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Bicapite, $KNa_2Mg_2(H_2PV^{5+}_{14}O_{42})\cdot 25H_2O$, a new polyoxometalate mineral with a bicapped Keggin anion from the Pickett Corral mine, Montrose County, Colorado, U.S.A.

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Abstract

Bicapite, $KNa_2Mg_2(H_2PV^{5+}_{14}O_{42})\cdot 25H_2O$, is a new mineral species (IMA2018-048) discovered at the Pickett Corral mine, Montrose County, Colorado, U.S.A. Bicapite occurs as square tablets up to about 0.2 mm on edge on montroseite-corvusite-bearing sandstone. Crystals are dark red-brown, often appearing black. The streak is orange, and the luster is vitreous. Bicapite is brittle, has a Mohs hardness of 1½, and displays one excellent cleavage on {100}. The measured density is 2.44(2) g/cm^3. Bicapite is uniaxial (+), $\omega = 1.785(5)$, $\varepsilon \approx 1.81$ (white light); pleochroism is red-brown; $E > O$, slight. The electron probe microanalysis and results of the crystal structure determination provided the empirical formula (based on 67 O apfu) $(K_{1.23}Na_{2.23}Mg_{1.48})_{\Sigma 4.94}[H_{2.51}P_{1.02}(V^{5+}_{13.91}Mo^{6+}_{0.07})_{\Sigma 13.98}O_{42}]\cdot 25H_2O$. Bicapite is tetragonal, $I4/m$, with $a = 11.5446(12)$ Å, $c = 20.5460(14)$ Å, $V = 2738.3(6)$ Å^3, and $Z = 2$. The strongest four lines in the diffraction pattern are [d in Å (I) (hkl)]: 10.14 (100) (002,101); 2.978 (29) (134,206); 2.809 (11) (305); and 2.583 (11) (420,008). The atomic arrangement of bicapite was solved and refined to $R_1 = 0.0465$ for 1008 independent reflections with $I > 2\sigma I$. The structural unit is a $[H_2PV^{5+}_{12}O_{40}(V^{5+}O)_2]^{7-}$ heteropolyanion composed of 12 distorted VO_6 octahedra surrounding a central PO_4 tetrahedron and capped on opposite sides by two VO_5 square pyramids; the structural unit is a modification of the α-isomer of the Keggin anion, $[XM_{12}O_{40}]^{n-}$. Charge balance in the structure is maintained by the $[KNa_2Mg_2(H_2O)_{25}]^{7+}$ interstitial complex. The name bicapite is in recognition of this being the only known mineral with a structure based on a bicapped Keggin anion. The discovery of bicapite and numerous other natural polyoxometalate compounds in the Colorado Plateau uranium/vanadium deposits make that the most productive region found to date for naturally occurring polyoxometalate compounds.

Keywords: Bicapite, new mineral, crystal structure, polyoxometalate, bicapped Keggin anion, Pickett Corral mine, Montrose County, Colorado, U.S.A.