

# Deposit Art Material for

## Structural variations in the brownmillerite series $\text{Ca}_2(\text{Fe}_{2-x}\text{Al}_x)\text{O}_5$ : Single-crystal X-ray diffraction at 25 °C and high-temperature X-ray powder diffraction ( $25\text{ °C} \leq T \leq 1000\text{ °C}$ )

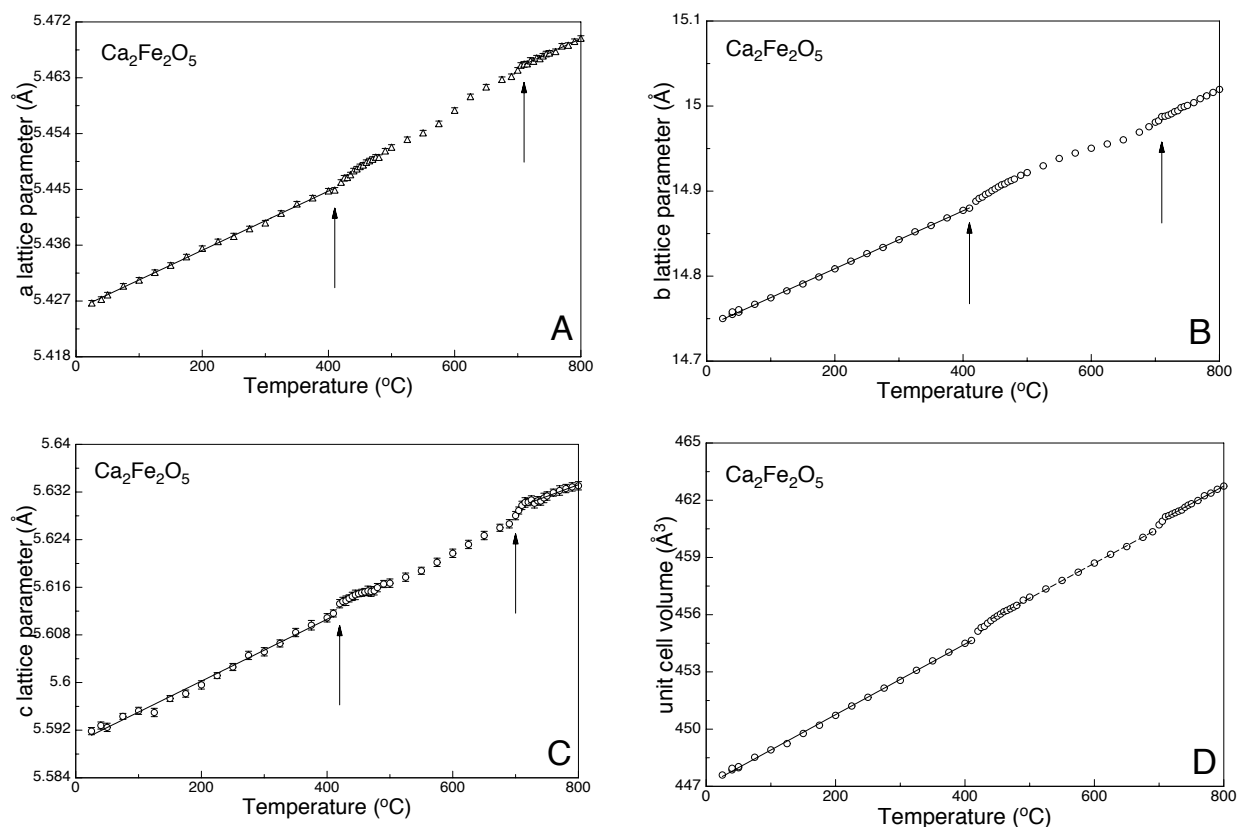
Günther J. Redhammer,<sup>1,\*</sup> Gerold Tippelt,<sup>2</sup> Georg Roth,<sup>1</sup> and Georg Amthauer<sup>2</sup>

<sup>1</sup>Institute of Crystallography, Rheinisch-Westfälische Technische Hochschule Aachen, Jägerstrasse 17/19, D-52056 Aachen, Germany

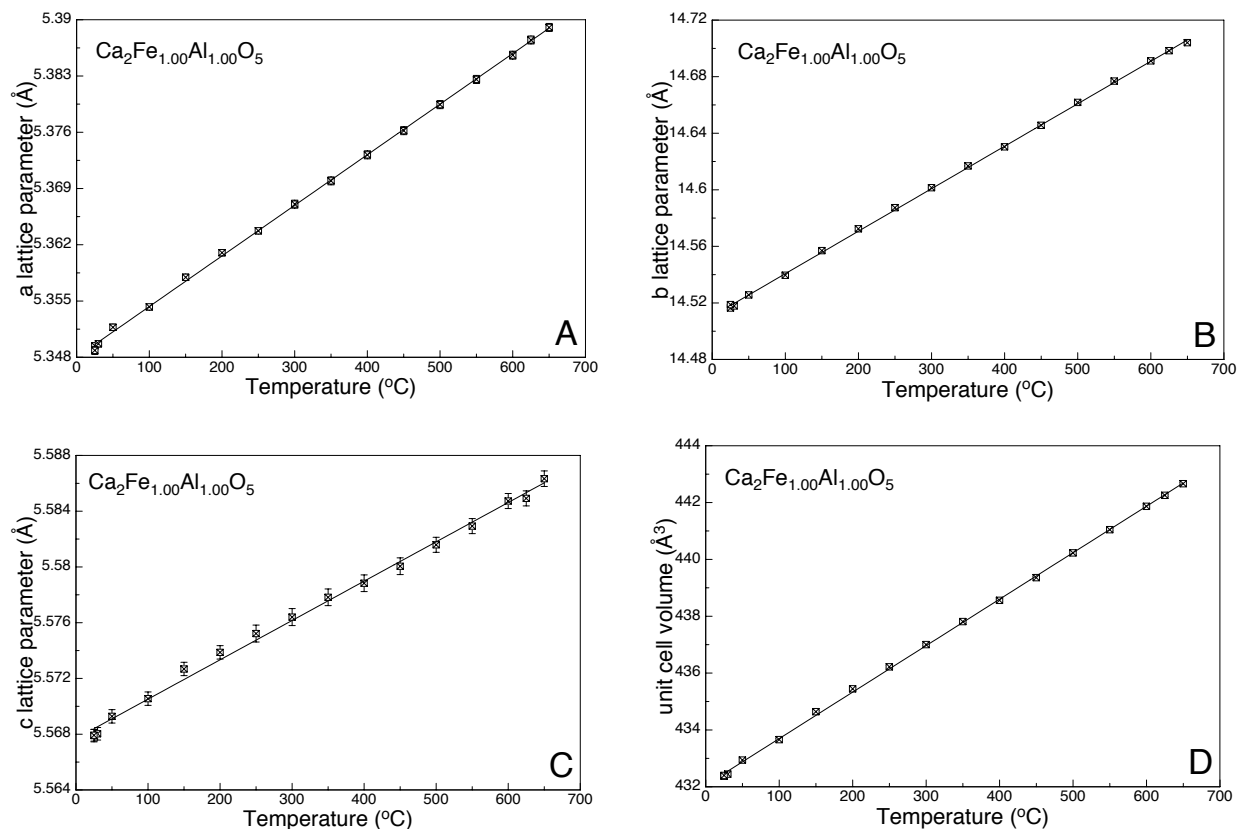
<sup>2</sup>Institute of Mineralogy, University of Salzburg, Hellbrunnerstrasse 34, A-5020 Salzburg, Austria

<sup>3</sup>Corresponding address: Neuhofen im Innkreis 224/1, A-4910 Ried im Innkreis, Austria

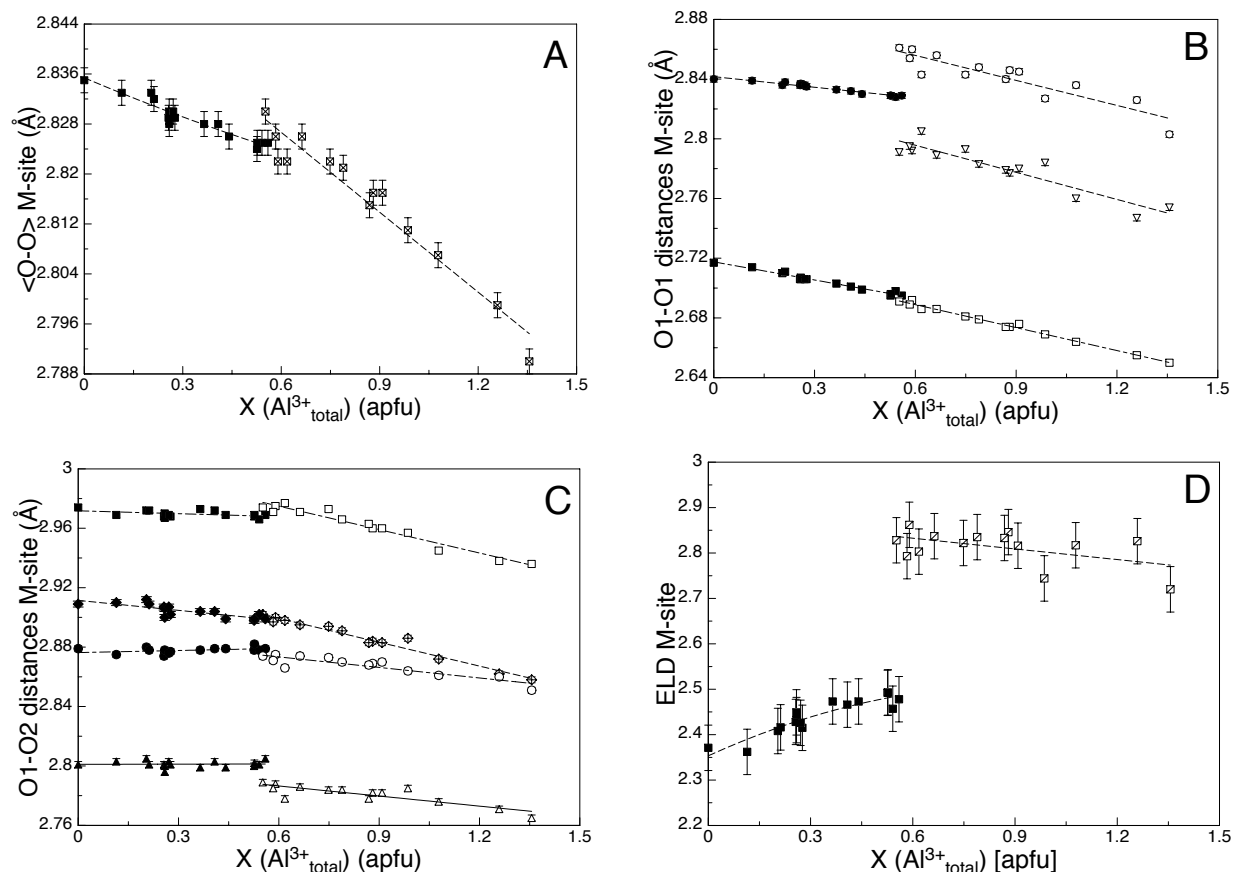
3 pages; deposit item AM-04-058



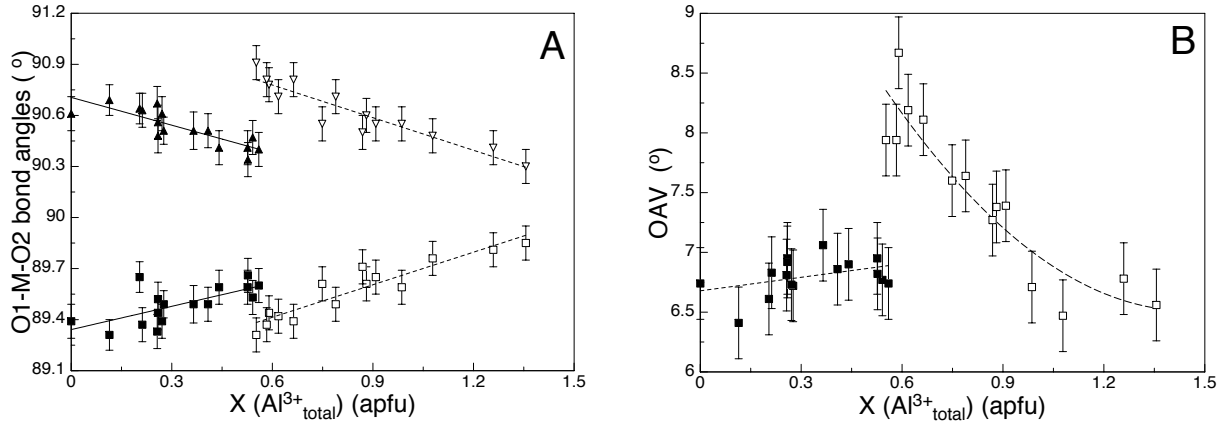
**DEPOSIT FIGURE 5.** Temperature-dependent evolution of the lattice parameters of  $\text{Ca}_2\text{Fe}_2\text{O}_5$  ( $x = 0.00$ ) as determined from powder X-ray diffraction data. Arrows indicate discontinuities related to the magnetic and the crystallographic phase transition  $\approx 430$  and  $724(2)$  °C, respectively. Estimated standard deviations are smaller than the symbols.



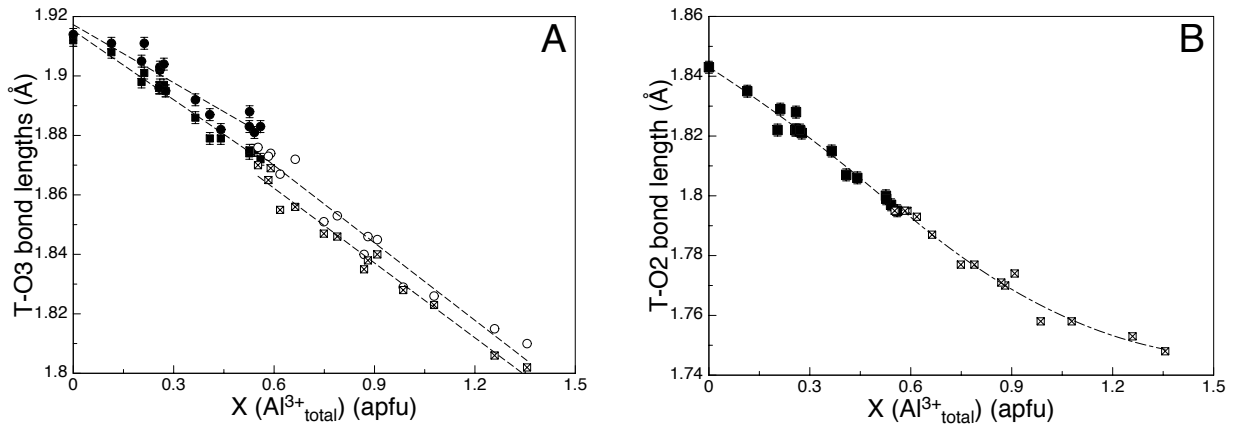
DEPOSIT FIGURE 6. Temperature-dependent evolution of the lattice parameters of  $\text{Ca}_2\text{FeAlO}_5$  ( $x = 1.00$ ) as determined from powder X-ray diffraction data.



Deposit Figure 10a-10d.



**DEPOSIT FIGURE 11.** O1-M-O2 bond angles (a) and quadratic octahedral angle variance (OAV, Robinson et al. 1971) for the  $\text{Ca}_2\text{Fe}_{2-x}\text{Al}_x\text{O}_5$  solid solution series at 25 °C. Regression curves are fitted to the data and serve as guides to the eye, and the filled and open symbols correspond to  $Pnma$  and  $I2mb$  symmetry of the samples.



**DEPOSIT FIGURE 13.** Individual (a–b) and average T-O bond lengths for samples of the  $\text{Ca}_2\text{Fe}_{2-x}\text{Al}_x\text{O}_5$  solid solution series at 25 °C. Regression curves are fitted to the data and serve as guides to the eye; if not visible, estimated standard deviations are smaller than the symbols, and the filled and open symbols correspond to  $Pnma$  and  $I2mb$  symmetry of the samples.

← **DEPOSIT FIGURE 10.** Average (a) and individual O-O atom distances, defining the edge of the  $(\text{Fe}^{3+}, \text{Al}^{3+})\text{O}_6$  octahedron as well as edge length distortion (ELD) for the  $\text{Ca}_2\text{Fe}_{2-x}\text{Al}_x\text{O}_5$  solid solution series at 25 °C. Regression lines are fitted to the data and serve as guides to the eye; if not visible, estimated standard deviations are smaller than the symbols, and the filled and open symbols correspond to  $Pnma$  and  $I2mb$  symmetry of the samples.