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99 - Sulfate adsorption on ferrihydrite studied by sulfur K-edge EXAFS spectroscopy and differential PDF analyses

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Sulfate adsorption on iron oxides is an important environmental chemical process. However, the adsorption topology has remained unclear. We have determined the S-Fe distances in the sulfate sorption complexes on ferrihydrite in 0.1 M NaNO $_3$ solution at pH 4 using sulfur K-edge X-ray absorption spectroscopy and differential X-ray pair distribution functions (d-PDF). The S XANES spectrum had a pre-edge peak characteristic of S-O-Fe linkages, suggesting sulfate inner-sphere complexes. S EXAFS fitting indicated a S-Fe inter-atomic distance of 3.16 \pm 0.06 Å. Fitting of the spectrum of K-jarosite resolved a S-Fe distance of 3.19 \pm 0.05 Å, in agreement with the 3.22 Å distance in the jarosite crystal structure, demonstrating the reliability of the S EXAFS fittings. The d-PDF analysis of the sorption samples revealed a S-Fe distance of 3.25 \pm 0.02 Å, consistent with the EXAFS result. Ongoing research and calculations are investigating the adsorption topology based on these results.

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