

BAVSIITE, $\text{Ba}_2\text{V}_2\text{O}_2[\text{Si}_4\text{O}_{12}]$, A NEW SILICATE MINERAL WITH SINGLE 4-RINGSWalter, F.¹ & Bojar, H.-P.¹¹Centre of Natural History – Mineralogy, Universalmuseum Joanneum, Weinzöttlstraße 16, A-8045 Graz, Austria
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Bavsiite from the type locality Gun Claim, Yukon Territory, Canada, occurs as millimetre sized sky-blue, platy crystals in a barium-rich low temperature skarn related to a porphyritic quartz monzonite stock. Associated minerals are alstonite, barite, celsian, diopside, fresnoite, suzukiite, walstromite, witherite and minerals from the cerchiarite group. Electron microprobe analyses yielded the empirical formula $\text{Na}_{0.02}\text{Ba}_{1.98}\text{Ti}_{0.16}\text{Fe}^{2+}_{0.03}\text{V}^{4+}_{1.80}\text{Al}_{0.05}\text{Si}_{4.00}\text{O}_{14}$ based on 14 oxygens per formula unit; the simplified chemical formula is $\text{Ba}_2\text{V}_2\text{Si}_4\text{O}_{14}$. Bavsiite is tetragonal, space group $I4/m$, $a = 7.043(1)$, $c = 11.444(2)$ Å, $V = 567.6(2)$ Å³, $Z = 2$. Least-squares refinement using anisotropic displacement parameters was carried out with the program SHELXL-2013 (SHELDRICK, 2015) and yielded $R1 = 0.0159$ based upon 312 unique reflections with $I > 2\sigma(I)$. The crystal structure of bavsiite comprises unbranched single $[\text{Si}_4\text{O}_{12}]^{8-}$ rings connected by $[\text{VO}_5]^{6-}$ square pyramids and BaO_{12} polyhedra. It can also be considered as cage-like $[\text{Si}_4\text{V}_2\text{O}_{18}]^{12-}$ clusters built by four SiO_4 tetrahedra and two VO_5 square pyramids (Fig. 1a). These clusters are cross-linked to form a pseudo-two-dimensional network (2D) parallel to the (001) plane, containing empty channels along the a axis (Fig. 1b). The 2D networks are held together by Ba^{2+} ions located in channels parallel to the c axis (Fig. 1c). Bavsiite is isotypic to synthetic $\beta\text{-BaVSi}_2\text{O}_7$ (LIU & GREEDAN, 1994) and polymorphic to orthorhombic suzukiite (BaVSi_2O_7). In the crystal structure of suzukiite (ITO et al., 2014) Si_4O_{12} chains along the c axis are linked by VO_5 square pyramids to form layers parallel to the ac plane, which are connected by barium atoms.

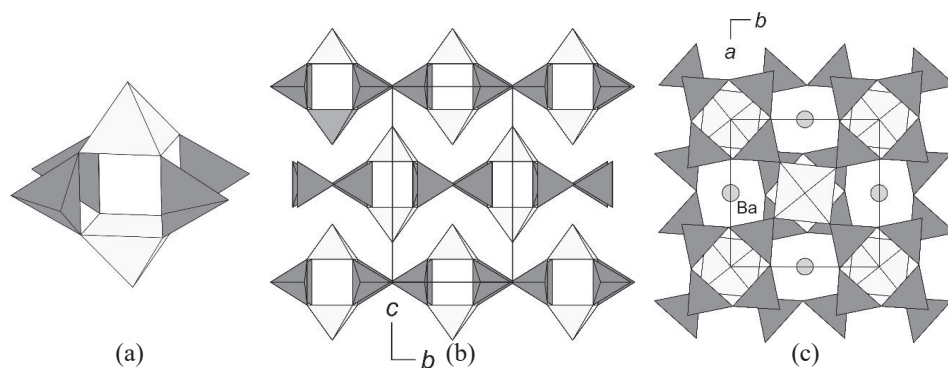


Figure 1. The crystal structure of bavsiite: (a) the cage-like $[\text{Si}_4\text{V}_2\text{O}_{18}]^{12-}$ cluster, (b) cross-linked clusters form a pseudo-two-dimensional network (2D) parallel to the (001) plane, Ba atoms are omitted for clarity and (c) projected along the (001) plane with Ba atoms in the channels along c .

ITO, M. et al. (2014): J. Miner. Petrol. Sci., 109, 222–227.

LIU, G., GREEDAN, J.E. (1994): J. Solid State Chem., 108, 267–274.

SHELDRICK, G.M. (2015): Acta Cryst., C71, 3–8.