

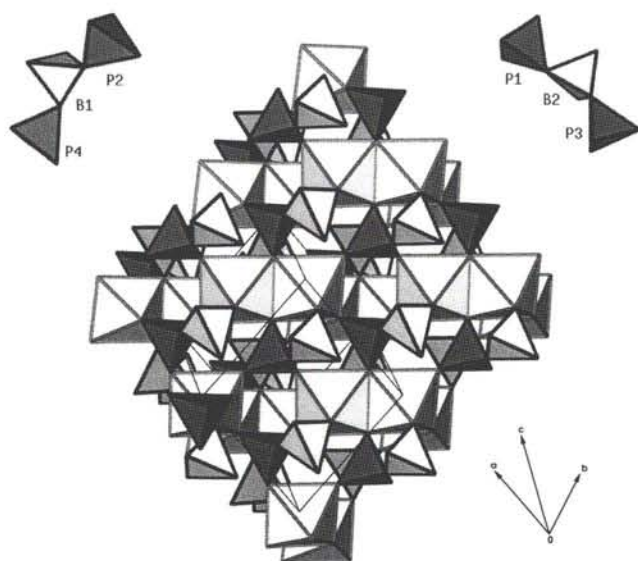
# Crystal structure of dimagnesium (monohydrogenmonophosphate-dihydrogenmonoborate-monophosphate), $Mg_2[BP_2O_7(OH)_3]$

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Dedicated to Prof. Dr. P. Böttcher on the occasion of his 60th birthday

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aspects (short interatomic O...O contacts) hydrogen bridges are supposed to be located between O1...O14 (257 pm) and O2...O2 (276 pm) or O16...O19 (275 pm), respectively. Based on general principles of borophosphate structural chemistry [2] the terminal corners of the  $BO_4$  groups are assumed to be protonated. The metrical transformation by applying matrix  $(-1 -1 0, 1 -1 0, 0 0 1)$  results in a pseudo monoclinic space group  $C2/m$ , in which the structure can not be refined. The existence of a centre of symmetry was also excluded.

Table 1. Data collection and handling.

Crystal:	colorless platelet, size 0.1 x 0.2 x 0.3 mm
Wavelength:	Mo $K\alpha$ radiation (0.71070 Å)
$\mu$ :	8.76 cm <sup>-1</sup>
Diffractometer, scan mode:	Siemens P4, $\omega$
2 $\theta$ <sub>max</sub> :	72.2°
$N(hkl)$ <sub>measured</sub> , $N(hkl)$ <sub>unique</sub> :	1535, 1535
Criterion for $I_{obs}$ , $N(hkl)$ <sub>gt</sub> :	$I_{obs} > 2 \sigma(I_{obs})$ , 1469
$N(param)$ <sub>refined</sub> :	161
Programs:	SHELXS-97 [3], SHELXL-97 [4]

## Abstract

$B_2H_6Mg_4O_{20}P_4$ , triclinic,  $P1$  (No. 1),  $a = 6.452(1)$  Å,  $b = 6.455(2)$  Å,  $c = 8.360(2)$  Å,  $\alpha = 82.50(1)^\circ$ ,  $\beta = 82.56(2)^\circ$ ,  $\gamma = 80.98(2)^\circ$ ,  $V = 338.8$  Å<sup>3</sup>,  $Z = 1$ ,  $R_g(F) = 0.042$ ,  $R_w(F^2) = 0.108$ ,  $T = 293$  K.

## Source of material

$Mg_2[BP_2O_7(OH)_3]$  was prepared by hydrothermal reaction of  $H_3BO_3$ ,  $MgHPO_4 \cdot 3H_2O$ , and  $MgCl_2 \cdot 6H_2O$  (molar ratio 1:1:2; conc. solution, pH = 0.5, (HCl)) at 433 K.

## Discussion

The crystal structure of  $Mg_2[BP_2O_7(OH)_3]$  contains two crystallographically independent trinuclear anions  $[(OH)O_2PO_{1/2}O_{1/2}B(OH)_2O_{1/2}O_{1/2}PO_3]^{4-}$  of corner sharing tetrahedra. This type of oligomeric tetrahedral anion is also present in the crystal structure of  $NaFe[BP_2O_7(OH)_3]$  [1]. Magnesium is in an octahedral coordination by O and OH corners of the oligomeric units. The octahedra share common edges to form infinite octahedral chains (figure) which are arranged in layers perpendicular to  $[111]$  and which are separated by layers containing the oligomeric tetrahedral anions (in the figure light:  $BO_4$ , dark:  $PO_4$ ). Hydrogen positions could not be determined. According to geometrical

Table 2. Atomic coordinates and displacement parameters (in Å<sup>2</sup>).

Atom	Site	x	y	z	$U_{iso}$
B(1)	1a	0.603(2)	0.741(1)	1.189(1)	0.020(2)
B(2)	1a	0.160(2)	0.295(1)	0.236(1)	0.020(2)
O(1)	1a	0.4083(9)	0.5385(8)	0.8587(6)	0.014(1)
O(2)	1a	-0.276(1)	-0.4114(9)	0.5458(7)	0.014(1)
O(3)	1a	0.008(1)	-0.1337(9)	0.5272(7)	0.014(1)
O(4)	1a	0.0358(9)	0.2106(8)	0.6268(6)	0.012(1)
O(5)	1a	0.689(1)	-0.1362(8)	0.7991(6)	0.012(1)
O(6)	1a	0.355(1)	-0.0722(8)	0.6127(7)	0.014(1)
O(7)	1a	0.784(1)	-0.3291(9)	1.0663(7)	0.017(1)
O(8)	1a	0.229(1)	0.1157(8)	0.3580(7)	0.016(1)
O(9)	1a	0.9718(9)	-0.4552(8)	0.8128(6)	0.013(1)
O(10)	1a	-0.336(1)	-0.1022(9)	0.2841(7)	0.025(1)
O(11)	1a	0.084(1)	-0.513(1)	0.3145(7)	0.026(1)
O(12)	1a	0.002(1)	0.2358(9)	1.1410(7)	0.025(1)
O(13)	1a	0.414(1)	0.817(1)	1.1109(7)	0.027(1)
O(14)	1a	-0.6397(9)	-0.5067(8)	0.5666(6)	0.016(1)
O(15)	1a	0.672(1)	0.227(1)	0.9384(8)	0.032(2)
O(16)	1a	0.312(1)	0.1768(9)	0.8787(7)	0.015(1)
O(17)	1a	-0.427(1)	-0.4577(9)	0.2960(7)	0.024(1)
O(18)	1a	0.360(1)	0.3276(9)	1.1297(7)	0.023(1)
O(19)	1a	1.035(1)	-0.1080(9)	0.8971(7)	0.013(1)
O(20)	1a	-0.327(1)	-0.7708(9)	0.4864(8)	0.029(1)

**Table 3.** Atomic coordinates and displacement parameters (in Å<sup>2</sup>).

Atom	Site	x	y	z	U <sub>11</sub>	U <sub>22</sub>	U <sub>33</sub>	U <sub>12</sub>	U <sub>13</sub>	U <sub>23</sub>
Mg(1)	1a	-0.3236(4)	-0.0871(4)	0.5361(3)	0.011(1)	0.014(1)	0.020(2)	0.002(1)	-0.003(1)	-0.004(1)
Mg(2)	1a	0.0438(4)	-0.4648(4)	0.5572(3)	0.011(2)	0.012(1)	0.015(1)	0.001(1)	-0.003(1)	0.000(1)
Mg(3)	1a	-0.0118(4)	0.2245(4)	0.8891(3)	0.014(2)	0.010(1)	0.019(1)	0.002(1)	-0.002(1)	-0.002(1)
Mg(4)	1a	0.3657(5)	0.8572(4)	0.8681(3)	0.013(1)	0.009(1)	0.014(1)	0.002(1)	-0.001(1)	-0.001(1)
P(1)	1a	0.1559(3)	0.0283(3)	0.5359(2)	0.012(1)	0.0079(9)	0.013(1)	-0.0016(8)	-0.0021(9)	0.0011(7)
P(2)	1a	0.8731(3)	-0.2546(3)	0.8889(2)	0.010(1)	0.0095(9)	0.012(1)	-0.0010(8)	0.0003(8)	-0.0024(8)
P(3)	1a	0.4387(3)	0.3152(3)	0.9509(2)	0.012(1)	0.0123(9)	0.0136(9)	-0.0017(9)	0.0009(8)	-0.0038(7)
P(4)	1a	-0.4143(3)	-0.5377(3)	0.4746(2)	0.012(1)	0.0095(9)	0.014(1)	-0.0027(8)	-0.0029(8)	0.0017(7)

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