A comparison of the Ca₃(PO₄)₂ and CaSiO₃ 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 Ca₃(PO₄)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 R3m and unit-cell parameters a = 5.2522(9) Å and c = 18.690(3) Å. The structure of tuite is characterized by three distinct polyhedra, PO₄, Ca₁O₁₂, and Ca₂O₁₀, that are translationally interconnected in the sequence of PO₄-Ca₂O₁₀-Ca₁O₁₂-Ca₂O₁₀-PO₄ along the c-axis.

Comparison of the CaSiO₃ and Ca₃(PO₄)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, Ca₃(PO₄)₂, whitlockite, close-packing, pseudowollastonite, wollastonite, perovskite, CaSiO₃