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Studies on Structural Phase Transitions on 1:3 Ordered Perovskites $Ba_{4-x}Sr_xNaSb_3O_{12}$

Q. Zhou, B. J. Kennedy

School of Chemistry, The University of Sydney, Sydney, NSW, Australia

As part of our ongoing studies of the structures and phase transitions in perovskites oxides, 25 members of the series of 1:3 ordered perovskites of the type $Ba_{4-x}Sr_xNaSb_3O_{12}$ have been synthesized and their structures determined using synchrotron X-ray and neutron powder diffraction techniques. At room temperature $Ba_4NaSb_3O_{12}$ has a cubic structure, where the Na and Sb cations are ordered but there is no tilting of the octahedra. As the average size of the A-site cation decreases tilting of the octahedra is introduced and ultimately $Sr_4NaSb_3O_{12}$ presents a monoclinic structure in space group $P2_1/n$. The powder neutron diffraction studies show that the two orthorhombic and tetragonal phases of *Cmca* and *P*4/*mnc* co-exist at room temperature for samples with *x* between 2 and 3.

Variable temperature synchrotron powder diffraction studies demonstrate that a discontinuous transition from orthorhombic *Cmca* to tetragonal *P*4/*mnc* occurs at ~350 ^oC for $Ba_{1.5}Sr_{2.5}NaSb_3O_{12}$, and again, a continuous transition to the cubic structure near 550 ^oC. These experimental results are consistent with a group theoretical analysis of the phase transition in 1:3 ordered perovskites.