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A new type of cubic-stacked layer structure in anthoinite, $AlWO_3(OH)_3$

Ian E. Grey,[1,*] Ian C. Madsen,[1] Stuart J. Mills,[2] Frederic Hatert,[3] Vanessa K. Peterson,[4] and Timothy J. Bastow[5]

[1]CSIRO Minerals, Box 312, Clayton South, Victoria 3169, Australia
[2]Department of Earth and Ocean Sciences, University of British Columbia, Vancouver, British Columbia V6T 1Z4, Canada
[3]Laboratoire de Minéralogie et de Cristallochimie, B-18, Université de Liège, B-4000 Liège, Belgium
[4]Bragg Institute, ANSTO, PMB 1, Menai, New South Wales 2234, Australia
[5]CSIRO Materials Science and Engineering, Private Bag 33, Clayton South, Victoria 3169, Australia

Abstract

Anthoinite, $AlWO_3(OH)_3$, from the Mt. Misobo Mine, Democratic Republic of the Congo, has triclinic symmetry with cell parameters $a = 8.196(1)$ Å, $b = 9.187(1)$ Å, $c = 11.316(1)$ Å, $\alpha = 92.82(1)°$, $\beta = 94.08(1)°$, $\gamma = 90.23(1)°$, space group $I\bar{1}$, $Z = 8$. The structure was solved by applying ab initio structure solution methods (Reverse Monte Carlo/Simulated Annealing) to both X-ray and neutron powder diffraction data and was refined using the Rietveld method. The structure is built up of two types of $M_4(O,OH)_{16}$ planar tetrameric clusters of edge-sharing octahedra, one containing predominantly Al and the other predominantly W. The Al-rich and W-rich clusters interconnect via corner sharing to form stepped layers parallel to (001). The layers are held together by strong hydrogen bonding. The structure can be described as a rocksalt derivative structure, with the close-packed anion layers parallel to (012), and with Al and W atoms ordered into one third of the octahedral sites within the cubic close-packed anion lattice. The structure is complicated by partial disorder between Al and W in the tetrameric clusters and associated disorder in the H atom sites. Infrared and ^{27}Al MAS NMR results are also presented for anthoinite.

Keywords: Structure of anthoinite, ab initio structure determination, new layer structure in $AlWO_3(OH)_3$, layer structure of anthoinite