



Combined X-ray and Neutron Powder Diffraction Study on B-Site Cation Ordering in Complex Perovskite $\text{La}_2(\text{Al}_{1/2}\text{MgTa}_{1/2})\text{O}_6$

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Complex perovskite $\text{La}_2(\text{Al}_{1/2}\text{MgTa}_{1/2})\text{O}_6$ (LAMT) crystallizes in a monoclinic unit cell with space group $P2_1/n$ at room temperature. Due to little scattering contrast between the neighbouring elements Mg and Al of the periodic table, conventional X-rays could not properly resolve the mixed occupation on the B-site. Hence, complementary neutron powder diffraction studies were carried out to verify the exact B-site cation ordering in the unit cell. In this specific configuration of the B-cations, with its occupancy ratio and the presence of a heavy element Ta as well as neighbouring elements Mg and Al, only the strategy of a combined Rietveld analysis using both the X-ray and neutron powder diffraction data simultaneously succeeded in elucidating an accurate B-site cation ordering in this complex perovskite system. A full occupancy of Mg on the 2c-Wyckoff position and each a half occupancy of Al and Ta on the 2d-Wyckoff position could be resolved for the rock-salt-type ordering of the B-site cations in the monoclinic unit cell of LAMT.

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Sitzung Einordnung: Mounting Posters, Beer and light Dinner

Track Klassifizierung: Advanced Materials & Processing