BaZn₂(AsO₄)₂·H₂O: A Framework Structure related to Feldspar

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In connection with crystal chemical studies of alkaline earth arsenates, $BaZn_2(AsO_4)_2$ ·H₂O was synthesized under hydrothermal conditions. Its crystal structure was investigated by single-crystal X-ray diffraction data from a merohedral twin.

BaZn₂(AsO₄)₂·H₂O crystallizes in space group $P2_1$: a = 5.291(1), b = 10.418(2), c = 8.055(2) Å, $\beta = 95.33(3)^{\circ}, Z = 2$. The feldspar-like framework consists of ZnO₄ and AsO₄ tetrahedra which share corners. The central atoms Zn and As are arranged alternatingly, thus all O atoms of the framework are linked to a Zn and an As atom. The tetrahedra are connected to four- and eight-membered rings which are arranged to form channels in the direction of the *a*-axis. Parallel to these channels only the same kinds of tetrahedra are stacked above each other. Topologically related - but not identical - are e.g., paracelsian, BaAl₂(SiO₄)₂ [1], danburite, CaB₂(SiO₄)₂ [2], and BaZn₂(AsO₄)₂ [3]. The [8]-coordinated Ba atom (BaO₈ forms a tetragonal antiprism) and the water molecules are located in cavities centred in the larger channels. The H₂O molecule is linked to two Ba atoms; the acceptors of the hydrogen bonds are framework O atoms. Financial support of the Austrian science foundation (FWF) is gratefully acknowledged (Grant P15875-N03).

[1] Chiari et al., Am. Mineral., 1985, **70**, 969. [2] Sugiyama, Takéuchi, Z. Kristallogr., 1985, **173**, 293. [3] Lucas et al., Canad. Mineral., 1998, **36**, 1045. Keywords: BaZn₂(AsO₄)₂·H₂O, hydrothermal synthesis, crystal chemistry of inorganic compounds