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A single-crystal neutron diffraction study of hambergite, $Be_2BO_3(OH,F)$

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Abstract

The crystal chemistry and crystal structure of hambergite from the Anjanabonoina mine, Madagascar [$Be_2BO_3(OH)_{0.96}F_{0.04}$, $Z = 8$, $a = 9.762(2)$, $b = 12.201(2)$, $c = 4.430(1)$ Å, $V = 527.6(2)$ Å^3, space group *Pbca*], were reinvestigated by means of electron microprobe analysis in wavelength-dispersive mode, secondary-ion mass spectrometry, single-crystal X-ray and neutron Laue diffraction. Chemical analyses show only a small amount of F (0.7–0.8 wt%, approximately 0.04 atoms per formula unit) substituting OH and no other substituent at a significant level. An anisotropic neutron structural refinement has been performed with final agreement index $R_1 = 0.0504$ for 76 refined parameters and 1430 unique reflections with $F_o > 4\sigma(F_o)$. The geometry of the hydroxyl group and hydrogen bonding in hambergite is now well defined: (1) only one independent H site was located and the O4-H distance, corrected for "riding motion," is ~0.9929 Å; (2) only one hydrogen bond appears to be energetically favorable, with a symmetry-related O4 as *acceptor* and with O4···O4 = 2.904(1) Å, H···O4 = 1.983(1) Å, and O4-H···O4 = 157.5(1)°. In other words, O4 sites act both as *donor* and as *acceptor* of the hydrogen bond, with a zigzag chain of H-bonds along [001]. The hydrogen-bonding scheme in hambergite found in this study is consistent with the pleochroic scheme of the infrared spectra previously reported, with two intensive modes ascribable to stretching vibrations of the hydroxyl group, at 3415 and 3520 cm^{-1}, respectively. The two modes suggest at least two distinct hydrogen-bonding environments, ascribable to the presence of oxygen and fluorine at the *acceptor* site.

Keywords: Hambergite, crystal chemistry, electron microprobe analysis in wavelength-dispersive mode, secondary-ion mass spectrometry, neutron Laue diffraction, hydrogen bonding