

Understanding the unique geochemical behavior of Sc in the interaction with clay minerals

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ABSTRACT

Regolith-hosted rare earth elements (REEs) deposits received great attention due to the increasing incorporation of REEs in modern technologies. In lateritic Sc deposits and ion-adsorption deposits (IADs), Sc behaves quite differently from REEs: REEs adsorb as outer-sphere complexes on clay surface in IADs, while Sc could enter the lattice of clay minerals in lateritic Sc deposits. The unique behavior of Sc has not been well understood yet. Here, by using first-principles molecular dynamics techniques, we show that the complexation mechanisms of Y^{3+} and Sc^{3+} on clay edge surfaces are distinctly different. Y^{3+} preferentially adsorbs on $Al(OH)_2SiO$ site with its coordination water protonated. Sc^{3+} is found to behave similarly to other first-row transition metals (e.g., Ni^{2+}) due to its smaller ionic radius and prefers adsorbing on the vacancy site, from where Sc^{3+} can be readily incorporated in the clay lattice. The H_2O ligands of Sc^{3+} get deprotonated upon complexation, providing new binding sites for further enrichment of Sc^{3+} . These processes prevent Sc^{3+} from being leached during weathering and lead to the formation of Sc-rich clay minerals found in lateritic deposits. Based on these results, it is revealed that the small ionic radius and high affinity to enter the vacancy on edge surfaces make Sc compatible with clay minerals and are the origin of its unique geochemical behavior.

Keywords: Scandium, rare earth elements, clay minerals, complexation mechanisms, first-principles molecular dynamics