Calderonite, a new lead-iron-vanadate of the brackebuschite group José González Del Tánago,^{1,*} Ángel La Iglesia,² Jordi Rius,³ and Soledad Fernández Santín¹

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ABSTRACT

Calderonite, ideally Pb₂Fe³⁺(VO₄)₂(OH), a new member of the brackebuschite group, has been found in the upper oxidation zone of two Pb-Zn hydrothermal deposits located at Santa Marta and Azuaga, Badajoz province, Spain. Brackebuschite and calderonite probably form a complete solid solution, locally with important substitution of Cu and Zn for Fe and Mn. The monoclinic cell parameters derived from powder X-ray diffraction (XRD) data are: a = 7.647(5) Å, b = 6.094(1) Å, c = 8.900(2) Å, $\beta = 112.0(2)^{\circ}$ and V = 384.5(4) Å³, and the six strongest lines, *d*-spacing (Å),(I),(*hkl*), are: 4.893(4)(011), 4.166(3)(002), 3.242(10) (Z11), 3.058(3)(020), 2.980(5) (T03) and 2.746(5)(003). Electron microprobe analyses (EMPA) show a certain degree of compositional variation not only between the Santa Marta and Azuaga samples but also among grains from the same locality. A representative formula of Santa Marta calderonite, determined from EMPA, based on 9 O atoms: is (Pb_{1.950}Ca_{0.004}Ba_{0.015})_{1.969}(Fe³⁺_{0.892}Cu_{0.059}Zn_{0.008}Al_{0.015})_{0.974} (V_{1.847}As_{0.008}Si_{0.039}P_{0.057})_{1.951}O_{7.507}(OH)_{1.493}. Fe³⁺ is principally substituted by Cu²⁺, and V⁵⁺ by Si⁴⁺. $\rho_c = 6.05$ g/cm³. The thermogravimetric analysis yields a weight loss of 1.91%, which corresponds to the 1.493 H needed to maintain the charge balance. Differential thermal analysis shows endothermic effects at 279 and 663 °C due to dehydroxylation.

A single-crystal XRD refinement was carried out on a selected crystal with cationic content determined by EMPA and starting atomic positions from brackebuschite. Final R-value of 5.81% based on 952 reflections with $I > 2\sigma_I$, assuming $P2_I/m$ symmetry, the cell dimensions are a = 7.649 Å, b = 6.101 Å, c = 8.904 Å, $\beta = 112.23^{\circ}$.

Calderonite is red orange to red brown, semitransparent to translucent with vitreous luster and red streak and powder. The fracture is splintery. Optically, it is biaxial positive, with a $2V_x = 86^\circ$ and strong dispersion. In plane-polarized light, it is strongly pleochroic (X = light greenish brown, Y = brown, Z = reddish brown).