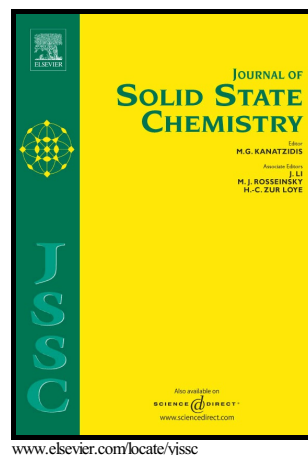


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Crystal and Magnetic Structure of Novel Brownmillerite, $\text{Ca}_2\text{Fe}_{0.875}\text{Cr}_{0.125}\text{GaO}_5$: An Approach towards Natural GMR Layers in Bulk Metal Oxides

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We present an in-depth study on the structure and magnetic properties of a novel layered oxide, $\text{Ca}_2\text{Fe}_{0.875}\text{Cr}_{0.125}\text{GaO}_5$. 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 $\text{Ca}_2\text{Fe}_{0.875}\text{Cr}_{0.125}\text{GaO}_5$

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