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Dukeite, $Bi_{24}^{3+}Cr_8^{6+}O_{57}(OH)_6(H_2O)_3$, a new mineral from Brejaúba, Minas Gerais, Brazil: Description and crystal structure

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ABSTRACT

Dukeite, $Bi_{24}^{3+}Cr_8^{6+}O_{57}(OH)_6(H_2O)_3$, space group $P31c$, a = 15.067(3), c = 15.293(4) Å, V = 3007(1) Å^3, Z = 2, is a new mineral found on a museum specimen labeled as originating from the São José Mine, Brejaúba, Minas Gerais, Brazil. The strongest seven lines of the X-ray powder-diffraction pattern [d in Å (I) (hkl)] are: 7.650 (50) (002), 3.812 (40) (004), 3.382 (100) (222), 2.681 (70) (224), 2.175 (40) (600), 2.106 (40) (226), 1.701 (50) (228). It occurs as groupings of tightly bound 1 × 0.3 mm^2 sized sheaves that are associated with pucherite, schumacherite, bismutite, and hechtsbergite. Individual acicular crystals do not exceed 100 μm in length by 1–2 μm in width. Crystals are yellow inclining to a dirty yellow-brown, possess a bright yellow streak, are transparent, brittle, resinous, and do not fluoresce under ultraviolet light. The estimated Mohs hardness is between 3 and 4, the calculated density (for the empirical formula) is 7.171 g/cm^3, and the mineral is slowly soluble in concentrated HCl. Electron-microprobe analyses yielded Bi_2O_3 85.06, CrO_3 11.65, V_2O_5 0.59, H_2O (calc.) [1.67], total [98.97] wt%. The empirical formula, derived from the crystal-structure analysis and electron-microprobe analyses, is $Bi_{23.95}^{3+}(Cr_{7.64}^{6+}V_{0.43}^{5+})\Sigma_{8.07}O_{56.84}(OH)_{6.16}\cdot 3.01\ H_2O$, based on O = 66. In reflected plane-polarized light in air it is gray to purplish gray with strong yellow internal reflections. Bireflectance is very weak. Measured reflectance values, in air and in oil, are tabulated: indices of refraction calculated from these at 590 nm are 2.33 and 2.37. The name honors Duke University, Durham, North Carolina, in whose collection the mineral was found and also recognizes the contribution of the Duke family to the advancement of scientific knowledge.

The crystal structure of dukeite was solved by direct methods and refined on the basis of F^2 using all unique reflections measured with Mo$K\alpha$ X-radiation on a CCD-equipped diffractometer. The final $R1$ index was 8.7%, calculated using 1033 observed reflections. It contains irregular layers of $Bi\phi_n$ polyhedra (ϕ: O, OH^-, H_2O) parallel to (001), separated and connected by CrO_4 tetrahedra to form a framework structure. One CrO_4 tetrahedron shares all of its vertices with $Bi\phi_n$ polyhedra, whereas the other three CrO_4 tetrahedra share only three vertices each with the $Bi\phi_n$ polyhedra on either side.