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Crystal Structures of Titanosilicates: Complimenting X-ray Powder Diffraction Techniques by Single Crystal Diffraction Methods. Akhilesh Tripathi¹, Dmitri G. Medvedev², Jose Delgado¹, Abraham Clearfield¹, ¹Dept. of Chemistry, ²Dept. of Nuclear Engineering, Texas A & M Univ., College Station, Texas 77843, USA.

Porous titanosilicates with tunnels and channels in the structure are excellent candidates for the removal of ¹³⁷Cs and ⁹⁰Sr from waste solutions at various US DOE sites. In order to optimize kinetics and capacity of ion exchange in these materials, we are studying the origin of selectivity for Cs⁺ and Sr²⁺ via structural characterizations.

Titanosilicates with the mineral pharmacosiderite topology (TSPs) generally crystallize as powders. Although, Cs⁺ exchange in TSPs retain the symmetry and space group of the parent form, Sr²⁺ exchange often results in either new phases or mixture of phases with different unit cell dimensions and symmetry thus making the task of solving the structure by ab initio methods complicated. One approach to circumvent this problem and to determine the position of Sr cations in the channels is synthesis of single crystals of heteroatom substituted pharmacosiderite phases. We have synthesized single crystals of pure germanate with TSP topology in the K-form and a Sr exchange in the single crystals has revealed the Sr sites. The Sr positions obtained from single crystal study can be used to build a model for structural characterization using Rietveld refinement technique on the X-ray powder diffraction data for the titanosilicate phase. Attempts to synthesize single crystal of some other substituted pharmacosiderite phases such as silicogermanate, vanadogermanate and vanadosilicate are in progress to detail the origin of Sr selectivity in titanosilicates.