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Mineralogy and crystal structure of bouazzerite from Bou Azzer, Anti-Atlas, Morocco: Bi-As-Fe nanoclusters containing Fe^{3+} in trigonal prismatic coordination

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ABSTRACT

Bouazzerite, $Bi_6(Mg,Co)_{11}Fe_{14}[AsO_4]_{18}O_{12}(OH)_4(H_2O)_{86}$, is a new mineral occurring in "Filon 7" at the Bou Azzer mine, Anti-Atlas, Morocco. Bouazzerite is associated with quartz, chalcopyrite, native gold, erythrite, talmessite/roselite-beta, Cr-bearing yukonite, alumopharmacosiderite, powellite, and a blue-green earthy copper arsenate related to geminite. The mineral results from the weathering of a Variscan hydrothermal As-Co-Ni-Ag-Au vein. The Bou Azzer mine and the similarly named district have produced many outstanding mineral specimens, including the world's best erythrite and roselite.

Bouazzerite forms monoclinic prismatic {021} crystals up to 0.5 mm in length. It has a pale apple green color, a colorless streak, and is translucent with adamantine luster. d_{calc} is 2.81(2) g/cm^3 (from X-ray structure refinement). The new mineral is biaxial with very weak pleochroism from yellow to pale yellow; the refractive indices measured on the (021) cleavage face range from n_{min} = 1.657 to n_{max} = 1.660; the Gladstone-Dale relationship provides a value of 1.65. The empirical chemical formula is $Bi_{6.14}Fe_{12.6}Mg_{8.45}Co_{0.48}Ni_{0.12}Ca_{0.23}(As_{17.0}Cr_{0.64}Si_{0.32})_{\Sigma=18.0}O_{174.6}H_{184}$. Bouazzerite is monoclinic, $P2_1/n$, Z = 2, with a = 13.6322(13) Å, b = 30.469(3) Å, c = 18.4671(18) Å, β = 91.134(2)°, and V = 7669.0(13) Å^3. The eight strongest lines in the X-ray powder diffraction pattern are [d in Å (I)(hkl)]: 11.79(100)(02$\bar{1}$), 10.98(80)(101/$\bar{1}$01), 10.16(80)($\bar{1}$20), 7.900(80)(02$\bar{2}$), 12.45(70)(1$\bar{1}$0), 15.78(60)(0$\bar{1}$1), 3.414(40)(3$\bar{3}$3/400), 3.153(40)(35$\bar{3}$/2$\bar{2}$5).

The crystal structure of bouazzerite is based upon $[Bi_3Fe_7O_6(OH)_2(AsO_4)_9]^{11-}$ anionic nanoclusters that are built around $[^{\text{trigonal prismatic}}Fe^{3+}(^{\text{octahedral}}Fe^{3+}_3(OH)O_{12})_2]^{29-}$ groups, containing one Fe^{3+} ion in trigonal prismatic coordination and six Fe^{3+} ions in octahedral coordination. The nanoclusters have a diameter of about 1.3 nm and are linked together by chains of $Mg(O,H_2O)_6$ octahedra. The resulting arrangement displays channels down [100] that contain structural water. Bouazzerite is the first mineral based upon Bi- and As-containing ferric nanoclusters. Its discovery provides a unique insight into transport mechanisms of toxic elements in the oxidation zones of sulfide mineral deposits in the form of complex Fe-As nanoparticles.

Keywords: Bouazzerite, new mineral, crystal structure determination, trigonal prismatic coordination, Bou Azzer province, Anti-Atlas, Morocco