

Testing Research Consulting

BGMN/Profex User Meeting 2019

New Features in Profex 4 Part 2

Nicola Döbelin RMS Foundation, Bettlach, Switzerland

- → GUI changes
- Search / Match
- Peak detection
- Interaction with QualX / Match!
- Electron-density maps
- Drawing crystal structures with Vesta / Mercury
- Customizing report layouts





Rietveld Refinement



Optimize structure model, repeat calculation

Minimize differences between calculated and observed pattern by least-squares method



Rietveld Refinement

Direct space



Reciprocal space

Spacial arrangement of electron clouds (Scattering factors)



Minimize difference between $|F_{obs}|$ and $|F_{calc}|$



Structure Solution



 $\begin{array}{l} \mathsf{F}_{\mathsf{hkl}} \text{ is a complex number} \\ \text{We measure the amplitude } |\mathsf{F}_{\mathsf{obs}}| \\ \text{but not the phase } \varphi_{\mathsf{obs}} \end{array}$



Fourier Synthesis

Direct space







Measured structure factor amplitudes | F_{obs}|

Reciprocal space



Fourier Synthesis

« F_{obs} Fourier map»: Calculated from ϕ_{calc} and $|F_{obs}|$:

$$\rho(x, y, z) = \frac{1}{V} \cdot \sum_{hkl} |F_{obs}| \cdot \cos[2\pi(hx + ky + lz) - \phi_{calc}]$$

« F_{calc} Fourier map»: Calculated from ϕ_{calc} and $|F_{calc}|$:

$$\rho(x, y, z) = \frac{1}{V} \cdot \sum_{hkl} |F_{calc}| \cdot \cos[2\pi(hx + ky + lz) - \phi_{calc}]$$

«Difference Fourier map»: Calculated from ϕ_{calc} and $|F_{obs}| - |F_{calc}|$:

$$\rho(x, y, z) = \frac{1}{V} \cdot \sum_{hkl} (|F_{obs}| - |F_{calc}|) \cdot \cos[2\pi(hx + ky + lz) - \phi_{calc}]$$



Difference Fourier Maps



Misfits ($|F_{obs}| \neq |F_{calc}|$) in the refinement (reciprocal space) can be visualized in the crystal structure (direct space)







© F	Profex 4.0.0-rc1908	826				- 0	×
<u>F</u> ile	<u>E</u> dit <u>V</u> iew P	roject	R <u>un R</u> e	esults	<u>I</u> nstru	ment <u>I</u> ools <u>W</u> indow <u>H</u> elp	
	🗔 🗑 🕻	lut	lut 💾	1		$ \begin{tabular}{lllllllllllllllllllllllllllllllllll$	<u>∧</u> <u>∨</u>
Proje	cts		1	ð ×	180	131-06.dia 180131-06.sav 🔀 180131-06.lst 🗵 Apatite-OH.str 🗵	
Nam	2			Status	1	SampleID: D18 0001 01-00-00c	^
> 18	30131-06			comple	2	% Theoretical instrumental function	
					3	VERZERR=RMS-D8-ADS-15-LynxEyeXE.geq	
					4	% Wavelength	
					5	LAMBDA=CU	
					6	% Phases	
					7	STRUC[1]=Apatite-OH.str	
					8	% Measured background	
<				>	9	UNI=RD3-D8-AD5-15-LýNXEýEXE-DKGT.Xý	
Plot (Options			đΧ	11	KU-IU	
	C	C	N	or	12	Valida = 180131-06 xv	
	Scan	Scaling	vertical	Uffset	13	Minimum Angle (2theta)	
\leq	l observed	1.00	0.00		14	WMIN=10	
\leq	l calculated	1.00	0.00		15	<pre>% Maximum Angle (2theta)</pre>	
\leq	l difference	1.00	-1449.40)	16	% WMAX=60	
M	Background	1.00	0.00		17	% Result list output	
\sim	Hydroxyapatite	1.00	0.00		18	LIST=180131-06.1st	
					19	<pre>% Peak list output</pre>	
					20	OUTPUT=180131-06.par	
					21	§ Diagram output	
_					22	DIAGRAMM=180131-06.dia	
<				>	23	§ Global parameters for zero point and sample displacement	*

Generate two more output files:

*.res: Contains the refined structure in ShelX format

*.fcf: Contains $|F_{obs}|$, $|F_{calc}|$, and φ_{calc} in ShelX format



Profex 4.0.0-rc190826	Profex 4.0.0-rc190826								
Eile Edit <u>V</u> iew Project R <u>u</u> n <u>R</u> esults Instrument <u>T</u> ools <u>W</u> indow <u>H</u> elp									
🗎 🗔 🗟 🕻 📖 🔚 🕼 🏷 🐨 🍪 🖉 👗		I ₿↓ Q (Reference Structures> ✓ X thr 为 (-0.000056 €) ♦							
Projects 🗗 🗙 180131-06.dia 180131-06.sav	180131-06.lst 🗵 Apatite-OH.str 🗵								
Name Status 1 % SampleID: D18_000 > 180131-06 comple 2 % Theoretical inst: 3 VERZERR=RMS-D8-ADS: % Wavelength LAMBDA=CU % Phases STUPUC Ullematica 0	01 01-00-00c rumental function -15-LynxEyeXE.geq	1. Place mouse cursor on the	^						
Plot Options 5 x Scan Scaling Vertical Offset 12 VAL 11 % Measured backgroit 9 UNT=RMS-D8-ADS-15-1 10 RU=10 11 % Measured data 12 VAL 13 % Minimum Angle (21)	Ц <u>U</u> ndo L <u>R</u> edo Ctrl+Y Си <u>т</u> у <u>С</u> ору	 structure file to be visualized Right-click Select «Add RESOUT 							
I colculated 1.00 0.00 14 WMIN=10 ✓ I calculated 1.00 0.00 15 % Maximum Angle (2: ✓ I difference 1.00 -1449.40 15 % Maximum Angle (2: ✓ Background 1.00 0.00 17 % Result list output ✓ Hydroxyapatite 1.00 0.00 18 LIST=180131-06.1st	Paste Delete Select All Ctrl+A	4. Repeat the refinement							
20 OUTPUT=180131-06.p. 21 % Diagram output 22 DIAGRAMM=180131-06 23 % Global paramete	Add STRUCOUT file	acement	~						
Refinement Protocol	Add RDBOUIT file	ters &	×						
4.8254190E+01 3.6899125E+01 3.1244113E+	Comment line	Value ESD	^						
<pre>.th pattern file named RMS-D8-ADS-15-LynxEyeXE-bkgr.xy: assuming free XY[E L-rho=7.04% th pattern file named RMS-D8-ADS-15-LynxEyeXE-bkgr.xy: assuming free XY[E chinement completed in 00:00:03.248 hh:mm:ss.ms</pre>									
٢	> <u>c</u>	0.68818 0.00002	~						
C:\xrd\S19_0007\Profex-E-density-maps\180131-06.sav	1 Proje	roject] λ = 1.5406 Å] 2θ = 31.121°] I = 565.648 cts] d = 2.871 Å							

Profex 4.0.0-rc190826	– O X	٦
File Edit View Project Run Results Instrument Tools Window Help		
		7
		<u>*</u>
Projects 🗗 🗙 180131-06.dia 180131-06.sav* 🔀 180131-06.lst 🗵 A	× ×	
Name Status 1 % SampleID: D18_0001 01-00-00c		•
> 180131-06 comple 2 % Theoretical instrumental function		
4 % Wavelength		
5 LAMBDA=CU		
6 % Phases		
7 STRUC[1]=Apatite-OH.str 8 ECEOUT[1]=Apatite-OH-180131-06 fcf		
9 RESOUT[1]=Apatite-OH-180131-06.res		
10 % Measured background		
Plot Options D X 11 UNT=RMS-D8-ADS-15-LynxEyeXE-bkgr.xy		
Scan Scaling Vertical Offset 12 R0=10		
V lobserved 1.00 0.00 14 VAL[1]=180131-06.xy		
Icalculated 1.00 0.00 15 % Minimum Angle (2theta)		
Background 100 000		
Hydroxyapatite 1.00 0.00 18 S WAX=60		
19 % Result list output		
20 LIST=180131-06.1st		
21 % Peak list output		
22 OUTPUT=180131-06.par		-
Refinement Protocol	Refined Parameters	×
4.8254190E+01 3.6899125E+01 3.1244113E+01 3.4753071E+01 4.7258928E-03	Parameter Value ESD	
lth pattern file named RMS-D8-ADS-15-LynxEyeXE-bkgr.xy: assuming free XY[E	> Statistics	
1-rho=7.04%	Global GOALs	
1th pattern file named RMS-D8-ADS-15-LynxEyeXE-bkgr.xy: assuming free XY[E		
Refinement completed in 00.00.03 248 hhymmiss ms	✓ Hydroxyapatite	
	A 0.94239 0.00002	
< >>	C 0.68818 0.00002	¥
C:\xrd\S19_0007\Profex-E-density-maps\180131-06.sav	1 Project $\lambda = 1.5406 \text{ Å}$ $2\theta = 31.121^{\circ}$ $I = 565.648 \text{ cts}$ $d = 2.871 \text{ Å}$	



Apatite-OH-180131-06.res

Apatite-OH-180131-06.fcf

TITL P6 3/m	n No.176 Hy	/droxyapa	atite			
CELL 1.5410	0 9.42393	9.42393	6.88182	90.000	90.00	0 120.000
ZERR 2.0	80000.0	0.00008	0.00006	0.000	0.00	0 0.000
LATT -1						
SYMM -Y, X-	-Y, Z					
SYMM -X+Y,	-X, Z					
SYMM -X, -Y	(, Z+0.5					
SYMM Y, -X+	Y, Z+0.5					
SYMM X-Y, X	K, Z+0.5					
SYMM -X, -Y	(, -Z					
SYMM Y, -X+	Y, -Z					
SYMM X-Y, X	K, -Z					
SYMM X, Y,	-Z+0.5					
SYMM -Y, X-	-Y, -Z+0.5					
SYMM -X+Y,	-X, -Z+0.5	5				
SFAC CA MG	РОН					
UNIT 6 4 6	26 2					
CA1 1	0.33333	0.66667	0.001	50 0.0	0000	0.00841
MG1 2	0.33333	0.66667	0.001	50 0.3	3333	0.00841
CA2 1	0.24680	0.99340	0.250	00 10.5	0000	0.00719
P1 3	0.39870	0.36850	0.250	00 10.5	0000	0.00605
01 4	0.32840	0.48480	0.250	00 10.5	0000	0.01208
02 4	0.58730	0.46510	0.250	00 10.5	0000	0.01284
03 4	0.34370	0.25790	0.070	20 11.0	0000	0.01899
04 4	0.00000	0.00000	0.195	00 0.1	6667	0.00000
H1 5	0.00000	0.00000	0.060	80 0.1	6667	0.03733
END						

	1	-1	0	18.90	5.76	180.00
	1	0	0	18.90	5.76	180.00
	-1	1	0	18.90	5.76	180.00
	-1	0	0	18.90	5.76	180.00
	0	1	0	18.90	5.76	180.00
	0	-1	0	18.90	5.76	180.00
	1	-1	1	15.58	12.83	180.00
	1	-1	-1	15.58	12.83	0.00
	1	0	1	15.58	12.83	0.00
	1	0	-1	15.58	12.83	180.00
	-1	1	1	15.58	12.83	0.00
	-1	1	-1	15.58	12.83	180.00
	-1	0	1	15.58	12.83	180.00
	-1	0	-1	15.58	12.83	0.00
	0	1	1	15.58	12.83	180.00
	0	1	-1	15.58	12.83	0.00
	0	-1	1	15.58	12.83	0.00
	0	-1	-1	15.58	12.83	180.00
	2	-1	0	31.55	41.80	180.00
	-2	1	0	31.55	41.80	180.00
	1	-2	0	31.55	41.80	180.00
	1	1	0	31.55	41.80	180.00
	-1	2	0	31.55	41.80	180.00
	-1	-1	0	31.55	41.80	180.00
	2	-2	0	31.20	14.56	180.00
	2	0	0	31.20	14.56	180.00





Draw atom labels

x=-infy=-infz=0.0000

-1.00













RMS





2. Electron density map



RMS







Where does the mismatch come from? → Compute Difference Fourier Map





RMS

- 1. Fix refinement of Ca1 position
- 2. Repeat the refinement
- 3. Re-calculate Difference Fourier Map
- 4. Check for improvement

PHASE=Hydroxyapatite // 01-074-0565 MineralName=Hydroxylapatite // Formula=Ca5 (PO4)3 (OH) // SpacegroupNo=176 HermannMauguin=P6 3/m // PARAM=A=0.9424 0.932976^0.951824 PARAM=C=0.6879 0.6810^0.6948 // RP=4 k1=0 PARAM=k2=0 0^0.0001 B1=ANISO^0.05 GEWICHT=SPHAR4 // GOAL=GrainSize(0,0,1) // GOAL=GrainSize(1,0,0) // GOAL:Hydroxyapatite=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1) E=(CA(0),MG(1)) Wyckoff=f x=0.3333 y=0.6667 z=0.0015 TDS=0.00664290 E=CA Wyckoff=h x=0.2468 y=0.9934 z=0.2500 TDS=0.00567436 E=P Wyckoff=h x=0.3987 y=0.3685 z=0.2500 TDS=0.00477426 E=O Wyckoff=h x=0.3284 y=0.4848 z=0.2500 TDS=0.00953535 E=O Wyckoff=h x=0.5873 y=0.4651 z=0.2500 TDS=0.01014069 E=O Wyckoff=i x=0.3437 y=0.2579 z=0.0702 TDS=0.01499127 E=O(0.5) Wyckoff=e x=0.0000 y=0.0000 z=0.1950 TDS=0.00000000 E=H(0.5) Wyckoff=e x=0.0000 y=0.0000 z=0.0608 TDS=0.02947459

Ca1 is completely substituted with Mg

(to generate a massive mismatch)





Instead of changing it back to 100% Ca, lets refine the Ca / Mg ratio:

E=(CA(0),MG(1)) Wyckoff=f x=0.3333 y=0.6667 z=0.0015 TDS=0.00664290

Step 1:Parametrize the site occupancy factors.Keep the site fully occupied but with variable Ca / Mg ratio.

E=(CA(**p**),MG(**1-p**)) **p=0** Wyckoff=f x=0.3333 y=0.6667 z=0.0015 TDS=0.00664290

Step 2: Refine p between 0 and 1.

E=(CA(**p**),MG(**1-p**)) **PARAM=p=0_0^1** Wyckoff=f x=0.3333 y=0.6667 z=0.0015 TDS=0.00664290

Step 3:Repeat the refinement.Recalculate the Difference Fourier Map.





Mismatch in diffraction pattern is gone



Difference Fourier Map

100% Mg substitution

Refined Mg substitution

Refined Mg substitution with range -2.38 to 2.38





Profex 4.0.0-rc190826	- 🗆 X
<u>F</u> ile <u>E</u> dit <u>V</u> iew Project R <u>u</u> n <u>R</u> esults <u>Instrument T</u> ools <u>W</u> indow <u>H</u> elp	
🗎 🗔 🗟 🗘 🔟 🛄 🕼 🕼 🐨 🐨 🚱 🖉 👗 🛨 🏠 🔳 💿 ▷ ▷ □ 🗇	$\texttt{L} Q = \texttt{CReference Structures} \times \texttt{th} \mathcal{H} = \texttt{C.000054} \text{C} \text{C}$
Projects 🗗 🗙 180131-06.dia 180131-06.sav 🗵 180131-06.lst 🗵	
Name Status 16 ************************************	*** ·
22 A=0.9423847+-0.0000074	Mg content on Cal
<pre> 23 C=0.6881820+-0.00000057 24 k2=0.000001029+-0.0000000097 25 GrainSize(0,0,1)=713+-53 </pre>	refined to 0.0
Plot Options D X 26 GrainSize (1, 0, 0) = 362+-11	
Scan Scaling Vertical Offset 27 GEWICHT=SPHR4, MeanValue (GEWICHT)=0.0589845 ✓ Iobserved 1.00 0.00 28 Bl=ANISOLIN, MeanValue (Bl)=0.0000454, sqrt3(det (Bl)) ✓ Icalculated 1.00 0.00 30 31 4 0.33333 0.6667 0.0015 E=(CA(1.0000), MG(0)) ✓ Hydroxyapatite 1.00 0.00 32 9=1.00000 33 ✓ Hydroxyapatite 1.00 0.00 34 6 0.2468 0.9934 0.2500 E=(CA(1.0000)) 36 6 0.3284 0.4684 0.2500 E=(O(1.0000)) 37 6 0.5873 0.4651 0.2500 E=(O(1.0000)) 37)=0.000935691
38 12 0.3437 0.2579 0.0702 E=(0(1.0000))	~
Refinement Protocol B × Refined Parameter	rs B X
5.2520274E-03 	Value ESD ^
	0.942385 0.000007
C	0.688182 0.000006
C:\xrd\S19_0007\Profex-E-density-maps\180131-06.lst 1 Pro	ject λ = 1.5406 A 2θ = 0.000° I = 0.000 cts d = 0.000 Å

Visualizing refined crystal structures

- 1. Refine structural parameters (atomic coordinates)
- 2. Export refined crystal structure data in CIF format
- 3. Import in structure visualization program



Works with any visualization program supporting CIF input files. Tested with: Vesta [1], Mercury [2], Diamond [3]

http://www.jp-minerals.org/vesta/en/
 https://www.ccdc.cam.ac.uk/solutions/csd-system/components/mercury/
 https://www.crystalimpact.com/diamond/Default.htm



Example «Profex-structure-visualization»:

- 1. Open Apatite-OH.str
- 2. Refine unit cell and profile parameters k2, B1, GEWICHT
- 3. Refine Mg substitution on both Ca sites
- 4. Refine all general atomic coordinates (except for H site)
- 5. Refine all TDS (except for H site)

```
PHASE=Hydroxyapatite // 01-074-0565
MineralName=Hydroxylapatite //
Formula=Ca5 (PO4)3 (OH) //
SpacegroupNo=176 HermannMauguin=P6 3/m //
PARAM=A=0.9424 0.932976^0.951824 PARAM=C=0.6879 0.6810^0.6948 //
RP=4 k1=0 PARAM=k2=0 0^0.0001 B1=ANISO^0.05 GEWICHT=SPHAR4 //
GOAL=GrainSize(0,0,1) //
GOAL=GrainSize(1,0,0) //
GOAL:Hydroxyapatite=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1)
E=(CA(p),MG(1-p)) PARAM=p=0 0^1 Wyckoff=f x=0.3333 y=0.6667 PARAM=z=0.0015 -0.0485^0.0515 PARAM=TDS=0.006643 0^0.02
E=(CA(p),MG(1-p)) PARAM=p=0 0^1 Wyckoff=h PARAM=x=0.2468 0.1968^0.2968 PARAM=y=0.9934 0.9434^1.0434 z=0.2500 PARAM=TDS=0.005674 0^0.02
E=P Wyckoff=h PARAM=x=0.3987 0.3487^0.4487 PARAM=y=0.3685 0.3185^0.4185 z=0.2500 PARAM=TDS=0.004774 0^0.02
E=O Wyckoff=h PARAM=x=0.3284 0.2784^0.3784 PARAM=y=0.4848 0.4348^0.5348 z=0.2500 PARAM=TDS=0.009535 0^0.02
E=O Wyckoff=h PARAM=x=0.5873 0.5373^0.6373 PARAM=y=0.4651 0.4151^0.5151 z=0.2500 PARAM=TDS=0.010141 0^0.02
E=O Wyckoff=i PARAM=x=0.3437 0.2937^0.3937 PARAM=y=0.2579 0.2079^0.3079 PARAM=z=0.0702 0.0202^0.1202 PARAM=TDS=0.014991 0^0.02
E=O(0.5000) Wyckoff=e x=0.0000 y=0.0000 PARAM=z=0.1950 0.1450^0.2450 TDS=0.00000000
E=H(0.5000) Wyckoff=e x=0.0000 y=0.0000 z=0.0608 TDS=0.029475
```



Profex 4.0.0-rc190c.	- 🗆 X
<u>File Edit View Project Kun Results</u> Instrument <u>I</u> ools <u>W</u> indow <u>H</u> elp	
📄 🗔 🕞 🗋 🛄 🛄 🧐 Export Global Parameters and GOALs Ctrl+E 💿 ▷ 🔊	□ □ ↓ Q ♡ <reference structures=""> ✓ × 計 功 0.000054 🕃 🔶 😤</reference>
Projects Export Local Parameters and GOALs Ctrl+Shift+E	
Name Export Chemical Composition	180131-06.dia
> 180131-06 Export Peak Integrals	
Export CFL files from RES file	I observed I calculated
2	I difference Background
Generate Report	Hydroxyapatite
	<u></u>
	© CIF Export ? X
Scan Scaling Vertical Offect	CIF Output Format
I observed 1.00 0.00	One single-phase CIF file per phase
I calculated 1.00 0.00	O One multi-phase CIF file per project
difference 1.00 -158.17 1000 - Background 1.00 0.00	O One global multi-phase CIF file
Hydroxyapatite 1.00 0.00	
	Experimental Data
	Temperature 295 K
Ontional information	Radiation source X-ray V
written to CIF file	
	OK Cancel







∕ ∻	VESTA								- 0	×		
<u>File</u>	<u>E</u> dit <u>V</u> iew <u>O</u> bjects	<u>U</u> tilities <u>H</u> elp										
	New Structure	Ctrl+N	1	下 Step (°): 180.0 🛧 🕹 🗧	\rightarrow Step (px):	50 + - j=	Step (%): 50					
	New <u>W</u> indow			VESTA								
	<u>O</u> pen	Ctrl+O	Ы									
	Save	Ctrl+S										
	Save <u>A</u> s	Ctrl+Shift+S										
	Export Data											
	Export <u>R</u> aster Image											
	Export Vector Image											
	Save Output <u>T</u> ext											
	<u>C</u> lose	Ctrl+W			,							
-	EXit	Ctrl+Q	E		🜲 Open							
	Show sections					. « S10 > P	rofex-structure-visualizat	tion 🗸	"Profex-stri	icture-visua	izatio	
	Show isosurfac	ces		Vis	S / I					n n		
	Style	iy			Organisieren 🔻	Neuer Ordner				i≡: ▼		
	Smooth shadir	ng			Name		Änderungs	datum	Тур	Größe		
	○ Wireframe	2			📔 180131-06-H	ydroxyapatite.cif	02.09.2019	13:50	CIF-Datei		4 KB	
	O Dot surface											
	Courtel abanas											
	Show shapes				R V							
	Style											
	Unicolor											
	O Custom color											
	○ Wireframe			OpenGL version: 4.5.0 - Video configuration: Int					2			
				Maximum supported width								
	Pro	perties		opensis depth burrer bit.		_			2			
	Boundary	Orientation				Datei <u>n</u> ame: 1	80131-06-Hydroxyapatite	cif	Crystallogr	aphic Inforn	nation F	F



Edit View Objects Utilities Help	— L	, ,
a Undo Ctrl+Z	▶ Step (°): 180.0 \uparrow \downarrow \leftarrow \rightarrow Step (px): 50 + - □ Step (%): 50	
Redo Ctrl+Shift+Z	180131-06-Hydroxyapatite.cif	
<u>E</u> dit Data >		
Bonds Ctrl+B		
Vectors		
Lattice Planes		
Q Preferences		
P opace mining		
O Polyhedral	Q Q Q Q	
() Wireframe		
€ U Stick		
Volumetric data	Bonds - 180131-00-Hydroxyapatite.cif	
Show sections	Dharey 1 🔺 100121 06 Hydrowyapatite	
Show isosurfaces	rindse i vilousi-ou-nyuroxyapane	
Surface coloring	Search bonds and atoms	
Style	Search mode Boundary mode	
Smooth shading	Search A2 bonded to A1 Do not search atoms beyond the boundary	
O Wireframe	O Search bonded to A1 Search additional atoms if A1 is included in the	e boundary
Obersunace	D Search additional atoms recursively if either A	1 or A2 is visible
Crystal shapes		
Show shapes	Search by label bow polyhedra	
Style	A1: P V A2: O V Min. length: 0 Max. le	ngth: 1.7
Unicolor		
O Custom color	No. Atom 1 Atom 2 Min. (Å) Max. (Å) Bound. Po	New
 Wireframe 	1 P 0 0 1.6 2	3
	Number of polygons a	Delete
Properties		Clear
Boundary Orientation		
	Output Comment	









PROI	^{T}LA				5°		
Sample Information							
D18_0001 01-00-00c							
File Name	ile Name 180131-06.dia						
Instrument configuration	RMS-D8-ADS-15-Lyn	RMS-D8-ADS-15-LynxEyeXE.geg					
Wavelength	CU (1.5406 Å)						
Directory	G:/Auftr_Proj/S-Auftra	aege/2019/S19_0007 XR	D-Kurs Freiberg/Example	s/Profex-custom-report			
Date of Refinement	Montag, 2. Septembe	Montag, 2. September 2019					
Operator	Doebelinn	Doebelinn					
Statistics	R _{WD} = 10.13	Rexp = 10.09	$x^2 = 1.0079$	GoF = 1.0040			

Global GOALs

Parameter	Value	ESD
QHydroxyapatite	1.000000	0.000000





PROFEX

Sample Information

D18_0001 01-00-00c							
File Name 180131-06.dia							
Instrument configuration	RMS-D8-ADS-15-LynxEyeXE.geq						
Wavelength	CU (1.5406 Å)						
Directory	G:/Auftr_Proj/S-Auftraege	G:/Auftr_Proj/S-Auftraege/2019/S19_0007 XRD-Kurs Freiberg/Examples/Profex-					
Date of Refinement	Montag, 2. September 20)19					
Operator	Doebelinn						
Statistics	R _{wp} = 10.13	R _{exp} = 10.09	$\chi^2 = 1.0079$ G				

Global GOALs

Parameter	Value	ESD
QHydroxyapatite	1.000000	0.000000

Diffraction Pattern





Sample Information

D18_0001 01-00-00c					
File Name	180131-06.dia	180131-06.dia			
Instrument configuration	RMS-D8-ADS-15-LynxEy	eXE.geq			
Wavelength	CU (1.5406 Å)				
Directory	G:/Auftr_Proj/S-Auftraege	/2019/S19_0007 XRD-Kur	s Freiberg/Examples/Profe	x-custon	
Date of Refinement	Montag, 2. September 2019				
Operator	Nicola Döbelin				
Statistics	R _{wp} = 10.13	R _{exp} = 10.09	$\chi^2 = 1.0079$	GoF = 1	

Global GOALs

Parameter	Value	ESD
QHydroxyapatite	1.000000	0.000000

Refined Chemical Composition

Phase	Phase Quantity (wt-%)	H2O (wt-%)	MgO (wt-%)	P2O5 (wt-%)
Hydroxyapatite	100.00	1.79	0.00	42.39
Weighted total	100.00	1.79	0.00	42.39

Document Release

	Name	Date / Signature
Operator		
Control		

Electronic reports/certificates distributed as PDF files do not contain original signatures and therefore are for information Printed and signed reports/certificates are the only valid documentation.



TECHNISCHE UNIVERSITÄT BERGAKADEMIE FREIBERG



RMS

Sample Information

D18_0001 01-00-00c							
File Name	180131-06.dia	180131-06.dia					
Instrument configuration	RMS-D8-ADS-15-Ly	RMS-D8-ADS-15-LynxEyeXE.geq					
Wavelength	CU (1.5406 Å)	CU (1.5406 Å)					
Directory	G:/Auftr_Proj/S-Auft	G:/Auftr_Proj/S-Auftraege/2019/S19_0007 XRD-Kurs Freiberg/Examples/Profex-custom-report					
Date of Refinement	Montag, 2. Septemb	Montag, 2. September 2019					
Operator	Nicola Döbelin	Nicola Döbelin					
Statistics	R _{wp} = 10.13	$R_{wp} = 10.13$ $R_{exp} = 10.09$ $\chi^2 = 1.0079$ GoF = 1.0040					

Global GOALs

Parameter	Value	ESD
QHydroxyapatite	1.000000	0.000000

Diffraction Pattern



General	BGMN - Refinement Report	
Text Editors		
✓ Graphs	Structure Header Style	
Appearance		
Fonts	1	<2 <> 븕 + -
Scan Styles		
Print and Export	Section	Text / Value
✓ BGMN	 Sample Information 	Sample Information
Backend Configuration	Operator Name	Doebelinn
Repositories	Refinement Statistics	
Peak Detection	Global GOALs	Global GOALs
Search-Match	 Diffraction Pattern 	Diffraction Pattern
Reference Structures	Aspect Ratio	1.4140
Favorites	Local GOALs	Local GOALs
Refinement Limits	Chemical Composition	Refined Chemical Composition
GOAL Management	Peak List	Peak List
Summary Tables		
Refinement Report	Double-click c	n items
Fullprof.2k		
Chemical Composition	to change the	e display text
Text Blocks		
	Fa 🛃	







A L	
T	
Section	Text / Value
✓ ✓ Sample Information	Sample Information
Operator Name	Nicola Döbelin
Refinement Statistics	
Global GOALs	Refined Phase Quantities
✓ ☑ Diffraction Pattern	Diffraction Pattern
Aspect Ratio	1.4140
Local GOALs	Local GOALs
Chemical Composition	Refined Chemical Composition
Peak List	Peak List

Insert / remove page break after selected item

Move selected item up/down





IGMN - Refinement Report		Insert / remove a custom HTML element
Structure Header Style Image: Section Image: Sample Information Image: Section Image: Operator Name Image: Section Image: Operator Name </th <th>Text / Value Sample Information Nicola Döbelin Refined Phase Quantities Diffraction Pattern 1.8000 Local GOALs</th> <th>Image: Custom HTML element ? × Name: Example ? × <hr/> Example for a custom html element</th>	Text / Value Sample Information Nicola Döbelin Refined Phase Quantities Diffraction Pattern 1.8000 Local GOALs	Image: Custom HTML element ? × Name: Example ? × <hr/> Example for a custom html element
		OK Cancel



Custom HTML element	?	×
Name: Example		
<hr/> Example for a custom html element <hr/>		
ОК	Can	cel

PROFEX

Sample Information

D18_0001 01-00-00c					
File Name	180131-06.dia	180131-06.dia			
Instrument configuration	RMS-D8-ADS-15-LynxEy	RMS-D8-ADS-15-LynxEyeXE.geq			
Wavelength	CU (1.5406 Å)				
Directory	G:/Auftr_Proj/S-Auftraege/2019/S19_0007 XRD-Kurs Freiberg/Examples/Profex-custom-report				
Date of Refinement	Montag, 2. September 2019				
Operator	Nicola Döbelin				
Statistics	$R_{wp} = 10.13$ $R_{exp} = 10.09$ $\chi^2 = 1.0079$ GoF = 1.0040				

Refined Phase Quantities

Parameter	Value	ESD
QHydroxyapatite	1.000000	0.000000



Example for a custom html element

RMS

Custom Refinement Reports – Banner

BGMN - Refinement Report Structure Header Style Logo:		Specif leave Profe>	y banne empty fo banner	r file or or defau	llt
Banners and span	appear at the to the to the entire page	cop of th ge width	າe repor າ	t	
	Sample Information				
	D18_0001 01-00-00c				
	File Name	180131-06.dia			
	Instrument configuration	RMS-D8-ADS-15-L	.ynxEyeXE.geq		
	Wavelength	CU (1.5406 Å)	Breeze (2010/E10, 0007 VD	D Kura Eraihara/Eurolo-	/Drefey austern senert
	Date of Refinement	Montag 2 Senter	ntraege/2019/519_0007 XR nber 2019	D-runs meiberg/Examples	armolex-custom-report
Banners must be saved	Operator	Nicola Döbelin			
	Statistics	R _{wp} = 10.13	R _{exp} = 10.09	$\chi^2 = 1.0079$	GoF = 1.0040
in SVG format (no other		I			
formats supported)					



Inkscape: Free software to create SVG graphs https://inkscape.org/de/



Create a new document of approximately 160x15 mm Save in default format (*.svg)



Custom Refinement Reports – Banner

go: D007 XRD-Kurs Freiberg/Examples/Profex-custom-report/rms-cmyk.svg E Sample Information D18_0001 01.00.00C File Name 180131-06.dia Instrument configuration RMS-D8-ADS-15-LynxEyeXE.geq Wavelength CU (1.5406 A) Directory G:/Auftrage/2019/S19_0007 XRD-Kurs Freiberg/Examples/Profex-custom-report Date of Refinement Montag. 2. September 2019 Operator Nicola Dobelin Statistics R_wn = 10.13 R_wn = 10.09 y ² = 1.0079 GeF = 1.0040	ructure Header Style						
Testing · Research · Consulting Testing · Research · Consulting Consulting	o: 0007 XRD-Kurs Freiberg/E	xamples/Profex-custom-report/rms-c	myk.svg				
Testing · Research · Consu Differention Differentiation Differentiation File Name 180131-06.dia Instrument configuration RMS-D8-ADS-15-LynxEyeXE.geq Wavelength CU (1.5406 Å) Directory G:/Auftr_Proj/S-Auftraege/2019/S19_0007 XRD-Kurs Freiberg/Examples/Profex-custom-report Date of Refinement Montag, 2. September 2019 Operator Statistics Run = 10.13 Run = 10.09 y2 = 1.0079 GoF = 1.0040	AS	••••• Testing • Rese	arch - Consulting				
Testing • Research • Consu Sample Information D18_0001 01-00-00c File Name 180131-06.dia Instrument configuration RMS-D8-ADS-15-LynxEyeXE.geq Wavelength CU (1.5406 Å) Directory G:/Auftr_Proj/S-Auftraege/2019/S19_0007 XRD-Kurs Freiberg/Examples/Profex-custom-report Date of Refinement Montag. 2. September 2019 Operator Nicola Dobelin Statistics Rwn = 10.13 Revn = 10.09 y² = 1.0079 GoF = 1.0040							
Sample Information D18_0001 01-00-00c File Name 180131-06.dia Instrument configuration RMS-D8-ADS-15-LynxEyeXE.geq Wavelength CU (1.5406 Å) Directory G:/Auftr_Proj/S-Auftraege/2019/S19_0007 XRD-Kurs Freiberg/Examples/Profex-custom-report Date of Refinement Montag, 2. September 2019 Operator Nicola Döbelin Statistics Rwn = 10.13 Resn = 10.09 y² = 1.0079 GoF = 1.0040			RMS		0 0	•••• Testing	• Research • Consulti
Sample Information D18_0001 01-00-00c File Name 180131-06.dia Instrument configuration RMS-D8-ADS-15-LynxEyeXE.geq Wavelength CU (1.5406 Å) Directory G:/Auftr_Proj/S-Auftraege/2019/S19_0007 XRD-Kurs Freiberg/Examples/Profex-custom-report Date of Refinement Montag, 2. September 2019 Operator Nicola Döbelin Statistics Rwn = 10.13 Rexn = 10.09 y2 = 1.0079 GoF = 1.0040							
Sample Information D18_0001 01-00-00c File Name 180131-06.dia Instrument configuration RMS-D8-ADS-15-LynxEyeXE.geq Wavelength CU (1.5406 Å) Directory G:/Auftr_Proj/S-Auftraege/2019/S19_0007 XRD-Kurs Freiberg/Examples/Profex-custom-report Date of Refinement Montag, 2. September 2019 Operator Nicola Döbelin Statistics Rwn = 10.13 Rexn = 10.09 y2 = 1.0079 GoF = 1.0040							
Sample Information D18_0001 01-00-00c File Name 180131-06.dia Instrument configuration RMS-D8-ADS-15-LynxEyeXE.geq Wavelength CU (1.5406 Å) Directory G:/Auftr_Proj/S-Auftraege/2019/S19_0007 XRD-Kurs Freiberg/Examples/Profex-custom-report Date of Refinement Montag, 2. September 2019 Operator Nicola Döbelin Statistics Rwn = 10.13 Rexn = 10.09 y² = 1.0079 GoF = 1.0040							
D18_0001 01-00-00c File Name 180131-06.dia Instrument configuration RMS-D8-ADS-15-LynxEyeXE.geq Wavelength CU (1.5406 Å) Directory G:/Auftr_Proj/S-Auftraege/2019/S19_0007 XRD-Kurs Freiberg/Examples/Profex-custom-report Date of Refinement Montag, 2. September 2019 Operator Nicola Döbelin Statistics Rwn = 10.13 Rexn = 10.09 y² = 1.0079 GoF = 1.0040							
File Name 180131-06.dia Instrument configuration RMS-D8-ADS-15-LynxEyeXE.geq Wavelength CU (1.5406 Å) Directory G:/Auftr_Proj/S-Auftraege/2019/S19_0007 XRD-Kurs Freiberg/Examples/Profex-custom-report Date of Refinement Montag, 2. September 2019 Operator Nicola Döbelin Statistics Rwn = 10.13 Rexn = 10.09 y² = 1.0079 GoF = 1.0040			Sample Information				
Instrument configuration RMS-D8-ADS-15-LynxEyeXE.geq Wavelength CU (1.5406 Å) Directory G:/Auftr_Proj/S-Auftraege/2019/S19_0007 XRD-Kurs Freiberg/Examples/Profex-custom-report Date of Refinement Montag, 2. September 2019 Operator Nicola Döbelin Statistics Rwn = 10.13 Rexn = 10.09 y² = 1.0079 GoF = 1.0040			Sample Information D18_0001 01-00-00c				
Wavelength CU (1.5406 Å) Directory G:/Auftr_Proj/S-Auftraege/2019/S19_0007 XRD-Kurs Freiberg/Examples/Profex-custom-report Date of Refinement Montag, 2. September 2019 Operator Nicola Döbelin Statistics Rwn = 10.13			Sample Information D18_0001 01-00-00c File Name	180131-06.dia			
Directory G:/Auftr_Proj/S-Auftraege/2019/S19_0007 XRD-Kurs Freiberg/Examples/Profex-custom-report Date of Refinement Montag, 2. September 2019 Operator Nicola Döbelin Statistics Rwn = 10.13 Rexn = 10.09 y² = 1.0079 GoF = 1.0040			Sample Information D18_0001 01-00-00c File Name Instrument configuration	180131-06.dia RMS-D8-ADS-15-Lyn	xEyeXE.geq		
Date of Refinement Montag, 2. September 2019 Operator Nicola Döbelin Statistics R _{wn} = 10.13 R _{exn} = 10.09 y² = 1.0079 GoF = 1.0040			Sample Information D18_0001 01-00-00c File Name Instrument configuration Wavelength	180131-06.dia RMS-D8-ADS-15-Lyn CU (1.5406 Å)	xEyeXE.geq		
Operator Nicola Döbelin Statistics R _{wn} = 10.13 R _{exn} = 10.09 y ² = 1.0079 GoF = 1.0040			Sample Information D18_0001 01-00-00c File Name Instrument configuration Wavelength Directory	180131-06.dia RMS-D8-ADS-15-Lyn CU (1.5406 Å) G:/Auftr_Proj/S-Auftra	xEyeXE.geq aege/2019/S19_0007 XRE	D-Kurs Freiberg/Example	es/Profex-custom-report
Statistics $R_{wn} = 10.13$ $R_{wn} = 10.09$ $y^2 = 1.0079$ GoF = 1.0040			Sample Information D18_0001 01-00-00c File Name Instrument configuration Wavelength Directory Date of Refinement	180131-06.dia RMS-D8-ADS-15-Lyn CU (1.5406 Å) G:/Auftr_Proj/S-Auftra Montag, 2. September	xEyeXE.geq aege/2019/S19_0007 XRE ar 2019	D-Kurs Freiberg/Example	s/Profex-custom-report
			Sample Information D18_0001 01-00-00c File Name Instrument configuration Wavelength Directory Date of Refinement Operator	180131-06.dia RMS-D8-ADS-15-Lyn CU (1.5406 Å) G:/Auftr_Proj/S-Auftra Montag, 2. Septembe Nicola Döbelin	xEyeXE.geq aege/2019/S19_0007 XRC ar 2019	D-Kurs Freiberg/Example	s/Profex-custom-report
			Sample Information D18_0001 01-00-00c File Name Instrument configuration Wavelength Directory Date of Refinement Operator Statistics	180131-06.dia RMS-D8-ADS-15-Lyn CU (1.5406 Å) G:/Auftr_Proj/S-Auftra Montag, 2. September Nicola Döbelin Rwp = 10.13	xEyeXE.geq aege/2019/S19_0007 XRE ar 2019 R _{exp} = 10.09	D-Kurs Freiberg/Example χ ² = 1.0079	es/Profex-custom-report GoF = 1.0040



BGMN - Refinement Report

Structure Header Style	
☑ Use Style Sheet:	
Style	
Font: Helvetica 10 pt	
Color of table header:	
Color of alternting rows:	
Color of table border:	

Style sheets are a technology used in web design (CSS) → Not covered here (https://www.w3schools.com/Css/)

Two options for colors / style:

- Specify a CSS file (enable «Use Styls Sheet»)
- Select table colors directly (disable «Use Style Sheet»)





Refined Phase Quantities

Parameter	Value	ESD
QHydroxyapatite	1.000000	0.000000

Refined Chemical Composition

Phase	Phase Quantity (wt-%)	H2O (wt-%)	MgO (wt-%)	P2O5 (wt-%)	CaO (wt-%)
Hydroxyapatite	100.00	1.79	0.00	42.39	55.82
Weighted total	100.00	1.79	0.00	42.39	55.82

Use a web browser to print reports to paper or PDF







Х

~ 👩

Mar

]== **|**