
XRD DIFFRAC.EVA: Quick Start Guide

Introduction

This guide is a quick introduction to the DIFFRAC.EVA software and how to use the program to solve crystalline phase identification. For detailed information and an in-depth guide refer to DIFFRAC.EVALUATION User Guide & Tutorial available in hard copy in the XRD lab or online in Cumulus.

Part 1: Opening Diffractogram in DIFFRAC.EVA

To open a diffractogram for evaluation:

1. Click **File > Import Scan** (*Figure 1*).
2. Select the Scan you want to open.
3. Click **Open**.
4. The Scan is now open and ready for evaluation.

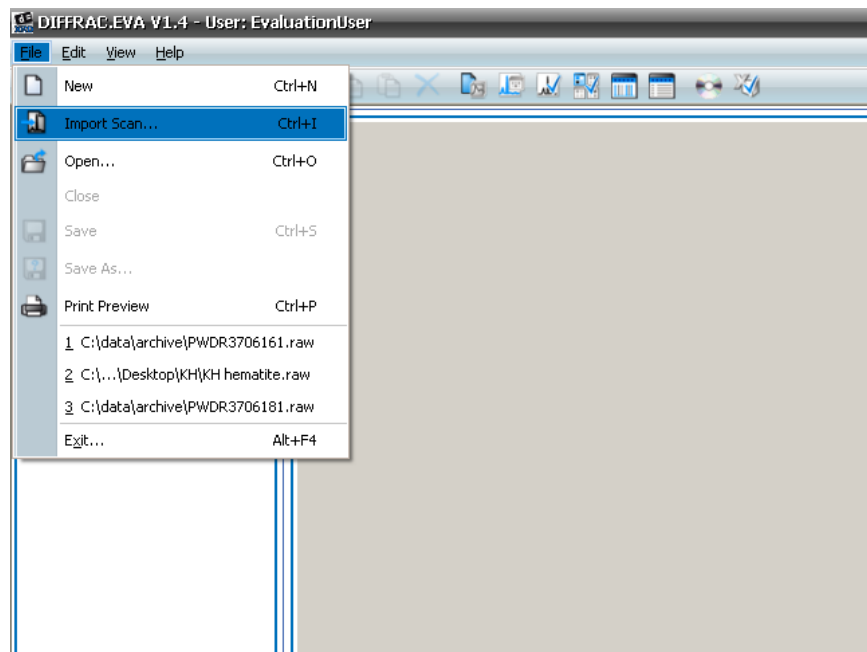


Figure 1. Open Scan.

Getting Acquainted

The DIFFRAC.EVA main screen has the following primary functional areas (*Figure 2*):

1. Toolbar
2. Data Command Panel
3. View Command Panel
4. View Window
5. Data/View Tree Panel

It is useful to have the **Data Command Panel** and **Data Tree Panel** open for view at all times (use the icons in the toolbar to open/close these views).

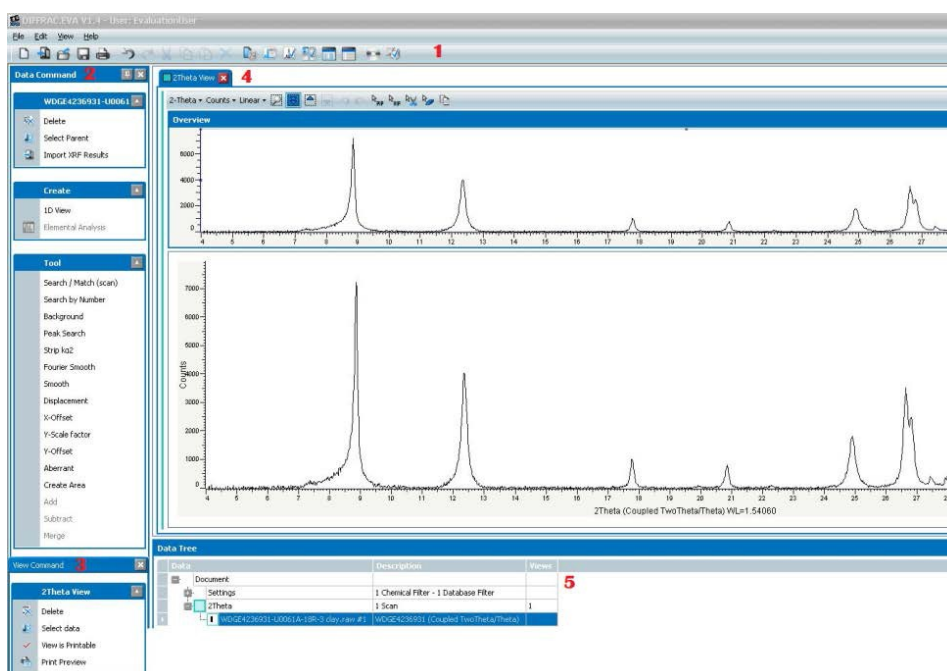


Figure 2. DIFFRAC.EVA Control Panel.

Part 2: Removing the Background

The first step in preparing a scan for search/match phase identification is to subtract the background (*Figure 3*). There are two methods for removing the background: a traditional method and an enhanced method.

Traditional method: is recommended for all scans; it gives an arc parabola but never submerges a complete peak.

Enhanced method: gives a smooth curve where some peaks may be under the background curve. This could be useful for crystallographic studies. See the EVA manual for greater detail.

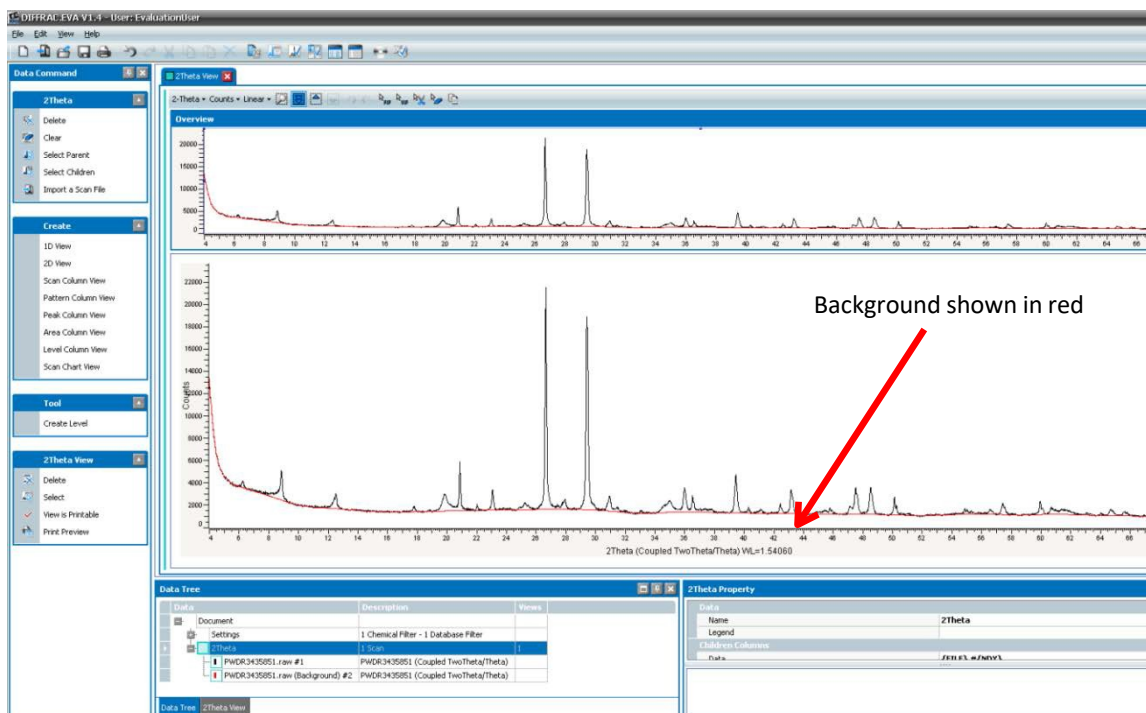


Figure 3. Background Highlighted.

1. Select **Data Command Panel > Tools > Background** to open the Background dialog box (*Figure 4*).
2. If needed, use the slider to adjust the curvature on background humps.
3. In the drop-down box, select **Background subtracted** option.
4. Close text box.

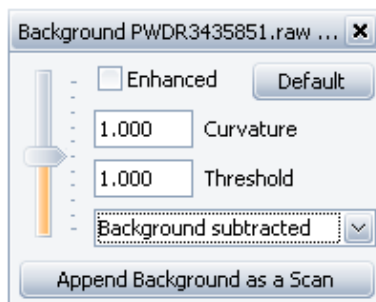


Figure 4. Background Dialog Box.

Part 3: Search Match

The Search Match tool attempts to match XRD scans with patterns found in the ICDD (International Centre for Diffraction Data) PDF database. The Search Match process tries to identify an unknown scan based on pattern recognition techniques. EVA can also find a reference pattern by its name or ICDD number.

Note: It is at the user's discretion to identify and choose the correct pattern matches.

1. Select **Search/Match (scan)** from **Data Command Panel > Tools**. Notice the Search/Match dialog box

has four tabs (*Figure 5*):

- Chemical Filter
 - Database Filter
 - Candidate List
 - Selected Candidates
2. Select desired search parameters (see suggestions below; *Figures 6, 7, 8*).
 3. Once the desired parameters are selected, click **Rebuild** to rebuild the database for your selections. After the database is rebuilt, click back onto **Candidate List** and click **Match**.

Search/Match Screen

In the *Criterion* field of the Candidate List Tab (*Figure 5*), begin the search with **2: Neutral**.

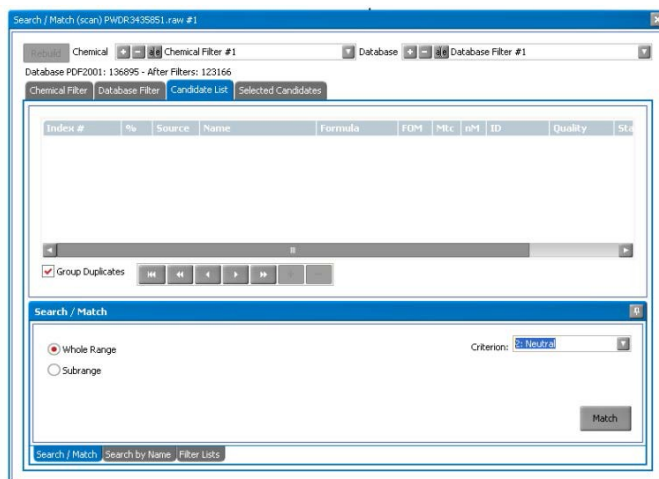


Figure 5. Search/Match Screen.

Chemical Filter Tab

A chemical filter can be set for any element in the periodic table (*Figure 6*).

- Green** = element is mandatory
- Red** = must be absent
- Blue** = at least one of the elements in blue must be present in the search result
- Gray** = not checked (absent or present)

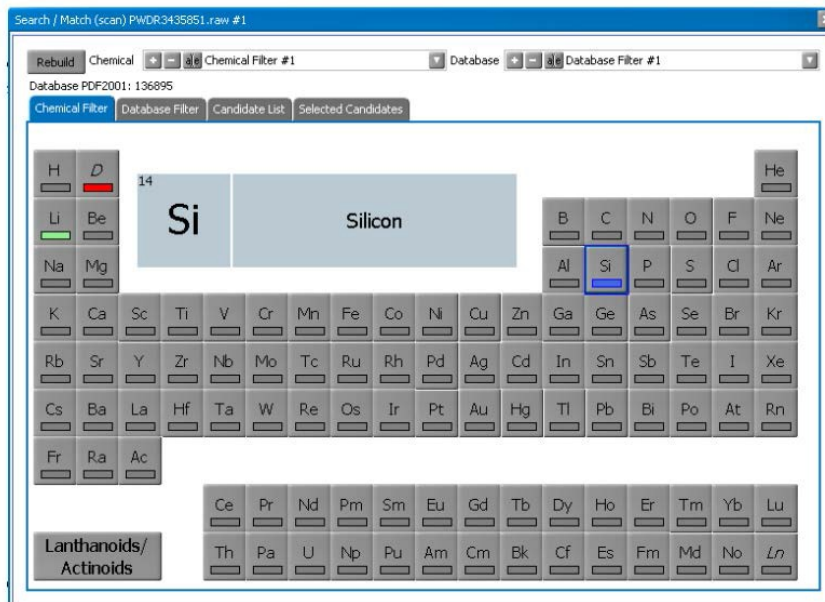


Figure 6. Chemical Filter Tab.

Database Filter Tab

Search/Match can be enhanced using database filters such as the following (*Figure 7*):

- Quality Marks:** degrees of pattern quality assigned by ICDD (recommended: *, Calculated, Indexed).
- Status:** recommended: Primary.
- Colors:** select the color of the mineral to be searched.
- Sources:** database section: select both.
- Subfiles:** select the group of patterns to be searched, for example, inorganics, zeolites, minerals, etc.
- Element # in Formula:** choose the minimum/maximum number of elements considered in the formula.
- Density:** enter a minimum/maximum density for the mineral being searched.

Filter	Value	Candidates
<input checked="" type="checkbox"/> Skip Non Ambient		126519
<input checked="" type="checkbox"/> Quality Marks		
<input type="checkbox"/> Blank		31798
<input type="checkbox"/> Low precision		17263
<input checked="" type="checkbox"/> Indexed		21944
<input checked="" type="checkbox"/> Star (*)		11901
<input checked="" type="checkbox"/> Calculated		53580
<input type="checkbox"/> Rietveld		404
<input type="checkbox"/> Quality Unknown		5
<input checked="" type="checkbox"/> Status		
<input checked="" type="checkbox"/> Colors		
<input checked="" type="checkbox"/> Sources		
<input checked="" type="checkbox"/> Subfiles		
<input checked="" type="checkbox"/> Element # in Formula		
<input checked="" type="checkbox"/> Density		

Figure 7. Database Filter Tab.

Candidate List Tab

Expand the table to see important information on the candidate (**Figure 8**), including

- Mtc**: number of reference pattern lines matching the unknown
- FOM**: Figure of Merit – a lower number is a better match
- Index #**: rank number of the pattern

Index #	No.	Source	Name	Formula	FOM	Mtc	IPR	ID	Quality	Status	I/Factor	Mineral
1	6	PDF2001	Polythionite-3T	K (Al Fe U) (Si Al) O10 (O H) F	2.91	15	1	PDF 43-1379	Star (*)	Primary	13.8	True
2	9	PDF2001	Polythionite-3T	K (U, Al)3 (Si, Al)4 O10	3.67	33	7	PDF 42-0612	Indexed	Primary		True
3	6	PDF2001	Polythionite-2M#1	K (U, Al)3 (Si, Al)4 O10 (F, O H)2	3.72	35	9	PDF 24-0594	Blank	Primary		True
4	6	PDF2001	Zirconolite-1M	K Al (Fe U) (Si Al) O10 F2	4.00	15	3	PDF 41-1462	Indexed	Deleted	13.8	True
5	27	PDF2001	Lithium Potassium Magnesium Nickel Fluoride Silicate	K U Mg Ni Si4 O10 F2	4.11	25	4	PDF 51-0046	Indexed	Primary		False
6	10	PDF2001	Trithionite-2M#2	K U (Al, U)2 (Si Al) O10 F2	4.30	30	10	PDF 43-0692	Indexed	Primary		True
7	29	PDF2001	Lithium Potassium Nickel Fluoride Silicate	K U Ni2 Si4 O10 F2	4.45	22	6	PDF 51-0047	Indexed	Primary		False

Figure 8. Candidate List Tab.

Part 4: Residual Scan – searching the minor phases

Minor phases are often difficult to identify because the patterns of the major peaks are higher on the list. Using the **Residue** tool will exclude the already matched patterns and increase the weight of the minor phases.

1. In **Search/Match** (scan) screen, choose the **Selected Candidates** tab.
2. Select the pattern you wish to exclude in your next search.
3. Select the **Residue** tool.
4. Adjust the width of the zone to exclude around the pattern peaks.
5. Click **Apply**.
6. Click back onto **Candidate List Tab** and click **Match**.
7. The candidates for the residual scan are listed in **Candidate List**

In addition, you can ‘cut’ the peaks out that you do not want included in a Search/Match.

1. Select the **Scissors** tool from the View Window toolbar.
2. Cut the peaks that you wish to exclude from the Search/Match.
3. Under **Search/Match** (scan) box, in the **Candidate List** tab, select **Match**.
4. The program will search the peaks left uncut.
5. To undo the cuts click the **Undo Arrow**.

Part 5: Peak Search

Peak Search detects peaks automatically and is useful for phases not identified with Search/Match or to export the pattern to another program.

1. Select the scan in the data tree.
2. Click **Peak Search** in the Tool List of the **Data Command Panel**. The **Peak Search** dialog box is displayed.
3. Move the slider to select the peaks you desire (*Figure 9*).
4. Once you are satisfied, click **Make Dif** to create a DIF pattern. The pattern list is created in the Data Tree and can be Search/Matched.
5. To select specific peaks click **Append to List** and a peak list is created in the Data Tree (*Figure 10*).
6. Highlight the peaks you want and click **Search/Match** (peak list) under Tool or **Make DIF Pattern** (which you can export to another program).

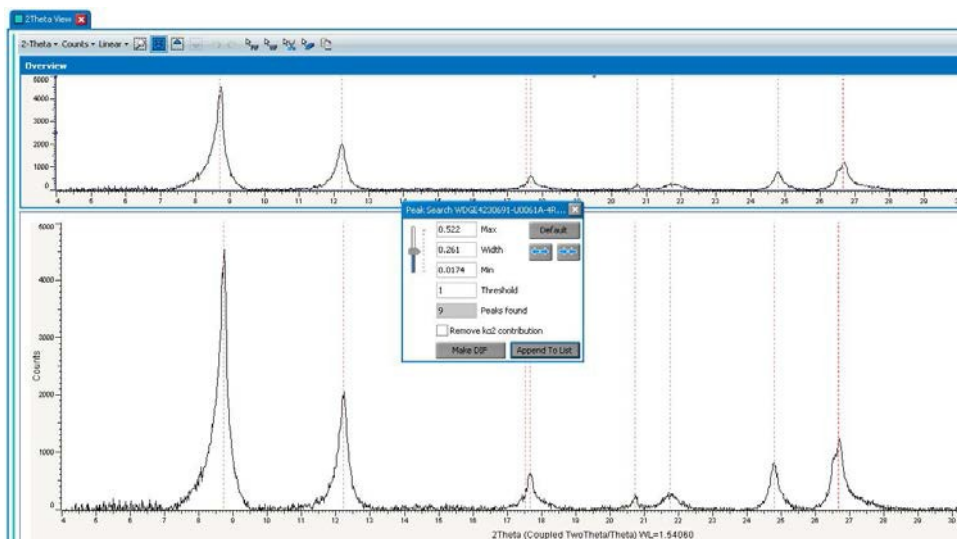


Figure 9. Peak Search.

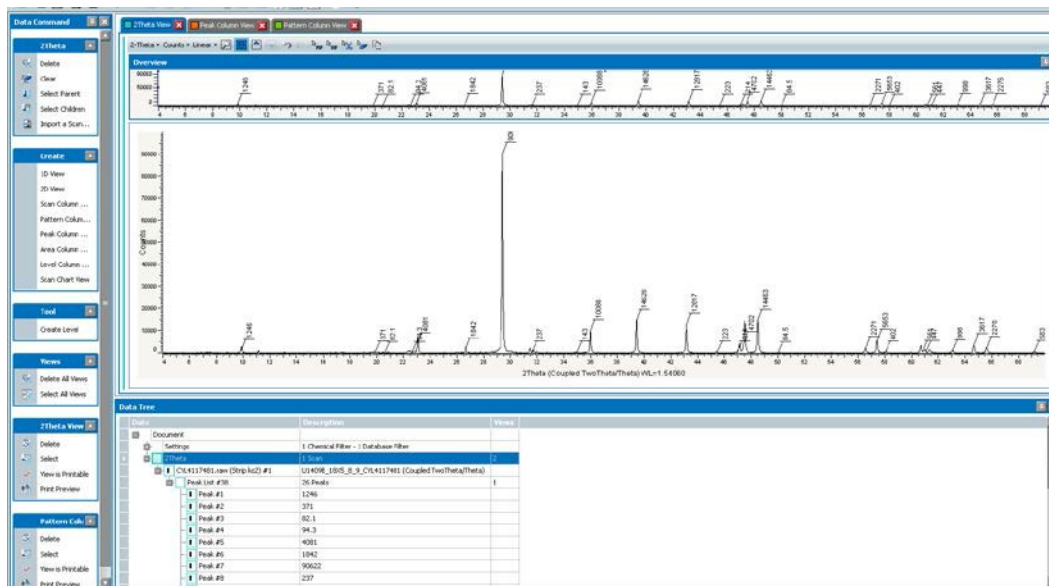
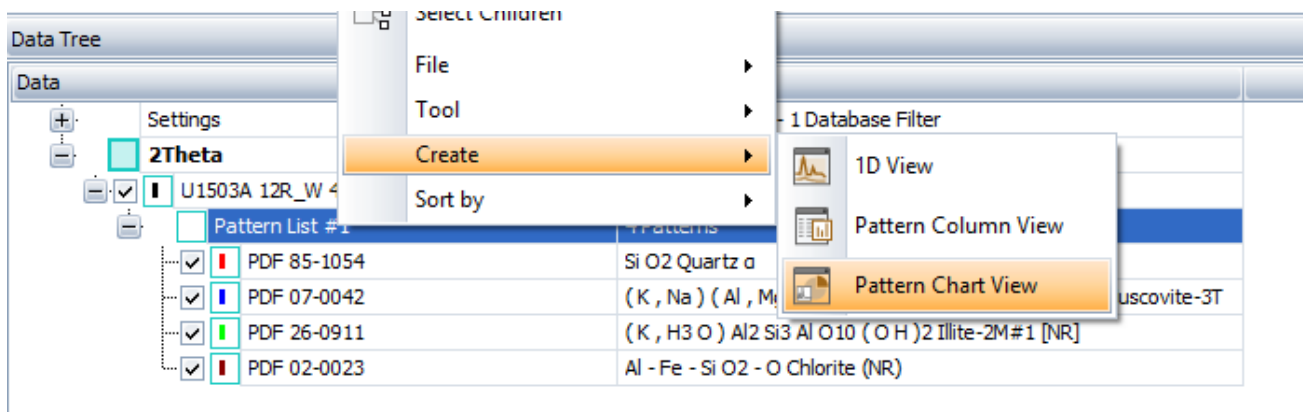


Figure 10. Peak Search with Append List.

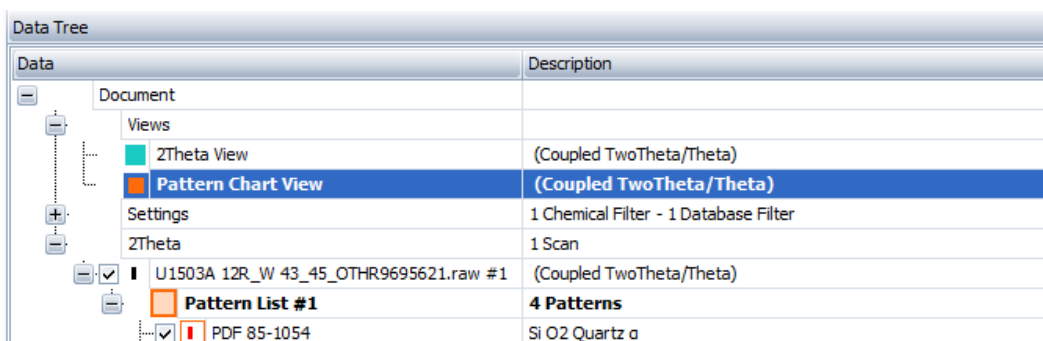
Part 6: Semi-Quantitative Analysis

Get an estimate of the percentage of each mineral in the scan by generating a Semi-Quantitative pie chart. EVA does this by using the relative intensities of the mineral peaks. For results to be as accurate as possible identify all phases in the diffractogram and that each mineral has an 'I/Icor' value.

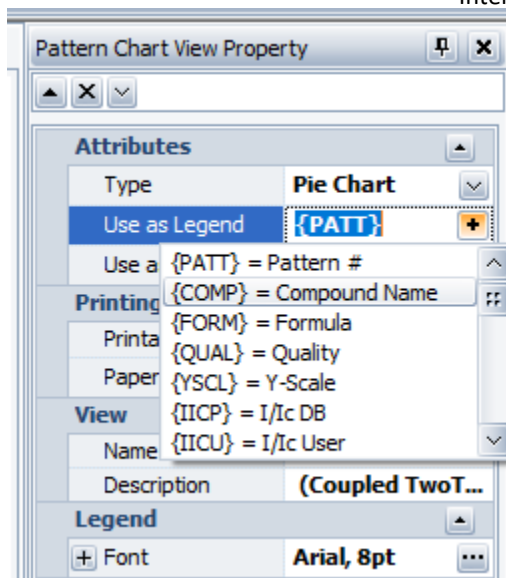
1. In the 'Data Tree' Panel right click on 'Pattern List' and select 'Create' > 'Pattern Chart View'. Again make sure all mineral phases have both been identified and have an I/Icor value before doing this.



2. A new tab with a pie chart indicating the percentages of present minerals appears. S-Q indicates 'Semi-Quantitative'.
3. Change the pie chart labels by selecting 'Pattern Chart View' in the Data Tree Panel under 'Views'



4. On the right hand side of the screen in the 'Pattern Chart Property View' Panel click on the '+' button next to 'Use as Legend'. This brings up all the legend options. Multiple components can be added.



5. Update the pie chart to show the new legend by selecting on the view again or on another scan.

Part 6: Printing in EVA

You can print any of the views in EVA.

Print Preview allows you to enter header and footers onto your print out, in addition to editing axis and labels.

You can also **Export** the print preview as an image *.PNG file or as a pdf.