. The interference of the X-rays scattered by a huge amount of atoms give information on the spatial arrangement of these atoms (crystallographic characterization by X-ray diffraction) – this effect is given by the term I_1 in the section Attenuation Formula.

But if we consider the individual atoms, this scattering creates a dispersion of the beam and thus a loss of intensity in a given direction.

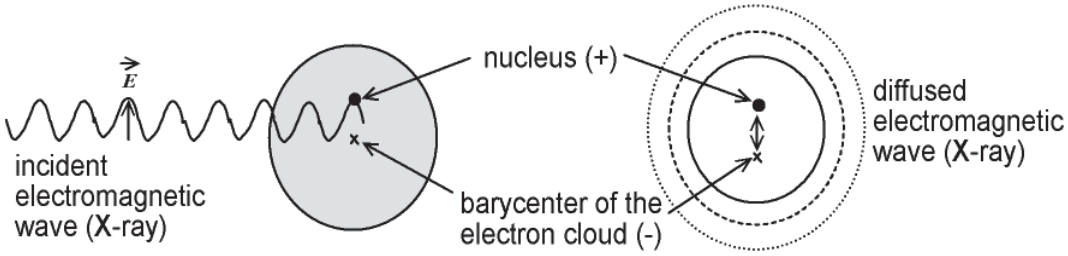


Fig.90: X-ray attenuation by elastic scattering — oscillating dipole, model of the elastically bound electron

The semi-classical model of the elastically-bound electron, which is used for the calculation of this effect, is not accurate near the absorption edges (because of the resonance of fine structures[7] and electron-hole interactions), nor for photons which energy is below 50 eV (because the scattering then involves valence orbitals or bands which are dependent on the structure and chemical bounds).

6 John William STRUTT Lord RAYLEIGH (1842-1919), Nobel prize in 1904

7 this effect is used in *EXAFS*: (extended X-ray absorption fine structure)

Attenuation by Inelastic Scattering

The X-photon can be inelastically diffused, i.e. it loses a part of its energy in the process (it is diffused with a bigger wavelength). This is the Compton[8] Effect: the photon ejects a peripheral electron, which is weakly bound to the nucleus. This mainly happen on high-Z atoms (the peripheral electrons are far from the nucleus, and the core electrons mask the charge of the nucleus).

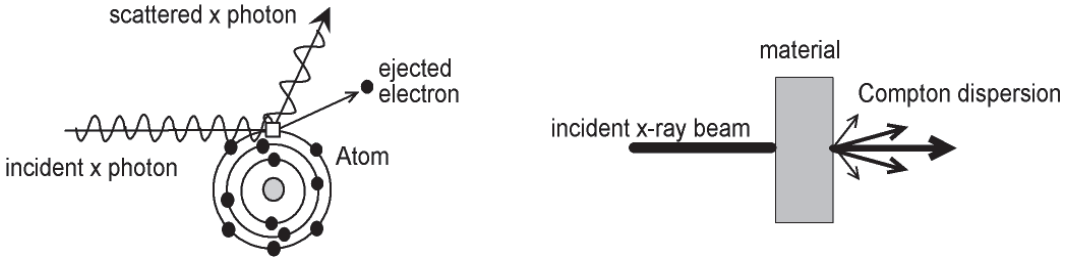


Fig.91: Compton Effect — collision between an X photon and a weakly bound electron

Attenuation Calculation

A monochromatic X radiation with a wavelength λ (and an energy E) hits a solid target with intensity I_0. Let us consider the contribution to the whole signal of a thin layer at the distance x under the surface of the sample. Before arriving on an elementary volume dV of this layer, the beam is attenuated; the attenuation depends on the path length and thus on the incidence angle ψ_1:

$$d^3I = \frac{I_0}{\sin\psi_1}\exp\left(-\mu\cdot\rho\cdot\frac{x}{\sin\psi_1}\right)\cdot dV$$

where μ is the attenuation coefficient for the wavelength λ, and ρ is the specific mass of the material. The coefficient $1/\sin\psi_1$ for I_0 comes from the spreading of the beam: the lower the angle ψ_1 (grazing), the wider is the irradiated surface for a given solid angle of the beam, so the lower is the surface density of received energy.

The scattered X-rays, which have the same wavelength, must travel through the sample towards the detector, with an angle ψ_2; thus:

$$d^3I' = d^3I\cdot F\cdot\exp\left(-\mu\cdot\rho\cdot\frac{x}{\sin\psi_2}\right)\cdot dV$$

where F is the scattering factor. Thus,

$$d^3I' = \frac{I_0}{\sin\psi_1}\cdot F\cdot\exp\left(-\mu\cdot\rho\cdot x\cdot\left(\frac{1}{\sin\psi_1}+\frac{1}{\sin\psi_2}\right)\right)\cdot dV$$

The integration on x for a sample which thickness is d gives:

$$I = \frac{I_0}{\sin\psi_1}\cdot F\cdot\frac{1-e^{-\beta\cdot\rho\cdot d}}{\beta}\cdot S = I_1\cdot\left(1-e^{-\beta\cdot\rho\cdot d}\right)$$

where S is the cross section of the beam (we assume the density of energy of the beam is uniform), I_1 is the intensity collected by the detector on a semi-infinite sample (infinite thickness), and

$$\beta = \frac{1}{\sin\psi_1}+\frac{1}{\sin\psi_2}$$

8 Arthur Holly COMPTON (1892-1962), Nobel prize in 1927

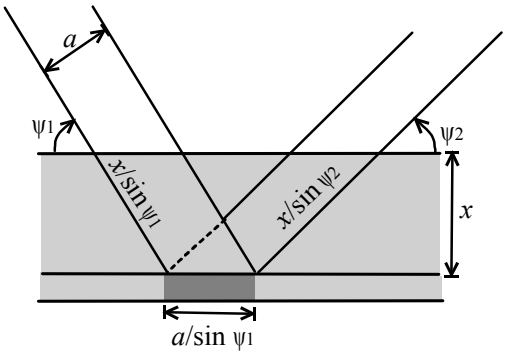


Fig.92: Absorption along the path

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Index