

Crystal structure of $\text{MgK}_{0.5}[\text{B}_6\text{O}_{10}](\text{OH})_{0.5}\cdot 0.5\text{H}_2\text{O}$, poly[dimagnesium potassium bis(hexaborate) hydroxide monohydrate]

Qi-Ming Qiu^{a*} and Jian-Biao Song^b

^aSchool of Science, China University of Geosciences, Beijing 100083, People's Republic of China, and ^bBeijing Chaoyang Foreign Language School, Beijing 100101, People's Republic of China. *Correspondence e-mail: qiuqiming890521@163.com

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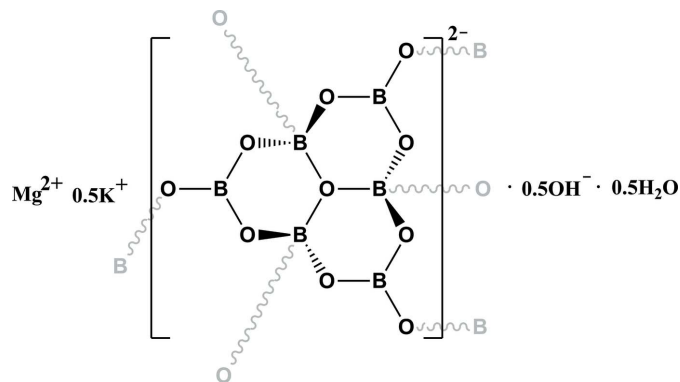
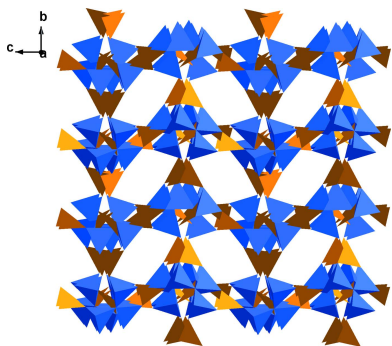
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The solvothermal reaction of H_3BO_3 , KCF_3SO_3 , $\text{Mg}(\text{CF}_3\text{SO}_3)_2$ and pyridine led to a new alkali- and alkaline-earth-metal borate, $\text{MgK}_{0.5}[\text{B}_6\text{O}_{10}](\text{OH})_{0.5}\cdot 0.5\text{H}_2\text{O}$. Its structure features an intricate three-dimensional framework built from $[\text{B}_6\text{O}_{13}]^{8-}$ clusters, thus resulting in a six-connected achiral net with high symmetry. Each $[\text{B}_6\text{O}_{13}]^{8-}$ building block is composed of three trigonal BO_3 and three tetrahedral BO_4 units, with these BO_4 units being further connected to neighboring BO_3 units, giving rise to an oxoboron cluster of the general formula $[\text{B}_6\text{O}_{10}]^{2-}$.

1. Chemical context

As inorganic materials, borates are an important class of non-linear optical crystals, mainly because they can easily crystallize in non-centrosymmetric space groups and such structures often show a large second-harmonic generation response (Qiu *et al.*, 2021a; Qui & Yang, 2021a). The combination of BO_3 -trigonal and BO_4 -tetrahedral units makes it possible to form a variety of isolated anionic clusters. Extended chains, layers and three-dimensional frameworks can be formed between clusters through the dehydration and condensation of the terminal hydroxyl groups of oxoboron clusters (Wang *et al.*, 2017). In addition, negatively charged oxoboron clusters can also combine with a variety of counter-cations, making the structure of borates more complex and diverse. Here, single crystals of $\text{MgK}_{0.5}[\text{B}_6\text{O}_{10}](\text{OH})_{0.5}\cdot 0.5\text{H}_2\text{O}$ with alkali- and alkaline-earth metals have been obtained under solvothermal conditions.



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2. Structural commentary

The asymmetric unit of the title compound consists of 2 B, 10/3 O, 1/3 Mg, 1/6 K, 1/6 OH, and 1/6 H₂O. The Mg, K, O4, O5 and O6 atoms are located on special positions with occupancy of 1/3 or 1/6, while the remaining B and O atoms are located at general positions with an occupancy of 1. Bond-valence-sum calculations show that Mg, K and B are consistent with the expected oxidation states (Brown & Altermatt, 1985; Brese & O’Keeffe, 1991). Three BO₄ units are joined together through corner-sharing of the O4 atom and three BO₄ units are connected with three neighboring BO₃ units to form a [B₆O₁₃]⁸⁻ oxoboron cluster (Fig. 1). To the best of our knowledge, this is the first example of a mixed alkali- and alkaline-earth-metal borate crystal with the [B₆O₁₃]⁸⁻ cluster anion. In this cluster, the B—O4 bonds are unique because their bond distances [1.529 (2) Å] are longer than other B—O bonds [1.359 (2)–1.453 (2) Å] in the BO₃ and BO₄ units. Each [B₆O₁₃]⁸⁻ unit is further connected to six other clusters by corner-sharing O atoms, resulting in a three-dimensional framework (Fig. 2).

3. Supramolecular features

In the title compound, the Mg and K atoms are six-coordinated, with Mg—O and distances in the range 2.332 (1)–2.374 (1) Å and K—O = 2.845 (1) Å. The three-dimensional structure is stabilized by a water cluster formed by O5—H5···O5, O5—H5···O6 and O6—H6A···O2 hydrogen bonds involving the water molecule, hydroxyl group and oxoboron cluster (Table 1). The channels of the compound are filled with ions/molecules (Mg²⁺, K⁺, OH⁻ and H₂O). The title structure is similar to previously reported analogues NH₄NaB₆O₁₀ (Wang *et al.*, 2014), K_{0.5}[B₆O₁₀]·H₂O·1.5H₂O (Qiu & Yang, 2021*b*), and NaRb_{0.5}[B₆O₁₀]·0.5H₂O (Qiu *et al.*, 2021*b*), so the simultaneous use of NH₄ and Na or K or Na and Rb or Mg and

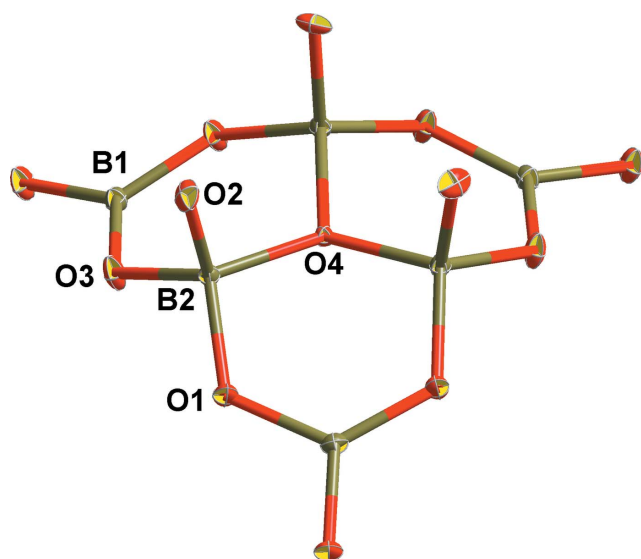


Figure 1
The asymmetric unit of the [B₆O₁₃]⁸⁻ oxoboron cluster. Displacement ellipsoids are drawn at the 50% probability level.

Table 1
Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O5—H5···O5 ⁱ	0.85	1.67	2.42 (3)	145
O6—H6A···O2 ⁱ	0.85	2.58	3.276 (15)	140
O5—H5···O6 ⁱ	0.85	1.78	2.484 (19)	139
O5—H5···O5 ⁱⁱ	0.85	2.30	3.06 (3)	150

Symmetry codes: (i) $y + \frac{1}{2}, -z + \frac{1}{2}, -x + 1$; (ii) $-x + 1, -y, -z + 1$.

K cations as templates has no effect on the crystallization of the oxoboron three-dimensional framework. However, after the introduction of Cl (Wu *et al.*, 2011) or Br (Al-Ama *et al.*, 2006), the new compounds crystallize in the trigonal space group *R3m* with a large second-harmonic generation response. The introduction of different anions can therefore play a key role in changing the crystalline structure to a non-centrosymmetric system.

4. Database survey

A search of the Cambridge Structural Database (CSD, version 5.43, update June 2022; Groom *et al.*, 2016) for the [B₆O₁₃]⁸⁻ oxoboron cluster gave 23 hits. The terminal oxygen atoms of this type of [B₆O_x] unit can be completely deprotonated [B₆O₁₃]⁸⁻, partially protonated [B₆O₁₁(OH)₂]⁶⁻ or completely protonated [B₆O₇(OH)₆]²⁻. Among the above 23 compounds, most of them are inorganic–organic hybrid solids, which contain transition-metal complexes and the [B₆O₇(OH)₆]²⁻ cluster (refcodes: CAFYIV, CAFYOB, Altahan *et al.*, 2021; CECWEM, Heller & Schellhaas, 1983; EMEHIP, Li *et al.*, 2016; HIXNAF, Jamai *et al.*, 2014; JOCCUC, JOCDAJ, Altahan *et al.*, 2019*a*; JUZLIC, Altahan *et al.*, 2020; MEBQUI, MEBRET, Altahan *et al.*, 2017; POJVIW, POJVOC, Altahan

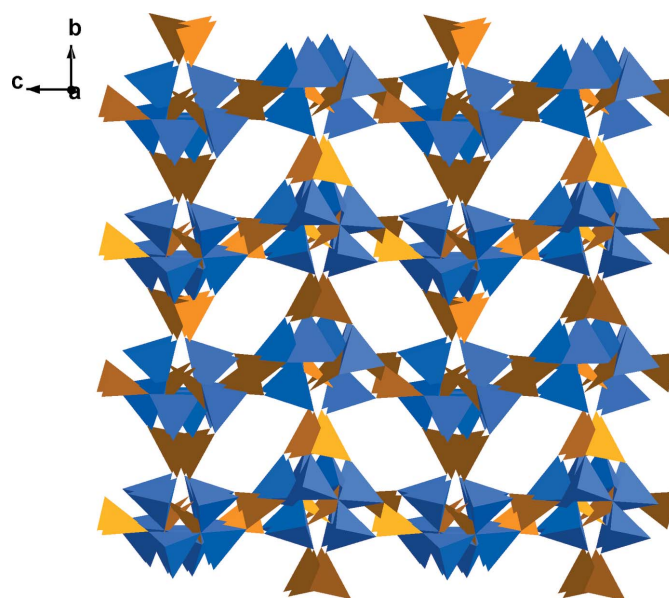


Figure 2
View of the three-dimensional supramolecular framework along the [100] direction. Color code: BO₃ trigonal, yellow, orange and brown; BO₄ tetrahedral, blue.

et al., 2019b; TAFROI, Natarajan *et al.*, 2003; VUVLOP, Jemai *et al.*, 2015; BATCUY, Jamai *et al.*, 2022; SAZVEY, Xin *et al.*, 2022). It is worth noting that this oxoboron cluster contains too many active hydroxyl groups and therefore tends to form isolated structures. In the crystal of [Cd(1,2-dap)]·[B₆O₁₁(OH)₂]·H₂O (1,2-dap = 1,2-diaminopropane, refcode: LOZZUY, Deng *et al.*, 2020) and Cd₃[B₆O₉(OH)₂]₂·2NO₃·4H₂O (refcode: ZUXLIQ, He *et al.*, 2020), partially protonated [B₆O₁₁(OH)₂]⁶⁻ was successfully extended to layered structures *via* B–O–B bonds. In the crystal of NaRb_{0.5}[B₆O₁₀]·0.5H₂O (refcode: UCEXOT, Qiu *et al.*, 2021b), each completely deprotonated [B₆O₁₃]⁸⁻ unit was linked to six nearest neighbors by bridging O atoms, leading to a 3D framework, similar to that of the title compound.

5. Synthesis and crystallization

A mixture of H₃BO₃ (0.618 g, 10 mmol), KCF₃SO₃ (0.188 g, 1 mmol) and Mg(CF₃SO₃)₂ (0.322 g, 1 mmol) was added to pyridine (3.0 mL). After stirring for 20 min, the resulting mixture was sealed in a 25 mL Teflon-lined stainless steel autoclave, heated at 488 K for 9 d, and then slowly cooled to room temperature and colorless block-shaped crystals MgK_{0.5}[B₆O₁₀](OH)_{0.5}·0.5H₂O were obtained (yield 56% based on H₃BO₃). Infrared (KBr pallet, cm⁻¹): 3190_{vs}, 1631_s, 1360_s, 1268_m, 1188_m, 1134_m, 1099_m, 964_s, 845_m, 781_m, 741_m, 718_m, 630_w, 564_w, 540_w, 480_w, 455_w.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Hydrogen atoms were positioned geometrically (O–H = 0.85 Å) and refined as riding with $U_{\text{iso}}(\text{H})$ 1.2 $U_{\text{eq}}(\text{O})$.

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Table 2

Experimental details.

Crystal data	
Chemical formula	Mg ₂ K[B ₆ O ₁₀] ₂ (OH)·H ₂ O
M_r	572.46
Crystal system, space group	Cubic, $Pa\bar{3}$
Temperature (K)	296
a (Å)	12.2966 (2)
V (Å ³)	1859.32 (9)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	0.47
Crystal size (mm)	0.10 × 0.08 × 0.08
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
T_{min} , T_{max}	0.762, 0.936
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	23808, 952, 828
R_{int}	0.056
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.714
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.116, 1.16
No. of reflections	952
No. of parameters	72
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.66, -0.64

Computer programs: *APEX2* and *SAINT* (Bruker, 2006), *SHELXT2018/3* (Sheldrick, 2015a), *SHELXL2018/3* (Sheldrick, 2015b), and *SHELXTL* (Sheldrick, 2008).

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Crystal structure of $\text{MgK}_{0.5}[\text{B}_6\text{O}_{10}](\text{OH})_{0.5}\cdot 0.5\text{H}_2\text{O}$, poly[dimagnesium potassium bis(hexaborate) hydroxide monohydrate]

Qi-Ming Qiu and Jian-Biao Song

Computing details

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINTE* (Bruker, 2006); data reduction: *SAINTE* (Bruker, 2006); program(s) used to solve structure: *SHELXT2018/3* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Poly[dimagnesium potassium bis(hexaborate) hydroxide monohydrate]

Crystal data

$\text{MgK}_{0.5}[\text{B}_6\text{O}_{10}](\text{OH})_{0.5}\cdot 0.5\text{H}_2\text{O}$

$M_r = 572.46$

Cubic, $P\bar{a}3$

$a = 12.2966$ (2) Å

$V = 1859.32$ (9) Å³

$Z = 4$

$F(000) = 1128$

$D_x = 2.045$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 5324 reflections

$\theta = 2.9\text{--}30.3^\circ$

$\mu = 0.47$ mm⁻¹

$T = 296$ K

Block, colorless

$0.10 \times 0.08 \times 0.08$ mm

Data collection

Bruker APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube, Bruker
(Mo) X-ray Source

φ and ω scans

Absorption correction: multi-scan
(SADABS; Krause et al., 2015)

$T_{\min} = 0.762$, $T_{\max} = 0.936$

23808 measured reflections

952 independent reflections

828 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.056$

$\theta_{\max} = 30.5^\circ$, $\theta_{\min} = 3.3^\circ$

$h = -16 \rightarrow 17$

$k = -16 \rightarrow 16$

$l = -16 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.039$

$wR(F^2) = 0.116$

$S = 1.16$

952 reflections

72 parameters

0 restraints

Hydrogen site location: difference Fourier map

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0658P)^2 + 0.9552P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.66$ e Å⁻³

$\Delta\rho_{\min} = -0.64$ e Å⁻³

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. The structure was solved by direct methods and refined by the full-matrix least-squares method on F^2 using the SHELXL programs (Bruker, 2006; Sheldrick, 2015a). All non-hydrogen atoms in the complex were refined anisotropically.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Mg	0.33884 (5)	0.33884 (5)	0.33884 (5)	0.0205 (3)	
K	0.500000	0.500000	0.500000	0.0257 (3)	
O1	0.52065 (8)	0.28854 (8)	0.29782 (8)	0.0110 (3)	
O2	0.22982 (9)	0.18931 (8)	0.38027 (8)	0.0118 (3)	
O3	0.36386 (8)	0.68000 (8)	0.55091 (8)	0.0113 (3)	
O4	0.18887 (7)	0.18887 (7)	0.18887 (7)	0.0057 (3)	
O5	0.4745 (13)	0.1216 (14)	0.5078 (12)	0.066 (4)	0.1667
H5	0.504419	0.061354	0.523614	0.099*	0.1667
O6	0.544 (2)	0.0524 (17)	0.5575 (10)	0.080 (6)	0.1667
H6A	0.548070	0.065436	0.625259	0.121*	0.1667
H6B	0.587560	0.097246	0.528419	0.121*	0.1667
B1	0.21526 (12)	0.22026 (12)	0.48534 (12)	0.0084 (3)	
B2	0.16682 (11)	0.13303 (11)	0.29771 (11)	0.0067 (3)	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mg	0.0205 (3)	0.0205 (3)	0.0205 (3)	0.0007 (2)	0.0007 (2)	0.0007 (2)
K	0.0257 (3)	0.0257 (3)	0.0257 (3)	0.0071 (2)	0.0071 (2)	0.0071 (2)
O1	0.0060 (4)	0.0113 (5)	0.0156 (5)	0.0015 (3)	−0.0031 (3)	−0.0047 (4)
O2	0.0141 (5)	0.0157 (5)	0.0055 (4)	−0.0039 (4)	0.0005 (3)	−0.0023 (3)
O3	0.0138 (5)	0.0134 (5)	0.0066 (4)	0.0060 (4)	−0.0017 (4)	−0.0027 (3)
O4	0.0057 (3)	0.0057 (3)	0.0057 (3)	0.0007 (3)	0.0007 (3)	0.0007 (3)
O5	0.058 (8)	0.074 (11)	0.067 (9)	0.005 (7)	0.011 (7)	−0.018 (8)
O6	0.123 (19)	0.101 (16)	0.017 (5)	0.029 (12)	−0.018 (7)	−0.002 (6)
B1	0.0094 (6)	0.0091 (6)	0.0065 (6)	0.0007 (5)	−0.0008 (5)	−0.0009 (5)
B2	0.0067 (6)	0.0067 (6)	0.0067 (6)	0.0003 (4)	0.0006 (4)	0.0005 (5)

Geometric parameters (\AA , $^\circ$)

Mg—O2 ⁱ	2.3319 (12)	O2—B1	1.3587 (16)
Mg—O2 ⁱⁱ	2.3319 (12)	O2—B2	1.4525 (16)
Mg—O2	2.3319 (12)	O3—B1 ^{vii}	1.3570 (18)
Mg—O1 ⁱ	2.3738 (10)	O3—B2 ^{viii}	1.4519 (16)
Mg—O1 ⁱⁱ	2.3738 (10)	O4—B2 ⁱ	1.5285 (15)
Mg—O1	2.3738 (10)	O4—B2 ⁱⁱ	1.5285 (15)
Mg—B1	2.7714 (15)	O4—B2	1.5285 (15)

Mg—B1 ⁱ	2.7715 (15)	O5—O6 ^{ix}	0.96 (2)
Mg—B1 ⁱⁱ	2.7715 (15)	O5—O6 ^x	1.27 (3)
Mg—K	3.4324 (11)	O5—O6	1.35 (3)
K—O3	2.8450 (10)	O5—H5	0.8500
K—O3 ⁱⁱⁱ	2.8450 (10)	O5—H6B	1.4451
K—O3 ⁱ	2.8450 (10)	O5—H6A ^{ix}	0.70 (3)
K—O3 ^{iv}	2.8450 (10)	O6—O6 ^{ix}	1.20 (3)
K—O3 ^v	2.8450 (10)	O6—O6 ^{xi}	1.20 (3)
K—O3 ⁱⁱ	2.8450 (10)	O6—H5	0.6476
O1—B1 ⁱⁱ	1.3821 (18)	O6—H6A	0.8500
O1—B2 ^{vi}	1.4531 (16)	O6—H6B	0.8500
O2 ⁱ —Mg—O2 ⁱⁱ	81.06 (5)	B1 ⁱⁱ —O1—B2 ^{vi}	123.77 (11)
O2 ⁱ —Mg—O2	81.06 (5)	B1 ⁱⁱ —O1—Mg	91.19 (8)
O2 ⁱⁱ —Mg—O2	81.06 (5)	B2 ^{vi} —O1—Mg	144.28 (8)
O2 ⁱ —Mg—O1 ⁱ	112.48 (4)	B1—O2—B2	136.70 (11)
O2 ⁱⁱ —Mg—O1 ⁱ	132.64 (4)	B1—O2—Mg	93.59 (8)
O2—Mg—O1 ⁱ	58.46 (3)	B2—O2—Mg	121.98 (8)
O2 ⁱ —Mg—O1 ⁱⁱ	58.46 (3)	B1 ^{vii} —O3—B2 ^{viii}	122.23 (11)
O2 ⁱⁱ —Mg—O1 ⁱⁱ	112.48 (4)	B1 ^{vii} —O3—K	125.09 (8)
O2—Mg—O1 ⁱⁱ	132.64 (4)	B2 ^{viii} —O3—K	110.32 (7)
O1 ⁱ —Mg—O1 ⁱⁱ	112.97 (3)	B2 ⁱ —O4—B2 ⁱⁱ	117.97 (4)
O2 ⁱ —Mg—O1	132.64 (4)	B2 ⁱ —O4—B2	117.97 (4)
O2 ⁱⁱ —Mg—O1	58.46 (3)	B2 ⁱⁱ —O4—B2	117.97 (4)
O2—Mg—O1	112.48 (4)	O6 ^{ix} —O5—O6	59 (2)
O1 ⁱ —Mg—O1	112.96 (3)	O6 ^x —O5—O6	89.1 (19)
O1 ⁱⁱ —Mg—O1	112.96 (3)	O6 ^{ix} —O5—H5	47.9
O2 ⁱ —Mg—B1	93.22 (5)	O6 ^x —O5—H5	67.1
O2 ⁱⁱ —Mg—B1	109.26 (5)	O6—O5—H5	22.1
O2—Mg—B1	29.29 (4)	O6 ^{ix} —O5—H6B	94.6
O1 ⁱ —Mg—B1	29.91 (4)	O6 ^x —O5—H6B	104.1
O1 ⁱⁱ —Mg—B1	123.25 (4)	O6—O5—H6B	35.2
O1—Mg—B1	121.16 (4)	H5—O5—H6B	50.4
O2 ⁱ —Mg—B1 ⁱ	29.30 (4)	O5 ^{xi} —O6—O6 ^{ix}	71 (3)
O2 ⁱⁱ —Mg—B1 ⁱ	93.22 (5)	O5 ^{xi} —O6—O6 ^{xi}	77 (3)
O2—Mg—B1 ⁱ	109.26 (5)	O6 ^{ix} —O6—O6 ^{xi}	101 (2)
O1 ⁱ —Mg—B1 ⁱ	121.16 (4)	O5 ^{xi} —O6—O5 ^{xii}	114 (2)
O1 ⁱⁱ —Mg—B1 ⁱ	29.90 (4)	O6 ^{ix} —O6—O5 ^{xii}	136.9 (16)
O1—Mg—B1 ⁱ	123.25 (4)	O6 ^{xi} —O6—O5 ^{xii}	45.7 (12)
B1—Mg—B1 ⁱ	114.20 (3)	O5 ^{xi} —O6—O5	107 (3)
O2 ⁱ —Mg—B1 ⁱⁱ	109.26 (5)	O6 ^{ix} —O6—O5	43.9 (9)
O2 ⁱⁱ —Mg—B1 ⁱⁱ	29.30 (4)	O6 ^{xi} —O6—O5	133.5 (16)
O2—Mg—B1 ⁱⁱ	93.22 (5)	O5 ^{xii} —O6—O5	134.5 (17)
O1 ⁱ —Mg—B1 ⁱⁱ	123.25 (4)	O5 ^{xi} —O6—H5	104.1
O1 ⁱⁱ —Mg—B1 ⁱⁱ	121.16 (4)	O6 ^{ix} —O6—H5	33.1
O1—Mg—B1 ⁱⁱ	29.91 (4)	O6 ^{xi} —O6—H5	103.9
B1—Mg—B1 ⁱⁱ	114.20 (3)	O5 ^{xii} —O6—H5	117.5
B1 ⁱ —Mg—B1 ⁱⁱ	114.20 (3)	O5—O6—H5	29.6

O2 ⁱ —Mg—K	131.38 (3)	O5 ^{xi} —O6—H6A	44.8
O2 ⁱⁱ —Mg—K	131.38 (3)	O6 ^{ix} —O6—H6A	101.0
O2—Mg—K	131.38 (3)	O6 ^{xi} —O6—H6A	103.2
O1 ⁱ —Mg—K	74.30 (3)	O5 ^{xii} —O6—H6A	111.4
O1 ⁱⁱ —Mg—K	74.30 (3)	O5—O6—H6A	111.4
O1—Mg—K	74.30 (3)	H5—O6—H6A	130.2
B1—Mg—K	104.19 (4)	O5 ^{xi} —O6—H6B	149.2
B1 ⁱ —Mg—K	104.19 (4)	O6 ^{ix} —O6—H6B	122.2
B1 ⁱⁱ —Mg—K	104.19 (4)	O6 ^{xi} —O6—H6B	122.0
O3—K—O3 ⁱⁱⁱ	65.411 (16)	O5 ^{xii} —O6—H6B	76.7
O3—K—O3 ⁱ	114.589 (16)	O5—O6—H6B	78.5
O3 ⁱⁱⁱ —K—O3 ⁱ	180.0	H5—O6—H6B	95.3
O3—K—O3 ^{iv}	65.410 (16)	H6A—O6—H6B	104.5
O3 ⁱⁱⁱ —K—O3 ^{iv}	114.590 (15)	O5 ^{xi} —O6—H5 ^{xi}	58.1 (15)
O3 ⁱ —K—O3 ^{iv}	65.410 (15)	O6 ^{ix} —O6—H5 ^{xi}	74 (3)
O3—K—O3 ⁱⁱ	114.590 (16)	O6 ^{xi} —O6—H5 ^{xi}	28.4 (18)
O3 ⁱⁱⁱ —K—O3 ⁱⁱ	65.410 (15)	O5 ^{xii} —O6—H5 ^{xi}	74 (3)
O3 ⁱ —K—O3 ⁱⁱ	114.590 (15)	O5—O6—H5 ^{xi}	114 (3)
O3 ^{iv} —K—O3 ⁱⁱ	180.0	H5—O6—H5 ^{xi}	87.3
O3 ^v —K—O3 ⁱⁱ	65.410 (16)	H6A—O6—H5 ^{xi}	97.8
O3—K—Mg ^v	76.32 (2)	H6B—O6—H5 ^{xi}	148.0
O3 ⁱⁱⁱ —K—Mg ^v	103.68 (2)	O3 ^{xiii} —B1—O2	123.87 (12)
O3 ⁱ —K—Mg ^v	76.32 (2)	O3 ^{xiii} —B1—O1 ⁱ	122.17 (12)
O3 ^{iv} —K—Mg ^v	103.68 (2)	O2—B1—O1 ⁱ	113.96 (12)
O3 ^v —K—Mg ^v	103.68 (2)	O3 ^{xiii} —B1—Mg	166.22 (10)
O3 ⁱⁱ —K—Mg ^v	76.32 (2)	O2—B1—Mg	57.12 (7)
O3—K—Mg	103.68 (2)	O1 ⁱ —B1—Mg	58.91 (7)
O3 ⁱⁱⁱ —K—Mg	76.32 (2)	O3 ^{xiv} —B2—O2	112.28 (11)
O3 ⁱ —K—Mg	103.68 (2)	O3 ^{xiv} —B2—O1 ^{xv}	109.48 (11)
O3 ^{iv} —K—Mg	76.32 (2)	O2—B2—O1 ^{xv}	110.35 (11)
O3 ^v —K—Mg	76.32 (2)	O3 ^{xiv} —B2—O4	109.12 (10)
O3 ⁱⁱ —K—Mg	103.68 (2)	O2—B2—O4	107.66 (11)
Mg ^v —K—Mg	180.000 (17)	O1 ^{xv} —B2—O4	107.83 (10)
O6 ^{ix} —O5—O6—O5 ^{xi}	-36 (3)	B1—O2—B2—O3 ^{xiv}	21.1 (2)
O6 ^x —O5—O6—O5 ^{xi}	-94.9 (17)	Mg—O2—B2—O3 ^{xiv}	-119.29 (10)
O6 ^x —O5—O6—O6 ^{ix}	-59 (2)	B1—O2—B2—O1 ^{xv}	-101.35 (17)
O6 ^{ix} —O5—O6—O6 ^{xi}	52 (3)	Mg—O2—B2—O1 ^{xv}	118.27 (10)
O6 ^x —O5—O6—O6 ^{xi}	-7 (5)	B1—O2—B2—O4	141.21 (14)
O6 ^{ix} —O5—O6—O5 ^{xii}	117 (3)	Mg—O2—B2—O4	0.84 (12)
O6 ^x —O5—O6—O5 ^{xii}	58 (4)	B2 ⁱ —O4—B2—O3 ^{xiv}	45.6 (2)
B2—O2—B1—O3 ^{xiii}	16.3 (2)	B2 ⁱⁱ —O4—B2—O3 ^{xiv}	-162.41 (10)
Mg—O2—B1—O3 ^{xiii}	163.52 (12)	B2 ⁱ —O4—B2—O2	-76.54 (15)
B2—O2—B1—O1 ⁱ	-163.39 (13)	B2 ⁱⁱ —O4—B2—O2	75.49 (15)

Mg—O2—B1—O1 ⁱ	-16.21 (12)	B2 ⁱ —O4—B2—O1 ^{xv}	164.40 (10)
B2—O2—B1—Mg	-147.18 (17)	B2 ⁱⁱ —O4—B2—O1 ^{xv}	-43.6 (2)

Symmetry codes: (i) y, z, x ; (ii) z, x, y ; (iii) $-y+1, -z+1, -x+1$; (iv) $-z+1, -x+1, -y+1$; (v) $-x+1, -y+1, -z+1$; (vi) $y+1/2, z, -x+1/2$; (vii) $-x+1/2, y+1/2, z$; (viii) $-y+1/2, -z+1, x+1/2$; (ix) $-y+1/2, z-1/2, x$; (x) $-z+1, x-1/2, -y+1/2$; (xi) $z, -x+1/2, y+1/2$; (xii) $y+1/2, -z+1/2, -x+1$; (xiii) $-x+1/2, y-1/2, z$; (xiv) $z-1/2, -x+1/2, -y+1$; (xv) $-z+1/2, x-1/2, y$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O5—H5 \cdots O5 ^{xii}	0.85	1.67	2.42 (3)	145
O6—H6A \cdots O2 ^{xii}	0.85	2.58	3.276 (15)	140
O6—H5 \cdots O6 ^{ix}	0.65	0.74	1.20 (3)	119
O6—H5 \cdots O6 ^x	0.65	1.23	1.84 (2)	158
O6—H5 \cdots O6 ^{xvi}	0.65	1.82	2.19 (3)	118
O6—H5 \cdots O5 ^{ix}	0.65	1.79	2.34 (3)	143
O6—H5 \cdots O5 ^x	0.65	2.09	2.484 (19)	121
O6—H5 \cdots O5	0.65	0.85	1.35 (3)	128
O5—H5 \cdots O6 ^{xii}	0.85	1.78	2.484 (19)	139
O5—H5 \cdots O6 ^{xi}	0.85	1.49	2.34 (3)	179
O5—H5 \cdots O6 ^{xvi}	0.85	1.82	2.30 (2)	114
O5—H5 \cdots O5 ^{xii}	0.85	1.67	2.42 (3)	145
O5—H5 \cdots O5 ^{xi}	0.85	1.28	1.88 (3)	122
O5—H5 \cdots O5 ^{xvi}	0.85	2.30	3.06 (3)	150

Symmetry codes: (ix) $-y+1/2, z-1/2, x$; (x) $-z+1, x-1/2, -y+1/2$; (xi) $z, -x+1/2, y+1/2$; (xii) $y+1/2, -z+1/2, -x+1$; (xvi) $-x+1, -y, -z+1$.