

Yttrium speciation in sulfate-rich hydrothermal ore-forming fluids

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Rare earth elements (REE) have gained importance due to their widening industrial applications and their use as geochemical tracers. REE sulfate complexes are some of the most stable REE aqueous species in hydrothermal fluids, and may be responsible for REE transport and deposition in a wide variety of geological environments, ranging from sedimentary basins to magmatic hydrothermal settings. However, the thermodynamic properties of most REE-sulfate complexes are derived from extrapolation of ambient temperature data, since direct information on REE-sulfate complexing under hydrothermal conditions is limited to a single study that derived formation constants for Nd, Sm and Er in sulfate solutions to 250 °C (Migdisov and Williams-Jones, 2008).

In this study, we employ *ab initio* molecular dynamics (MD) simulations to calculate the speciation and thermodynamic properties of yttrium(III) in sulfate and chloride solutions at temperatures and pressures up to 500 °C and 800 bar. The MD results were complemented by *in situ* X-ray absorption spectroscopy (XAS) measurements. Our results show that yttrium(III) forms complexes with sulfate with both monodentate and bidentate structures over the investigated temperature range (200 °C to 500 °C). In simulation boxes containing both chloride and sulfate, yttrium(III) bonds with less sulfate and forms mixed Y-Cl-SO₄ complexes. The thermodynamic properties for yttrium(III) sulfate complexes derived from MD enable a better modelling of REE transport in hydrothermal systems.

Migdisov, A. A., & Williams-Jones, A. E.
(2008). *Geochimica et Cosmochimica Acta*, 72(21),
5291-5303.