The Crystal Structure of α -La₂Mo₂O₉ and the Structural Origin of the Oxide Ion Migration Pathway

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Supplementary Data

1. Time-of-flight neutron powder diffraction data

Figure 1: Rietveld fit of the single crystal structural model of La₂Mo₂O₉ to neutron powder diffraction data collected on a 10 g sample using the SIRIUS time of flight diffractometer at

the High Energy Accelerator Research Organization (KEK). Time of flight range shown corresponds to a d-spacing range of 0.74 to 2.47 Å. 36 parameters were refined: 15 background terms, 11 terms describing peak shape, instrumental parameters and scale factors, 4 unit cell parameters and a single overall isotropic temperature factor for $\text{La}_2\text{Mo}_2\text{O}_9$; 4 unit cell parameters and a single overall isotropic temperature factor for a minor $\text{La}_2\text{Mo}_3\text{O}_{12}$ impurity, included as a second phase). Final agreement factors obtained: $R_{\text{wp}} = 3.97\%$, $R_{\text{Bragg}} = 2.03\%$.

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2. Spread of bond valence sums in the freely refined structure

Figure 2: Bond Valence sums for the 96 cations in the freely refined structure (Mo in yellow, La in green). Error bars are plotted as ± 1.5 esd's based on standard uncertainties in M-O bond lengths.