

Crystal chemistry of the new mineral brandholzite, $\text{Mg}(\text{H}_2\text{O})_6[\text{Sb}(\text{OH})_6]_2$, and of the synthetic analogues $\text{M}^{2+}(\text{H}_2\text{O})_6[\text{Sb}(\text{OH})_6]_2$ ($\text{M}^{2+} = \text{Mg}, \text{Co}$)

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ABSTRACT

Brandholzite, a new magnesium antimony hydroxide hydrate mineral, $\text{Mg}(\text{H}_2\text{O})_6[\text{Sb}(\text{OH})_6]_2$, has been discovered in Au-Sb-Quartz veins of the former mining district of Brandholz-Goldkronach, Fichtelgebirge, Germany. The new mineral is associated with stibnite and antimony-ochers and forms colorless, platelike crystals up to ~1 mm in size. Natural as well as synthetic samples obtained by slow evaporation of an aqueous solution exhibit $\{10\bar{1}0\}$ twinning, leading to a pronounced $\bar{3}1m$ pseudo-symmetry. The crystal structures of brandholzite and its synthetic analogue were investigated using single crystal X-ray CCD data: trigonal, space group $P3$, $Z = 6$, $a = 16.119(1)$ Å, $c = 9.868(1)$ Å, $R1 = 0.034$ for 14788 $F_o > 4\sigma(F_o)$ (brandholzite), and $a = 16.113(1)$ Å, $c = 9.868(1)$ Å, $R1 = 0.029$ for 16624 $F_o > 4\sigma(F_o)$ (synthetic analogue) and 525 variable parameters each. The structures are isotypic with bottinoite, $\text{Ni}(\text{H}_2\text{O})_6[\text{Sb}(\text{OH})_6]_2$, and are built up by nearly regularly shaped, isolated $\text{Mg}(\text{H}_2\text{O})_6$ and $\text{Sb}(\text{OH})_6$ octahedra which are interconnected by hydrogen bonds only. The strongest lines in the powder pattern are [d -value (Å), l , hkl]: 4.636, 100, (300); 3.392, 70, (302); 4.946, 50, (002); 2.356, 40, (332). At 589 nm, the mineral is optically uniaxial negative with refractive indices $n_{\omega} = 1.570(2)$ and $n_e = 1.569(2)$. The crystal structure of the pseudo-isotypic synthetic compound $\text{Co}(\text{H}_2\text{O})_6[\text{Sb}(\text{OH})_6]_2$ was also investigated: trigonal, space group $P3$, $a = 16.105(1)$, $c = 9.851(1)$, $Z = 6$, $R1 = 0.051$ for 13516 reflections with $F_o > 4\sigma(F_o)$ and 525 parameters. Compared to the Mg-antimonates and bottinoite, a significant rotation of some $\text{Sb}(\text{OH})_6$ octahedra is observed in $\text{Co}(\text{H}_2\text{O})_6[\text{Sb}(\text{OH})_6]_2$.