

Bamfordite, $\text{Fe}^{3+}\text{Mo}_2\text{O}_6(\text{OH})_3\cdot\text{H}_2\text{O}$, a new hydrated iron molybdenum oxyhydroxide from Queensland, Australia: Description and crystal chemistry

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ABSTRACT

Bamfordite from the abandoned W-Mo-Bi mines at Bamford, Queensland, Australia, is a new hydrated iron molybdate with a unique structure. This mineral formed by oxidation of molybdenite, MoS_2 , in the presence of strongly acidic solutions. It occurs as microcrystalline aggregates of tabular triclinic crystals between 0.005 and 0.05 mm long. The aggregates are apple-green with an earthy luster and greenish yellow streak. Crystals are transparent, with pale to moderate yellow-green pleochroism. They show principal forms $\{001\}$, $\{100\}$, $\{010\}$, $\{110\}$, $\{1\bar{1}0\}$, and prominent (100) cleavage traces. The Mohs hardness is 2–3 and the measured density is 3.620 g/cm^3 (calculated density is 3.616 g/cm^3). Crystals are biaxial negative and length slow, with RIs of $\alpha = 1.91$, $\beta = 2.03$, and $\gamma = 2.11$, and $2V \approx 90^\circ$. Chemical analysis yielded an empirical formula of $\text{Fe}_{1.00}^{3+}\text{Mo}_{2.01}\text{W}_{0.03}\text{P}_{0.02}\text{O}_{10}\text{H}_{4.62}$, calculated on the basis of ten O atoms. The simplified formula is $\text{Fe}^{3+}\text{Mo}_2\text{O}_6(\text{OH})_3\cdot\text{H}_2\text{O}$, chosen on the basis of crystal-structure determination and Mössbauer spectroscopy results. Unit-cell parameters calculated both from the X-ray powder and single-crystal diffraction data are $a = 5.889(5)$, $b = 7.545(5)$, $c = 9.419(5) \text{ \AA}$; $\alpha = 71.46(4)^\circ$, $\beta = 83.42(4)^\circ$, $\gamma = 72.78(4)^\circ$; $V = 378.9(4) \text{ \AA}^3$; $Z = 2$; $P1$ or $P\bar{1}$. The crystal structure was solved in $P1$ using direct methods and Fourier techniques. The final refinement based on 1486 observed reflections [$I > 2.00 \sigma I$] converged to $R = 0.05$ and $R_w = 0.038$. The bamfordite crystal structure contains groups of four MoO_6 octahedra, linked by edge-sharing, which in turn are linked through corner-sharing to pairs of FeO_6 octahedra thereby forming infinite sheets parallel to (100). These sheets are stepped and linked by hydrogen bonding. No other molybdenum oxides have this or a similar structure, instead molybdates such as wulfenite, PbMoO_4 , are based on tetrahedrally coordinated molybdenum.