

The synthesis and crystal structure of CaAlFSiO₄, the Al-F analog of titanite

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ABSTRACT

Aluminum-rich titanites [Ca(Ti,Al)(O,F)SiO₄] with $X_{Al} > 0.53$ [$X_{Al} = Al/(Al+Ti)$], including the pure end-member CaAlFSiO₄, were synthesized for the first time in a high-pressure experimental study. The crystal structure of CaAlFSiO₄ was determined by Rietveld analysis of an X-ray powder diffraction pattern. CaAlFSiO₄ is monoclinic, belongs to the space group *A2/a*, and has the unit-cell dimensions $a = 6.9149(2)$ Å, $b = 8.5064(1)$ Å, $c = 6.4384(2)$ Å, and $\beta = 114.684(2)^\circ$. The unit-cell volume is less than 93% of CaTiOSiO₄, 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 CaTiOSiO₄ and CaAlFSiO₄. The similarity of the crystal structures of titanite and CaAlFSiO₄ explains why in natural Al-rich titanite the end-member CaAlFSiO₄ generally dominates over the hypothetical end-member CaAlOHSiO₄, which under geological conditions is stable in a different crystal structure.