



# Full-Pattern Search-Match using the Crystallography Open Database: an internet tool



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## The NANOAIR project

The air quality is one of the major concerns for health. There is a need for continuous monitoring of the particulates especially in the submicron range. An European project named Nanoair has been concluded successfully which aim was to develop a mobile instrument for qualitative and quantitative analysis of breathable particles using XRD and SAXS.

Nanoair was granted by FP7-RTD (Grant agreement N° 222333)

## Goal of the project and general idea

Build a complete portable system that collect the dust, with automated analysis to obtain particle sizes (by SAXS), phase identification and quantification along with crystallites/microstrains (by XRD/Rietveld) and finally store all data and results online and the samples locally for reference. The idea is to use the Rietveld method also for the search-match step, as we are in any case limited to phases with known crystal structure usable in the Rietveld quantification. A Full Pattern Search-Match method has been developed and tested using the COD as an archive of crystal structures ([www.crystallography.net](http://www.crystallography.net)).

### Information card for 2105483

2105482 << 2105483 >> 2105484

**Preview**



**Coordinates** 2105483.cif  
**Structure factors** 2105483.hkl  
**Original IUCr paper** HTML

**Structure parameters**

Formula	-CS H12 N2 O 5 -
Calculated formula	-CS H12 N2 O 5 -
Title of publication	Methylthioureas and their morpholine and dioxane adducts, hydrogen-bonding patterns
Authors of publication	Jones, Peter G.; Thomas, Christina; Teschmit, Nicole; Thomas, Lena
Journal of publication	Acta Crystallographica Section B
Year of publication	2013
Journal volume	69
Journal issue	4
Pages of publication	405 - 413
a	6.847 ± 0.0004 Å
b	7.0982 ± 0.0004 Å
c	8.6412 ± 0.0003 Å
α	106.676 ± 0.005°
β	105.448 ± 0.005°
γ	90.679 ± 0.004°
Cell volume	386 ± 0.04 Å <sup>3</sup>
Cell temperature	100 ± 2 K

## WWW.CRYSTALLOGRAPHY.NET

Crystallography Open Database



Open-access collection of crystal structures of organic, inorganic, metal-organic compounds and minerals, excluding biopolymers

All data on this site have been placed in the public domain by the contributors.

COD Advisory Board thanks The Research Council of Lithuania for their financial support of the publication "Crystallography Open Database (COD): an open-access collection of crystal structures and platform for world-wide collaboration".

Nucleic Acids Research, (2012) EDE version

We thank Crystal Impact GmbH for their financial support of the publication "Crystallography Open Database - an open-access collection of crystal structures".

J. Appl. Crystallogr. (2009) EDE version

Currently there are 241466 entries in the COD.  
Latest deposited structure: 2110550 on 2013-11-06 at 12:23:17 UTC

CFI's Donators



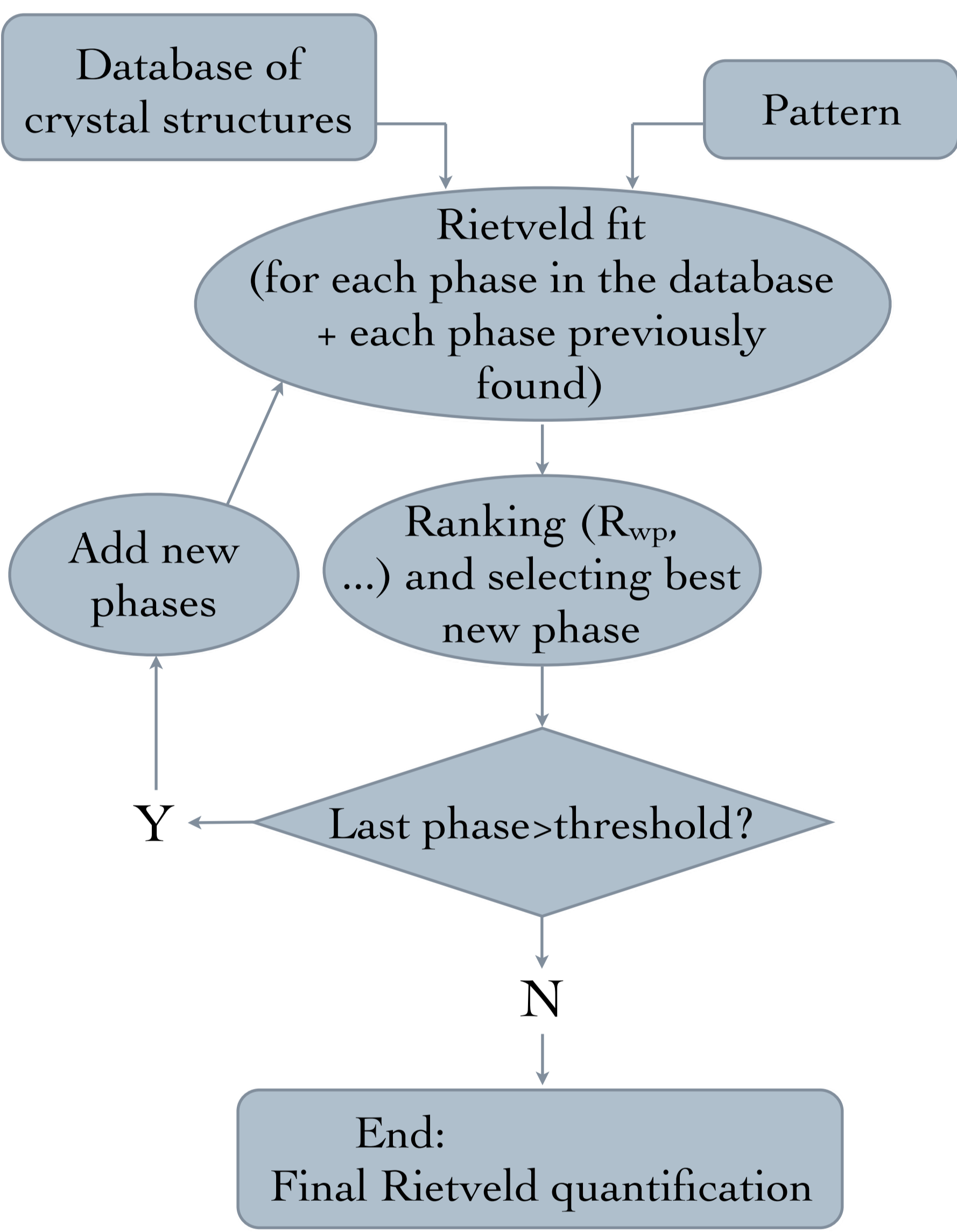
Advisory Board

Daniel Chateigner, Xiaolong Chen, Marco Ciriotti, Robert J. Downs, Sushil G. Ghoshal, Arnel Le Bail, Luca Lutterotti, Yoshihiko Masahashi, Peter Moeck, Miguel Quintero Olmosbal, Hareesh Rajan, Alexandre F.T. Yokochi

## The FPSM (Full Pattern Search-Match method)

Developed inside the Nanoair project for the portable instrument

- Pro:**
- No user intervention, automatic analysis
  - No peaks location/detection required (works with nano materials/particles)
  - Full Rietveld quantitative analysis provided
  - Works also for neutron and electron diffraction
- Cons:**
- Only phases with known crystal structure are ready to be used (unknown structures require a list of peaks and calibrated intensities, PONKS)
  - Available databases are still incomplete
  - If no elemental composition provided → requires > 20 minutes on 12 cores computer
  - Good ranking algorithm required for very small phase amount



Full Profile Search Match

Up L. Lutterotti using COD

The "FPSM method" uses a Rietveld-like fitting procedure to test all possible crystal structures from a database rank them and find the most probable in your diffraction pattern. In the end a Rietveld phase quantification is done with the phases identified. Be aware that if a phase is not present in the database (COD) it cannot be found nor quantify, so this method is limited to only the phases for which a crystal structure has been determined and has been updated in the database. This page has been constructed for your reference, so people to use the method and not on their data. To use it you need to upload a diffraction pattern in proper format: the .azw or .hkl file format with an .info file. The latter contains the alpha coordinate of space for (hkl), the second column the intensity corrected for incident intensity for (hkl). You need also to specify some additional instrument characteristics (scattering geometry etc.). If the selected instrumental broadening function match the one of your instrument, then a reasonable analysis of crystallite size and microstrain is reported.

See paper: L. Lutterotti, H. Pillière, C. Fontugne, P. Boulay, D. Chateigner (2013), submitted to J. Appl. Cryst.

Diffraction pattern and sample composition

Upload diffraction pattern: Choose file to be selected

Structure database: CODstructures set1

Atomic elements in the sample: O Ca F Zn

Crystallization: none

Experiment details

Radiation: X-ray tube: Cu

Other: none

Wavelength (Å): 1.54056

Instrument geometry: Bragg-Brentano (theta-theta)

Detector: Debye-Scherrer

Transmission

Instrument broadening function: Median

Search and quantify

DISCLAIMER

Your uploaded file will not be stored locally in our server and is only kept in memory during the computation. We have no access, nor interest in keeping your experimental data or results. The FPSM method will not be able to find a phase if it is not present in the database. At the moment the database is constructed using all phases in the COD. So it is extremely important to contribute and donate updated crystal structures to the COD to make it more complete. If you are willing to give us some feedback on the analysis or results, or want to contribute to maintain the service, send us email to: l.lutterotti@ing.unita.it, d.chateigner@inel.fr, with the diff.

inel CiMap UNICEN CNRS ENSICAEN CFI

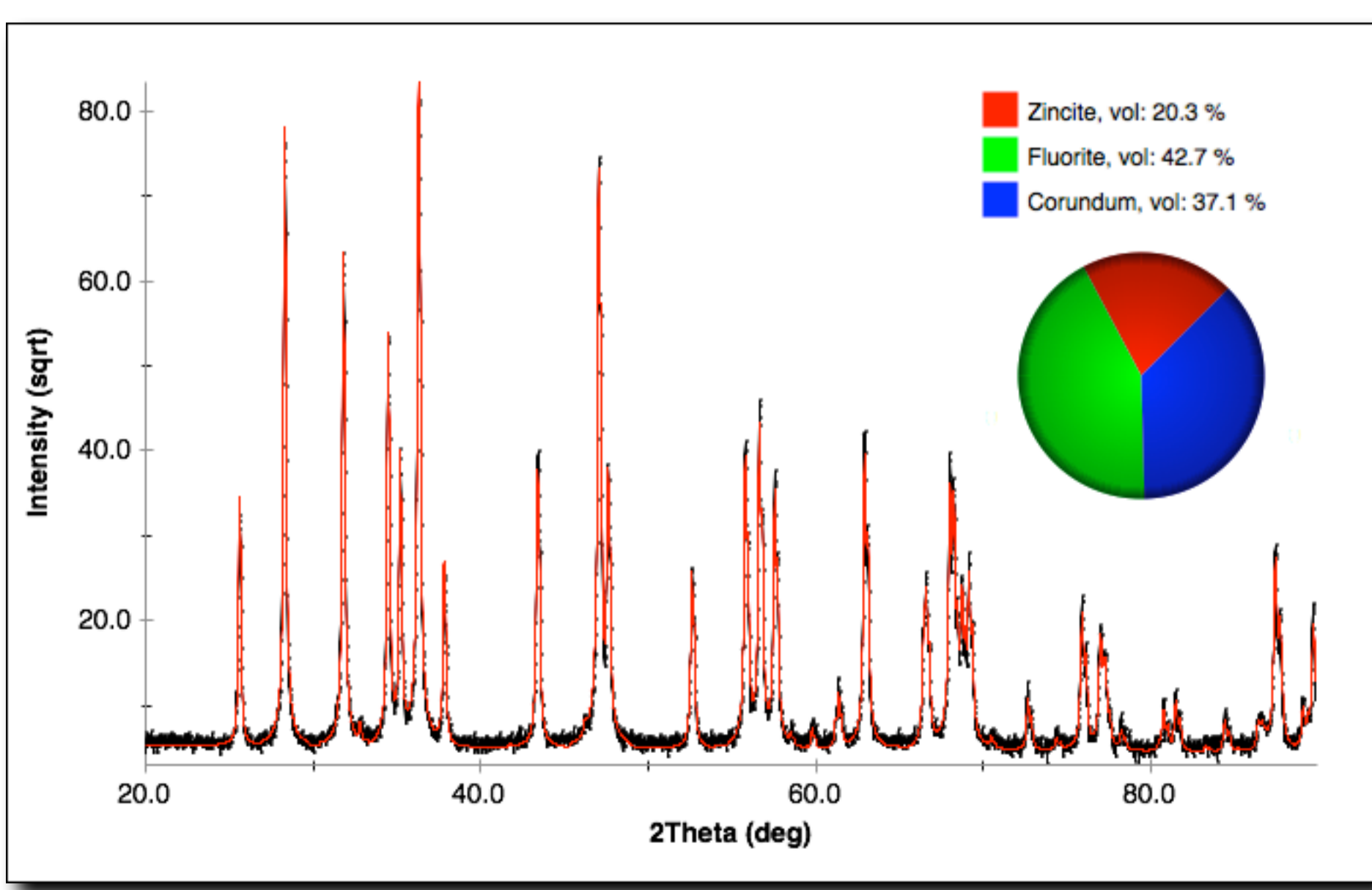
The first version of the FPSM method and program has been developed inside the Nanoair project by L. Lutterotti with INEL, the web version being a professional version at UNICEN/ENSICAEN. It is Open under request of UNICEN/ENSICAEN.

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An open internet version has been set up at: <http://cod.iutcaen.unicaen.fr>  
<http://nanoair.ing.unita.it:8080/sfpm>  
search and quantification is limited by the time required (or better server response time) so it should be used restricting the composition as much as possible to speed up computation. A limited number of concurrent connections are supported also. INEL SAS can be inquired for the full version.

## Testing FPSM using the COD

Sample cpd1h from quantitative analysis Round-Robin  
<http://www.iucr.org/resources/commissions/powder-diffraction/projects/qarr>



Phase (wt%)	FPSM	Round-Robin
ZnO	29	29.6
CaF	33.9	34.3
Al <sub>2</sub> O <sub>3</sub>	37.1	36.1

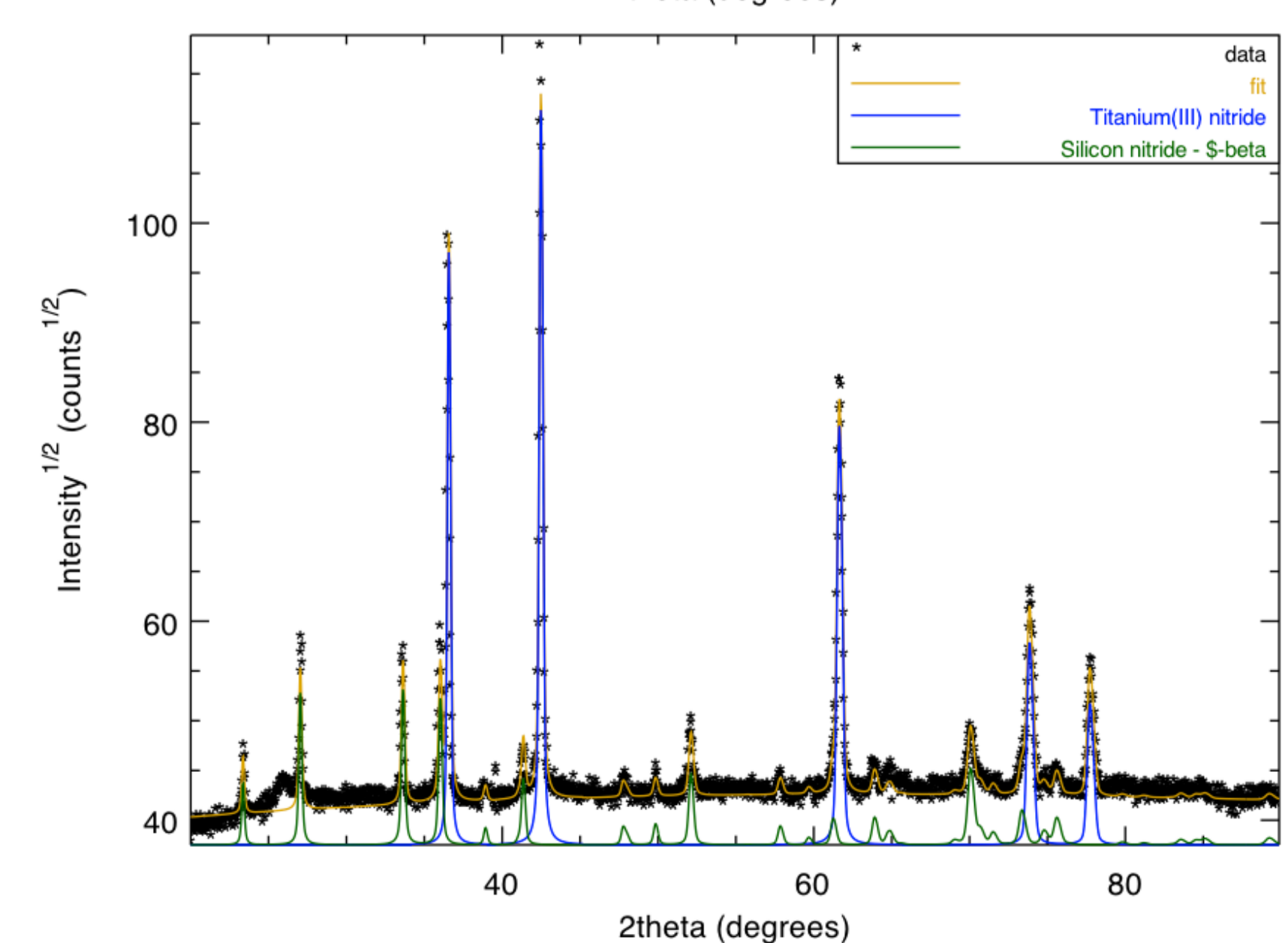
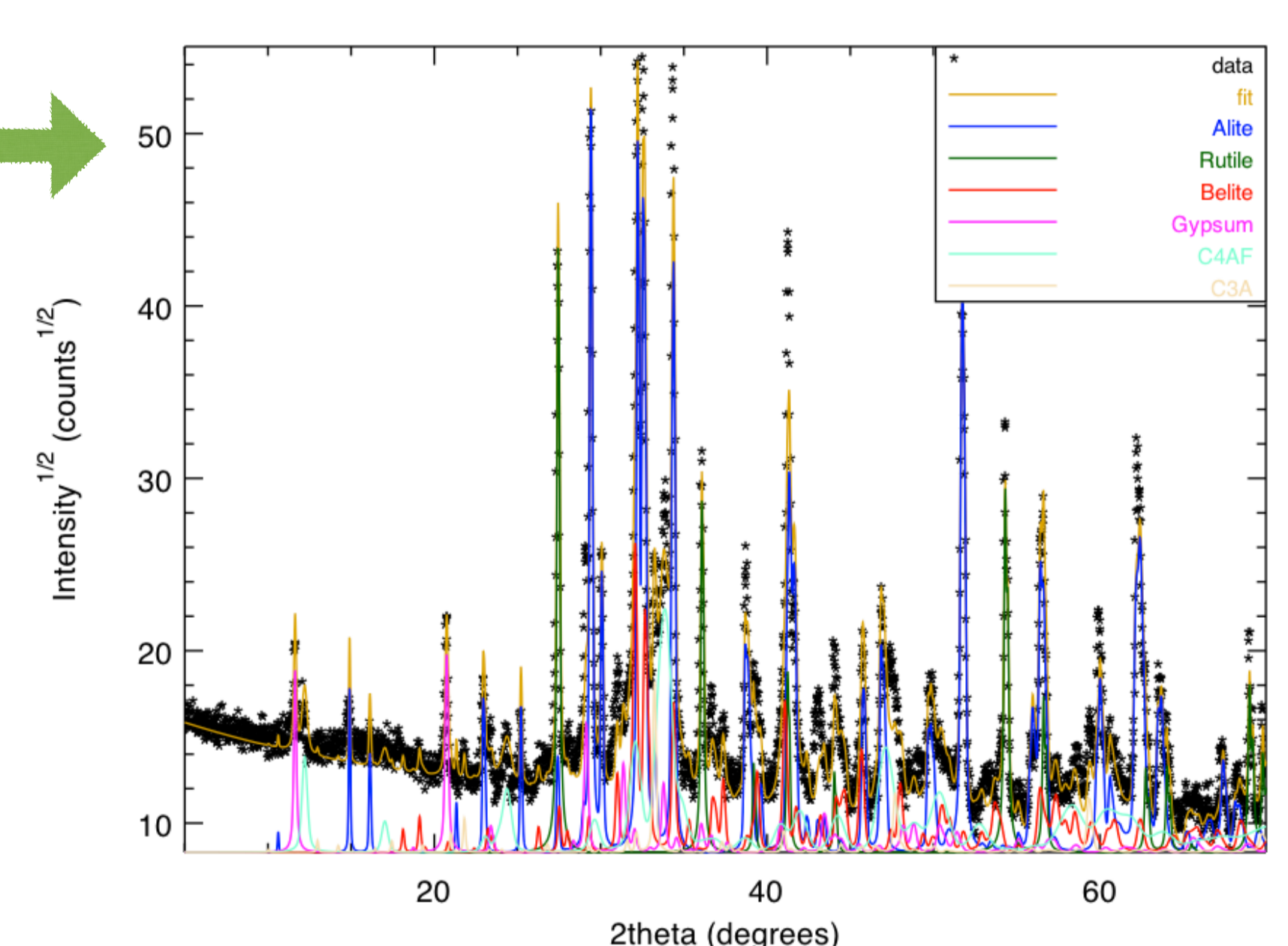
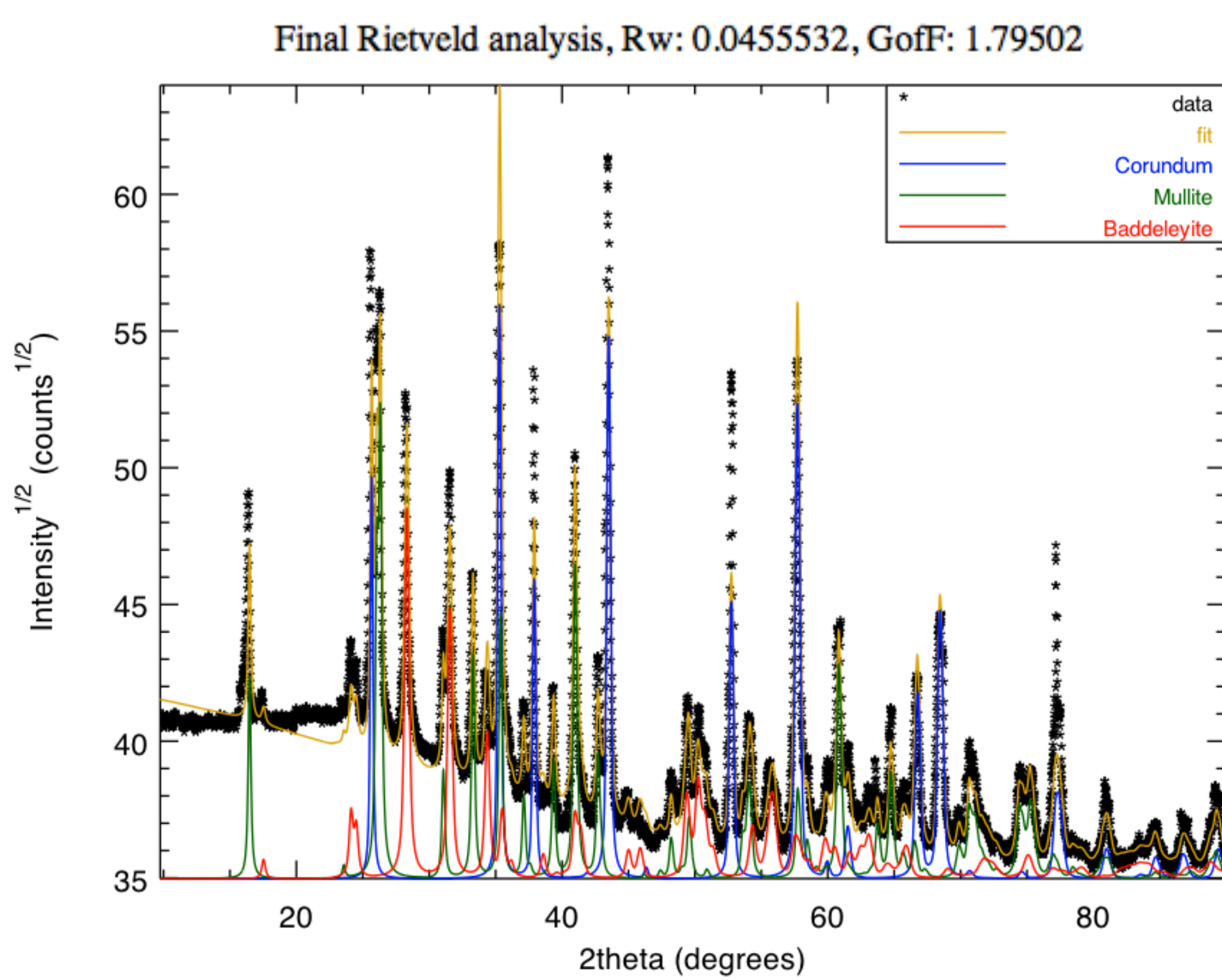
Total computation time (12 cores, 2.93GHz, COD, inorganic):

- No composition restriction: **565 secs**
- Only Al, Ca, F, Zn, O, Mg, Na, Si, Cl: **19 secs**

name	vol. (%)	wt. (%)	crystallites (Å)	microstrain
Alite	52.3359	50.1148	2722.86	0.000913623
Rutile	8.7909	11.3199	1382.41	4.9784e-05
Belite	14.6584	14.8578	1014.1	0.00145265
Gypsum	7.28186	5.03503	881.992	0.00175863
C4AF	14.4548	16.3939	485.795	0.00705494
C3A	2.47814	2.27862	1426.2	0.00125916

Some additional phases (cement phases) can be user added to the database if not present in the COD

Phase ID	name	vol. (%)	wt. (%)	crystallites (Å)	microstrain
9009672	Corundum	41.0726	45.1467	730.664	0.00137145
9005502	Mullite	53.5784	46.2318	515.483	0.000527227
9005833	Baddeleyite	5.34905	8.62151	371.805	0.00203445



Phase ID	name	vol. (%)	wt. (%)	crystallites (Å)	microstrain
1101045	Titanium(III) nitride	50.0729	62.8891	1682.09	0.00122093
1001246	Silicon nitride - S-beta	49.9271	37.1109	800.99	0.00129495

Final Rietveld analysis, R<sub>w</sub>: 0.0601521, Goff: 2.66024