Crystal structure of sodium aluminum (monohydrogenmonophosphate-dihydrogenmonoborate-monophosphate), $NaAl[BP_2O_7(OH)_3]$

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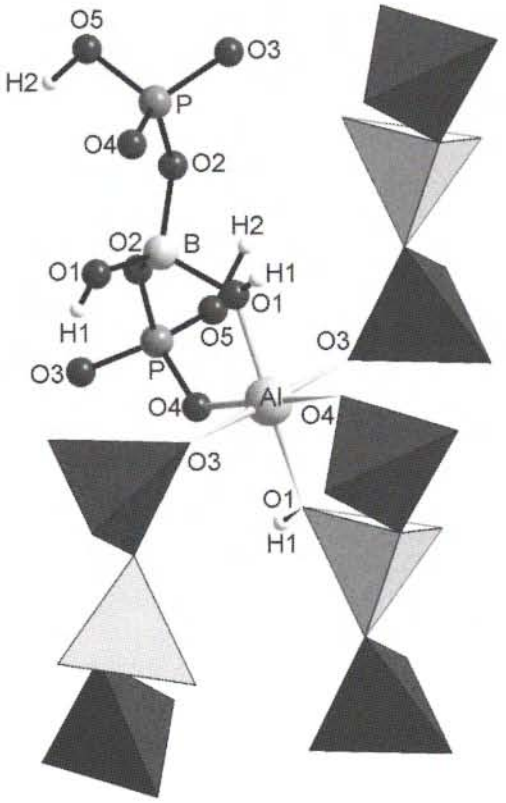

Abstract

$AlBH_3NaO_{10}P_2$, monoclinic, $C12/c1$ (No. 15), a = 10.497(2) Å, b = 7.993(2) Å, c = 9.077(2) Å, β = 117.26(3)°, V = 677.0 Å^3, Z = 4, $R_{gt}(F)$ = 0.049, $wR(F^2)$ = 0.077, T = 293 K.

Source of material

$NaAl[BP_2O_7(OH)_3]$ was prepared by hydrothermal treatment of 2.12 g $Al(H_2PO_4)_3$, 2.61 g $Na_2B_4O_7 \cdot 10H_2O$ and 3.63 g H_3PO_4 (85%) (conc. solution, pH 1.5) in teflon autoclaves (degree of fill 75%) at 438 K for two weeks.

Discussion

The crystal structure of $NaAl[BP_2O_7(OH)_3]$ (B:P < 1; [1]) contains isolated anions $[(OH)O_2PO_{1/2}\text{-}O_{1/2}B(OH)_2O_{1/2}\text{-}O_{1/2}PO_3]^{4-}$ of corner sharing tetrahedra. The crystal structure is an isotype of $NaFe[BP_2O_7(OH)_3]$ [2]. Aluminum is octahedrally coordinated by O (3,4) and OH (1) of four neighbouring oligomeric units. Hydrogen bridges (symmetric arrangement) are formed between O5 positions (O5···H2···O5; O5···H2 = 1.249 Å).

Table 1. Data collection and handling.

Crystal:	colourless, transparent prism, size 0.1 × 0.1 × 0.05 mm
Wavelength:	Ag K_α radiation (0.56086 Å)
μ:	4.59 cm^{-1}
Diffractometer, scan mode:	Stoe IPDS, 200 exposures, Δφ = 1°
$2\theta_{max}$:	43.98°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	3405, 847
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 455
$N(param)_{refined}$:	74
Programs:	SHELXL-97 [3], DIAMOND [4]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(1)	8*f*	0.478(7)	0.170(9)	1.071(8)	0.02
H(2)	4*d*	1/4	1/4	1/2	0.02

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Na	4*e*	1/2	0.3659(5)	3/4	0.020(2)	0.020(2)	0.026(2)	0	0.010(2)	0
Al	4*c*	1/4	1/4	0	0.008(1)	0.007(1)	0.010(1)	0.0009(9)	0.0043(9)	-0.0001(9)
B	4*e*	1/2	0.033(1)	1/4	0.004(3)	0.005(4)	0.009(3)	0	0.005(3)	0
P	8*f*	0.2255(1)	0.0656(2)	0.6822(2)	0.0075(6)	0.0062(7)	0.0075(6)	0.0007(6)	0.0040(5)	0.0000(6)
O(1)	8*f*	0.4323(4)	0.1365(5)	1.1000(4)	0.007(2)	0.012(2)	0.008(2)	0.001(2)	0.003(2)	0.004(1)
O(2)	8*f*	0.3919(4)	0.0796(5)	0.7579(4)	0.010(2)	0.006(2)	0.014(2)	0.000(2)	0.006(2)	-0.002(2)
O(3)	8*f*	0.1805(4)	0.0961(5)	0.8163(4)	0.007(2)	0.009(2)	0.011(2)	0.000(2)	0.006(1)	-0.000(2)
O(4)	8*f*	0.1783(4)	-0.1085(5)	0.6098(4)	0.011(2)	0.007(2)	0.014(2)	-0.003(1)	0.007(1)	-0.003(1)
O(5)	8*f*	0.1611(4)	0.2010(5)	0.5462(4)	0.012(2)	0.014(2)	0.012(2)	-0.002(2)	0.005(2)	0.005(2)

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