

Synthesis and Characterization of Sr₁₂Al₁₄O₃₃

Claudia Rawn¹, Katherine (Katie) Loughlin², Michael Koehler³

¹University of Tennessee Knoxville ²University of Tennessee, Knoxville, ³University of Tennessee, Knoxville

crawn@utk.edu

Ca₁₂Al₁₄O₃₃ has many interesting and potentially exploitable properties that arise from its crystal structure. The compound is known for being a room-temperature inorganic electride, and depending on the processing conditions, it can have near-metallic electrical conductivity. The unit cell is cubic, space group $I4\bar{3}d$ (no. 220), with a lattice parameter of ~ 12 Å and contains two formula units. The Ca, Al, and majority of the O create a framework of twelve cages per unit cell, within which the remaining two O are occluded. Isostructural compounds with different cation combinations may result in larger cages and enhanced properties. Using wet chemical methods and initially dissolving Al(NO₃)₃ • 9H₂O and SrCl₂ • 6H₂O in deionized H₂O, Sr₁₂Al₁₄O₃₃ has been synthesized, but attempts to eliminate secondary phases have not succeeded. Room temperature and high temperature X-ray diffraction data have been used to track the phase evolution. One consideration based on the synthesis is that Cl⁻, with a significantly larger ionic radius than O²⁻, is being occluded; the replacement of the divalent O with monovalent Cl would allow for more cages to be filled. However, the cage occupant is difficult to interrogate due to the low occupancy.