

Indium (In) speciation and equilibrium In isotope fractionation between chloride-rich aqueous solution and minerals

DR. HAOCHE DUAN¹ AND FANG HUANG²

¹School of Earth and Space Sciences, University of Science and Technology of China

²University of Science and Technology of China

Presenting Author: duanhc@ustc.edu.cn

Understanding the behavior of indium during magmatic-hydrothermal and atmosphere-hydrosphere interactions requires the speciation of indium (In) in aqueous fluids associated with their isotope effects. Nonetheless, little attention has been paid to In³⁺ speciation and equilibrium indium isotope fractionation. We explore indium speciation in neutral aqueous solutions and examine reduced partition function ratios ($\ln b$) of ¹¹⁵In/¹¹³In in aqueous solutions and In-bearing minerals using the first-principles calculation. The results demonstrate that the most abundant species in aqueous solutions are InCl₃(H₂O)₅, [InCl₂(H₂O)₂]⁺, and [InCl₂(H₂O)₂]⁺·[(H₂O)₂Cl₂Na]⁺ species. The proportion of aqueous In³⁺ species fluctuates with indium contents, demonstrating that cation concentration could influence the ligand ratios. The 10³ln*b* decreases in the order dzhalindite > InCl₃(H₂O)₅ > laforetite > roquesite > cadmoindite > yixunite > indite > damiaoite > [InCl₂(H₂O)₂]⁺ ≈ [InCl₂(H₂O)₂]⁺·[(H₂O)₂Cl₂Na]⁺ > native indium. The study of equilibrium indium isotope fractionation factors not only provides new insights into the equilibrium indium isotope fractionation, but it also has a lot of potential in geological and supergene processes.