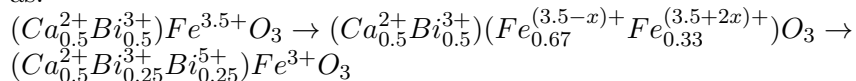


Abstract Submitted
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Successive coupled charge, magnetic, and structural transitions in $\text{Ca}_{0.5}\text{Bi}_{0.5}\text{FeO}_3$ FABIO DENIS ROMERO, YOSHITERU HOSAKA, NORIYA ICHIKAWA, TAKASHI SAITO, University of Kyoto, GRAHAM MCNALLY, J. PAUL ATTFIELD, University of Edinburgh, YUICHI SHIMAKAWA, University of Kyoto — Stoichiometric $\text{Ca}_{0.5}\text{Bi}_{0.5}\text{FeO}_3$ containing high-valent $\text{Fe}^{3.5+}$ adopting the perovskite structure was prepared under a high oxygen pressure and shows two successive phase transitions on cooling at 240 K and 200 K. Mössbauer spectroscopy and neutron powder diffraction data indicate that these transitions are associated with charge changes to relieve the instability of $\text{Fe}^{3.5+}$. The first transition is due to charge disproportionation of the iron centers while the second is due to intermetallic charge transfer between A-site Bi and B-site Fe. The transitions can be described as:



In the intermediate temperature phase, one third of B-sites ($\text{Fe}^{(3.5+2x)+}$) do not contribute to the magnetic scattering while the remaining spins couple antiferromagnetically. The lowest temperature magnetic structure is simple G-type antiferromagnetic resulting from a structure containing only Fe^{3+} . Competing intermetallic and disproportionation charge instabilities result in a variety of electronic, magnetic, and structural ground states.

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