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Hanjiangite, a new barium-vanadium phyllosilicate carbonate mineral from the Shiti barium deposit in the Dabashan region, China

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Abstract

Hanjiangite, ideal formula $Ba_2Ca(V^{3+}Al)[Si_3AlO_{10}(OH)_2]F(CO_3)_2$, is a new mineral found in the Shiti barium deposit in the Dabashan region, China. Hanjiangite was collected from lenticular witherite ore bodies and witherite-barite-quartz veins cutting carbonaceous slates. It is found as disseminations in both settings. It occurs as thin, euhedral, tetragonal, tabular crystals, and anhedral grains. Grain size commonly varies from 0.05 to 4 mm and occasionally reaches 15 mm. It is yellow-green or dark green, with one well-developed or perfect cleavage on {001}. Other physical properties are: brittle, transparent to translucent, nonfluorescent, vitreous luster, greenish white streak, hardness 4 in the Mohs scale, splintery fracture, and a measured density of 3.69 g/cm^3. Hanjiangite is biaxial (–), $\alpha = 1.615$, $\beta = 1.655$, $\gamma = 1.700$ (589 nm), and displays strong pleochroism from pale yellow-green to dark green. It is monoclinic, with unit-cell parameters refined from single-crystal X-ray diffraction: $a = 5.2050(12)$, $b = 9.033(2)$, $c = 32.077(8)$ Å, $\beta = 93.49(8)°$, $V = 1505.4(8)$ Å^3, $Z = 4$, space group $C2$. The strongest seven lines of the X-ray powder-diffraction pattern [d in Å(I)(hkl)] are: 15.866(7)(002), 5.340(91)(006), 4.010(10)($\bar{1}$14), 3.209(23) (027), 2.676(100) ($\bar{1}$ 1 10), 2.294(29)($\bar{1}$37), and 2.008(11)($\bar{2}$28). Chemical analysis by a combination of electron microprobe, HF combustion, IR absorption, thermogravimetric analysis (TGA) and crystal-structure refinement gives SiO_2 19.64, TiO_2 1.12, Al_2O_3 11.19, MgO 0.54, CaO 4.91, BaO 34.89, V_2O_3 9.93, Cr_2O_3 1.75, Na_2O 0.20, K_2O 0.06, MnO 0.01, FeO 0.02, NiO 0.01, SrO 0.34, Y_2O_3 0.85, La_2O_3 0.14, Nd_2O_3 0.26, F 1.80, Cl 0.04, CO_2 10.37, H_2O 1.30, F=O –0.76, Cl=O –0.01, sum 98.60 wt%. The empirical formula is $(Ba_{1.98}Na_{0.06}K_{0.01})_{\Sigma 2.05}(Ca_{0.76}Mg_{0.12}Y_{0.06}Sr_{0.03}\ La_{0.01}Nd_{0.01})_{\Sigma 0.99}(V_{1.15}Al_{0.75}Cr_{0.20}Ti_{0.12})_{\Sigma 2.22}[(Si_{2.84}Al_{1.16})_{\Sigma 4.00}O_{10}][(OH)_{1.25}O_{0.77}]_{\Sigma 2.02}(F_{0.82}Cl_{0.01})_{\Sigma 0.83}(CO_3)_{2.05}$ based on 19 anions per formula unit. A single-crystal X-ray structure determination (sample 2005st-17) was carried out with a Smart APEX CCD system using Mo$K\alpha$ ($\lambda = 0.71073$ Å) radiation. The structure was solved using direct methods, and refined with the SHELXTL PC (Bruker AXS Inc.) package. Anisotropic refinement using all measured independent data and reflections with $I > 2\sigma(I)$ resulted in an R_1 factor of 0.08 and wR^2 of 0.20. The crystal structure is composed of alternating T-O-T and $Ba_2Ca(CO_3)_2F$ layers. The $Ba_2Ca(CO_3)_2F$ layer occurs between the T-O-T layers. The T site contains both Si and Al, and the O site both V^{3+} and Al. The interlayer hosts not only Ba (like in chernykhite) but also Ca atoms and (CO_3) groups. While the coordination of the cations in the TOT layer is obvious, the coordinations of Ca and Ba in the interlayer are not straight forward. A hanjiangite has three polytypes, namely 1M-type, 2M-type, and 3T-type.

Keywords: New mineral, hanjiangite, electron-microprobe data, single-crystal X-ray diffraction, crystal structure, Shiti barium deposit, Ankang County, China