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Anion ordering in complex perovskite oxynitrides $\text{AM}_{0.2}\text{Ta}_{0.8}\text{O}_{2.8}\text{N}_{0.2}$ ($\text{A} = \text{Sr}, \text{Ba}$; $\text{M} = \text{Li}, \text{Na}$)

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Oxynitride-type complex perovskites, $\text{AM}_{0.2}\text{Ta}_{0.8}\text{O}_{2.8}\text{N}_{0.2}$ ($\text{A} = \text{Sr}, \text{Ba}$; $\text{M} = \text{Li}, \text{Na}$), were synthesized by the ammonolytic heating of a layered perovskite, $\text{A}_5\text{Ta}_4\text{O}_{15}$, with $0.5\text{M}_2\text{CO}_3$. A Rietveld refinement of the synchrotron X-ray and neutron powder diffraction patterns confirmed the complete structural transformation from a hexagonal layered-perovskite to a three-dimensional perovskite type, as well as the stabilization of alkali cations on the octahedral sites rather than on the dodecahedral sites in the latter. In all four compounds, M^+ and Ta^{5+} were disordered completely despite a charge difference as much as 4. The crystal symmetry of the average structure depended on the size of the dodecahedral cation; simple cubic for $\text{BaM}_{0.2}\text{Ta}_{0.8}\text{O}_{2.8}\text{N}_{0.2}$, and body-centered tetragonal for $\text{SrM}_{0.2}\text{Ta}_{0.8}\text{O}_{2.8}\text{N}_{0.2}$. This trend coincides with the symmetry transition from BaTaO_2N ($\text{Pm}\bar{3}\text{m}$) to SrTaO_2N (I4/mcm). In both $\text{SrM}_{0.2}\text{Ta}_{0.8}\text{O}_{2.8}\text{N}_{0.2}$, nitrogen atom preferentially occupied the c-axial 4a site of the tetragonal cell. Solid state magic angle spinning nuclear magnetic resonance spectroscopy showed that $\text{SrNa}_{0.2}\text{Ta}_{0.8}\text{O}_{2.8}\text{N}_{0.2}$ and $\text{BaNa}_{0.2}\text{Ta}_{0.8}\text{O}_{2.8}\text{N}_{0.2}$ exhibited marked downfield shifts of ^{23}Na , manifesting an octahedral coordination. On the other hand, the ^7Li NMR of $\text{SrLi}_{0.2}\text{Ta}_{0.8}\text{O}_{2.8}\text{N}_{0.2}$ and $\text{BaLi}_{0.2}\text{Ta}_{0.8}\text{O}_{2.8}\text{N}_{0.2}$ indicated a highly symmetrical coordination environment of Li.

Keywords

Oxynitride, Complex perovskite, Neutron diffraction, Rietveld refinement, Anion order

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