Proton conducting oxides are currently accumulating considerable attention due to their potential as efficient electrolytes in various electrochemical technologies, including intermediate temperature solid oxide fuel cells [1]. An important material is the brownmillerite structured oxide $\text{Ba}_2\text{In}_2\text{O}_5$, which may be described as an oxygen deficient variant of the perovskite structure, with alternating layers of $\text{In}_2\text{O}_3$ octahedra and $\text{In}_2\text{O}_3$ tetrahedra. Like many other oxygen-deficient oxides, $\text{Ba}_2\text{In}_2\text{O}_5$ transforms upon hydration into a hydrogen-containing material, $\text{Ba}_2\text{In}_2\text{O}_5(\text{H}_2\text{O})$, which show proton conducting properties. In this contribution, I will report on detailed investigations of the local structure and dehydration mechanism of $\text{Ba}_2\text{In}_2\text{O}_5(\text{H}_2\text{O})$, using a combination of variable temperature Raman spectroscopy together with inelastic neutron scattering and computer simulations [2,3]. The results suggest that $\text{Ba}_2\text{In}_2\text{O}_5(\text{H}_2\text{O})$ evolves upon heating from a perovskite-like structure for the fully hydrated material ($x=1$) at room temperature, through a partially hydrated intermediate phase, appearing at ca. 370 °C, to an essentially fully dehydrated ($x \approx 0$) brownmillerite material at 600 °C. The dehydration process appears to be a two-stage mechanism characterized by a homogenous release of protons below the hydrated-to-intermediate phase transition, whereas at higher temperatures a preferential desorption of protons originating in the nominally tetrahedral layers is observed.


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