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The nature of disorder in montmorillonite by simulation of X-ray powder patterns

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ABSTRACT

The planar disorder of Ca-montmorillonite (Fuller's earth) has been investigated using structural simulations of X-ray powder patterns. A standard sample was fully characterized using chemical, microscopic, and diffraction methods. Earlier models of disorder taken from the literature and newly formulated combined models were used to generate simulated powder patterns to be compared with the experimental spectrum.

A new model of disorder with random shifts of $-\mathbf{a}/3$ and $\pm\mathbf{b}/3$, with a total density of defects of 75%, gives the best fit to the observed data. Thus, the sample cannot be classified as a turbostratic structure (fully disordered) and consequently turbostratic disorder does not invariably apply to all smectite samples. These findings open a debate on the nature and application of turbostratic disorder: is it possible for smectite samples to have intermediate degrees of disorder between a fully disordered stacking (turbostratic) and a highly faulted but well-defined stacking or is the result obtained for the Ca-montmorillonite just an exception?

This model of disorder is useful for the quantitative phase analysis by X-ray powder diffraction based on the Rietveld method, which can now benefit from a more reliable initial structure model for Ca-montmorillonite and which will improve the accuracy of the weight-fraction estimates.