

The structure of schwertmannite, a nanocrystalline iron oxyhydroxysulfate

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ABSTRACT

Schwertmannite is a poorly crystalline mineral that forms ochre rusts and precipitates in acid mine environments. Despite its ubiquity and its role as scavenger of important contaminants such as arsenic or selenium, its structure has not been yet determined. Here, a structure for schwertmannite is presented based on pair distribution function (PDF) data, X-ray diffraction (XRD) analyses, and density functional theory (DFT) calculations. We propose a structure formed by a deformed frame of iron octahedra similar to that of akaganeite. Simulations of X-ray diffraction patterns unveil the presence of long-range order associated with the position of the sulfate molecules, providing a useful way to discern two types of sulfate complexes in the structure. The simulations suggest that two sulfate molecules per unit cell are present in the structure forming one outer sphere and one inner sphere complex inside the channels formed by iron octahedra. Knowledge of the positions of the sulfates in the structure will help to better understand exchange processes with oxyanions of trace contaminants, such as arsenate, chromate, or selenate, that strongly influence their biogeochemical cycling in mining ecosystems.

Keywords: Schwertmannite, diffraction, structure, X-ray, pair distribution function, DFT, iron, sulfate