Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Intersite charge transfer in the A-site-ordered $LaCu_3Fe_4O_{12}$ perovskite YOUWEN LONG, Institute for Chemical Research, Kyoto University, NAOAKI HAYASHI, Graduate School of Human and Environmental Studies, Kyoto University, TAKASHI SAITO, MASAKI AZUMA, Institute for Chemical Research, Kyoto University, SHIGETOSHI MURANAKA, Graduate School of Human and Environmental Studies, Kyoto University, YUICHI SHIMAKAWA, Institute for Chemical Research, Kyoto University — A novel transition metal oxide $LaCu_3Fe_4O_{12}$ was prepared at 10 GPa and 1400 K. It crystallizes an A-site-ordered perovskite structure, which has a general chemical formula $A'A_3B_4O_{12}$, with space group Im-3. Bond valence sum calculations and Mössbauer spectra confirm the change of charge combination at 393 K from a high-temperature $La^{3+}Cu_3^{2+}Fe_4^{3.75+}O_{12}$ with unusually high oxidation $Fe^{3.75+}$ ions at the B site to a low-temperature $La^{3+}Cu_3^{3+}Fe_4^{3+}O_{12}$ with exceptional Cu^{3+} ions at the A site. The results strongly suggest an unusual intermetallic charge transfer between the A-site Cu and B-site Fe ions. The simultaneous valence change ($3Cu^{2+}$-$3e^-$ $\rightarrow 3Cu^{3+}$ and $4Fe^{3.75+}$+$3e^-$ $\rightarrow 4Fe^{3+}$) caused by the $A-B$-site charge transfer leads to a first-order and reversible isostructural phase transition accompanied by an anomalous volume contraction as large as 1.0%. Meanwhile, a paramagnetic metal to antiferromagnetic insulator transition is also induced by the $A-B$-site charge transfer.

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Date submitted: 19 Dec 2008 Electronic form version 1.4