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Synthesis and structural characterization of the hexagonal anti-perovskite Na_2CaVO_4F

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A high-resolution neutron powder diffraction technique was used to observe and refine the structural details of the ordered hexagonal oxyfluoride Na_2CaVO_4F. Polycrystalline samples were prepared via solid-state synthesis using stoichiometric amounts of high pure starting materials. The structural changes between 25°C and 750°C revealed that the two structural subunits contained within this material exhibit different behavior when heated. There is an expansion of the face-shared FNa_4Ca_2 octahedra while the VO_4 tetrahedra due to increased thermal disorder reveal marginal bond contractions. The bond valence method is employed to compare observed and ideal bond distances and point to a structural instability at 750°C. The Echidna high-resolution powder diffractometer located at the OPAL Research Reactor of the Australian Nuclear Science and Technology Organization (ANSTO) was used for both room temperature and temperature-dependent studies whereby diffraction data was collected using a neutron beam with a wavelength of 1.6215(1) Å using a Ge (335) monochromator. All preliminary structural information was collected using a benchtop X-ray diffractometer using Cu-Kα (1.54059 Å) over the range of 3-149° 2-theta. Both X-ray and neutron diffraction data was refined using the GSAS suite of programs.

Biography

Robert L Green has earned his BS from Morehouse College, an MS from Purdue University and his PhD from the University of South Carolina in Chemistry. For the majority of his 12 years career in higher education, he has devoted time to promoting STEM education to both K-12 teachers and students underserved communities. He is a Member of the American Chemical Society and is the Founder of the Florida Polytechnic University Chapter of the National Society of Black Engineers (NSBE).

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