

Crystal structure of $Ln_{1/3}\text{NbO}_3$ ($Ln = \text{Nd}, \text{Pr}$) and phase transition in $\text{Nd}_{1/3}\text{NbO}_3$

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The crystal structure of the A-site deficient perovskite $Ln_{1/3}\text{NbO}_3$ ($Ln = \text{Nd}, \text{Pr}$) at room temperature has been determined, for the first time, as orthorhombic in space group $Cmmm$ using high resolution neutron powder diffraction. Pertinent features are the alternation of unoccupied layers of A-sites and layers partly occupied by Ln cations, as well as out-of-phase tilting of the NbO_6 octahedra around an axis perpendicular to the direction of the cation/vacancy ordering. The phase transition behaviour of $\text{Nd}_{1/3}\text{NbO}_3$ has also been studied *in situ*. This compound undergoes a continuous phase transition at around 650°C to a tetragonal structure in space group $P4/mmm$ due to the disappearance of the octahedra tilting. The analysis of spontaneous strains shows that this phase transition is tricritical in nature.