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The synthesis and crystal structure of $CaAlFSiO_4$, the Al-F analog of titanite

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ABSTRACT

Aluminum-rich titanites [Ca(Ti,Al)(O,F)SiO_4] with $X_{Al} > 0.53$ [X_{Al} = Al/(Al+Ti)], including the pure end-member $CaAlFSiO_4$, were synthesized for the first time in a high-pressure experimental study. The crystal structure of $CaAlFSiO_4$ was determined by Rietveld analysis of an X-ray powder diffraction pattern. $CaAlFSiO_4$ is monoclinic, belongs to the space group *A*2/*a*, and has the unit-cell dimensions a = 6.9149(2) Å, b = 8.5064(1) Å, c = 6.4384(2) Å, and β = 114.684(2)°. The unit-cell volume is less than 93% of $CaTiOSiO_4$, which is consistent with the natural occurrence of Al-rich titanite in high-*P* rocks. Although previous studies suggested that titanite with $X_{Al} > 0.5$ is possibly not stable, this study demonstrates that complete solid solution occurs between $CaTiOSiO_4$ and $CaAlFSiO_4$. The similarity of the crystal structures of titanite and $CaAlFSiO_4$ explains why in natural Al-rich titanite the end-member $CaAlFSiO_4$ generally dominates over the hypothetical end-member $CaAlOHSiO_4$, which under geological conditions is stable in a different crystal structure.