Crystal structure of aluminum *catena*-[monohydrogenborate-dihydrogenborate-bis(monohydrogenphosphate)] monohydrate, $\text{Al}[\text{B}_2\text{P}_2\text{O}_7(\text{OH})_5] \cdot \text{H}_2\text{O}$

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Abstract

$\text{AlB}_2\text{O}_{13}\text{H}_7\text{P}_2$, monoclinic, $C12/c1$ (No. 15), $a = 18.994(4) \text{ \AA}$, $b = 6.704(1) \text{ \AA}$, $c = 6.910(1) \text{ \AA}$, $\beta = 99.03(3)^\circ$, $V = 869.0 \text{ \AA}^3$, $Z = 4$, $R_{\text{gt}}(F) = 0.055$, $wR_{\text{ref}}(F^2) = 0.142$, $T = 293 \text{ K}$.

Source of material

$\text{Al}[\text{B}_2\text{P}_2\text{O}_7(\text{OH})_5] \cdot \text{H}_2\text{O}$ was synthesized under mild hydrothermal conditions. Mixtures of 2.12 g $\text{Al}(\text{H}_2\text{PO}_4)_3$, 1.66 g H_3BO_3 and 2.36 g H_3PO_4 (85%, conc. solution, pH 1.0) were treated in teflon autoclaves (degree of fill 70%) at 438 K for six days. The starting materials were all analytical-grade purity.

Discussion

In the last few years an increasing interest in microporous materials has developed. Compounds like borophosphates have come to attention because they show a rich crystal chemistry [1]. Until now only one Al borophosphate has been reported [2]. The structure of the title compound is related to the structure of $\text{Fe}[\text{B}_2\text{P}_2\text{O}_7(\text{OH})_5]$ [3], which without consideration of the crystal water in the structure of $\text{Al}[\text{B}_2\text{P}_2\text{O}_7(\text{OH})_5] \cdot \text{H}_2\text{O}$ would be an isotype. The structure of the title compound is characterized by isolated $\text{AlO}_2(\text{OH})_4$ octahedra sharing O corners with hydrogen-

phosphate and common OH corners with hydrogenborate groups from the anionic non-branched vierer-single-chains $[\text{B}_2\text{P}_2\text{O}_7(\text{OH})_5]^{3-}$, which are built of corner sharing $\text{BO}_3(\text{OH})$ and $\text{PO}_3(\text{OH})$ tetrahedra. Symmetric hydrogen bridges are formed between O1 positions of adjacent polyanions, $d[\text{O}(1) \cdots \text{O}(1)] = 2.48 \text{ \AA}$. The condensation of the borophosphate anions with Al-coordination octahedra via common corners results in an overall three-dimensional framework which contains elliptical channels running along the [001] direction. Water molecules are positioned within the open channels and are fixed through hydrogen bridges between O4 and O5, $d[\text{O}(4) \cdots \text{O}(4)] = 2.82 \text{ \AA}$. The bond distances $d(\text{Al} \cdots \text{O})$ amount to 1.844 Å and 1.906 Å, the value of $d(\text{Al} \cdots \text{OH})$ increases to 1.926 Å. The distance $d(\text{O}5 \cdots \text{H}1) = 3.52 \text{ \AA}$ is too long for the formation of a hydrogen bridge. The bond distances in the anionic borophosphate chains correspond to respective values in aluminum borophosphates [2].

Table 1. Data collection and handling.

Crystal:	transparent prism, size $0.1 \times 0.2 \times 0.6 \text{ mm}$
Wavelength:	Mo K_α radiation ($0.71073 \text{ \AA}$)
μ :	6.85 cm^{-1}
Diffractometer, scan mode:	Enraf Nonius CAD4, $\omega/2\theta$
$2\theta_{\text{max}}$:	59.54°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	4507, 1056
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 900
$N(\text{param})_{\text{refined}}$:	98
Programs:	SHELXS-97 [4], SHELXL-97 [5], DIAMOND [6]

Table 2. Atomic coordinates and displacement parameters (in $\text{\AA}^2$).

Atom	Site	x	y	z	U_{iso}
H(1)	4e	1/2	0.32(2)	1/4	0.10(4)
H(2)	8f	0.176(4)	0.06(1)	0.67(1)	0.04(2)
H(3)	8f	0.536(3)	0.87(1)	1.225(9)	0.04(2)
H(4)	8f	0.170(5)	-0.12(2)	0.61(1)	0.11(3)

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Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
P(1)	8f	0.33442(5)	0.1277(2)	0.9116(1)	0.0109(5)	0.0100(5)	0.0086(5)	−0.0010(4)	0.0018(3)	−0.0002(4)
Al(1)	4d	1/4	1/4	1/2	0.0108(8)	0.0083(8)	0.0067(7)	0.0003(6)	0.0020(6)	0.0005(6)
O(1)	8f	0.4544(2)	0.3308(5)	1.3599(4)	0.014(1)	0.018(2)	0.012(1)	−0.003(1)	0.003(1)	0.000(1)
O(2)	8f	0.3766(2)	0.2542(4)	1.0768(4)	0.014(1)	0.012(1)	0.008(1)	−0.003(1)	0.000(1)	0.000(1)
O(3)	8f	0.3118(2)	0.2702(4)	0.7448(4)	0.014(1)	0.014(1)	0.006(1)	−0.002(1)	−0.000(1)	−0.001(1)
O(4)	8f	0.3899(2)	−0.0226(5)	0.8517(4)	0.013(1)	0.011(1)	0.018(1)	−0.001(1)	0.005(1)	−0.001(1)
O(5)	4e	1/2	0.7806(8)	1/4	0.021(2)	0.028(3)	0.034(3)	0	0.009(2)	0
O(6)	8f	0.1722(2)	0.1671(5)	0.6293(4)	0.012(1)	0.011(2)	0.014(1)	−0.000(1)	0.007(1)	0.002(1)
O(7)	8f	0.2745(2)	0.0145(4)	0.9800(4)	0.016(1)	0.008(1)	0.012(1)	−0.001(1)	0.005(1)	0.001(1)
B(1)	8f	0.3849(2)	0.2349(7)	0.2904(6)	0.011(2)	0.010(2)	0.008(2)	0.001(2)	0.001(2)	0.000(2)

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