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The crystal structure of piergorite-(Ce), $Ca_8Ce_2(Al_{0.5}Fe^{3+}_{0.5})_{\Sigma1}(\square,Li,Be)_2Si_6B_8O_{36}(OH,F)_2$: A new borosilicate from Vetralla, Italy, with a modified hellandite-type chain

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ABSTRACT

Piergorite-(Ce) is a new mineral found at Tre Croci, Vetralla, Italy with simplified formula $Ca_8Ce_2(Al_{0.5}Fe^{3+}_{0.5})_{\Sigma1}(\square,Li,Be)_2Si_6B_8O_{36}(OH,F)_2$. It occurs as strong intergrowths of small crystals, colorless to pale yellow, associated with sanidine, mica, magnetite, rutile, titanite, and other Th-U-REE bearing minerals, in miarolitic cavities of a syenitic ejectum. Piergorite-(Ce) is biaxial negative, $n_\alpha = 1.717$ (1), $n_\beta = 1.728$ (1), and $n_\gamma = 1.735$ (1), $2V_{meas} = 68(2)°$, $X = \mathbf{b}$, and $Z \wedge \mathbf{c} = 7(1)°$. Crystals show tabular habit and a very good {010} cleavage; twinning along the $(30\bar{1})$ plane produces "L" forms. The three strongest lines in the simulated powder diffraction pattern (d_{obs}, I, hkl) are: 2.65 Å, 100.0, (213, $\bar{4}$13); 1.91 Å, 48.3, (223, $\bar{4}$23, 821); 2.90 Å, 44.9, ($\bar{6}$03, $\bar{6}$12). The structure was solved by Patterson synthesis from X-ray diffraction data [monoclinic, space group $P2/a$, $a = 28.097(3)$ Å, $b = 4.777(1)$ Å, $c = 10.236(2)$ Å, $\beta = 96.81(1)°$, $V = 1364.2(7)$ Å^3, Z = 2] and was refined to a final $R_{obs} = 0.059$ for 6480 Fo with $I_o > 3\sigma(I_o)$. The structure shows similarities with the hellandite group because Si and B tetrahedra form chains along **c**. Hellandite structure is characterized by a single chain of five-membered rings, whereas piergorite-(Ce) shows a double chain of five-membered rings interconnected by a single octahedral site to form a three-dimensional framework containing five independent eightfold-coordinated M sites and a partly occupied T-cavity.

Keywords: New mineral, piergorite-(Ce), borosilicate, crystal structure, SIMS, hellandite