

Title

In Situ Spectroscopic Investigation on Arsenate Surface Speciation at the Hematite-Water Interface.

TSNo

s02-arai134604-O

PaperType

O

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Keywords

ARSENATE	HEMATITE
ADSORPTION	

abstract

Arsenate (As(V)) is a ubiquitous toxic metalloid in oxic terrestrial/aquatic environments due to indigenous and anthropogenic inputs. In order to accurately predict the transport of As(V) in subsurface environments, detailed mechanistic information (i.e., stoichiometric reactions and surface complexes) is needed to better understand As(V) reactions at soil mineral-water interfaces. In this study, we investigated As(V) coordination environments at the hematite-water interface as a function of pH and loading level. The As(V) adsorption (8 g L⁻¹ and [As(V)]₀ = 0.45 mmol) on the hematite surface increased from 60 % to @100 % with decreasing pH from 9 to 4. Extended X-ray absorption fine structure (EXAFS) spectroscopic analysis of the As(V) sorption samples revealed two As-Fe distances of ~3.30 and ~3.50 angstroms at a loading level 0.63-1.46 micro-mol/m² at pH 4.5-8, indicating the formation of different inner-sphere bidentate binuclear complexes on edge-sharing and face-sharing iron octahedral sites. In situ Attenuated Total Reflectance Fourier transform infrared spectroscopy (ATR-FTIR) will be used to further investigate the molecular symmetry of As(V) surface complexes with respect to surface coordination and protonation.

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