American Mineralogist, Volume 91, pages 1927–1931, 2006

Hydroxylellestadite from Cioclovina Cave (Romania): Microanalytical, structural, and vibrational spectroscopy data

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ABSTRACT

Electron-microprobe analyses of hydroxylellestadite from the Cioclovina Cave (Romania) gave the composition $Ca_{10.27}[(SiO_4)_{2.53}(SO_4)_{2.17}(PO_4)_{1.27}]_{\Sigma=5.97}[(OH)_{1.66}F_{0.21}Cl_{0.16}]_{\Sigma=2.03}$. The mineral is translucent to transparent, light orange, slightly fluorescent, has a vitreous luster and <1.5 mm in length. A single-crystal X-ray structure investigation gave the average space-group symmetry $P6_3/m$ [$R1(F) = 0.038$ for 783 reflections up to $2\theta_{MoK\alpha} = 70°$ and 42 variables, $a = 9.496(2)$, $c = 6.920(2)$ Å, $V = 540.4$ Å^3, and $Z = 2$]. Some atoms exhibit large anisotropic displacements. Ordering of atoms along with a symmetry reduction is not verified. Fourier-transformed infrared (FT-IR) and micro-Raman spectra exhibit a distinct contribution from $(PO_4)^{3-}$ modes along with the characteristic $(SO_4)^{2-}$ and $(SiO_4)^{4-}$ modes. The occurrence is quite unusual and suggests that an intense thermal process affected a restricted area within the cave. Hydroxylellestadite is associated with berlinite, another high-temperature mineral. It is likely to have formed within highly phosphatized, silicate-rich, carbonate-mudstone sediments heavily compacted and thermally transformed due to in situ bat guano combustion.

Keywords: Hydroxylellestadite, britholite group, bat guano combustion, cave minerals, Cioclovina Cave, Romania