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Structure and electronic properties of the $\text{La}_4\text{Ni}_3\text{O}_8$ KONSTANTIN LOKSHIN, TAKESHI EGAMI, University of Tennessee — The $\text{Ni}^{1+}/\text{Ni}^{2+}$ states of nickelates have the identical ($3d^9/3d^8$) electronic configuration as $\text{Cu}^{2+}/\text{Cu}^{3+}$ in the high temperature superconducting cuprates, and are expected to show interesting properties. However, $\text{La}_4\text{Ni}_3\text{O}_8$, has infinite NiO_2 layers with Ni valence 1.33 and demonstrate a magnetic transition at 105 K, which has not been explained unambiguously yet. Here we report X-rays and Neutron diffraction evidences clarifying the nature of the transition. The observed structural changes around 105 K suggest that the magnetic transition in $\text{La}_4\text{Ni}_3\text{O}_8$ originates from Jahn Teller effect that accompanies with high spin – low spin transition. Thus, at low temperature the structural motive, electronic configuration and the spin state of $\text{Ni}^{1+}/\text{Ni}^{2+}$ nickelates are identical to $\text{Cu}^{2+}/\text{Cu}^{3+}$ cuprates.

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