

PROFEX

OPEN SOURCE XRD AND RIETVELD REFINEMENT



# New features in Profex 4.1

The screenshot displays the PROFEX software interface. On the left, a 'Files' panel lists 'vaterite.cif', 'Aragonite.cif', and 'Calcite.cif', with 'Calcite.cif' selected. The main window is split into two panes: 'STR File' and 'Source File'. The 'STR File' pane contains the following text:

```
1 PHASE=Calcite // amcsd_0009873
2 Reference=amcsd_0009873 //
3 Formula=Ca_C_O3 //
4 SpacegroupNo=167 HermannMauguin=R-32/c Setting=1 UniqueAxis=c Lattice=Trigonal //
5 PARAM=A=0.499100_0.494109^0.504091 PARAM=B=0.499100_0.494109^0.504091
  PARAM=C=1.706200_1.689138^1.723262 //
6 RP=4 k1=0 k2=0 PARAM=B1=0_0^0.01 GEWICHT=SPHAR4 //
7 GOAL:Calcite=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1) //
8 E=CA Wyckoff=b x=0.000000 y=0.000000 z=0.000000 TDS=0.007969
9 E=C Wyckoff=a x=0.000000 y=0.000000 z=0.250000 TDS=0.007580
10 E=O Wyckoff=e x=0.257300 y=0.000000 z=0.250000 TDS=0.013063
11
```

The 'Source File' pane is currently empty. Below the panes are navigation buttons (+, -, play, refresh, save). The 'Messages' panel shows an 'hkl Plot' with a graph of Intensity [%] versus Diffraction Angle [° 2θ]. The y-axis ranges from 0 to 100, and the x-axis ranges from 0 to 50. A legend indicates a density of  $\rho = 2.7090 \text{ g/cm}^3$ . The plot shows a sharp peak at approximately 29.5° 2θ. At the bottom, there are icons for file operations and a dropdown menu set to 'CuKα1 (1.540598 Å)'.

## Major improvements of CIF structure import:

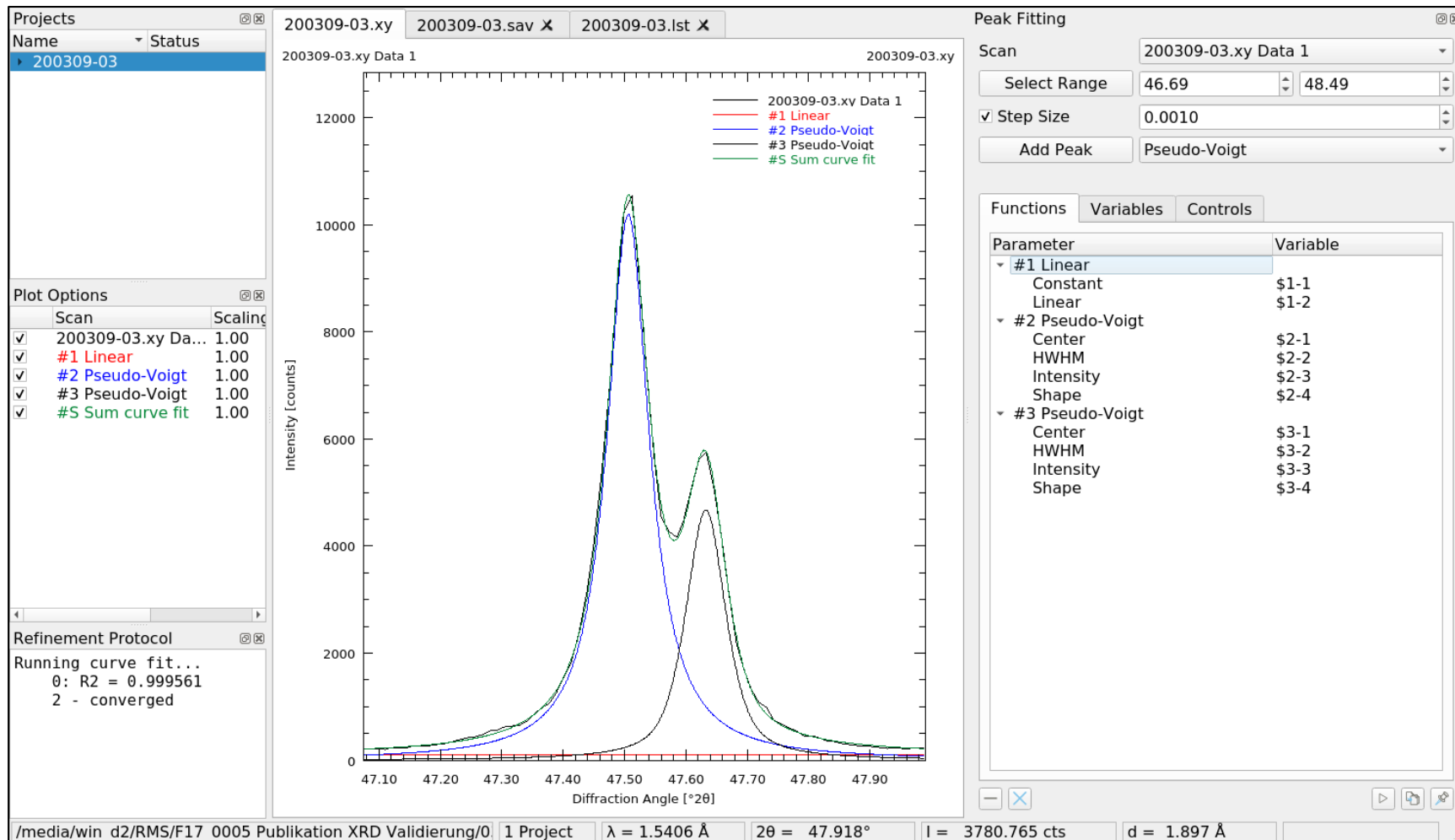
- Automatic recognition of missing Wyckoff symbols
- Improved detection of unit cell settings
- Automatically index new structure files

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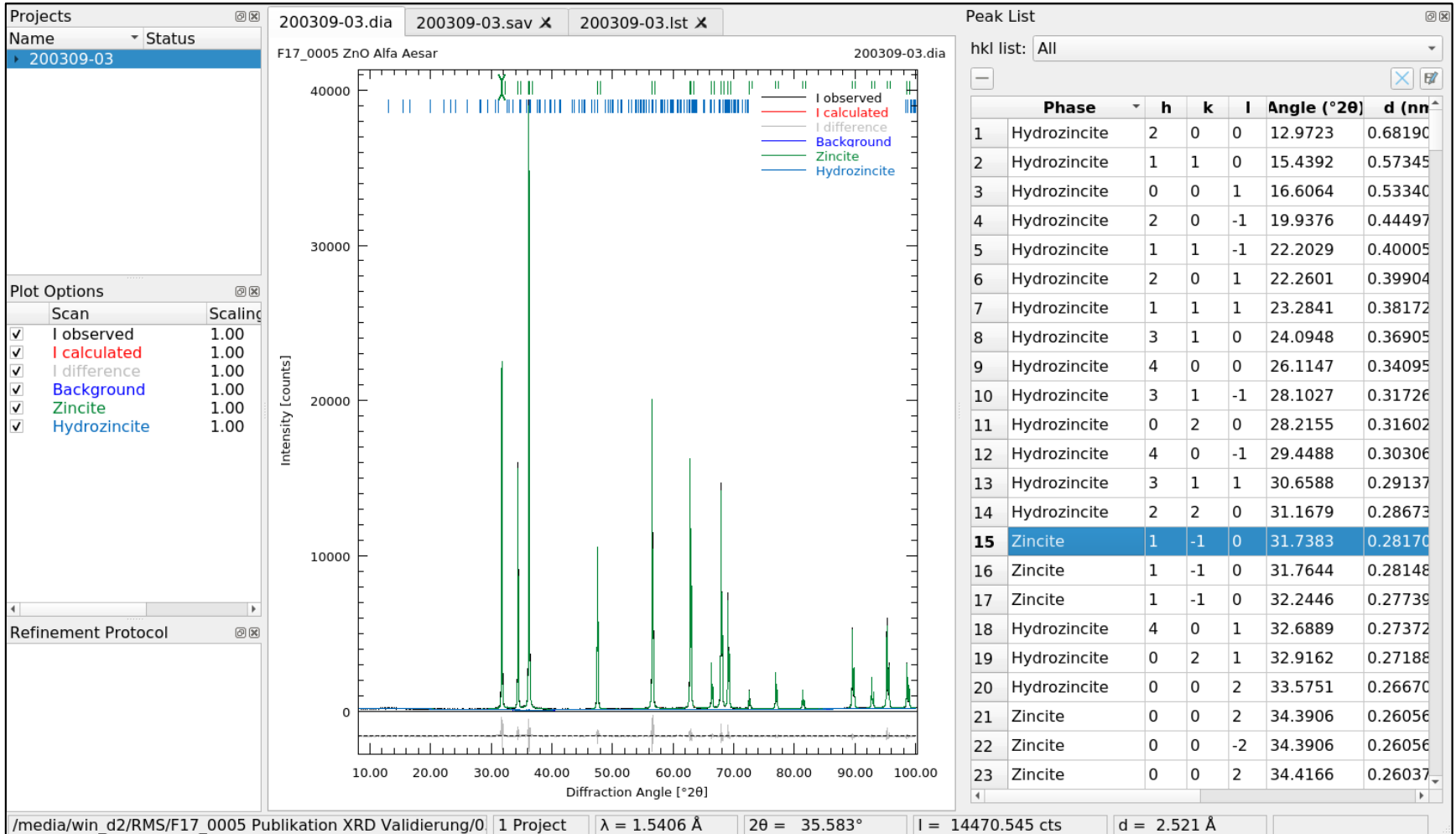
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A new module for generic peak fitting:

- Gaussian, Lorentzian, Pseudo-Voigt, Pearson-VII peak functions
- Split functions for asymmetric peaks
- Polynomial background functions



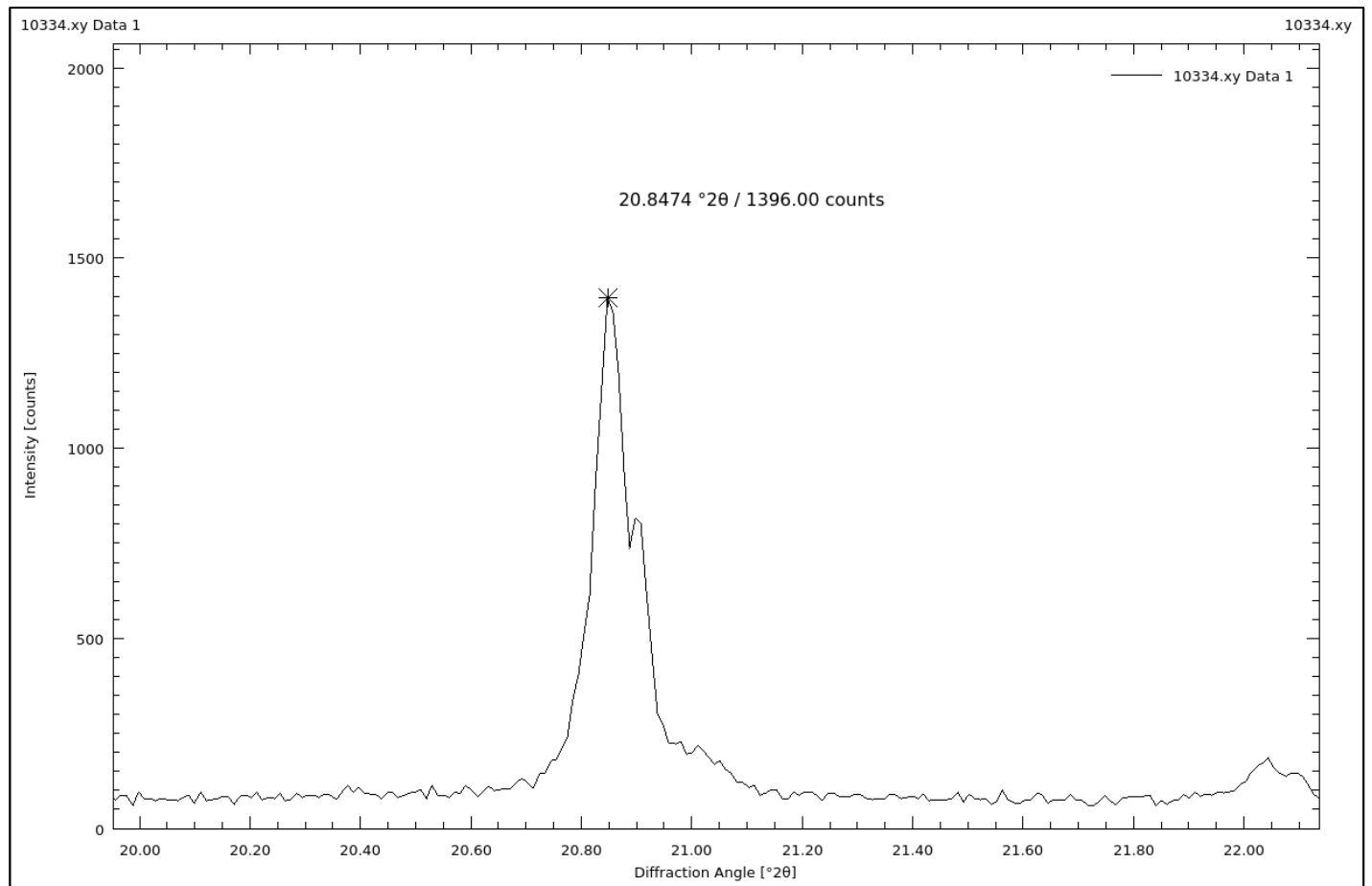
Peak list to analyze refined peak data  
(from BGMN \*.par file)



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New „data inspection“ cursor („i“ key)



More options to improve phase matching (reduce false-positive phase matches)

Restrict unit cell variability

Restrict crystallinity for residual searches

The screenshot displays the PROFEX Search/Match Phases window. It features three tabs: Database, Controls, and Results. The Results tab is active, showing a list of search results with columns for File and FoM. The FoM values are color-coded: green for the highest (0.044702), blue for the next (0.043461), and red for the lowest (0.041582). The list includes files like Microlnt1.str, Kaolinite1A.str, and Muscovite2M1.str. Below the list, the Instrument section shows settings for RMS-D8-ADS-15-LynxEyeXE with characteristic radiation 'cu' and synchrotron radiation '0.0500000 nm'. The Refinement section includes 'Number of iterations' set to 10, 'Minimum angle' at 8.00, and 'Maximum angle' at 52.00. The 'Unit cell variability' dropdown is set to 'Strict' and is highlighted with a red box. The 'Sample properties' section has 'Crystallinity' set to 'High', also highlighted with a red box. A blue line connects the 'Restrict unit cell variability' text to the 'Unit cell variability' dropdown. Another blue line connects the 'Restrict crystallinity for residual searches' text to the 'Crystallinity' dropdown.

File	FoM
Microlnt1.str	0.044702
Kaolinite1A.str	0.043461
Muscovite2M1.str	0.041582

**Search/Match Phases**

Database Controls Results

Score List

Instrument

Instrument configuration: RMS-D8-ADS-15-LynxEyeXE

Characteristic radiation: cu

Synchrotron radiation: 0.0500000 nm

Refinement

Number of iterations: 10

Minimum angle: 8.00

Maximum angle: 52.00

Unit cell variability: Strict

Sample properties

Crystallinity: High

+ many more improvements:

- Performance improvements of the user interface
- Support for Malvern/PANalytical XRDML v2.0 files
- Fixed wrong sorting of projects and wrong order of batch refinements
- Fixed wrong assignment of sample ID
- Fixed wrong calculation of chemical composition when goals are normalized to 100%
- Progress dialog for various „Apply to all projects“ functions
- Major internal code modernization

