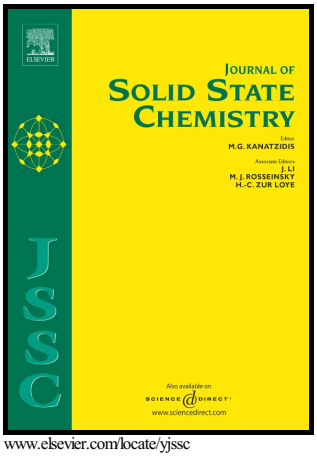

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Crystal and Magnetic Structure of Novel Brownmillerite, $Ca_2Fe_{0.875}Cr_{0.125}GaO_5$: An Approach towards Natural GMR Layers in Bulk Metal Oxides

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We present an in-depth study on the structure and magnetic properties of a novel layered oxide, $Ca_2Fe_{0.875}Cr_{0.125}GaO_5$. Structural studies from laboratory X-ray diffraction, synchrotron powder X-ray diffraction and neutron powder diffraction reveal that the compound crystallizes in an orthorhombic Brownmillerite phase with *Pnma* space group having Fe/Cr – octahedral layers and Ga – tetrahedral layers with around 9.0 % of Fe occupying tetrahedral sites. The temperature evolution of Neutron powder diffraction confirms the absence of any structural changes in the range 300 to 6 K. Magnetic characterizations show antiferromagnetic ordering at room temperature and the co-existence of antiferromagnetic and ferromagnetic phases at low temperature. The magnetic structure derived from neutron powder diffraction is a *G*-type antiferromagnetic. The ordered magnetic moments at 6 K on the octahedral and tetrahedral sites are 3.15 (2) μ_B/cation and 0.93 (4) μ_B/cation, respectively oriented in the *ac*-plane.

Graphical Abstract legend

Rietveld refined X-ray diffraction pattern at 300 K and magnetic structure obtained from Neutron diffraction at 6 K for $Ca_2Fe_{0.875}Cr_{0.125}GaO_5$