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

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Abstract

$\text{AlBHKO}_9\text{P}_2$, monoclinic, $P12_1/c1$ (No. 14), $a = 9.255(4)$ Å, $b = 8.190(1)$ Å, $c = 9.323(1)$ Å, $\beta = 102.89(3)^\circ$, $V = 688.9$ Å³, $Z = 4$, $R(P) = 0.113$, $R(I) = 0.059$, $T = 295$ K.

Source of material

$\text{KAl}[\text{BP}_2\text{O}_8(\text{OH})]$ was prepared under mild hydrothermal conditions from a mixture of 2.54 g $\text{Al}(\text{H}_2\text{PO}_4)_3$, 2.44 g $\text{K}_2\text{B}_4\text{O}_7 \cdot 4\text{H}_2\text{O}$, 2.35 g K_2HPO_4 and 5.01 g H_3PO_4 (85%, pH 1.5). The molar ratio of K : Al : B : P amounted to 5 : 1 : 4 : 10. The syntheses were carried out in teflon autoclaves (degree of fill 90%) at 438 K for 6 days. The starting materials were all analytical-grade purity. Chemical composition was confirmed by ICP-AES analyses.

Experimental details

The position of the H atom was not determined.

Discussion

During the past few years compounds with open framework structures like borophosphates have drawn much attention and show a rich crystal chemistry [1]. Systems including a p-block metal have not been intensively studied up to now, though some compounds with Al and Ga have been reported recently [2,3].

The title compound $\text{KAl}[\text{BP}_2\text{O}_8(\text{OH})]$ is an isotype of $\text{CsFe}[\text{BP}_2\text{O}_8(\text{OH})]$ [4] and $\text{RbFe}[\text{BP}_2\text{O}_8(\text{OH})]$ [5]. The anionic partial structure contains open-branched vierer-einfach-chains $[\text{BP}_2\text{O}_8(\text{OH})]^{4-}$ running along the [001] direction. The chains are formed by alternating hydrogenborate and phosphate tetrahedra sharing common corners. One further phosphate tetrahedron is linked to each borate tetrahedron. Bond lengths and angles within the anionic chains are consistent with related borophosphates [4,5]. Al^{3+} is coordinated octahedrally ($\text{AlO}_5(\text{OH})$) by oxygen atoms of three neighbouring tetrahedral chains. Thereby a 3-D linkage of tetrahedra and octahedra is established. K^+ is coordinated irregularly by nine oxygen atoms and one OH function. Bond distances Al—O range

from 1.835 Å to 1.980 Å, the bond distance Al—OH is increased to 2.031 Å.

Table 1. Data collection and handling.

Powder:	white
Wavelength:	Cu $K\alpha$ radiation (1.54051 Å)
μ :	12.9 cm ⁻¹
Diffractometer, scan mode:	STOE STADIP, Debye-Scherrer
$2\theta_{\text{max}}$, stepwidth:	80°, 0.02°
$N(\text{points})_{\text{measured}}$:	3750
$N(hkl)_{\text{measured}}$:	414
$N(\text{param})_{\text{refined}}$:	61
Programs:	FULLPROF [6], DIAMOND [7]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{iso}
K	4e	0.1919(4)	0.5950(4)	0.5666(4)	0.037(1)
Al	4e	0.2007(5)	0.1507(6)	0.4339(6)	0.027(3)
B	4e	0.328(2)	0.567(2)	0.187(2)	0.022(7)
P(1)	4e	0.0737(5)	0.4398(6)	0.2086(4)	0.003(3)
P(2)	4e	0.4174(5)	0.2454(6)	0.2226(5)	0.012(4)
O(1)	4e	0.087(1)	0.007(1)	0.3052(9)	0.017(4)
O(2)	4e	0.0835(9)	0.3466(9)	0.0784(9)	0.017
O(3)	4e	0.1033(8)	0.3390(8)	0.346(1)	0.017
O(4)	4e	0.1852(9)	0.590(1)	0.2337(8)	0.017
O(5)	4e	0.3153(9)	0.5474(1)	0.0289(8)	0.017
O(6)	4e	0.3483(8)	0.137(1)	0.3171(8)	0.017
O(7)	4e	0.3632(8)	0.223(1)	0.059(1)	0.017
O(8)	4e	0.410(1)	0.417(1)	0.2821(9)	0.017
O(9)	4e	0.5939(9)	0.213(1)	0.2516(9)	0.017

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