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LETTER

Crystal structure of uchucchacuaite, $AgMnPb_3Sb_5S_{12}$, and its relationship with ramdohrite and fizélyite

H. YANG,[1,*] R.T. DOWNS,[1] S.H. EVANS,[1] M.N. FEINGLOS,[2] AND K.T. TAIT[3]

[1]Department of Geosciences, University of Arizona, 1040 East 4th Street, Tucson, Arizona 85721, U.S.A.
[2]Duke University Medical Center, Box 3921, Durham, North Carolina 27710-0001, U.S.A.
[3]Department of Natural History, Royal Ontario Museum, 100 Queen's Park, Toronto, Ontario M5S 2C6, Canada

ABSTRACT

Uchucchacuaite, ideally $AgMnPb_3Sb_5S_{12}$, was originally reported as orthorhombic, with possible space group *Pmmm*, *P*222, or *Pmm*2, and unit-cell parameters $a = 12.67$, $b = 19.32$, and $c = 4.38$ Å obtained from powder X-ray diffraction data (Moëlo et al. 1984a). Using single-crystal X-ray diffraction, we examined two uchucchacuaite samples, one from the type locality, Uchucchacua, Peru, and the other from Hokkaido, Japan (designated as R100213 and R070760, respectively). Our results show that uchucchacuaite is isostructural with ramdohrite and fizélyite, with monoclinic symmetry ($P2_1/n$) and the unit-cell parameters $a = 19.3645(11)$, $b = 12.7287(8)$, $c = 8.7571(6)$ Å, $\beta = 90.059(3)°$ for R100213 and $a = 19.3462(7)$, $b = 12.7251(5)$, $c = 8.7472(3)$ Å, $\beta = 90.017(2)°$ for R070760. Both samples are pervasively twinned and the twin refinements yielded the final R_1 factors of 0.037 and 0.031 for R100213 and R070760, respectively. The chemical compositions determined from electron microprobe analysis are $Ag_{0.99}(Mn_{0.92}Pb_{0.03}Sb_{0.02}Bi_{0.01})_{\Sigma=0.98}Pb_{3.00}Sb_{5.00}S_{12.00}$ for R100213 and $Ag_{1.00}(Mn_{0.82}Sb_{0.11}Ag_{0.04}Bi_{0.02})_{\Sigma=0.99}Pb_{2.98}Sb_{5.00}S_{12.00}$ for R070760. The key structural difference among uchucchacuaite, ramdohrite, and fizélyite lies in the cations occupying the M2 site, which can be expressed with a general structural formula as $Ag(M^{2+}_{2y}Ag_{½–y}Sb_{½–y})Pb_3Sb_5S_{12}$, where M^{2+} represents divalent cations with $0 \le y \le ½$. From the current list of IMA-defined minerals, we consider M = Cd with $y = 0.125$ for ramdohrite, M = Pb with $y = 0.25$ for fizélyite, and M = Mn with $y = 0.5$ for uchucchacuaite. Associated with the variation in the average M2 cation size from fizélyite (1.078 Å) to ramdohrite (0.955 Å) and uchucchacuaite (0.83 Å) is the significant decrease in the average M2-S bond distance from 2.917 to 2.834, and 2.654 Å, respectively, as well as corresponding variations in the unit-cell *b* dimension from ~13.23 to 13.06 and 12.73 Å.

Keywords: Uchucchacuaite, fizélyite, ramdohrite, andorite series, sulfosalts, crystal structure, single-crystal X-ray diffraction