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Evidence on the structure of synthetic schwertmannite

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ABSTRACT

Evidence from transmission electron microscopy (TEM) and electron nanodiffraction (END) provides a new understanding of schwertmannite, an iron oxyhydroxysulfate mineral. The ball-and-whisker, or "hedge-hog," morphology of schwertmannite particles makes a complete structural interpretation difficult, but no evidence for a "modified" akaganeite structure was found in this study. END analyses suggest that most schwertmannite whiskers have a structure consistent with the maghemite-like structural component previously described by Janney et al. (2000a) for ferrihydrite. Some sections of whiskers also contain the previously described highly disordered ferrihydrite structural component (Janney et al. 2000a), and more amorphous regions. Under certain conditions in an electron microscope, schwertmannite particles transformed to crystalline cubic and hexagonal phases. During this process, sulfate and OH/H_2O were ejected from the structure, confirming sulfate to be structurally incorporated. The existence in schwertmannite whiskers of such structural components may seem unlikely, as it contradicts previous conclusions concerning the octahedral coordination of Fe^{3+} and the location of sulfate in the structure. It has been hypothesized, however, that the incorporation of OH/H_2O and sulfate may permit an octahedral coordination of Fe^{3+} in a cubic-close-packed arrangement. Unfortunately, the thickness of the schwertmannite aggregates precludes determination of whether they consist solely of whiskers (containing the maghemite-like/highly disordered/amorphous structural components) radiating from a central point or if a structurally distinct material resides within the core of these aggregates. This study provides a new perspective of the schwertmannite structure, and its relationship to ferrihydrite, as both contain similar structural components.