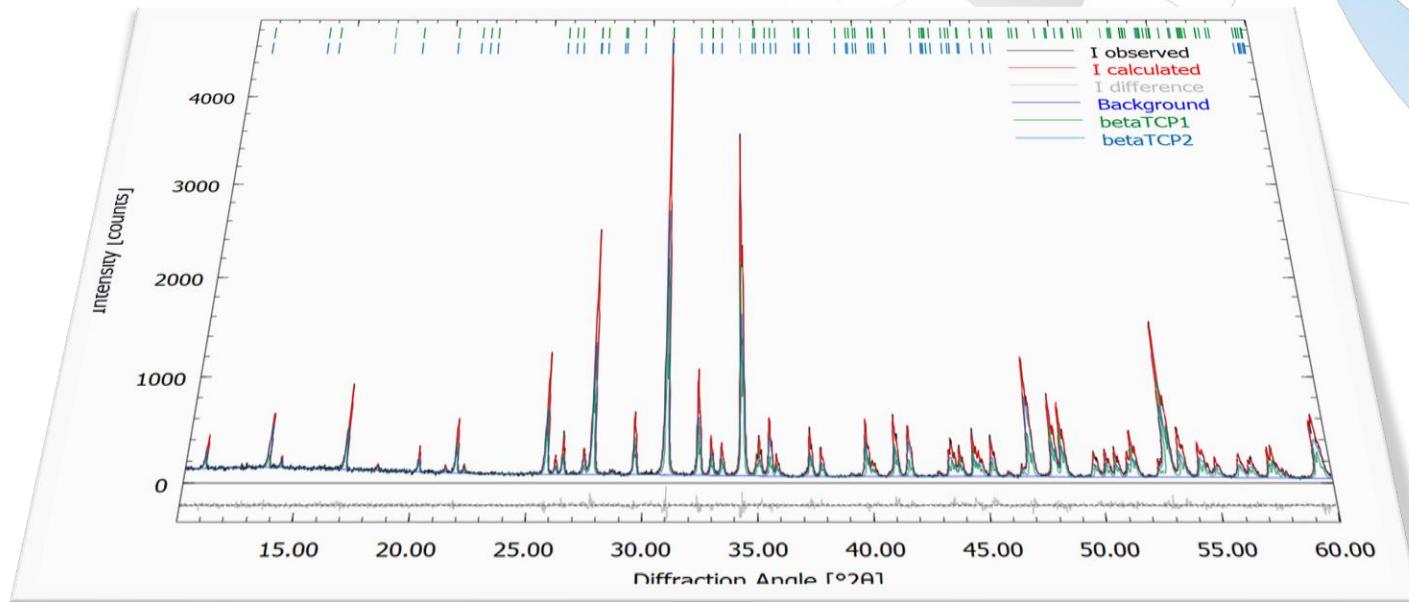
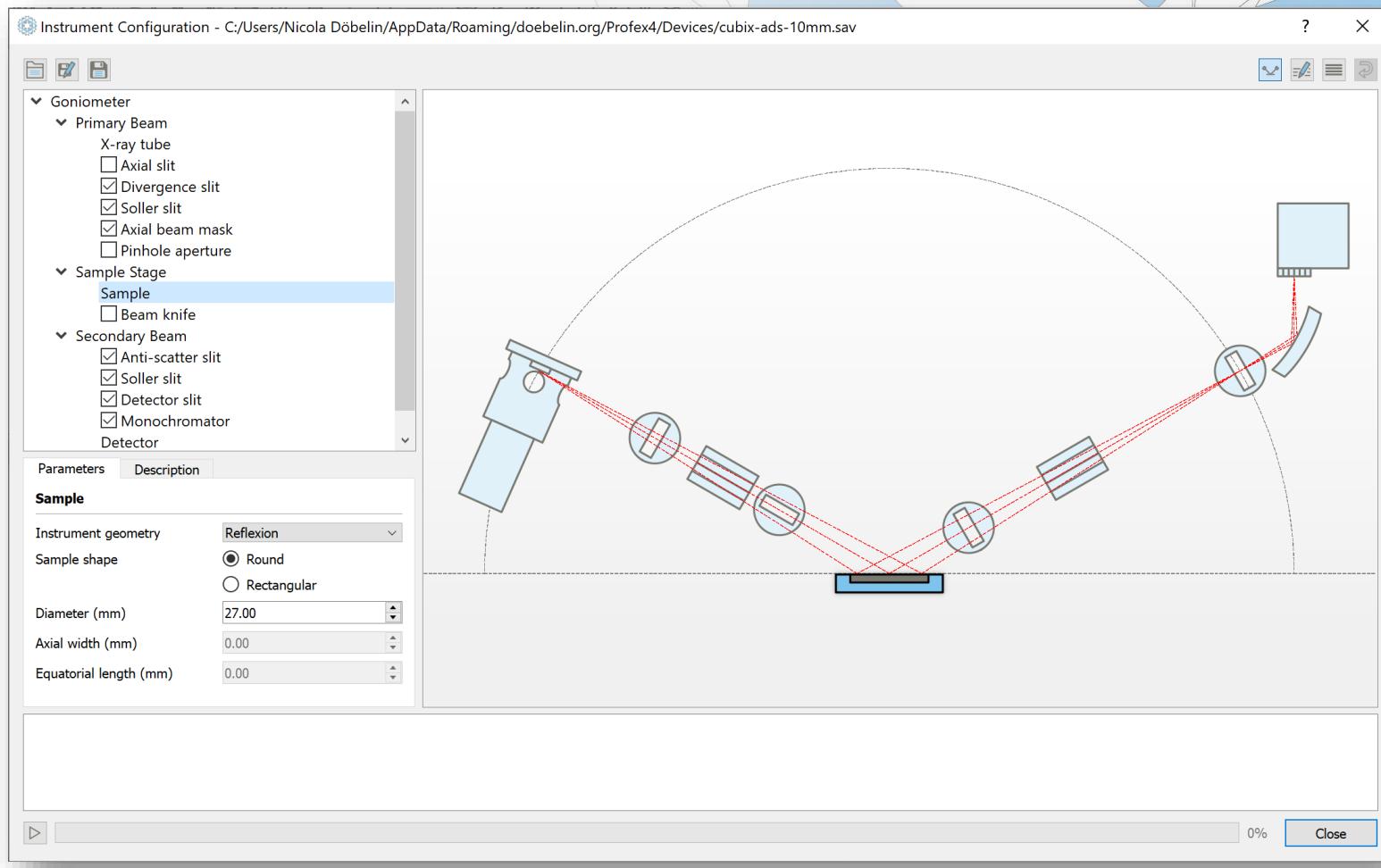


New Features in Profex 4.2



New graphical instrument editor



Chemical restrictions in Search-Match module

Search/Match Phases

Phases **Restrictions** Controls Results

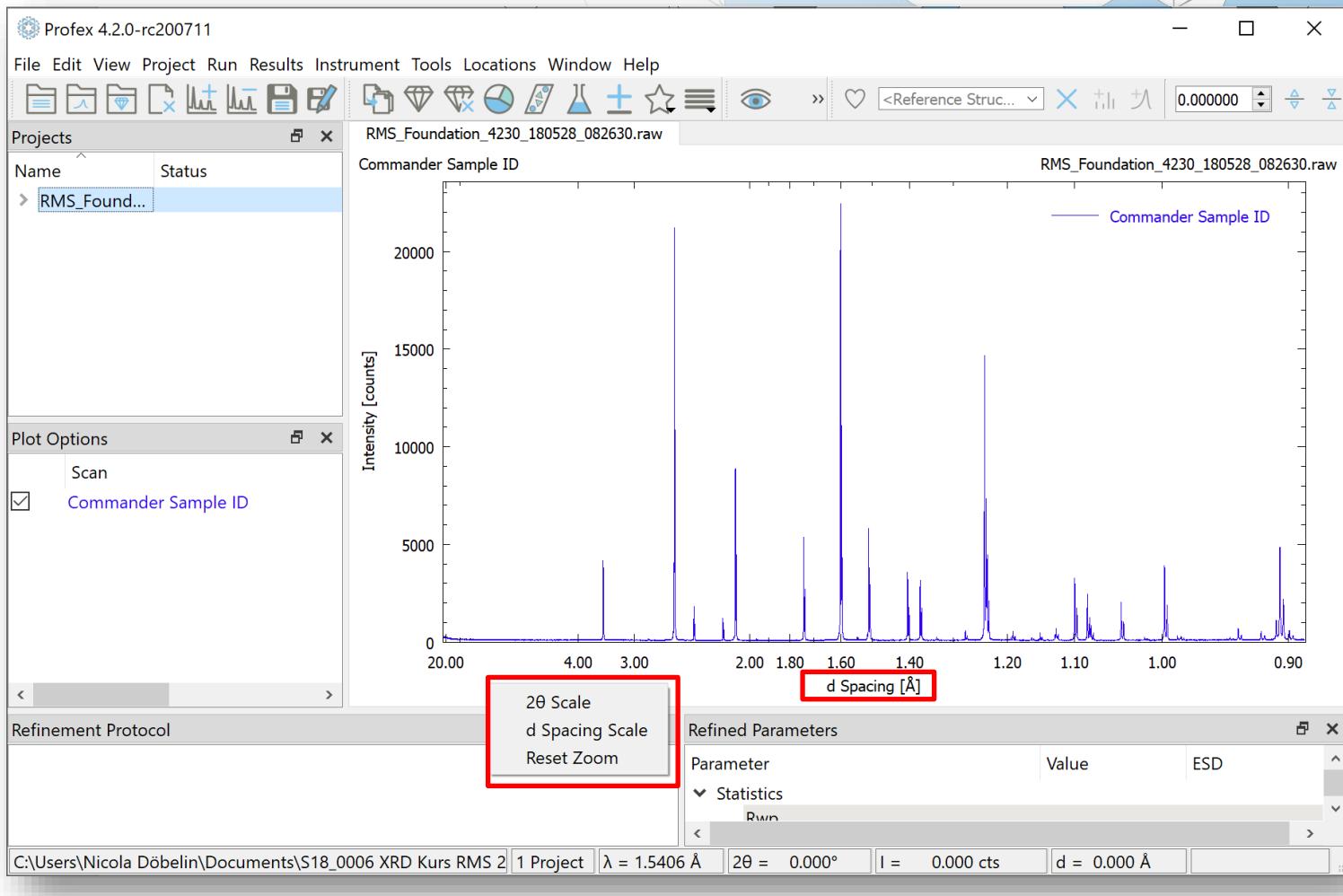
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	
1	H																	He	
2	Li	Be																	
3	Na	Mg																	
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
6	Cs	Ba	*	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
7	Fr	Ra	**																
L			*	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb		
A			**	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf						

Change all

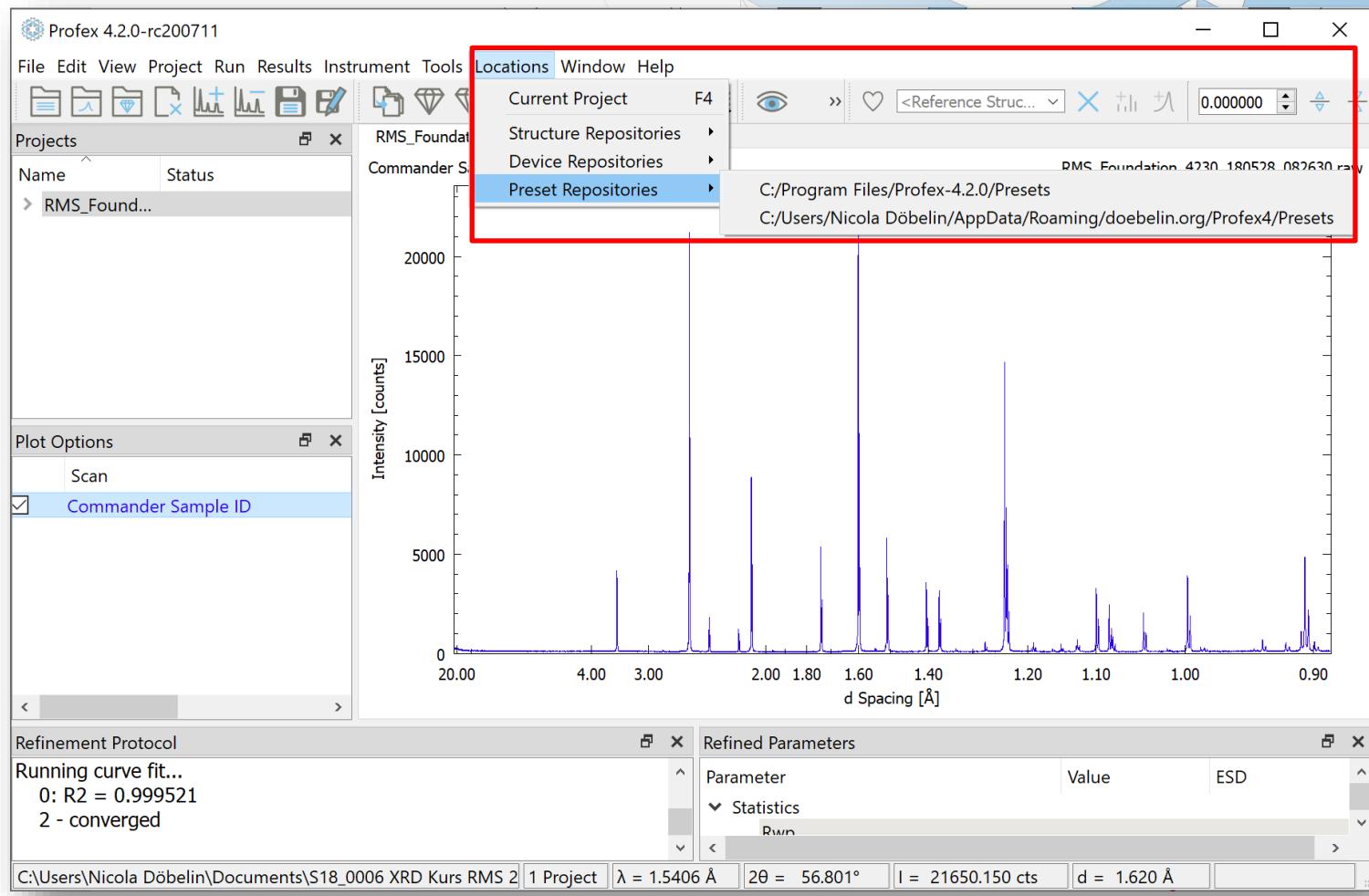
Optional At least one Discard optional

Mandatory Discarded

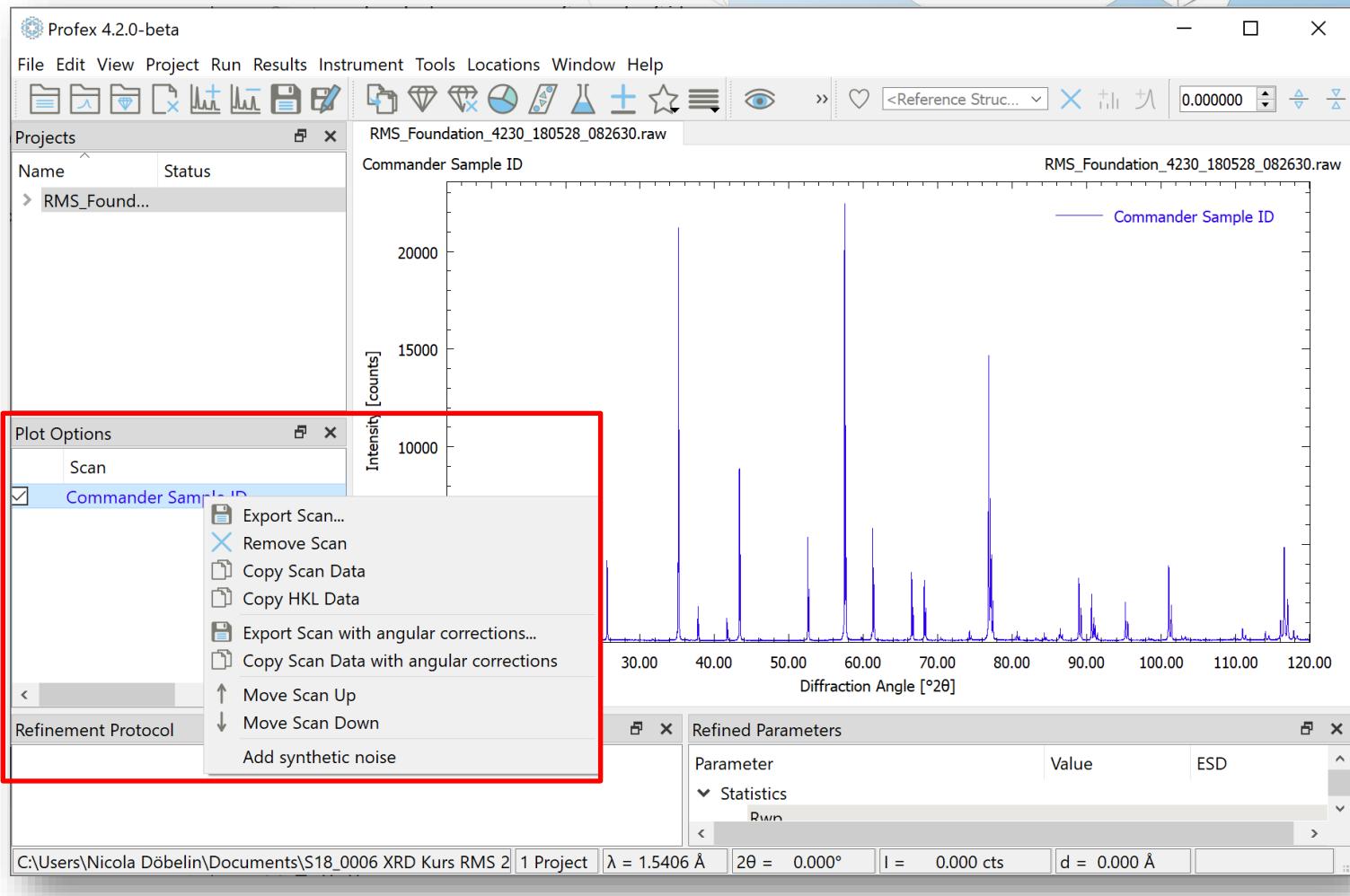
Change x-axis unit to d-spacing



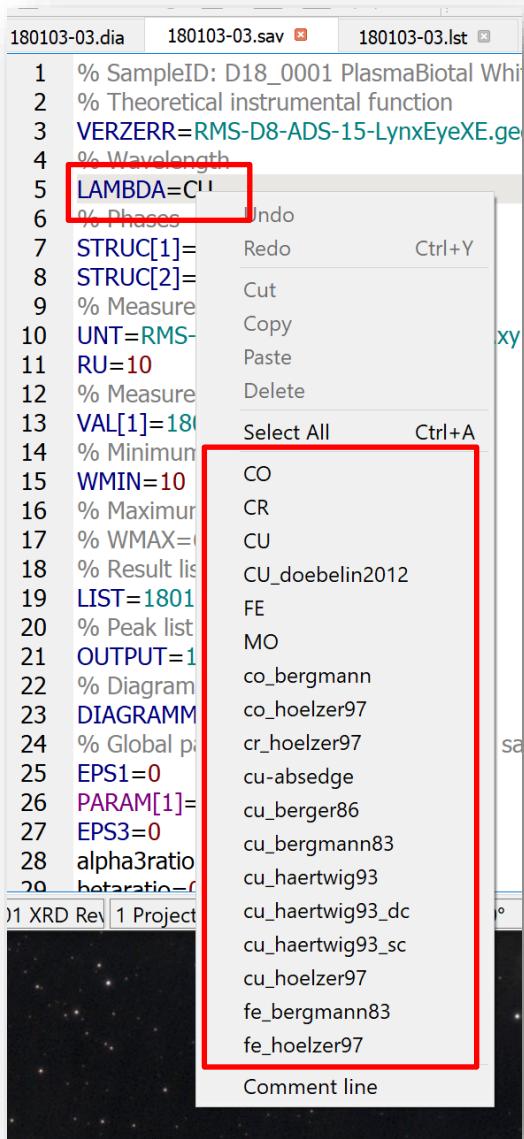
New menu „Locations“ for direct access to repositories



More scan export functions



Select wavelength file from mouse context menu



Right-click on „LAMBDA“ keyword

Improved CIF and XML structure import

Import Structure Files

Files

STR File Source File

Clinoptilolite.cif

```
1 PHASE=ClinoptiloliteCa //
2 Formula=Al2.74_Ca1.78_H21.94_K1.28_Na1.78_O45.58_Si15.26 //
3 SpacegroupNo=12 HermannMauguin=C12/m1 Setting=1 CellChoice=1 UniqueAxis=b Lattice=Monoclinic //
4 PARAM=A=1.763300_1.745667^1.780933 PARAM=B=1.794100_1.776159^1.812041
PARAM=C=0.740000_0.732600^0.747400 //
5 PARAM=BETA=116.390000_115.226100^117.553900 //
6 RP=4 k1=0 k2=0 PARAM=B1=0_0^0.01 GEWICHT=SPHAR4 //
7 GOAL:ClinoptiloliteCa=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1) //
8 E=(SI(0.8700),AL(0.1300)) Wyckoff=j x=0.178900 y=0.170500 z=0.095300 TDS=0.011171
9 E=(SI(0.6700),AL(0.3300)) Wyckoff=j x=0.213100 y=0.410400 z=0.503000 TDS=0.011474
10 E=(SI(0.9000),AL(0.1000)) Wyckoff=j x=0.208000 y=0.190700 z=0.715200 TDS=0.011237
11 E=(SI(0.9200),AL(0.0800)) Wyckoff=j x=0.065400 y=0.298900 z=0.412900 TDS=0.011283
12 E=(SI(0.9100),AL(0.0900)) Wyckoff=g x=0.000000 y=0.216000 z=0.000000 TDS=0.011640
13 E=(NA(0.5000),CA(0.5000)) Wyckoff=i x=0.147800 y=0.000000 z=0.666100 TDS=0.058006
14 E=(NA(0.3900),CA(0.3900)) Wyckoff=i x=0.540400 y=0.000000 z=0.216700 TDS=0.037669
15 E=K(0.6400) Wyckoff=i x=0.734400 y=0.000000 z=0.025200 TDS=0.087203
16 E=O Wyckoff=i x=0.697300 y=0.000000 z=0.457100 TDS=0.025813
17 E=O Wyckoff=j x=0.232000 y=0.121200 z=0.613800 TDS=0.024212
18 E=O Wyckoff=j x=0.182500 y=0.156500 z=0.885000 TDS=0.026624
```

Messages hkl Plot

Intensity [%]

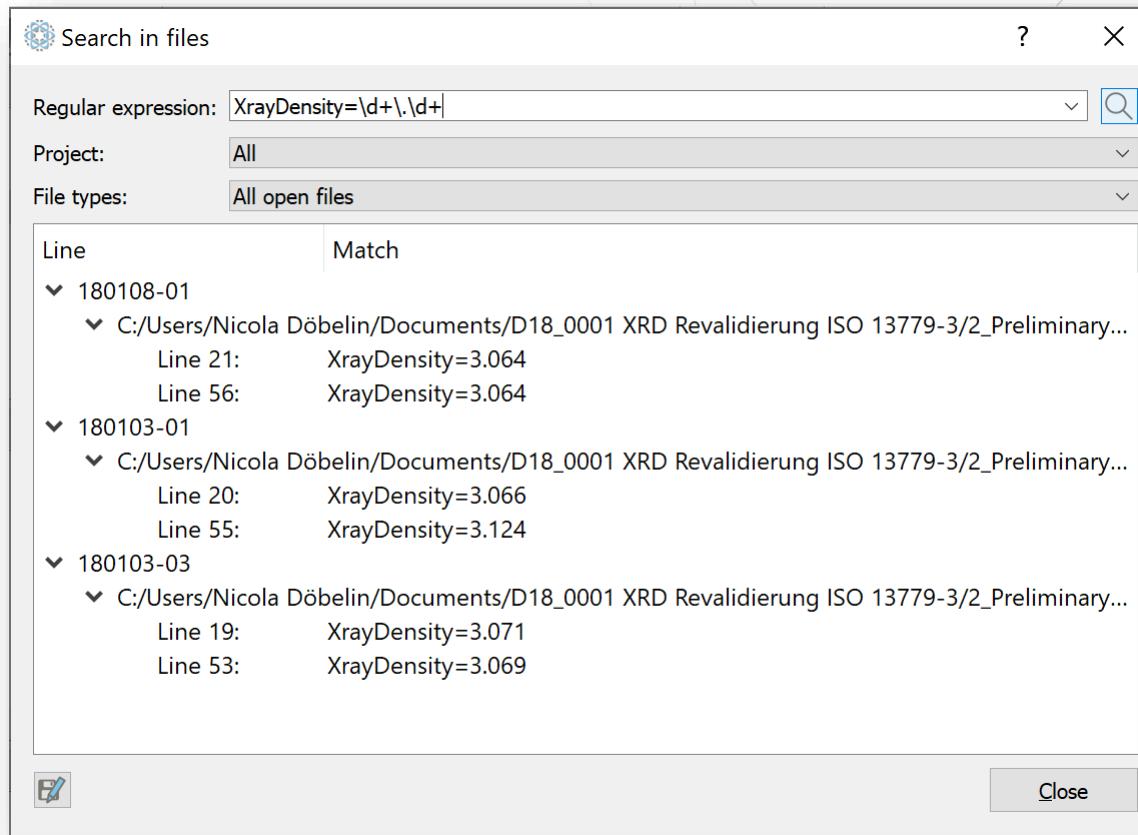
Diffraction Angle [° 2θ]

$\rho = 2.2080 \text{ g/cm}^3$

CuKa1 (1.540598 Å)

Close

New dialog „Edit → Search in files“:
Searches regular expressions in all open
files and projects



Improved BGMN backend auto-detection

Support for multiple repositories

The screenshot displays two overlapping preference dialog boxes from the Profex software interface.

Left Dialog: BGMN - Configuration

- General Options:**
 - Use bundled BGMN installation
 - Use custom BGMN installation
- Executable Selections:**
 - BGMN executable: [Empty Text Box]
 - MakeGEQ executable: [Empty Text Box]
 - Geomet executable: [Empty Text Box]
 - Teil executable: [Empty Text Box]
 - Eflech executable: [Empty Text Box]
- Refinement Options:**
 - Convert raw scans to XY format
 - Spectral line cursor shows all wave
 - Normalize quantity GOALs to 100%
 - Create report after refinement

Right Dialog: BGMN - Repositories

- Structure file repositories:**
 - C:/Program Files/Profex-4.2.0/Structures
 - C:/Users/Nicola Döbelin/AppData/Roaming/doebelin.org/Profex4/Structures
- Device file repositories:**
 - C:/Program Files/Profex-4.2.0/Devices
 - C:/Users/Nicola Döbelin/AppData/Roaming/doebelin.org/Profex4/Devices
- Presets repositories:**
 - C:/Program Files/Profex-4.2.0/Presets
 - C:/Users/Nicola Döbelin/AppData/Roaming/doebelin.org/Profex4/Presets

Buttons at the bottom: OK and Cancel

+ many bug fixes

- more shortcuts in text editors
- improved nonlinear curve fitting dialog
- uses scroll areas in dock widgets
- activates scans when curves are selected in peak fit dialog
- fixed wrong display of theta in SVG export
- fixed persistent wait cursor at program start
- shows B_1 and b_2^2 in peak list
- removed graph flickering when running search-match
- automatically sets up user repositories outside of the application bundle