American Mineralogist, Volume 103, pages 1497–1501, 2018

Segerstromite, $Ca_3(As^{5+}O_4)_2[As^{3+}(OH)_3]_2$, the first mineral containing $As^{3+}(OH)_3$, the arsenite molecule, from the Cobriza mine in the Atacama Region, Chile

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Abstract

A new mineral species, segerstromite, ideally $Ca_3(As^{5+}O_4)_2[As^{3+}(OH)_3]_2$, has been discovered at the Cobriza mine in the Sacramento district in the Copiapó Province, Chile. Crystals of segerstromite occur as tetrahedra, dodecahedra (up to 0.50 × 0.50 × 0.50 mm), or in blocky aggregates. Associated minerals include talmessite, vladimirite, and Sr-bearing hydroxylapatite. Similar to the associated minerals, segerstromite is a secondary mineral. The new mineral is colorless in transmitted light, transparent with a white streak and vitreous luster. It is brittle and has a Mohs hardness of ~4.5. No cleavage, parting, or twinning was observed. The measured and calculated densities are 3.44(3) and 3.46 g/cm^3, respectively. Optically, segerstromite is isotropic, with n = 1.731(5). It is insoluble in water or hydrochloric acid. An electron microprobe analysis yielded an empirical formula (based on 14 O apfu) $Ca_{2.98}(AsO_4)_{2.00}[As(OH)_3]_{2.00}$.

Segerstromite is cubic, with space group $I2_13$ and unit-cell parameters a = 10.7627(2) Å, V = 1246.71(4) Å^3, and Z = 4. Its crystal structure is constructed from three different polyhedral units: distorted CaO_8 cubes, rigid $As^{5+}O_4$ arsenate tetrahedra, and neutral $As^{3+}(OH)_3$ arsenite triangular pyramids. The Ca-groups form layers of corrugated crankshaft chains that lie parallel to the cubic axes. These chains are linked by the isolated $As^{5+}O_4$ and $As^{3+}(OH)_3$ groups. Segerstromite is the first known crystalline compound that contains the $As^{3+}(OH)_3$ arsenite molecule, pointing to a new potential approach to remove highly toxic and mobile $As^{3+}(OH)_3$ from drinking water.

Keywords: New mineral, segerstromite, arsenate/arsenite, crystal structure, X-ray diffraction, Raman spectrum