American Mineralogist, Volume 103, pages 1319–1328, 2018

Discreditation of bobdownsite and the establishment of criteria for the identification of minerals with essential monofluorophosphate (PO_3F^{2-})

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Abstract

Bobdownsite, IMA number 2008-037, was approved as a new mineral by the Commission on New Minerals, Nomenclature and Classification (CNMNC) as the fluorine end-member of the mineral whitlockite. The type locality of bobdownsite is in Big Fish River, Yukon, Canada, and bobdownsite was reported to be the first mineral with essential monofluorophosphate (PO_3F^{2-}). The type specimen of bobdownsite has been reinvestigated by electron probe microanalysis (EPMA), and our data indicate that fluorine abundances are below detection in the mineral. In addition, we conducted detailed analysis of bobdownsite from the type locality by gas chromatography isotope ratio mass spectrometry, Raman spectroscopy, EPMA, and NMR spectroscopy. These data were compared with previously published data on synthetic monofluorophosphate salts. Collectively, these data indicate that bobdownsite is indistinguishable from whitlockite with a composition along the whitlockite-merrillite solid solution. Bobdownsite is therefore discredited as a valid mineral species. An additional mineral, krásnoite, has been purported to have monofluorophosphate components in its structure, but reexamination of those data indicate that F^- in krásnoite forms bonds with Al, similar to OH^- bonded to Al in perhamite. Consequently, krásnoite also lacks monofluorophosphate groups, and there are currently no valid mineral species with monofluorophosphate in their structure. We recommend that any future reports of new minerals that contain essential monofluorophosphate anions be vetted by abundance measurements of fluorine, vibrational spectroscopy (both Raman and FTIR), and where paramagnetic components are permissibly low, NMR spectroscopy. Furthermore, we emphasize the importance of using synthetic compounds containing monofluorophosphate anions as a point of comparison in the identification of minerals with essential monofluorophosphate. Structural data that yield satisfactory P-F bond lengths determined by X-ray crystallography, coupled with direct chemical analyses of fluorine in a material do not constitute sufficient evidence alone to identify a new mineral with essential monofluorophosphate.

Keywords: Merrillite, whitlockite, apatite, krásnoite, fluorine, SIMS standard, NMR spectroscopy, hydrogen isotopes