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Arsenate sorption on schwertmannite

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ABSTRACT

The sorption mechanism of arsenate [As(V)] on schwertmannite was investigated by means of batch sorption experiments as a function of As(V) concentration in acidic solution at 25 °C. Structural simulation indicated that the surface sites of schwertmannite comprised various O atom (or hydroxyl) and SO_4 groups. Sorption experiments showed that the reactive sites for As(V) sorption are surface-coordinated SO_4 groups rather than surface hydroxyl groups, as reported in earlier studies. The As(V) sorption mechanism involves ligand exchange with surface-adsorbed and structural SO_4. The results of the sorption experiments also suggested monodentate As(V) coordination at the surface-adsorbed SO_4 sites [$(Fe_1)_2SO_4$] and bidentate As(V) coordination at the structural SO_4 sites [$(Fe_3)_2SO_4$]. The overall ligand-exchange reaction was

$$0.61\ (Fe_1)_2SO_4 + 0.39\ (Fe_3)_2SO_4 + 1.61\ H_2AsO_4^- \rightarrow 1.22\ Fe_1H_2AsO_4 + 0.39\ (Fe_3)_2HAsO_4 + 0.39\ H^+ + SO_4^{2-}$$

where the 1 and 3 in Fe_1 and Fe_3 are coordination numbers. The equilibrium constant derived for the exchange reaction, $\log K_{EX} = 4.96$, describes the observed As(V) sorption behavior. Nanocrystalline materials like schwertmannite are widespread in nature and typically contain significant amounts of anionic impurities, such as sulfate and silicate. Our results indicate that the effects of impurities can be significant and should be considered in order to gain a realistic understanding of sorption processes in natural systems.