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Structural reinvestigation of getchellite $As_{0.98}Sb_{1.02}S_{3.00}$

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ABSTRACT

The crystal structure of getchellite, $As_{0.98}Sb_{1.02}S_{3.00}$, from the type-locality (the Getchell mine, Humboldt County, Nevada), monoclinic, $P2_1/a$, a = 11.949(3), b = 9.028(1), c = 10.130(2) Å, β = 116.15(1)°, V = 980.9(4) Å^3, Z = 8, was solved by direct methods and refined with full-matrix least-squares techniques to R = 0.058 and Rw = 0.062 for 505 observed reflections [$I_o > 5\sigma(I_o)$] collected using Mo$K\alpha$ radiation. The structure is made up of (As,Sb)S_3 trigonal pyramids forming an eight-membered $(As,Sb)_8S_8$ ring; the sheets formed by the eight-membered rings are connected to each other by S1 and S6 atoms are parallel to (001). The sheet structure is responsible for the cleavage and twin planes of getchellite. The cations predominantly occupy the M2 site in natural getchellite, because the M2S_6 polyhedron has the most distorted (irregular) geometry compared with other metal polyhedra in the structure. The amount of As incorporated at the M1 sites correlates strongly with M2 site composition. An important feature of As^{3+} sulfide minerals is that the crystal structures are composed of a 3-dimensional network consisting not only of AsS_3 pyramids but also containing trigonal pyramids of other constituent cations because the structures are governed strongly by the stereochemical requirement of As^{3+} cations for MS_3 trigonal pyramids.