The crystal structure of vicanite-(Ce), a borosilicate showing an unusual $(Si_3B_3O_{18})^{15-}$ polyanion

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ABSTRACT

The crystal structure of holotype vicanite-(Ce) has been solved and refined to $R = 1.8\%$ for 1398 observed reflections with the aid of a new crystal from the same locality (Tre Croci, Vetralla, Italy), found more than 10 years after the first. The new unit formula is $(Ca,REE,Th)_{15}Fe^{3+}(SiO_4)_3$ $(Si_3B_3O_{18})(BO_3)(As^{5+}O_4)(As^{3+}O_3)_x(NaF_3)_{1-x}F_7 \cdot 0.2H_2O$ with x = 0.4. The structure is trigonal, $R3m$, Z = 3, $a = 10.8112(2)$, $c = 27.3296(12)$ Å, and layered along [001] with three distinct layers.

Layer A at z ca. 0 (1/3, 2/3) contains an $Fe(SiO_4)_6$ group and a threefold B_3O_9 borate ring. Each tetrahedron of the ring shares one oxygen atom with one Si tetrahedron, forming an unusual $Si_3B_3O_{18}^{15-}$ polyanion.

Layer B at z ca. 1/9 (4/9, 7/9) contains an AsO_4 tetrahedron and a BO_3 triangle.

Layer C at z ca. 2/9 (5/9, 8/9) represents the disordered part of the structure, containing two very close (0.85 Å) $As^{3+}O_3^{3-}$ and NaF_3^{2-} polyhedra, the occurrence of which is mutually exclusive and statistically disordered.

A 3-dimensional network of M-(O,F)$_n$ polyhedra (M = Ca, REE, Th; $8 < n < 10$) provide connections among neighboring layers.