

QUANTITATIVE ANALYSIS OF PHASES WITH PARTIAL OR NO KNOWN CRYSTAL STRUCTURE

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The method of quantitative analysis of phases with Partial Or No Known Crystal Structure, PONKCS [1], allows the accurate quantification of compounds, where the classic Rietveld method or other classic quantification methods fail. Amorphous phases, disordered phases, or phases with unknown crystal structures (e.g. new polymorphs) can be quantified with the same or even higher accuracy as for well-defined crystalline phases.

With PONKCS, crystal structure information is replaced by measured intensities from a reference sample, requiring calibration using an internal standard. As a result, extremely accurate results can be also obtained in cases, where classic Rietveld analysis cannot be applied at all.

The methodology and examples will be discussed.

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