

The crystal structure of feitknechtite (β -MnOOH) and a new MnOOH polymorph

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ABSTRACT

Studies suggest that feitknechtite (β -MnOOH) is a prevalent, and perhaps necessary, intermediate phase during the synthesis of birnessite-like phases, the abiotic oxidation of Mn^{2+} , and the transformation of biogenic hexagonal phylломanganates to more complex Mn oxides in laboratory and natural systems. Researchers have generally described feitknechtite as consisting of pyrochroite-like (or cadmium iodide-like) Mn-O octahedral layers, but a detailed crystal structure has not been reported. We used TEM/SAED and powder XRD and Rietveld refinements to derive the unit cell and, for the first time, report a complete structure description for feitknechtite (β -MnOOH). Rietveld refinements were also completed for three natural feitknechtite/hausmannite samples, and time-resolved synchrotron XRD experiments were used to follow the thermal transformation of feitknechtite to hausmannite. Additionally, we identified and report the structure for a second, and perhaps novel, MnOOH polymorph (proposed designation ϵ -MnOOH), mixed with the synthetic feitknechtite, that is similar to β -MnOOH but with a different layer stacking.

Keywords: Feitknechtite, manganese oxide, Beta-MnOOH, Rietveld, birnessite