



New Features in Profex 3.5

Nicola Döbelin May 2015

New Mouse and Keyboard Actions Press «Shift» or «Help → Mouse and Keyboard Actions» to show overview

Mouse and keyboard actions				
1	Mouse and Keyboard actions			
	Left Mouse Button	Zoom		
	Ctrl + Left Mouse Button Drag view			
	Double Click	Load reference structure with strongest peak at click position		
	Ctrl + Double Click	Print current coordinates to refinement protocol console		
	Right Mouse Button	Reset zoom		
	Middle Mouse Button	Scale intensity of reference lines		
	Scroll Wheel	Zoom horizontally		
	Ctrl + Scroll Wheel	Zoom vertically		
	C key	Toggle cross hair cursor on / off		
	N key	Toggle noise cursor on / off		
	S key	Toggle spectral line cursor on / off		
		ОК		

Profession



New Cursors Spectral Line Cursor (press «s» to toggle on/off)





Tungsten Peaks

Spectral line cursor can be used to identify Tungsten peaks caused by tube aging



Activate Tungsten lines in
«Edit → Preferences → Graphs → Show characteristic Tungsten lines with spectral lines cursor»

Save existing refinement as Preset



Profex



Grid Lines

Show Major and/or Minor Grid Lines «Edit → Preferences → Graphs → Show Major / Minor Grid Lines»



Improved Y-axis scaling «Edit \rightarrow Preferences \rightarrow Scans \rightarrow Y-axis scaling





Profex

Create STR files from ICDD XML Files

Profestant

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File Edit Tools Window Help					
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Save PDF Card Stort S Save Grapn Eixed Slit Intensity	«File → Save PDF Card»				
Print Preview PDF Card Strg+P ar need of card.nesty Print Graph 20 d(Å) I h k I	750				
221 8.168350 449 Close All .8547 6.881000 5 Close .8331 5.962600 54 Image: Close .8009 4.71000 70 Fixed Slit Intensity 21.7423 4.08410 116 Image: Close 25.3383 3.512120 8 Image: Close 25.8748 3.440500 307 Image: Close All 25.8748 3.440500 307 Image: Close All 25.8748 3.440500 307 Simulated Profile 28.953 3.087350 211 Raw Diffraction Data (PD3) 3.7403 2.816810 999 PDF Experimental Physical Crystal Optical Structure Miscellaned PDF #: 04-011-1880 S S S S S	xrd PDF Card - 04-014-2292.xml DF Card - 04-014-2292.xml 150				
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Weight %: Ca40.62 O40.54 P18.84					
Atomic %: Ca24.39 O60.98 P14.63					
ANX: A6B10X25					

Create STR files from ICDD XML Files

In Profex: «File \rightarrow Import ICDD XML...»



Profest

Create STR files from ICDD XML Files

Select space group setting

Profestant

No space group setting found	Complete STR file
Choose the correct Setting for Space Group "P-1"	ि ि ि
HermannMauguin=P-1 Setting=1 Lattice=Triclinic 🔻	STR File Source File XML File
OK Cancel	<pre>PHASE=Hydrogen_Calcium_Phosphate // Reference=04-009-2424 // Formula=H4_Ca_(_P_04_)2 // SpacegroupNo=2 Setting=1 HermannMauguin=P-1 Lattice=Triclinic // PARAM=ALPHA=109.870000_108.771300^110.968700 PARAM=BETA=93.680000_92.743200^ RP=4 kl=0 k2=0 PARAM=B1=0_0^0.01 GEWICHT=SPHAR6 // GOAL:Hydrogen_Calcium_Phosphate=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1) GOAL=GrainSize(1,1,1) // E=CA Wyckoff=i x=0.313900 y=0.419000 z=0.187700 TDS=0.01025760 E=P Wyckoff=i x=0.256900 y=0.159600 z=0.517100 TDS=0.01195880 E=H Wyckoff=i x=0.84800 y=0.012300 z=0.237000 TDS=0.01030710 E=O Wyckoff=i x=0.180200 y=0.188800 z=0.767100 TDS=0.01030710 E=O Wyckoff=i x=0.641100 y=0.112600 z=0.161000 TDS=0.01207520 E=O Wyckoff=i x=0.00000 y=0.500000 z=0.500000 TDS=0.02396460 E=P Wyckoff=i x=0.916700 y=0.331600 z=0.35100 TDS=0.02396460 E=P Wyckoff=i x=0.916700 y=0.331600 z=0.35100 TDS=0.022396460 E=P Wyckoff=i x=0.916700 y=0.370800 z=0.586000 TDS=0.02282510 E=O Wyckoff=i x=0.916700 y=0.370800 z=0.386000 TDS=0.02882510 E=W Wyckoff=i x=0.602600 y=0.370800 z=0.40300 TDS=0.02189270 E=H Wyckoff=i x=0.602600 y=0.370800 z=0.40300 TDS=0.02189270 E=H Wyckoff=i x=0.602600 y=0.370800 z=0.40300 TDS=0.02189270 E=H Wyckoff=i x=0.882000 y=0.370800 z=0.40300 TDS=0.02189270 E=H Wyckoff=i x=0.882000 y=0.370800 z=0.40300 TDS=0.02189270 E=H Wyckoff=i x=0.602600 y=0.370800 z=0.40300 TDS=0.02189270 E=H Wyckoff=i x=0.425900 y=0.370800 z=0.40300 TDS=0.02189270 E=H Wyckoff=i x=0.425900 y=0.370800 z=0.40300 TDS=0.02189270 E=H Wyckoff=i x=0.425900 y=0.370800 z=0.40300 TDS=0.02882510 E=O Wyckoff=i x=0.425900 y=0.370800 z=0.40300 TDS=0.02882510 E=O Wyckoff=i x=0.425900 y=0.370800 z=0.40300 TDS=0.01283800 E=O Wyckoff=i x=0.425900 y=0.318900 z=0.512200 TDS=0.01283800 E=O Wyckoff=i x=0.425900 y=0.318900 z=0.512200 TDS=0.01283300 *</pre>
Add Files	Save STR Qose