Online Material for

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

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OM1. Complexation structures of Y^{3+} and Sc^{3+} on clay (110) surface

Y^{3+} and Sc^{3+} were initially placed on the (AlOH)(AlSiO) site and vacancy site on (110) surface. During the simulation, Y^{3+} initially complexed on the vacancy site gradually transferred to the $(AlOH)_2SiO$ site (Fig. OM1a). The average Y^{3+}-O distance was 2.33 Å. On this site, Y^{3+} was seven-fold coordinated (i.e., four H_2O ligands, two AlOHs, and one SiO) in a pentagonal bipyramid cage. Y^{3+} was tilted away from the mid-plane of the clay TOT sheet on this site. On the (AlOH)(AlSiO) site, Y^{3+} was eight-fold coordinated with six H_2Os and two AlOHs in a square antiprism geometry (Fig. OM1b). The average Y^{3+}-O distance on this site was 2.38 Å.

On the vacancy site, one water ligand of Sc^{3+} dissociated spontaneously during the simulation and the resulting structure was a slightly irregular octahedron where Sc^{3+} was six-coordinated with four surface O atoms, one OH, and one H_2O (Fig. OM1c). The average distance between Sc^{3+} and apical O, O of AlOH, O of H_2O ligand, and OH were 2.31 Å, 2.14 Å, 2.08 Å, and 1.92 Å, respectively. On the (AlOH)(AlSiO) site, Sc^{3+} was six-fold coordinated with four H_2Os, one apical O, and one AlOH (Fig. OM1d). Sc^{3+} exhibited a regular octahedron coordination geometry and located at the mid-plane of the clay TOT sheet. The average Sc^{3+}-O distance was 2.13 Å.

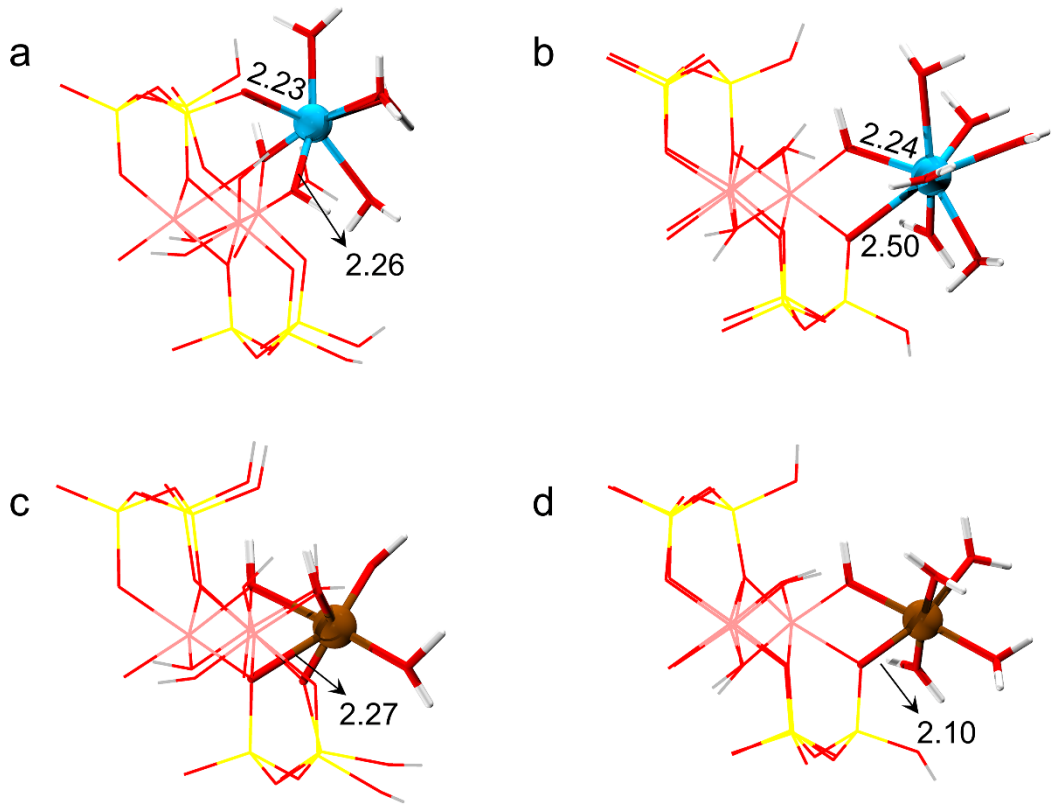

FIGURE OM1. Complexation structures of Y^{3+} and Sc^{3+} on clay (110) surface. **(a)** and **(b)** complexation structures of Y^{3+} on the $(AlOH)_2SiO$ site and the (AlOH)(AlSiO) site, respectively. **(c)** and **(d)** complexation structures of Sc^{3+} on the vacancy site and the (AlOH)(AlSiO) site, respectively. For clarity, only the nearest three Al octahedrons and Si tetrahedrons are shown. O = red, H = white, Si = yellow, Al = pink, Y = cyan, Sc = brown.