

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 ($25\text{ °C} \leq T \leq 1000\text{ °C}$)

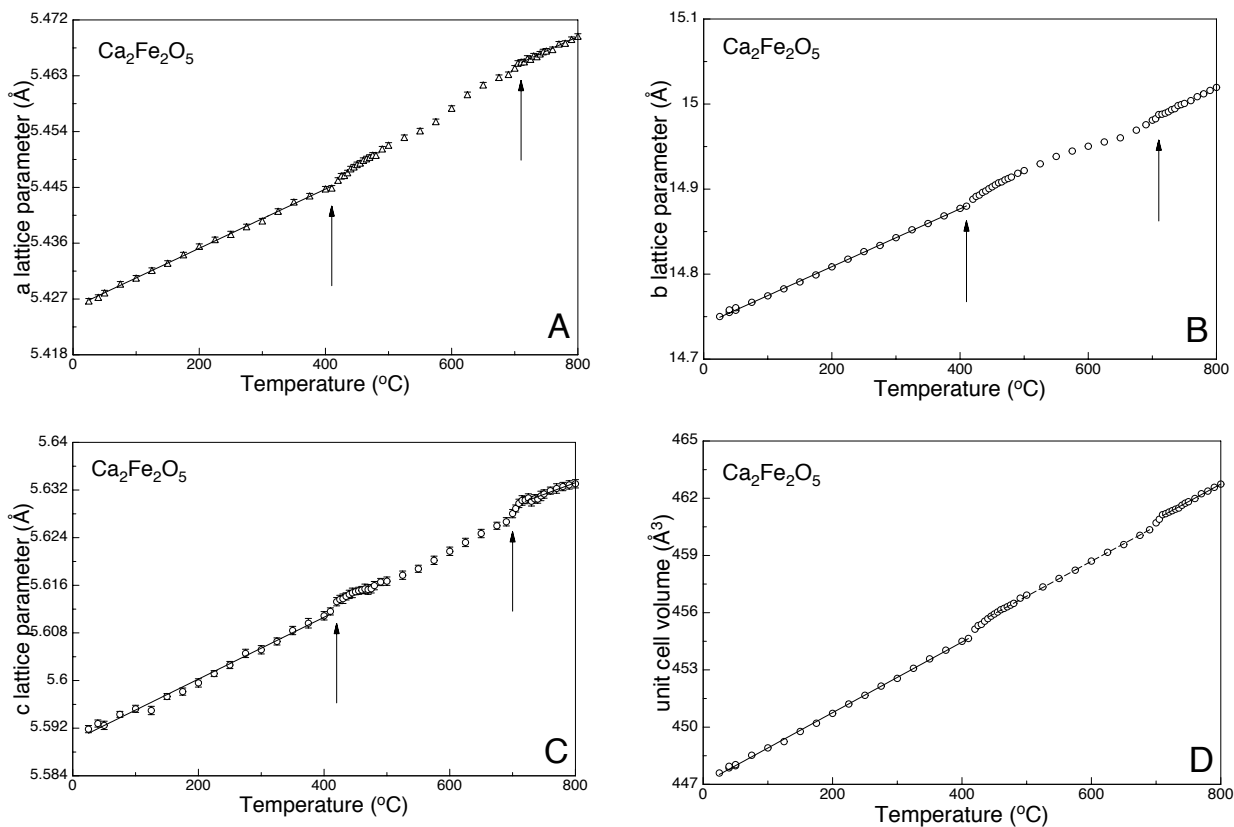
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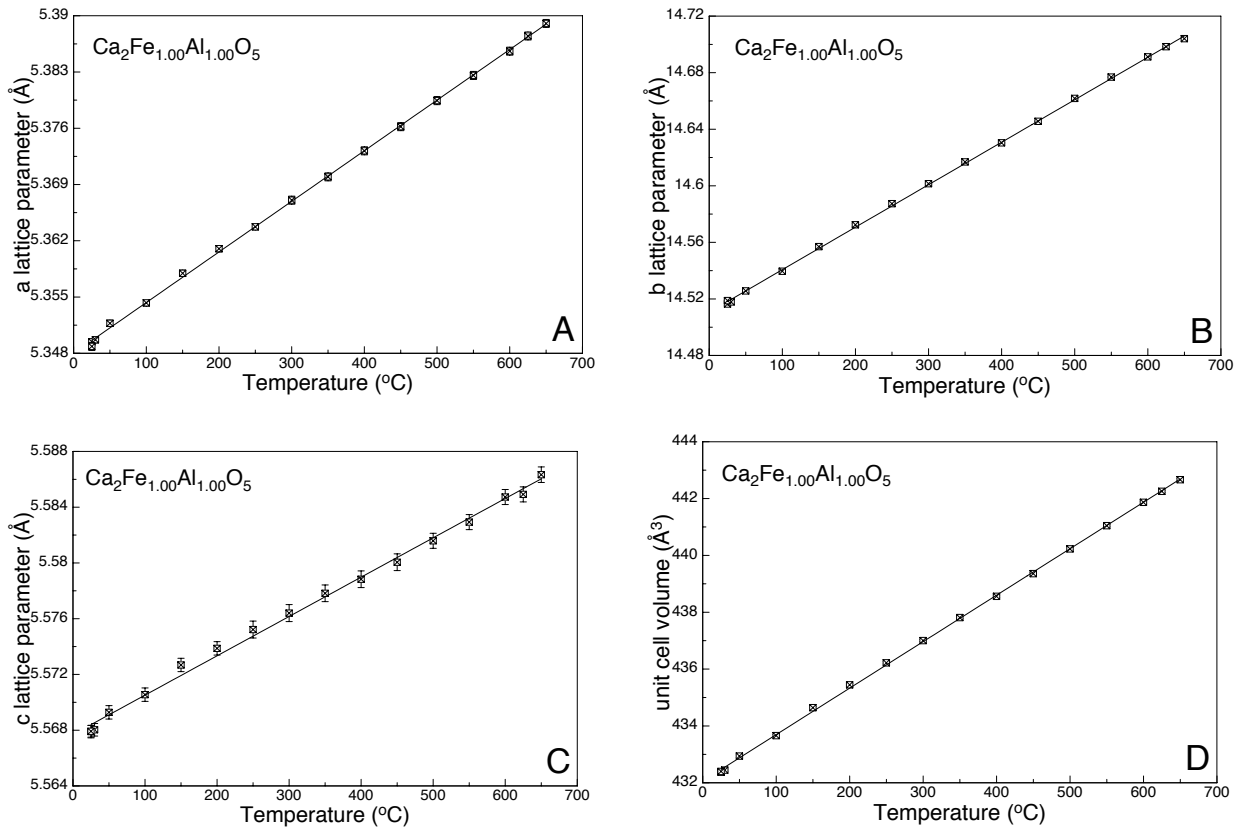
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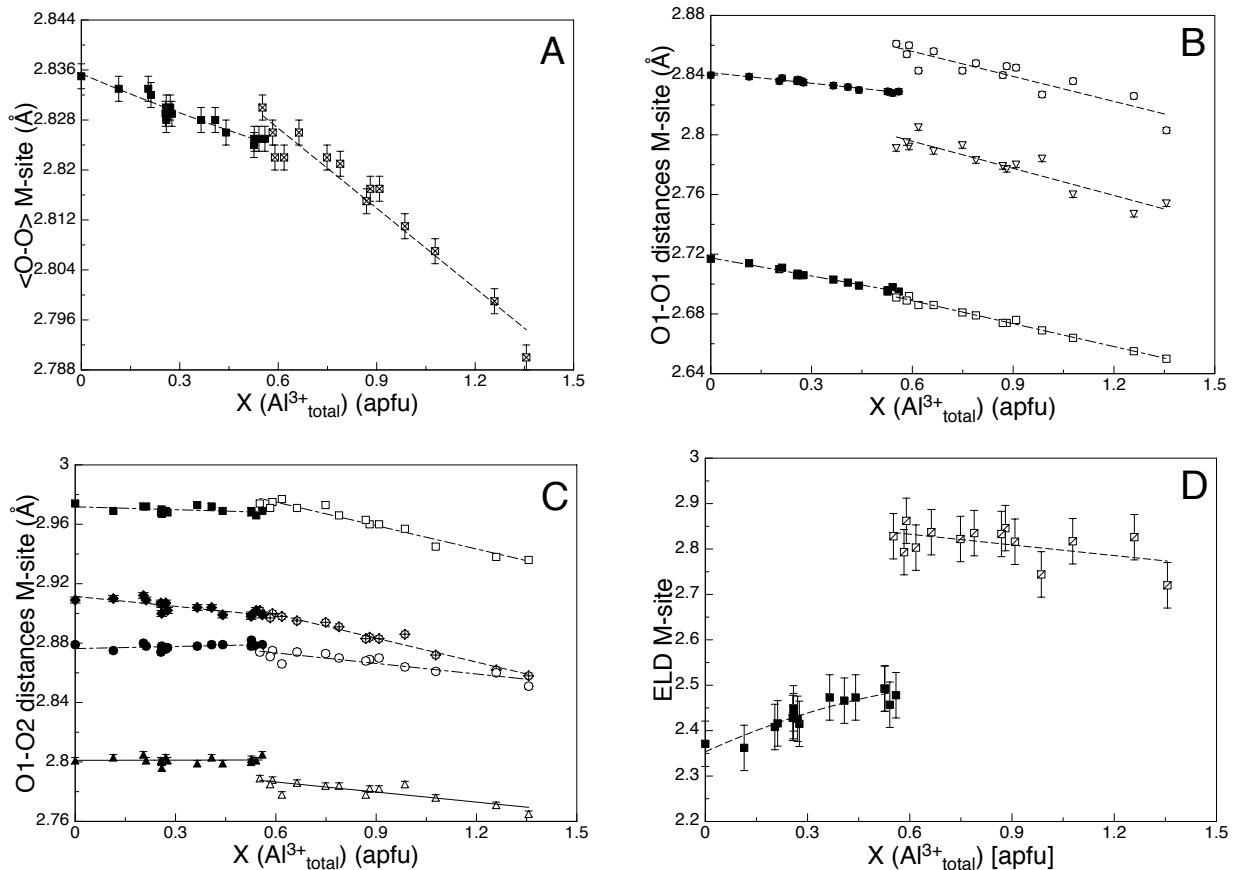
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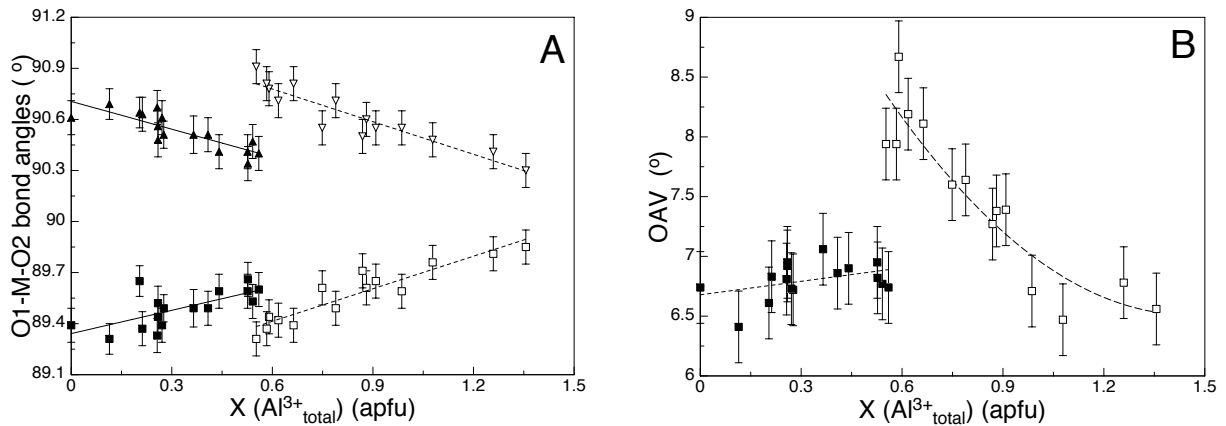
DEPOSIT FIGURE 5. Temperature-dependent evolution of the lattice parameters of $\text{Ca}_2\text{Fe}_2\text{O}_5$ ($x = 0.00$) as determined from powder X-ray diffraction data. Arrows indicate discontinuities related to the magnetic and the crystallographic phase transition ≈ 430 and $724(2)$ °C, respectively.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



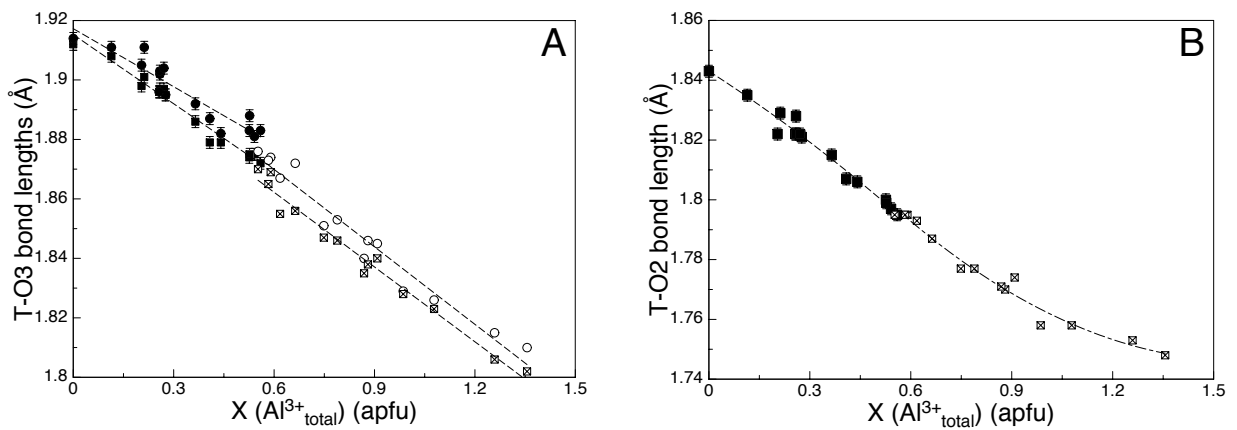
DEPOSIT FIGURE 6. Temperature-dependent evolution of the lattice parameters of $\text{Ca}_2\text{FeAlO}_5$ ($x = 1.00$) as determined from powder X-ray diffraction data.



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.