Neutron diffraction in gemology: Single-crystal diffraction study of brazilianite, \( \text{NaAl}_3(\text{PO}_4)_2(\text{OH})_4 \)

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**ABSTRACT**

The chemical composition and the crystal structure of a gem-quality brazilianite from the Telírio pegmatite, near Linópolis, Minas Gerais, Brazil, \( \text{NaAl}_3(\text{PO}_4)_2(\text{OH})_4 \), \( a = 11.2448(5) \) Å, \( b = 10.1539(6) \) Å, \( c = 7.1031(3) \) Å, \( \beta = 97.351(4) ^\circ \), \( V = 804.36(7) \) Å³, space group \( P2_1/n \), \( Z = 4 \), have been reinvestigated by means of electron microprobe analysis in wavelength-dispersive mode, single-crystal X-ray and neutron diffraction. The chemical analysis shows that brazilianite from Telírio Claim approaches almost ideal composition. The neutron anisotropic structural refinement was performed with final agreement index \( R_1 = 0.0290 \) for 211 refined parameters and 2844 unique reflections with \( F_o > 4\sigma(F_o) \), the X-ray refinement led to \( R_1 = 0.0325 \) for 169 refined parameters and 2430 unique reflections with \( F_o > 4\sigma(F_o) \). The building-block units of the brazilianite structure consist of chains of edge-sharing \( \text{AlO}_4(\text{OH})_2 \) and \( \text{AlO}_3(\text{OH})_3 \) octahedra. Chains are connected, via corner-sharing, by P-tetrahedra to form a three-dimensional framework, with Na atoms located in distorted cavities running along [100]. Five independent H sites were located, here labeled as H(1), H(2a), H(2b), H(3), and H(4). The configuration of the OH groups, along with the complex hydrogen-bonding scheme, are now well defined. The O-H distances corrected for “riding motion” range between \( \sim \)0.992 and \( \sim \)1.010 Å, the O···O distances between \( \sim \)2.67 and \( \sim \)2.93 Å, and the O-H···O angles between \( \sim \)151° and \( \sim \)174°. The H(2a) and H(2b) are only \( \sim \)1.37 Å apart and mutually exclusive (both with site occupancy factor of 50%). The differences between the crystal structure of brazilianite and wardite [ideally NaAl_3(PO_4)_2(OH)_4·2H_2O] are discussed. This work fulfills the need for accurate crystal-chemical data for this gem mineral.

**Keywords:** Brazilianite, crystal chemistry, single-crystal neutron diffraction, hydrogen bonding