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Leucostaurite, $Pb_2[B_5O_9]Cl{\cdot}0.5H_2O$, from the Atacama Desert: The first Pb-dominant member of the hilgardite group, and micro-determination of boron in minerals by PIGE

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Abstract

Leucostaurite is a new nanoporous lead borate discovered in samples from the Mina Asunción, Sierra Gorda, Atacama Desert, Chile, preserved since 1912 in the collections of the Natural History Museum of Bern, Switzerland. Leucostaurite formed via the oxidation of base-metal ores in the presence of B-rich brines. The mineral name is derived from the Greek "*leukos*" (white) and "*stauros*" (cross), and alludes to the white or transparent, colorless cruciform twinned crystals. Leucostaurite forms thin-tabular {010}, striated //[100], interpenetrated twinned crystals, and sheaf-like aggregates up to 0.8 mm on a paralaurionite and boleite matrix. The streak is white and the luster adamantine. Leucostaurite shows a weak, light-yellow fluorescence under short-wavelength UV but no fluorescence under long-wavelength UV light. The mineral is brittle, Mohs hardness ~4, with perfect cleavage parallel to {010} and good cleavage parallel to {100}; calculated density is 5.071 g/cm^3. Leucostaurite is biaxial, $2V$ (meas) ~30°, dispersion: r > v, strong. Optic sign and refractive indices could not be measured, but the average index calculated from the Gladstone-Dale relationship is 1.849. The empirical formula based on Pb + Sr + Ca = 2 atoms per formula unit (apfu), 1 H apfu and B + Si = 5 apfu, is $(Pb_{1.967}Sr_{0.026}Ca_{0.007})_{\Sigma 2.000}(B_{4.983}Si_{0.017})_{\Sigma 5.000}(Cl_{1.073}I_{0.004})_{\Sigma 1.077}O_{8.971}{\cdot}0.5H_2O$, which simplifies to $Pb_2[B_5O_9]Cl{\cdot}0.5H_2O$. The boron content was measured on two crystal fragments using proton-induced γ-ray emission spectroscopy; the analytical value [26.7(3) wt% B_2O_3] is within error of the stoichiometric value of 26.5 wt% B_2O_3. Leucostaurite is orthorhombic, space group *Pnn*2, a = 11.376(2), b = 11.505(2), c = 6.5558(7) Å, V = 858.1(2) Å^3, Z = 4. The seven strongest lines measured in the X-ray powder diffraction pattern are [d in Å/I_{rel} in %]: 4.04/100; 2.84/100; 5.71/80; 2.019/70; 3.29/40; 2.55/40; 1.877/40. The crystal structure of leucostaurite (R_1 = 6.2%) contains a hilgardite-type three-dimensional $[B_5O_9]^{3-}$ framework. Leucostaurite is the first mineral of the hilgardite group with orthorhombic (*Pnn*2) symmetry. However, several borates synthesized for their non-linear optical properties are structurally and chemically closely related to leucostaurite. For example in $Na_{0.5}Pb_2(B_5O_9)Cl(OH)_{0.5}$, one type of channels contains Cl^- ions, the other contains OH^-, Cl^-, and Na^+ ions; in leucostaurite these channels are occupied by Cl^- ions, and Cl^- ions + H_2O groups, respectively.

Keywords: Leucostaurite, new mineral, crystal structure, Mina Asunción, Sierra Gorda, Atacama Desert, Chile