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A multi-domain gem-grade Brazilian apatite

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Abstract

A gem-grade apatite from Brazil of general composition $(Ca,Na)_{10}[(P,Si,S)O_4]_6(F,Cl,OH)_2$ has been studied using single-crystal X-ray and neutron diffraction together with synchrotron powder X-ray diffraction. Earlier electron microscopy studies had shown the nominally single-phase apatite contains an abundant fluorapatite (F-Ap) host, together with chloro-hydroxylapatites (Cl/OH-Ap) guest phases that encapsulate hydroxylellestadite (OH-El) nanocrystals. While the latter features appear as small (200–400 nm) chemically distinct regions by transmission electron microscopy, and can be identified as separate phases by synchrotron powder X-ray diffraction, these could not be detected by single-crystal X-ray and neutron analysis. The observations using neutron, X-ray and electron probes are however consistent and complementary. After refinement in the space group $P6_3/m$ the tunnel anions F^- are fixed at $z = ¼$ along <001>, while the anions Cl^- and OH^- are disordered, with the suggestion that O-H···O-H··· hydrogen-bonded chains form in localized regions, such that no net poling results. The major cations are located in the $4f\ A^FO_6$ metaprism (Ca+Na), $6h\ A^TO_6X$ tunnel site (Ca only), and $6h\ BO_4$ tetrahedron (P+Si+S). The structural intricacy of this gem stone provides further evidence that apatite microstructures display a nano-phase separation that is generally unrecognized, with the implication that such complexity may impact upon the functionality of technological analogues.

Keywords: Apatite, X-ray diffraction, Laue neutron diffraction, synchrotron X-ray diffraction