Crystal structure of rubidium aluminum *catena*-[monohydrogen-monoborate-bis(monophosphate)], $\text{RbAl}[\text{BP}_2\text{O}_8(\text{OH})]$

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Abstract

$\text{AlBHO}_9\text{P}_2\text{Rb}$, monoclinic, $P12_1/c1$ (No. 14), $a = 9.244(1) \text{ \AA}$, $b = 8.403(1) \text{ \AA}$, $c = 9.394(2) \text{ \AA}$, $\beta = 103.388(7)^\circ$, $V = 709.9 \text{ \AA}^3$, $Z = 4$, $R_{\text{gt}}(F) = 0.059$, $wR_{\text{ref}}(F^2) = 0.141$, $T = 295 \text{ K}$.

Source of material

$\text{RbAl}[\text{BP}_2\text{O}_8(\text{OH})]$ was synthesized under mild hydrothermal conditions. The reactions were carried out with mixture of RbCl (1.813 g), $\text{Al}(\text{H}_2\text{PO}_4)_3$ (3.179 g), H_3BO_3 (0.618 g) and 4 ml 85% H_3PO_4 with molar ratio of $\text{Rb} : \text{Al} : \text{B} : \text{P} = 1.5 : 1 : 1 : 3.6$. The mixture was filled in a teflon autoclave ($V = 20 \text{ ml}$). The degree of filling is about 50%. The autoclave was placed in an oven with subsequent heating at 413 K for 7 days. The starting materials were all of analytical-grade purity.

Discussion

Despite the systematic investigations on borophosphates with the main group elements, Ga and In, reported recently [1–6], there is only one compound, $\text{NaAl}[\text{BP}_2\text{O}_7(\text{OH})_3]$ [7], reported until now in the respective Al system. The crystal structure of the title compound is isotypic to $\text{RbV}[\text{BP}_2\text{O}_8(\text{OH})]$, $(\text{NH}_4)\text{Ga}[\text{BP}_2\text{O}_8(\text{OH})]$ and $\text{CsAl}[\text{BP}_2\text{O}_8(\text{OH})]$ [8–10]. The crystal structure is characterized by isolated $\text{AlO}_5(\text{OH})$ octahedra sharing common O corners with five phosphate tetrahedra and a common (OH) corner with a hydrogenborate group to form a three-dimensional framework structure. The anionic partial structure contains open-branched vierer-single chains $[\text{BP}_2\text{O}_8(\text{OH})]^{4-}$, which are formed by alternating hydrogenborate and phosphate tetrahedra sharing common O corners. Rubidium cations reside in the open elliptical channels running along the a axis. The Al—O and Al—OH bond distances range from 1.851 Å to 2.017 Å. Bond lengths and angles of hydrogenborate and phosphate tetrahedra within the anionic chains are consistent with other borophosphates [1–6].

Table 1. Data collection and handling.

Crystal:	colorless prism, size $0.07 \times 0.07 \times 0.25 \text{ mm}$
Wavelength:	Mo K_α radiation ($0.71073 \text{ \AA}$)
μ :	75.78 cm^{-1}
Diffractionmeter, scan mode:	Rigaku AFC7-CCD, 600 images, $\Delta\phi = 0.6^\circ$, $60-\omega$ scan, $\Delta\omega = 0.6^\circ$, $\chi = 90^\circ$
$2\theta_{\text{max}}$:	64.64°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	8318, 2055
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2\sigma(I_{\text{obs}})$, 1872
$N(\text{param})_{\text{refined}}$:	131
Programs:	SHELXL-97 [11], DIAMOND [12]

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

Atom	Site	x	y	z	U_{iso}
H(1)	4e	0.13(2)	0.06(2)	0.51(1)	0.05

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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
Rb(1)	4e	0.30899(9)	0.39218(9)	0.44143(8)	0.0268(4)	0.0203(4)	0.0181(4)	−0.0048(3)	0.0048(3)	−0.0040(3)
P(1)	4e	0.4297(2)	0.9336(2)	0.2952(2)	0.0054(6)	0.0061(6)	0.0050(7)	−0.0010(5)	0.0005(5)	−0.0002(5)
P(2)	4e	0.0852(2)	0.7373(2)	0.2795(2)	0.0029(6)	0.0057(6)	0.0086(7)	−0.0006(4)	0.0003(5)	0.0001(5)
Al(1)	4e	0.2972(2)	0.8476(2)	0.5698(2)	0.0069(8)	0.0073(8)	0.0065(9)	−0.0006(6)	0.0013(6)	0.0002(6)
B(1)	4e	0.1651(7)	0.0519(8)	0.3020(8)	0.007(3)	0.006(3)	0.014(3)	−0.002(2)	0.002(2)	−0.001(2)
O(1)	4e	0.3104(5)	0.0726(5)	0.2679(5)	0.005(2)	0.007(2)	0.012(2)	0.000(1)	0.003(2)	0.003(1)
O(2)	4e	0.9163(5)	0.6970(5)	0.2499(5)	0.004(2)	0.007(2)	0.019(2)	−0.001(1)	0.001(2)	−0.003(2)
O(3)	4e	0.1540(5)	0.7207(5)	0.4406(5)	0.015(2)	0.011(2)	0.007(2)	−0.004(2)	−0.002(2)	0.000(2)
O(4)	4e	0.4208(5)	0.9890(5)	0.6944(5)	0.007(2)	0.011(2)	0.010(2)	−0.004(2)	0.001(2)	−0.005(2)
O(5)	4e	0.0844(5)	0.9125(5)	0.2293(5)	0.010(2)	0.007(2)	0.013(2)	−0.000(2)	−0.001(2)	0.001(2)
O(6)	4e	0.3968(5)	0.6697(5)	0.6591(5)	0.010(2)	0.007(2)	0.011(2)	0.002(1)	0.002(2)	0.003(2)
O(7)	4e	0.1586(5)	0.6303(5)	0.1874(5)	0.011(2)	0.011(2)	0.012(2)	0.002(2)	0.005(2)	−0.000(2)
O(8)	4e	0.4182(5)	0.8444(5)	0.4330(5)	0.011(2)	0.012(2)	0.008(2)	0.001(2)	0.003(2)	0.001(2)
O(9)	4e	0.1907(5)	0.0375(5)	0.4631(5)	0.010(2)	0.011(2)	0.010(2)	0.001(2)	0.005(2)	−0.000(2)

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