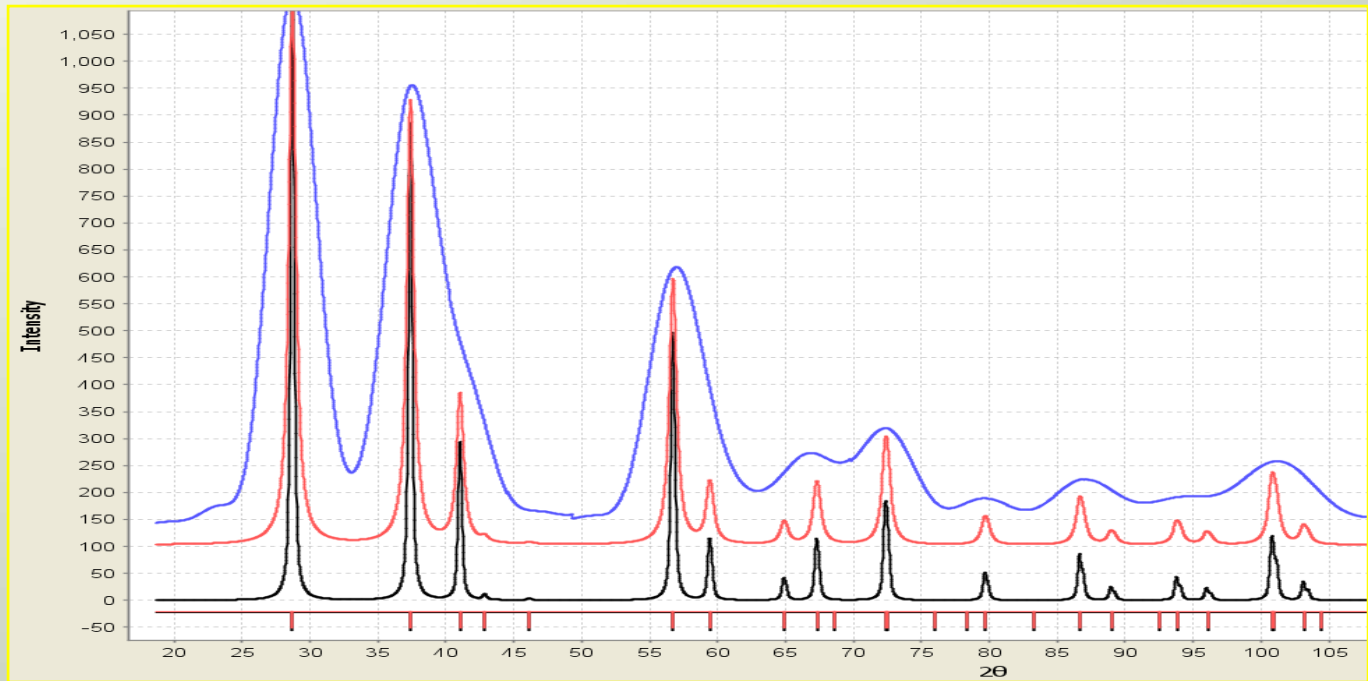


Digital Pattern Simulations

Pattern Simulations



Pattern Simulations

What?

Digital powder patterns can be calculated for all entries in the Powder Diffraction File.

Multiple patterns can be plotted to simulate experimental data.

Pattern Simulations

Why?

Digital pattern calculations can be varied to account for instrumental and experimental conditions normally present in a diffraction experiment.

By using digital patterns, reference data can be adjusted to more closely simulate experimental data for either phase identification or quantitative analysis.

Pattern Simulations

How?

The Powder Diffraction File (PDF) contains 3 basic types of data. Therefore, the simulations use 3 different algorithms to calculate a digital pattern from each type. In the PDF, the software automatically elects the appropriate algorithm based on the information available from the entry data.

Each algorithm can be adjusted for common experimental and instrumental factors.

Pattern Simulations

From Main Menu

Select “**Edit**” from the Tool Bar.

Use drag down menu to select “**Preferences**”.

Select “**Diffraction**” from the Preferences drag down menu.

Select either “**Experimental**” or “**Calculated**”.

This changes all experimental or calculated patterns in a simulation.

From a PDF Entry

Select either “**Experimental Diffraction Pattern** or **Calculated Diffraction Pattern**” from the Tool Bar.

This will produce a digital pattern for the *selected PDF entry*.

Select “**Edit**” from the Tool Bar of the pattern.

Select “**Preferences**” from the Edit drag down menu.

This changes only the selected pattern in the simulation.

From a PDF Entry

PDF Card - 04-003-1024

File Edit d-Spacings Tools Window Help

Wavelength: Cu Kα1 1.54056Å

Intensity: Fixed Slit Variable Slit Integrated

2θ	d(Å)	I	h	k	l
28.6797	3.110070	999	1	1	0
37.3549	2.405320	490	1	0	1
41.0068	2.199150	92	2	0	0
42.8151	2.110360	126	1	1	1
46.1089	1.966980	44	2	1	0
56.6654	1.623040	466	2	1	1
59.3853	1.555030	129	2	2	0
64.8534	1.436500	56	0	0	2

PDF #: 04-003-1024 Status: Primary QM: Star (5)

Pressure/Temperature: Ambient

Chemical Formula: MnO₂

Weight %: Mn63.19 O36.81

Atomic %: Mn33.33 O66.67

ANX: _____

Compound Name: Manganese Oxide

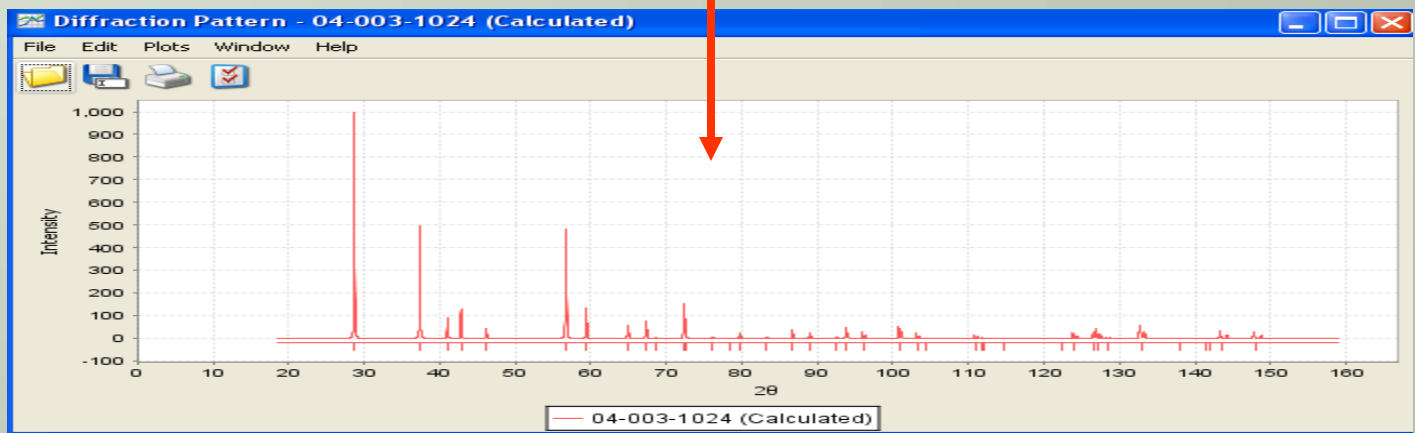
Mineral Name: _____

Common Name: manganese(IV) oxide



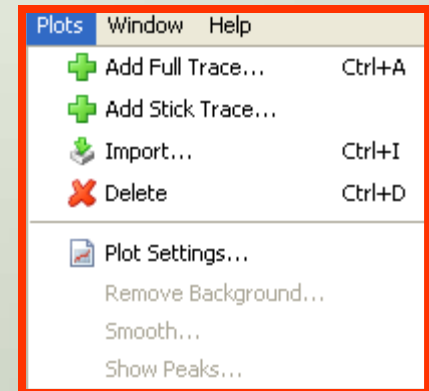
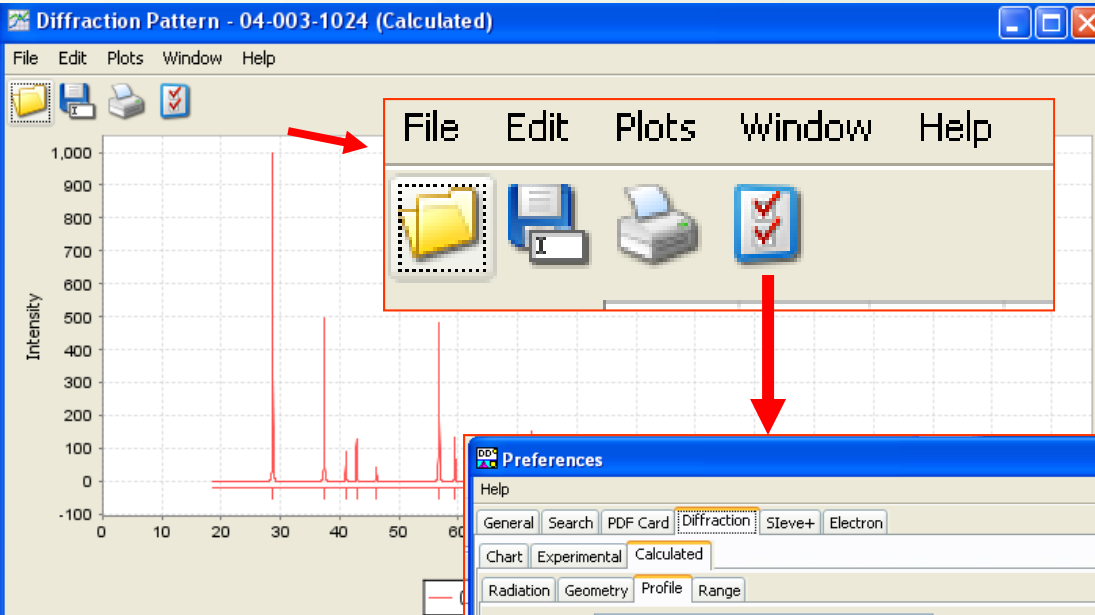
From an entry, select the Graph icon.

This will produce a digital diffraction pattern using default settings.

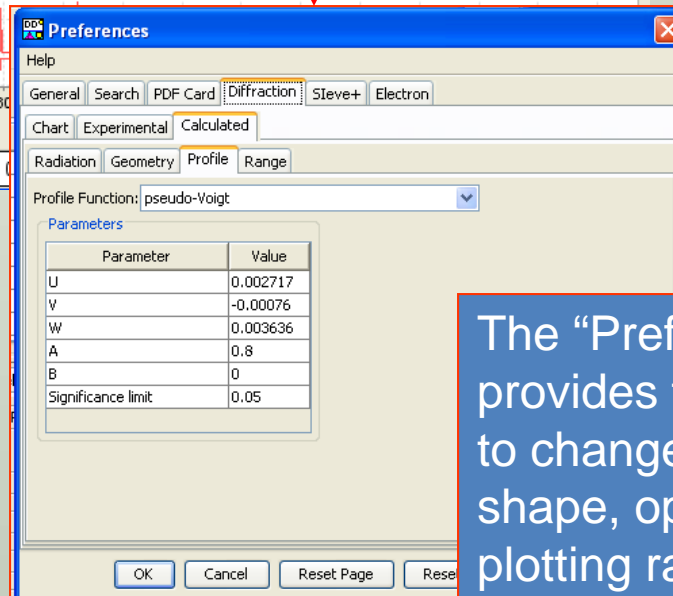


Digital Pattern Toolbar

Custom Settings



The "Plots" Menu lets you Add or Delete additional patterns and change their settings (color, scale, etc.).



The "Preferences" Menu provides the user with options to change wavelength, peak shape, optical geometry and plotting range.

Pattern Simulations From an Entry

Options for the addition of multiple phases, instrument and specimen factors, wavelengths. Options for import/export and graphic display calculations.

PDF Card - 04-003-1024

File Edit d-Spacings Tools Help

d-Spacings

Wavelength: Cu Ka1 1.54056Å

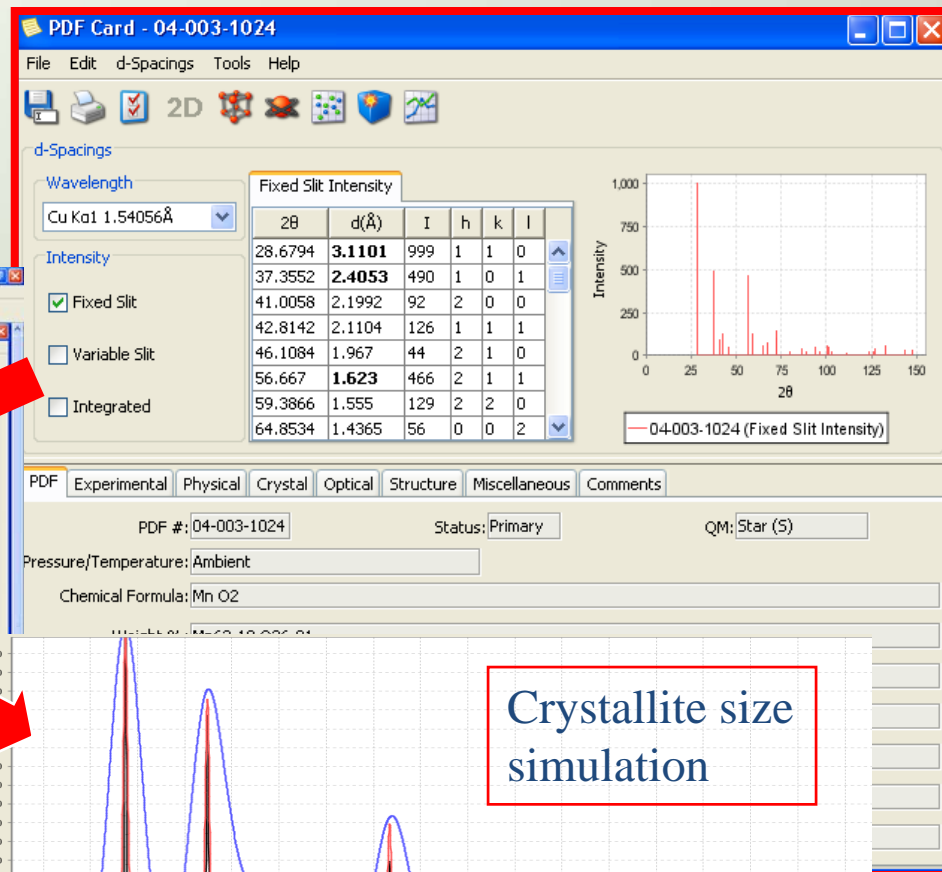
2θ	d(Å)	I	h	k	l
28.6794	3.1101	999	1	1	0
37.3552	2.4053	490	1	0	1
41.0058	2.1992	92	2	0	0
42.8142	2.1104	126	1	1	1
46.1084	1.967	44	2	1	0
56.667	1.623	466	2	1	1
59.3866	1.555	129	2	2	0
64.8534	1.4365	56	0	0	2

Intensity: Fixed Slit, Variable Slit, Integrated

PDF #: 04-003-1024 Status: Primary QM: Star (5)

Pressure/Temperature: Ambient

Chemical Formula: Mn O2



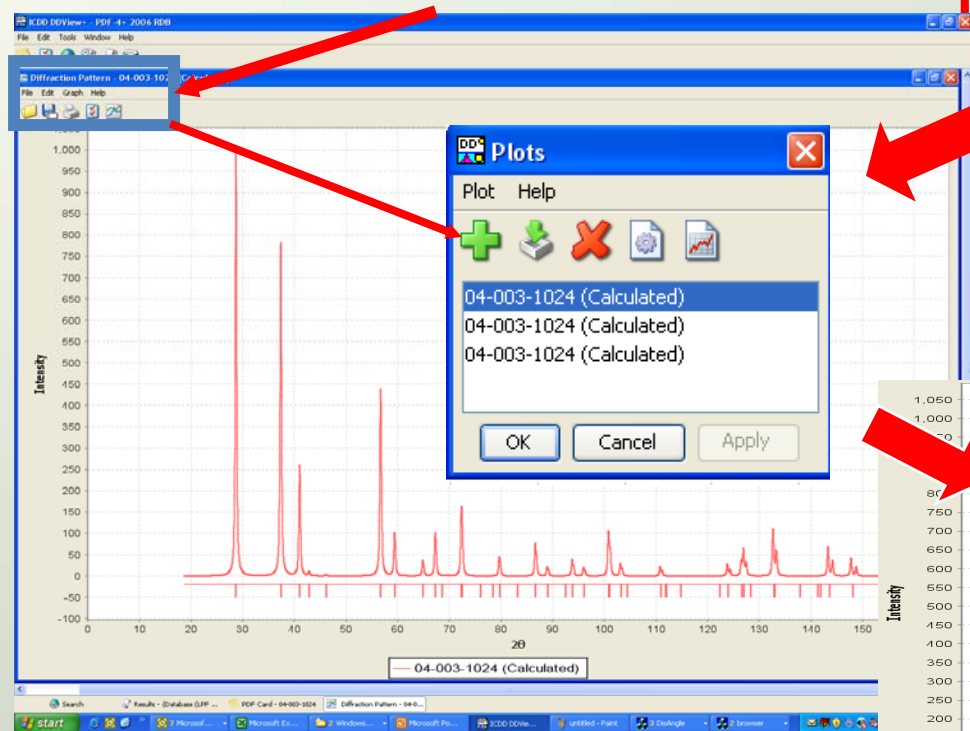
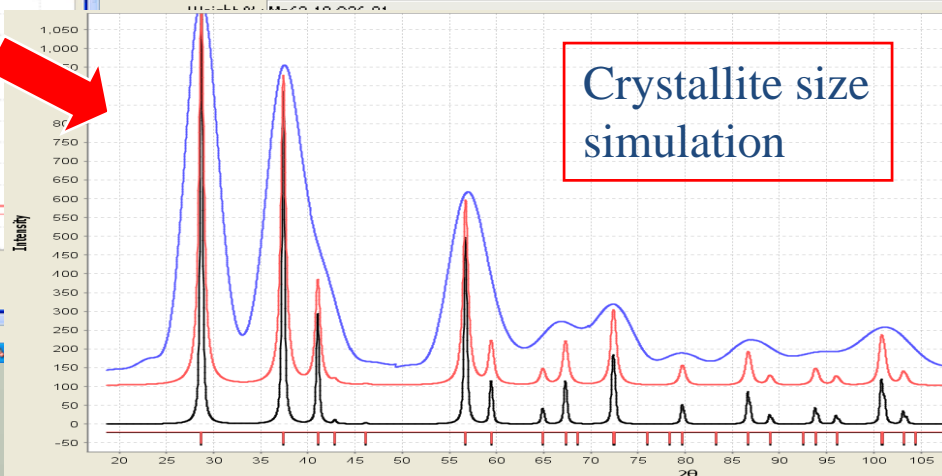
ICDD DDView - PDF 4- 2006.R06

Diffraction Pattern - 04-003-1024

Intensity vs 2θ plot showing experimental data (red) and calculated pattern (black).

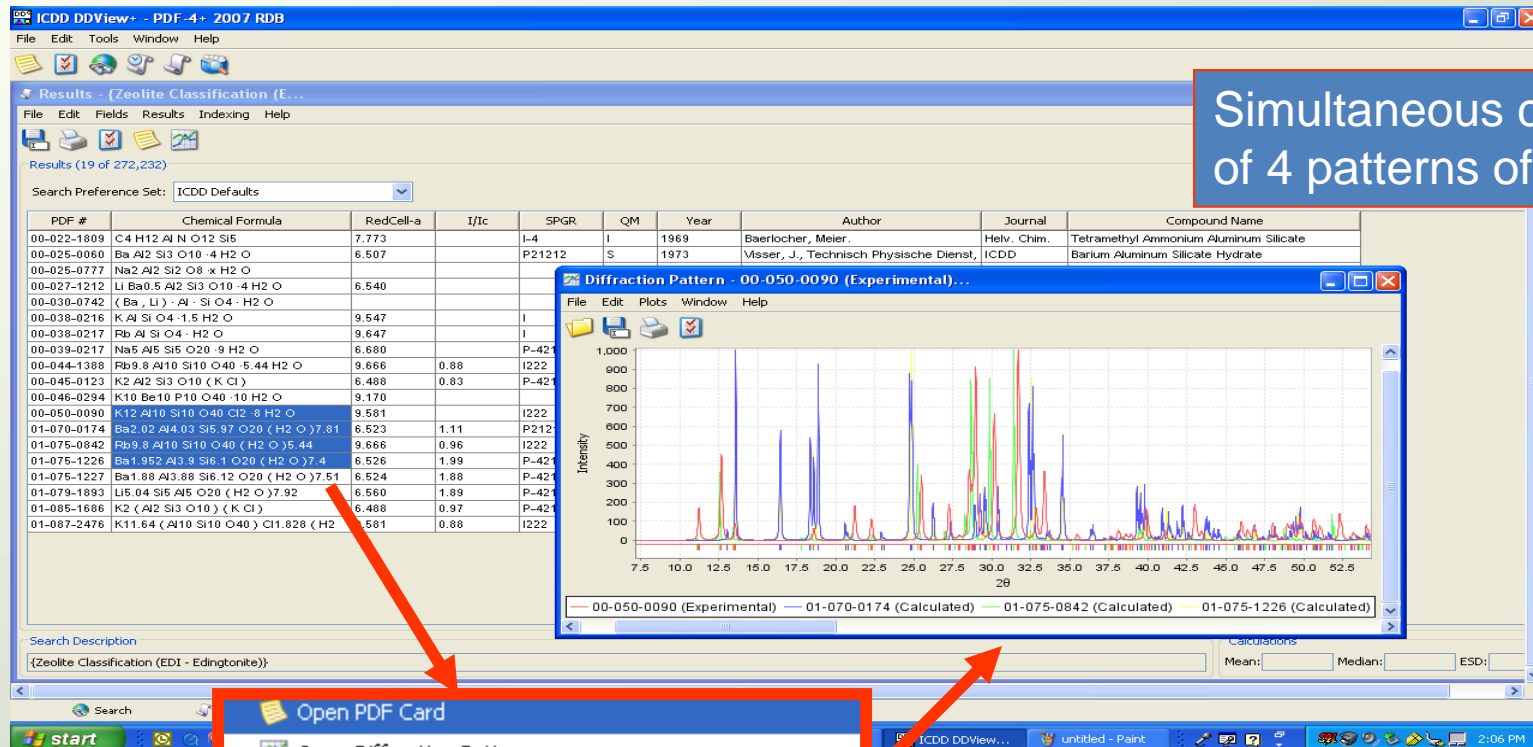
Plots dialog box:

- Plot Help
- Buttons: + (Add), - (Remove), X (Delete), [Icon], [Icon]
- List: 04-003-1024 (Calculated), 04-003-1024 (Calculated), 04-003-1024 (Calculated)
- Buttons: OK, Cancel, Apply

Multi-Pattern Simulations

From the Results Form



ICDD DDView+ - PDF-4+ 2007 RDB

Results - (Zeolite Classification (E...))

Search Preference Set: ICDD Defaults

PDF #	Chemical Formula	RedCell-a	I/Ic	SPGR	QM	Year	Author	Journal	Compound Name
00-022-1809	C4 H12 Al N O12 Si5	7.773		I-4	I	1969	Baerlocher, Meier.	Helv. Chim.	Tetramethyl Ammonium Aluminum Silicate
00-025-0060	Ba Al2 Si3 O10 · 4 H2 O	6.507		P21212	S	1973	Visser, J., Technisch Physische Dienst,	ICDD	Barium Aluminum Silicate Hydrate
00-025-0777	Na2 Al2 Si2 O8 · x H2 O	6.540							
00-027-1212	Li Ba0.5 Al2 Si3 O10 · 4 H2 O								
00-030-0742	(Ba, Li) · Al · Si O4 · H2 O								
00-038-0216	K Al Si O4 · 1.5 H2 O	9.547		I					
00-038-0217	Rb Al Si O4 · H2 O	9.647		I					
00-039-0217	Na5 Al5 Si5 O20 · 9 H2 O	6.680		P-421					
00-044-1388	Rb9.8 Al10 Si10 O40 · 5.44 H2 O	9.666	0.88	I222					
00-045-0123	K2 Al2 Si3 O10 (K Cl)	6.488	0.83	P-421					
00-046-0294	K10 Be10 P10 O40 · 10 H2 O	9.170							
00-050-0090	K12 Al10 Si10 O40 Cl2 · 8 H2 O	9.581		I222					
01-070-0174	Ba2.02 Al4.03 Si5.97 O20 (H2 O)7.81	6.523	1.11	P21212					
01-075-0842	Rb9.8 Al10 Si10 O40 (H2 O)5.44	9.666	0.96	I222					
01-075-1226	Ba1.952 Al3.9 Si6.1 O20 (H2 O)7.4	6.526	1.99	P-421					
01-075-1227	Ba1.88 Al3.88 Si6.12 O20 (H2 O)7.51	6.524	1.88	P-421					
01-079-1893	Li5.04 Si5 Al5 O20 (H2 O)7.92	6.560	1.89	P-421					
01-085-1686	K2 (Al2 Si3 O10) (K Cl)	6.488	0.97	P-421					
01-087-2476	K11.64 (Al10 Si10 O40) Cl1.828 (H2	5.81	0.88	I222					

Diffraction Pattern - 00-050-0090 (Experimental)...

Intensity vs 2θ plot showing experimental data (red) and calculated patterns for 01-070-0174 (blue), 01-075-0842 (green), and 01-075-1226 (yellow).

Context Menu:

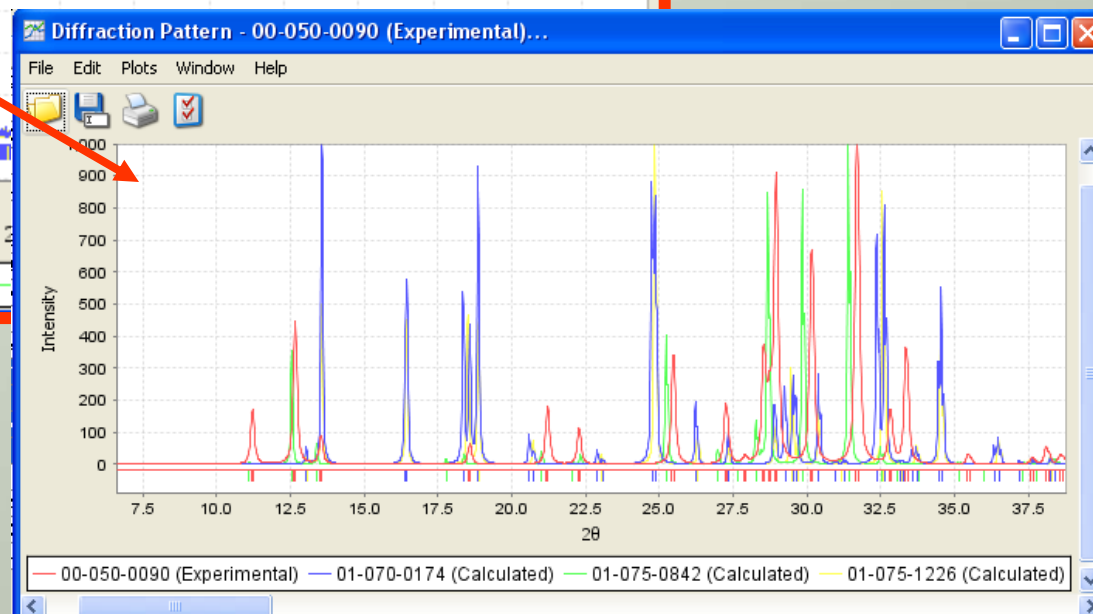
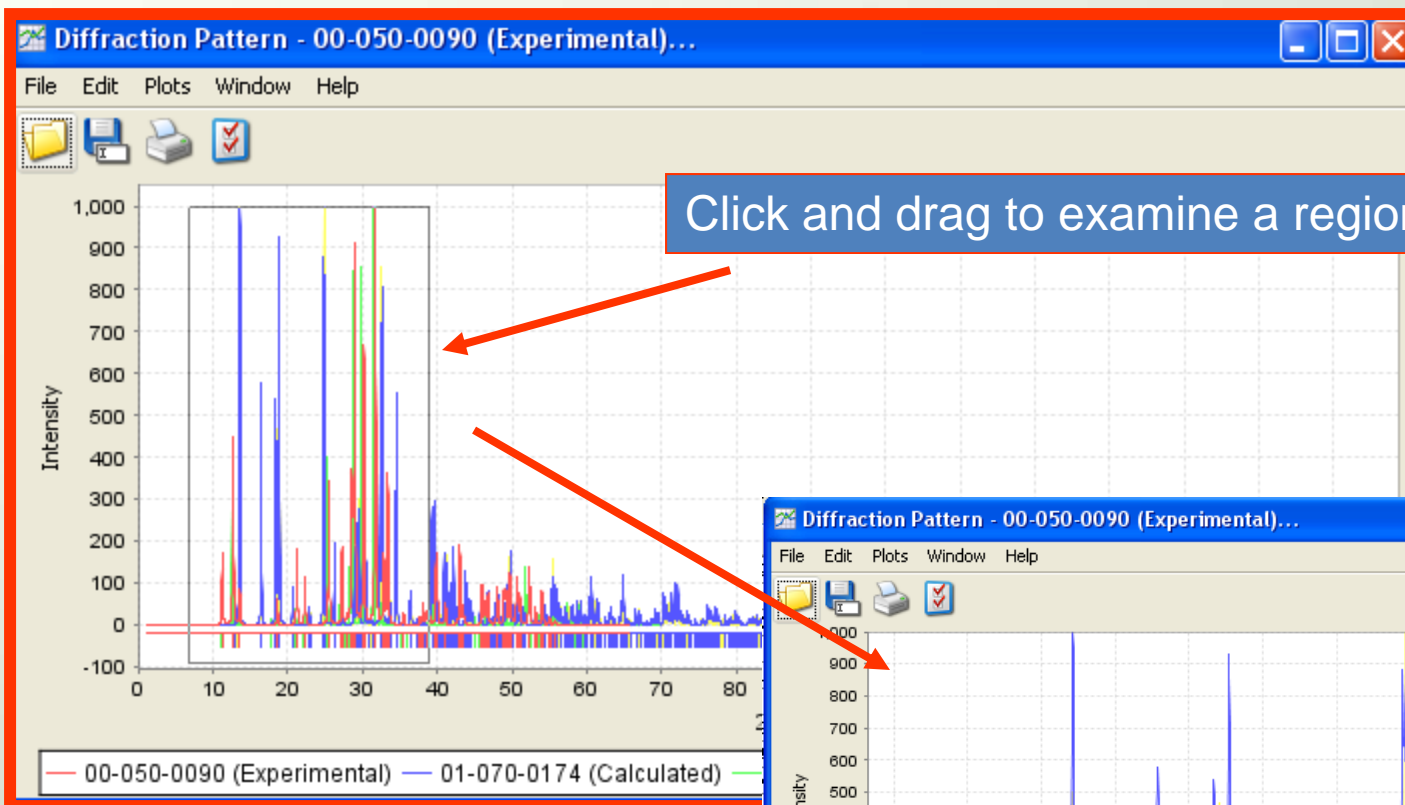
- Open PDF Card
- Open Diffraction Pattern
- Open Diffraction Pattern with Experimental Data
- View Chemical Formula
- Copy Chemical Formula (Ctrl+C)
- Select All
- Graph Fields...

Simultaneous comparison of 4 patterns of Edingtonite

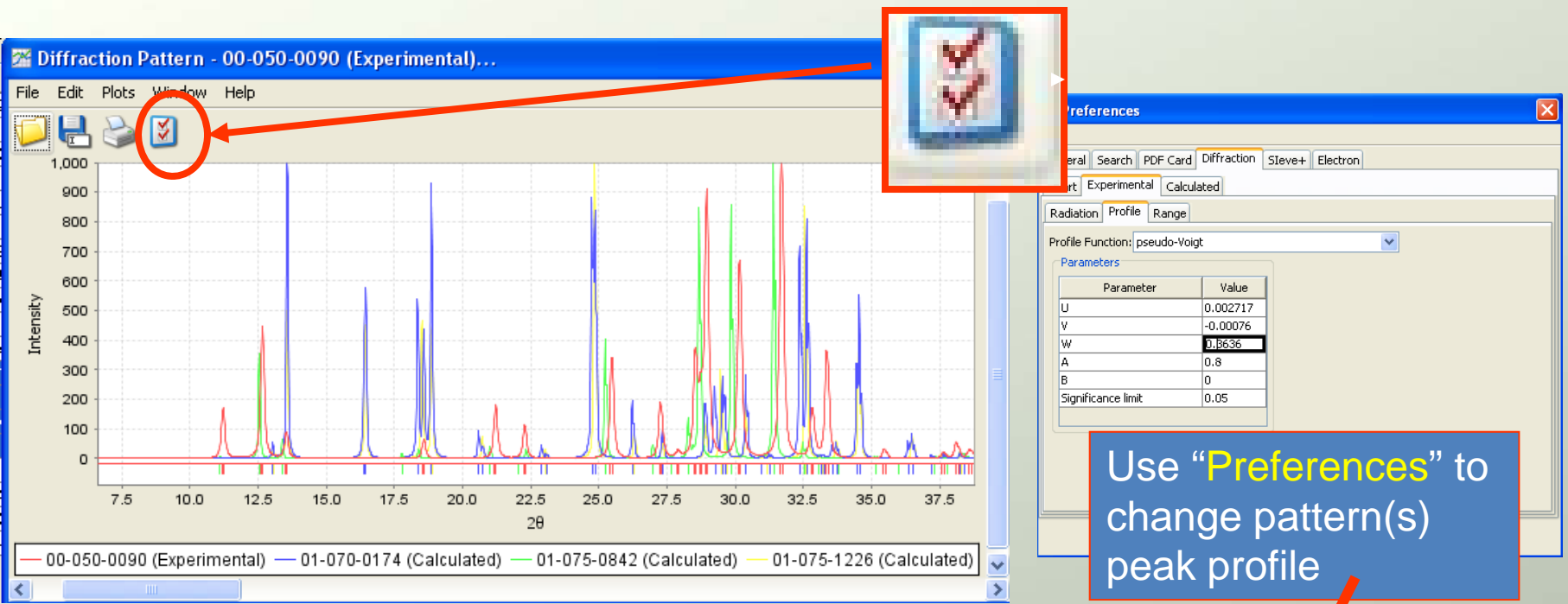
- 1) Highlight a selection
- 2) Right click brings up a menu
- 3) Select **Open Diffraction Pattern**

Note: Shift and Ctrl keys highlight selections

Multi-Pattern Simulations



Multi-Pattern Simulations



Diffraction Pattern - 00-050-0090 (Experimental)...

File Edit Plots Window Help

Intensity

7.5 10.0 12.5 15.0 17.5 20.0 22.5 25.0 27.5 30.0 32.5 35.0 37.5

2θ

— 00-050-0090 (Experimental) — 01-070-0174 (Calculated) — 01-075-0842 (Calculated) — 01-075-1226 (Calculated)

Preferences

General Search PDF Card Diffraction Sieve+ Electron

Plot: Experimental Calculated

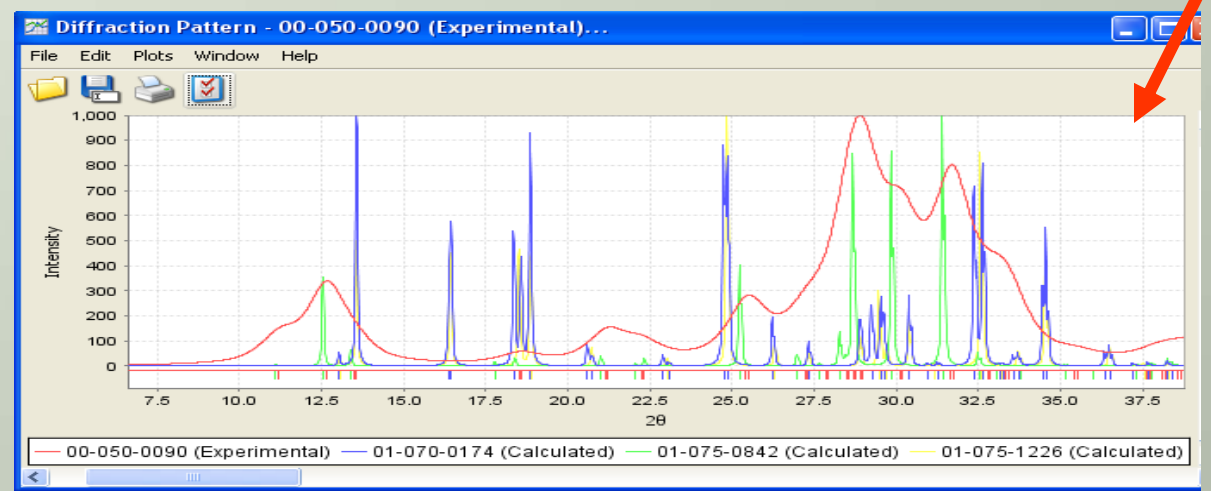
Radiation Profile Range

Profile Function: pseudo-Voigt

Parameters

Parameter	Value
U	0.002717
V	-0.00076
W	0.0636
A	0.8
B	0
Significance limit	0.05

Use "Preferences" to change pattern(s) peak profile



Simulations with Experimental Data

The digital pattern module can be used interactively with the program Sleve+. (See the Identification – PDF-4 Sleve+ tutorial).

The program Sleve+ will search the database to find matches for experimental data based on Fink, Hanawalt or Long 8 search algorithms.

Sleve+ will examine the peak heights of the reference data and scale them to the experimental data. This scale factor is then input automatically into the digital plotting routines.

Sieve+ and Experimental Data

GOM	PDF #	Compound Name	Chemical Formula	L1	L2	L3	L4	L5	L6	L7	L8	I/Ic	Pat. GOM	Integral In
886	00-002-0571	Magnesium Silicate Hydrate	3 Mg O · 4 Si O ₂ · H ₂ O	9.300000	4.600000	3.110000	2.600000	2.480000	2.220000	1.720000	1.520000		212	4.95
886	00-003-0881	Magnesium Silicate Hydroxide	Mg ₃ Si ₄ O ₁₀ (OH) ₂	9.300000	4.580000	3.130000	2.620000	2.490000	2.220000	1.720000	1.530000		171	7.03
886	00-009-0474	Calcium Cerium Silicate Hydroxide	Ca ₂ Ce ₃ (Si O ₄) (Si ₂ O ₇) (O, O H...	9.300000	5.070000	4.620000	3.500000	3.340000	2.960000	2.830000	2.670000		182	4.47
886	00-013-0118	Calcium Uranyl Silicate Hydrate	Ca ₃ (U O ₂) ₄ Si ₁₀ O ₃₅ · 24 H ₂ O	9.300000	5.070000	4.620000	4.470000	3.570000	3.340000	3.210000	3.037000		224	9.17
886	00-014-0155	Potassium Magnesium Vanadium Oxid...	K Mg V ₅ +5 O ₁₄ · 8 H ₂ O	9.300000	8.200000	7.400000	7.000000	5.000000	4.100000	3.310000	3.130000		212	16.4
886	00-028-2010	Fluorene	C ₆ H ₄ C H ₂ C ₆ H ₄	9.300000	5.100000	4.780000	4.590000	4.240000	4.150000	3.350000	2.590000		206	7.18
886	00-029-1659	Diazepam	C ₁₆ H ₁₃ Cl N ₂ O	9.300000	6.680000	6.470000	5.130000	5.030000	4.680000	3.893000	3.729000		220	18.18
886	00-031-0273	Calcium Iron Magnesium Aluminum Ph...	Ca Fe Mg ₂ Al ₂ (P O ₄) ₄ (O H) ₂ · 8 H...	9.300000	5.590000	4.920000	4.850000	4.660000	3.487000	2.946000	2.789000		228	11.15

Matches Filter Filter Description

Select... {Subfile/Subclass (Mineral Or Pharmaceutical)}

Experiment

Search Line(s): 9.29134 Å D1 Range: 9.145 - 9.438 Å Rotation: 1 of 8

Preferences

Search Window: 0.15 ° Match Window: 0.15 °

Search Method: LongS Lowest Allowable GOM: 500




Wavelength: Cu Kα1 1.54056 Å

Phases (6)

# ▲	Accepted	PDF #	Compound Name	Int. Ratio	Int. %	I/Ic	Time
1	<input checked="" type="checkbox"/>	04-008-8528	Calcium Carbonate	0.834	34	3.25	127.6s
2	<input checked="" type="checkbox"/>	04-002-3211	Potassium Chloride	0.783	31	6.07	21.2s
3	<input checked="" type="checkbox"/>	01-070-8072	Zinc Oxide				
4	<input checked="" type="checkbox"/>	00-009-0080	Calcium Hydroxide Phosphate				
5	<input checked="" type="checkbox"/>	01-086-1155	Titanium Oxide				
6	<input type="checkbox"/>	00-003-0881	Magnesium Silicate Hydroxide				

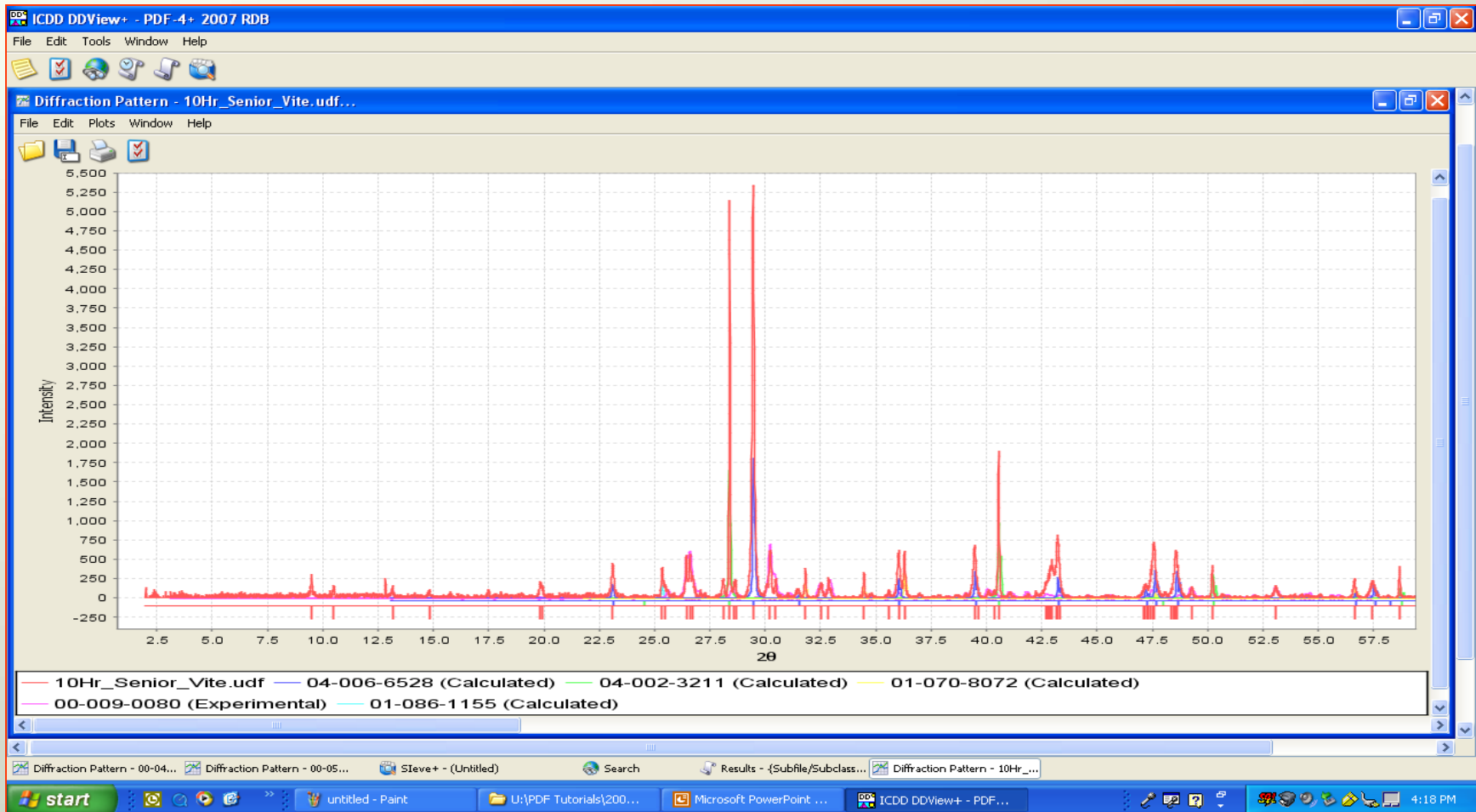
Lines (40 of 57)

Ex d(Å) ▼	Ex I	P1 d(Å)	P1 I	P2 d(Å)	P2 I	P3 d(Å)	P3 I	P4 d(Å)
9.29134	4							
8.41404	3							
6.72086	2							6.74000
5.96723	1							
4.47349	3							4.48000
4.45305	2							
3.84620	8	3.847720	10					
3.51236	6							
3.49085	2							3.48000
3.36829	10							3.37000
3.34751	10							3.35000
3.33210	4							3.33000
3.17173	4							
3.14155	96			3.143300	100			
3.11907	3							3.13000
3.11106	4							3.10000
3.02987	100	3.029430	100					
2.95613	10							2.95800

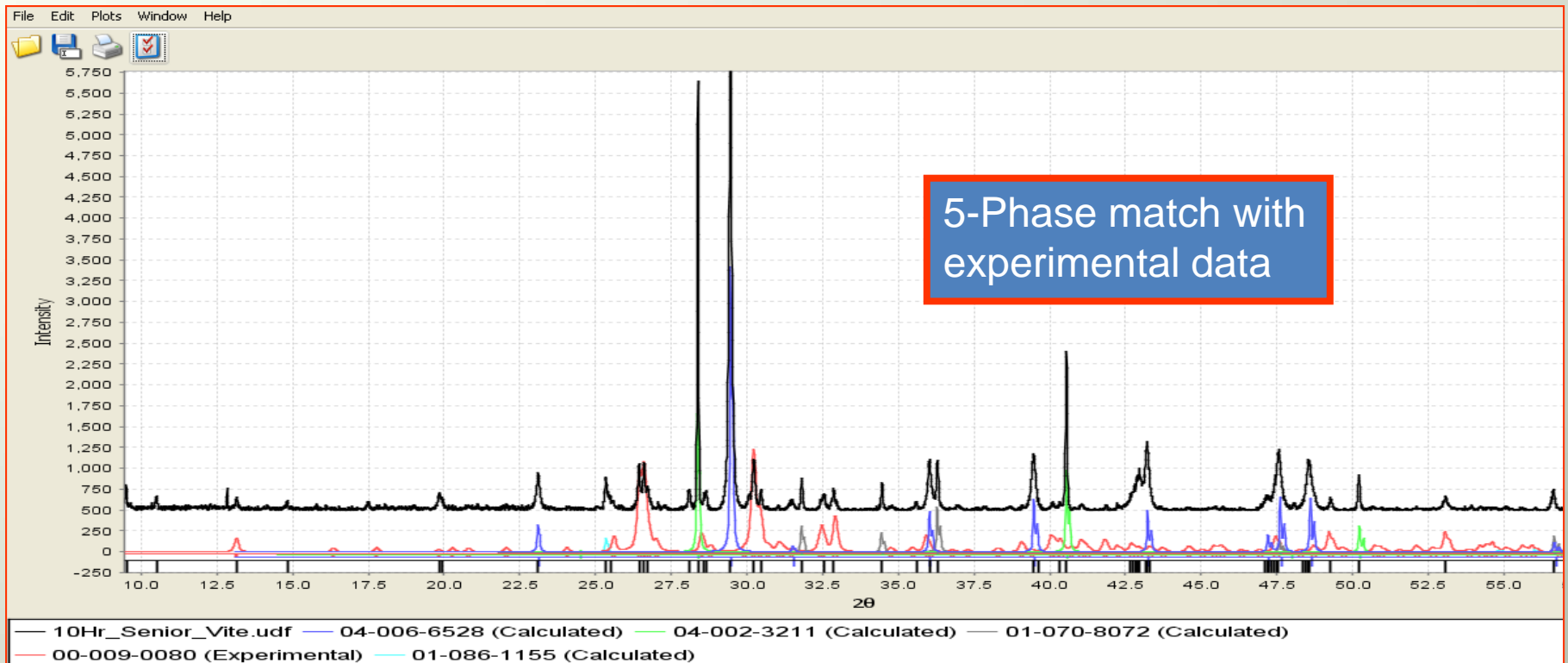
-  Open PDF Card
-  Open Diffraction Pattern
-  Open Diffraction Pattern with Experimental Data

- 1) After Sieve search
- 2) Right click on highlighted results
- 3) Open with experimental data

Experimental Data and Digital Pattern Simulations



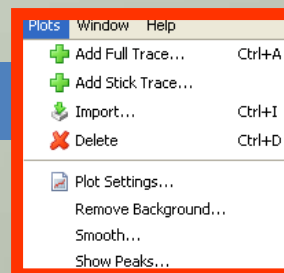
Adjust Scale, Plot, and Offset Experimental Data



Used Preferences



and Plots



to adjust fit

Digital Patterns

- Can simulate crystallite size and other experimental conditions
- Useful for comparing data mining results
- Can be used to compare multiphase simulations with experimental results



Thank you for viewing our tutorial.

Additional tutorials are available at the ICDD website
(www.icdd.com).

International Centre for Diffraction Data

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Newtown Square, PA 19073

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Fax: 610.325.9823