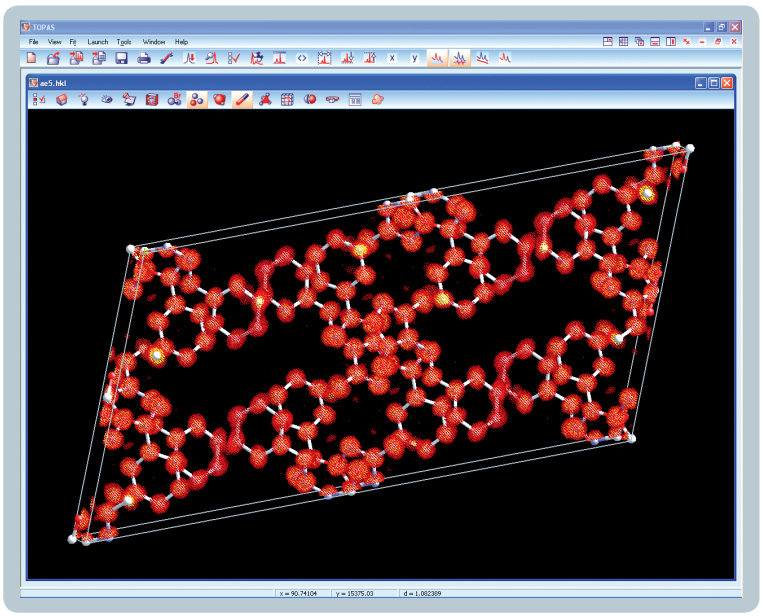
TOPAS

New!
Version 4

Total Pattern Analysis Solutions

Charge Flipping - 3D Fourier Maps - VCT - PONKCS



TOPAS V4 comes with a series of exciting new innovations, offering new and important capabilities specifically for crystal structure and quantitative phase analysis.

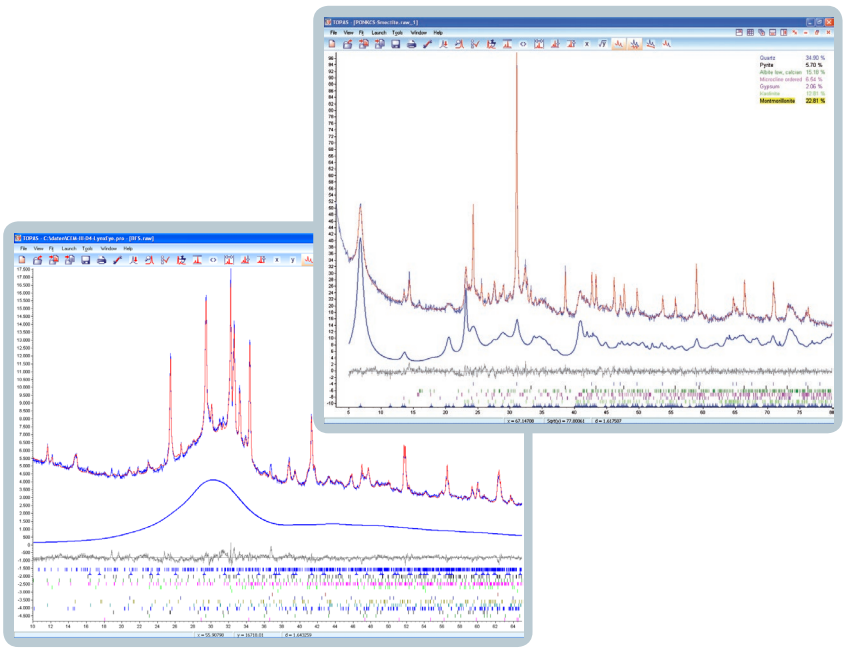
The highlights are:

Structure analysis:

- The **Charge Flipping** method for ab-initio structure determination [1, 2].
- **3D Fourier maps** for completion of partial structure models including advanced atom picking capabilities.
- **VCT:** Support of Variable Counting Time data to compensate the natural intensity fall-off towards higher angles 2Θ with X-ray diffraction

Quantitative phase analysis:

The **PONKCS method** [3] for accurate quantification of compounds, where the classic Rietveld method cannot be applied. Amorphous phases, disordered phases, or phases with unknown crystal structures can be quantified with the same accuracy as for well-defined crystalline phases.



TOPAS V4 - What's New?

Graphical user interface:

- Completely new graphical user interface with Windows XP look & feel
- The Structure Viewer window is now combined with the Rigid Body Editor

Structure analysis:

- The Charge Flipping method
- 3D Fourier maps
- Support of Variable Counting Time data
- The Cloud method - an atomic position averaging technique for the visual display of atomic movements
- Torsion angle penalties to complement distance and angle restraints

New fundamental parameters:

- Support of position sensitive detectors (LynxExe, VÅNTEC-1)
- Support of capillary geometry
- Beam overflow correction (peak shape and intensity)

General:

- Support of scattering factors of atoms / ions with Z>92
- Support of user-defined scattering factors
- Double precision for absolutely everything achieving greater stability for refinements with many parameters or high correlations
- The bootstrap method of error determination
- Bootstrap errors for fractional coordinates that are a function of a rigid body

References:

[1] Coelho, A. A. (2007): A Charge Flipping algorithm incorporating the tangent formula for solving difficult structures. - Acta Cryst., A36, 400–406.

[2] Oszlányi, G. & Süto A. (2004): Ab initio structure solution by charge flipping. - Acta Cryst., A60, 134-141.

[3] Scarlett, N.V.Y. & Madsen, I.C. (2006): Quantification of phases with partial or no known crystal structure. - Powder Diffraction, 21(4), 278-284

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