BGMNWrapper – a tool for efficient parametric Rietveld refinements of clay samples

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X-ray powder diffraction (XRD) in combination with the Rietveld method became one of the most common methods used for quantitative analysis of clay mineral mixtures. The development of structural based disorder models for disordered layer stacks additionally allows the refinement of disorder parameters like stacking vectors or stacking probabilities [1], even in mixtures of several disordered minerals. The correct choice of structure models is essential for a successful Rietveld refinement. However, this is difficult in case of coexisting clay minerals, even with detailed examinations like pre-treatments by intercalations or heating procedures. One way to verify the uniqueness and also to reduce the number of refineable parameters is the parametric Rietveld refinement [2]. This means that different measurements of a sample under different conditions will be fitted in one overall refinement by the connection of the structural models via external parameters, for example the swelling behaviour.

One of the Rietveld programs which is capable to apply disorder models in a parametric refinement procedure is BGMN [3]. BGMN was implemented in the graphical user interface Profex [4]. The combination of BGMN and Profex allows a user-friendly quantification of large sample series as well as the examination of one-dimensional patterns of oriented mounts. Unfortunately, Profex has not been designed to support parametric refinements in BGMN.

The modification and connection of input text files is required in the background of the refinement procedure to allow parametric refinements in BGMN. Therefore, the software BGMNWrapper has been developed. BGMNWrapper allows the parallel display of several refinements (graphics and text), the transfer of parameters from one refinement to others and to switch between individual refinements and parametrical refinements. Parametric refinements of one set of measurements can automatically be transferred to other sample series. The various possibilities of BGMNWrapper will be demonstrated on typical clay samples, measured as bulk and as oriented mounts in air-dried and ethylene glycol intercalated conditions.

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