

A comparison of the $\text{Ca}_3(\text{PO}_4)_2$ and CaSiO_3 systems, with a new structure refinement of tuite synthesized at 15 GPa and 1300 °C

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ABSTRACT

Tuite, the high-pressure γ -form of the $\text{Ca}_3(\text{PO}_4)_2$ system, has been synthesized from chlorapatite at 15 GPa and 1300 °C using a multi-anvil apparatus. Its crystal structure was determined with single-crystal X-ray diffraction. It is isostructural with palmierite, with space group $R\bar{3}m$ and unit-cell parameters $a = 5.2522(9)$ and $c = 18.690(3)$ Å. The structure of tuite is characterized by three distinct polyhedra, PO_4 , Ca1O_{12} , and Ca2O_{10} , that are translationally interconnected in the sequence of PO_4 - Ca2O_{10} - Ca1O_{12} - Ca2O_{10} - PO_4 along the **c** axis.

Comparison of the CaSiO_3 and $\text{Ca}_3(\text{PO}_4)_2$ polymorphic systems shows a striking resemblance in the evolution of atomic packing arrangements as the polymorphic density increases. In both cases, the Ca atoms are progressively incorporated into the (Ca+O) close-packed monolayers, consistent with the hypothesis that close packing is a consequence of volume decrease as density increases. Based on this observation, we predict a possible high-pressure post-tuite phase.

Keywords: Tuite, $\text{Ca}_3(\text{PO}_4)_2$, whitlockite, close-packing, pseudowollastonite, wollastonite, perovskite, CaSiO_3