

Supplementary Data

Effects of bond-character on the electronic structure of Brownmillerite-phase oxides, $\text{Ca}_2\text{B}'_x\text{Fe}_{2-x}\text{O}_5$ ($\text{B}' = \text{Al}, \text{Ga}$); an X-ray absorption and electron energy loss spectroscopic study

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Table S1. Lattice constants and space-groups of the different $\text{Ca}_2\text{Fe}_2\text{O}_5$, $\text{Ca}_2\text{Al}_x\text{Fe}_{2-x}\text{O}_5$, and $\text{Ca}_2\text{Ga}_x\text{Fe}_{2-x}\text{O}_5$ samples examined by XANES and EELS.

Material	Space-group ^a	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)
$\text{Ca}_2\text{Fe}_2\text{O}_5$	Pnma	5.425(1)	14.750(4)	5.593(2)
$\text{Ca}_2\text{Al}_{0.2}\text{Fe}_{1.8}\text{O}_5$	Pnma	5.412(2)	14.702(4)	5.593(2)
$\text{Ca}_2\text{Al}_{0.4}\text{Fe}_{1.6}\text{O}_5$	Ibm2	5.3931(7)	14.636(2)	5.5918(7)
$\text{Ca}_2\text{Al}_{0.8}\text{Fe}_{1.2}\text{O}_5$	Ibm2	5.365(2)	14.551(3)	5.578(2)
$\text{Ca}_2\text{AlFeO}_5$	Ibm2	5.345(1)	14.508(2)	5.562(2)
$\text{Ca}_2\text{Ga}_{0.5}\text{Fe}_{1.5}\text{O}_5$	Pnma	5.4095(6)	14.721(2)	5.601(1)
$\text{Ca}_2\text{GaFeO}_5$	Pnma	5.394(2)	14.696(4)	5.599(2)
$\text{Ca}_2\text{Ga}_{1.5}\text{Fe}_{0.5}\text{O}_5$	Pnma	5.3727(8)	14.676(2)	5.5860(8)

^aThe change in space-group from Pnma to I2mb with *x* in $\text{Ca}_2\text{Al}_x\text{Fe}_{2-x}\text{O}_5$ was observed to occur at a slightly lower, although similar, value than that reported previously (*x* = 0.47).³⁰ The change in space-group from Pnma to I2mb is easily identified owing to the presence of (131) and (151) reflections in powder patterns from the former but not the later.³⁰