

Lithium diaquamagnesium catena-borodiphosphate(V) monohydrate, $\text{LiMg}(\text{H}_2\text{O})_2[\text{BP}_2\text{O}_8]\cdot\text{H}_2\text{O}$, at 173 K

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Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{Mg}-\text{O}) = 0.003$ Å; H-atom completeness 67%; disorder in main residue; R factor = 0.037; wR factor = 0.093; data-to-parameter ratio = 17.9.

The crystal structure of $\text{LiMg}(\text{H}_2\text{O})_2[\text{BP}_2\text{O}_8]\cdot\text{H}_2\text{O}$ consists of tubular structural units, built from tetrahedral $\infty^1\{[\text{BP}_2\text{O}_8]^{3-}\}$ borophosphate ribbons and $(\text{LiO}_4)_n$ helices running along [001], which are interconnected by $\text{MgO}_4(\text{H}_2\text{O})_2$ octahedra, forming a three-dimensional network structure with one-dimensional channels along [001] in which the water molecules are located. The water molecule in the channel is significantly displaced by up to 0.3 Å from the special position $6b$ (..2) to a half-occupied general position. Mg, B and one Li atom all lie on twofold axes. Of the two Li positions, one is at a special position $6b$ (..2), while the other is at a general position; both are only half-occupied.

Related literature

For $\text{NaMg}(\text{H}_2\text{O})_2[\text{BP}_2\text{O}_8]\cdot\text{H}_2\text{O}$ and $\text{KMg}(\text{H}_2\text{O})_2[\text{BP}_2\text{O}_8]\cdot\text{H}_2\text{O}$, see: Kniep *et al.* (1997). For $\text{LiCu}(\text{H}_2\text{O})_2[\text{BP}_2\text{O}_8]\cdot(\text{H}_2\text{O})$ and $\text{LiZn}(\text{H}_2\text{O})_2[\text{BP}_2\text{O}_8]\cdot\text{H}_2\text{O}$, see: Boy & Kniep (2001*a,b*). For $\text{LiCd}(\text{H}_2\text{O})_2[\text{BP}_2\text{O}_8]\cdot\text{H}_2\text{O}$, see: Ge *et al.* (2003).

Experimental

Crystal data

$\text{LiMg}(\text{H}_2\text{O})_2[\text{BP}_2\text{O}_8]\cdot\text{H}_2\text{O}$
 $M_r = 286.05$
Hexagonal, $P6_322$
 $a = 9.4139$ (1) Å
 $c = 15.7113$ (3) Å
 $V = 1205.82$ (3) Å³

$Z = 6$
Mo $K\alpha$ radiation
 $\mu = 0.67$ mm⁻¹
 $T = 173$ (2) K
 $0.16 \times 0.07 \times 0.07$ mm

Data collection

Oxford Diffraction Gemini R Ultra
CCD area-detector
diffractometer
Absorption correction: numerical
(*CrysAlis RED*; Oxford

Diffraction, 2005)
 $T_{\min} = 0.900$, $T_{\max} = 0.954$
3404 measured reflections
1343 independent reflections
1142 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.092$
 $S = 1.06$
1343 reflections
75 parameters
H-atom parameters not refined

$\Delta\rho_{\text{max}} = 0.74$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.55$ e Å⁻³
Absolute structure: Flack (1983),
410 Friedel pairs
Flack parameter: -0.1 (2)

Table 1

Selected geometric parameters (Å, °).

P1—O3	1.501 (2)	B1—O2 ^{iv}	1.469 (3)
P1—O4	1.5033 (19)	Li1—O3 ^v	2.113 (12)
P1—O1 ⁱ	1.558 (2)	Li1—O5 ^v	2.135 (2)
P1—O2 ⁱⁱ	1.5632 (17)	Li1—O6 ^{vi}	2.35 (2)
Mg1—O4 ⁱ	2.042 (2)	Li2—O6 ^{vii}	1.82 (2)
Mg1—O3 ⁱⁱⁱ	2.0590 (17)	Li2—O4 ^{vii}	2.08 (2)
Mg1—O5	2.179 (2)	Li2—O6 ^{viii}	2.08 (2)
B1—O1 ⁱⁱ	1.461 (3)	Li2—O5 ^{ix}	2.10 (2)
B1 ^x —O1—P1 ^x	128.00 (16)	P1—O3—Mg1	130.05 (11)
B1—O2—P1 ⁱⁱ	130.40 (17)		

Symmetry codes: (i) $y, -x + y + 1, z + \frac{1}{6}$; (ii) $x - y + 1, -y + 2, -z$; (iii) $-x + y, y, -z + \frac{1}{2}$; (iv) $-y + 2, -x + 2, -z + \frac{1}{6}$; (v) $-y + 1, -x + 1, -z + \frac{1}{6}$; (vi) $x - y, x, z - \frac{1}{6}$; (vii) $-x + y + 1, y, -z + \frac{1}{2}$; (viii) $y, x, -z + \frac{1}{3}$; (ix) $y, -x + y, z + \frac{1}{6}$; (x) $x - y + 1, x, z - \frac{1}{6}$.

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O5—H1 \cdots O4 ⁱⁱⁱ	0.86	2.09	2.852 (3)	148
O5—H2 \cdots O2 ⁱⁱ	0.88	1.98	2.779 (3)	151
O5—H2 \cdots O3 ^v	0.88	2.46	3.198 (3)	142

Symmetry codes: (iii) $-x + y, y, -z + \frac{1}{2}$; (v) $-y + 1, -x + 1, -z + \frac{1}{6}$; (xi) $y - 1, -x + y, z + \frac{1}{6}$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2005); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1997–2004) and *ATOMS* (Dowty, 2004); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2074).

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supplementary materials

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Lithium diaquamagnesium *catena*-borodiphosphate(V) monohydrate, $\text{LiMg}(\text{H}_2\text{O})_2[\text{BP}_2\text{O}_8]\cdot\text{H}_2\text{O}$, at 173 K

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Comment

In the last decade, much attention has been paid to the large family of borophosphates with the general formula $AM(\text{H}_2\text{O})_2[\text{BP}_2\text{O}_8]\cdot y\text{H}_2\text{O}$ ($A^I=\text{Li, Na, K, NH}_4^+$; $M^{II}=\text{Mg, Mn, Fe, Co, Ni, Cu, Zn, Cd}$)(where $y = 0.5-1$) due to their chiral structure property and potential applications for catalysts (Kniep *et al.*, 1997; Ewald *et al.*, 2007). Many combinations between monovalent A cations and divalent M cations are available. At the M site, most of the known compounds in this family apply transition metal ions, while only two magnesium components, $\text{NaMg}(\text{H}_2\text{O})_2[\text{BP}_2\text{O}_8]\cdot\text{H}_2\text{O}$ as well as $\text{KMg}(\text{H}_2\text{O})_2[\text{BP}_2\text{O}_8]\cdot\text{H}_2\text{O}$, are listed for the inclusion of alkaline-earth metals (Kniep *et al.*, 1997). Whereas at the A site, up to date, only three Li-based borophosphates are known, *e.g.* $\text{LiCu}(\text{H}_2\text{O})_2[\text{BP}_2\text{O}_8]\cdot(\text{H}_2\text{O})$ (Boy & Kniep, 2001*a*), $\text{LiZn}(\text{H}_2\text{O})_2[\text{BP}_2\text{O}_8]\cdot\text{H}_2\text{O}$ (Boy & Kniep, 2001*b*) and $\text{LiCd}(\text{H}_2\text{O})_2[\text{BP}_2\text{O}_8]\cdot\text{H}_2\text{O}$ (Ge *et al.*, 2003). Therefore herein we report on a new member of this family with the combination of Li and Mg, $\text{LiMg}(\text{H}_2\text{O})_2[\text{BP}_2\text{O}_8]\cdot\text{H}_2\text{O}$.

The crystal structure of the title compound contains infinite one-dimensional helical borophosphate ribbons $\infty^1\{[\text{BP}_2\text{O}_8]^{3-}\}$, arranged around 6_5 screw axes, which are built up from four-membered rings of corner-sharing PO_4 and BO_4 tetrahedra (Fig. 1 & 2). There are two partially occupied Li positions. Li1, located at the outside of ribbons (Fig. 2), is fixed by an irregular arrangement of five oxygen atoms from adjacent phosphate groups (O3) and water molecules (O5, O6). Li2 is tetrahedrally coordinated by four oxygen atoms that originated from phosphate groups (O4) and two water molecules (O5, O6)(Fig. 3). The resulting distorted tetrahedra, $(\text{Li}_2\text{O}_4)_n$, located at the free thread of the borophosphate ribbons, are also wound around 6_5 screw axes to form helices *via* corner-sharing oxygen atoms which further connect the above infinite one-dimensional borophosphate ribbons by sharing common oxygen corners to develop into a tubular structure where water molecules (O6) with a disorder mode reside in. The magnesium site is octahedrally coordinated by four oxygen atoms from phosphate tetrahedra (O3, O4) and two water molecules (O5) which are located between the adjacent tubes and connect the neighbouring tubes to form a three-dimensional framework.

Experimental

Transparent, colorless single crystals of the title compound were hydrothermally synthesized. A mixture of $\text{MgCl}_2\cdot 6\text{H}_2\text{O}$ (0.5344 g), $\text{LiOH}\cdot\text{H}_2\text{O}$ (5.042 g), H_3BO_3 (1.568 g) and 10 ml (85%) H_3PO_4 in an approximate molar ratio $\text{Mg}:\text{Li}:\text{B}:\text{P} = 1:46:10:65$, are dissolved in 5 ml distilled water while stirring. The resulting solution (pH = 1.5) was transferred into a Teflon-lined autoclave (internal volume 30 ml, degree of filling 67%) and held at 463 K for four days under autogenous pressure. Then the autoclave was cooled to room temperature by turning off the power. Products were filtered off, washed with distilled water and dried at room temperature. Crystals with hexagonal bipyramidal morphology were selected for single-crystal diffraction after checking under a polarizing microscope and identifying by X-ray powder diffraction.

Refinement

The hydrogen atoms connected with O5 are located from the difference Fourier maps and fixed the positions and displacement parameters assigned as 0.05. The hydrogen positions for O6 are not determined due to the connecting water molecule in disorder mode. The occupancy of O6 was fixed to 0.5 in the last cycles of refinement because its refined value was close to 50%.

Figures

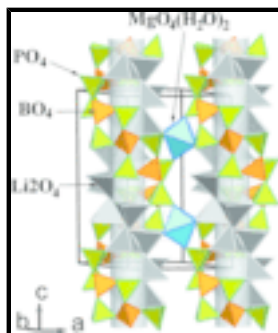


Fig. 1. Helical arrangements in the crystal structure of $\text{LiMg}(\text{H}_2\text{O})_2[\text{BP}_2\text{O}_8]\cdot\text{H}_2\text{O}$, Green tetrahedra: PO_4 , Orange tetrahedra: BO_4 , grey tetrahedra: Li_2O_4 .

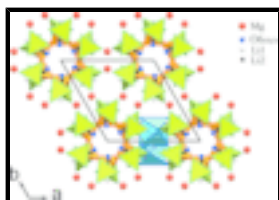


Fig. 2. The crystal structure of $\text{LiMg}(\text{H}_2\text{O})_2[\text{BP}_2\text{O}_8]\cdot\text{H}_2\text{O}$ plotted in projection along $[001]$

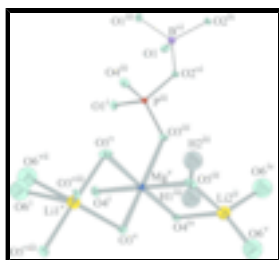


Fig. 3. The coordination environment of the metal atoms in $\text{LiMg}(\text{H}_2\text{O})_2[\text{BP}_2\text{O}_8]\cdot\text{H}_2\text{O}$, with displacement ellipsoids drawn at the 50% probability level. (symmetry codes: (i) $y, x, -1/3 - z$; (ii) $x - y, 1 - y, -z$; (iii) $x, 1 + x - y, -1/6 - z$; (iv) $1 - x, 1 - y, -1/2 + z$; (v) $-x + y, 1 - x, -2/3 + z$; (vi) $1 + x - y, x, -1/6 + z$; (vii) $y, 1 - x + y, -5/6 + z$; (viii) $-x + y, y, -1/2 - z$; (ix) $1 + x - y, 2 - y, -z$)

Lithium diaquamagnesium catena-borodiphosphate(V) monohydrate

Crystal data

$\text{LiMg}(\text{H}_2\text{O})_2[\text{BP}_2\text{O}_8]\cdot\text{H}_2\text{O}$

$M_r = 286.05$

Hexagonal, $P6_522$

Hall symbol: $P\ 65\ 2\ (0\ 0\ 1)$

$a = 9.41390\ (10)\ \text{\AA}$

$b = 9.41390\ (10)\ \text{\AA}$

$c = 15.7113\ (3)\ \text{\AA}$

$\alpha = 90^\circ$

$Z = 6$

$F_{000} = 864$

$D_x = 2.364\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3404 reflections

$\theta = 2.8\text{--}32.6^\circ$

$\mu = 0.67\ \text{mm}^{-1}$

$T = 173\ (2)\ \text{K}$

$\beta = 90^\circ$ Hexagonal bipyramidal, colourless
 $\gamma = 120^\circ$ $0.16 \times 0.07 \times 0.07$ mm
 $V = 1205.82(3) \text{ \AA}^3$

Data collection

Oxford Diffraction CCD area-detector diffractometer	1343 independent reflections
Radiation source: fine-focus sealed tube	1142 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.033$
$T = 173(2)$ K	$\theta_{\text{max}} = 32.6^\circ$
326 images, $\Delta\omega = 1^\circ$, Exp time: 40 s. scans	$\theta_{\text{min}} = 2.8^\circ$
Absorption correction: numerical (CrysAlis RED; Oxford Diffraction, 2005)	$h = -7 \rightarrow 14$
$T_{\text{min}} = 0.900$, $T_{\text{max}} = 0.954$	$k = -13 \rightarrow 14$
3404 measured reflections	$l = -22 \rightarrow 8$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters not refined
$R[F^2 > 2\sigma(F^2)] = 0.037$	$w = 1/[\sigma^2(F_o^2) + (0.0493P)^2]$
$wR(F^2) = 0.092$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{\text{max}} < 0.001$
1343 reflections	$\Delta\rho_{\text{max}} = 0.74 \text{ e \AA}^{-3}$
75 parameters	$\Delta\rho_{\text{min}} = -0.55 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none
Secondary atom site location: difference Fourier map	Absolute structure: Flack (1983), 410 Friedel pairs
	Flack parameter: $-0.1(2)$

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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)
P1	0.61413 (8)	0.82894 (8)	0.08573 (4)	0.00616 (14)	

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Mg1	0.44657 (8)	0.89313 (15)	0.2500	0.0080 (3)	
O1	0.8112 (2)	0.7888 (2)	-0.06431 (11)	0.0096 (4)	
O2	0.7643 (2)	1.1783 (2)	0.01261 (10)	0.0074 (4)	
O3	0.4841 (2)	0.8559 (2)	0.12481 (11)	0.0113 (4)	
O4	0.6190 (3)	0.6808 (2)	0.11749 (11)	0.0116 (4)	
O5	0.1958 (3)	0.7110 (3)	0.21628 (13)	0.0168 (5)	
B1	0.8496 (2)	1.1504 (2)	0.0833	0.0082 (7)	
O6	0.8943 (11)	0.8068 (7)	0.2666 (4)	0.0528 (18)*	0.50
Li1	0.2395 (13)	0.7605 (13)	0.0833	0.027 (3)*	0.426 (18)
Li2	0.893 (3)	0.750 (3)	0.3456 (13)	0.027 (3)*	0.287 (9)
H1	0.1273	0.6655	0.2575	0.050*	
H2	0.1925	0.6306	0.1868	0.050*	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0073 (3)	0.0063 (3)	0.0050 (2)	0.0035 (2)	0.0006 (2)	-0.0002 (2)
Mg1	0.0081 (4)	0.0074 (6)	0.0084 (5)	0.0037 (3)	0.0018 (4)	0.000
O1	0.0103 (9)	0.0091 (9)	0.0108 (8)	0.0060 (8)	-0.0029 (7)	-0.0014 (7)
O2	0.0090 (9)	0.0091 (9)	0.0045 (7)	0.0048 (8)	-0.0006 (6)	0.0004 (6)
O3	0.0124 (9)	0.0166 (11)	0.0067 (8)	0.0087 (8)	0.0006 (7)	-0.0030 (7)
O4	0.0186 (10)	0.0074 (9)	0.0098 (7)	0.0073 (8)	-0.0013 (8)	0.0012 (7)
O5	0.0132 (11)	0.0124 (10)	0.0160 (9)	-0.0002 (9)	0.0040 (8)	-0.0044 (8)
B1	0.0100 (14)	0.0100 (14)	0.0065 (15)	0.0063 (16)	-0.0018 (13)	-0.0018 (13)

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

P1—O3	1.501 (2)	B1—O1 ⁱ	1.461 (3)
P1—O4	1.5033 (19)	B1—O2 ^{ix}	1.469 (3)
P1—O1 ⁱ	1.558 (2)	B1—O2	1.469 (3)
P1—O2 ⁱⁱ	1.5632 (17)	O6—O6 ⁱⁱⁱ	0.549 (14)
P1—Li2 ⁱⁱⁱ	2.94 (2)	Li1—O3 ^x	2.113 (12)
Mg1—O4 ⁱ	2.042 (2)	Li1—O5 ^x	2.135 (2)
Mg1—O4 ^{iv}	2.042 (2)	Li1—O6 ^{vi}	2.35 (2)
Mg1—O3 ^v	2.0590 (17)	Li1—O6 ^{iv}	2.35 (2)
Mg1—O3	2.0590 (17)	Li1—Li2 ^{iv}	2.40 (3)
Mg1—O5	2.179 (2)	Li2—O6 ⁱⁱⁱ	1.82 (2)
Mg1—O5 ^v	2.179 (2)	Li2—O4 ⁱⁱⁱ	2.08 (2)
Mg1—Li2 ^{vi}	3.07 (2)	Li2—O6 ^{vii}	2.08 (2)
Mg1—Li2 ^{vii}	3.07 (2)	Li2—O5 ^{xi}	2.10 (2)
Mg1—Li1 ^{viii}	3.128 (4)	Li2—Li2 ^{vii}	2.36 (4)
Mg1—Li1	3.128 (4)	Li2—O6 ⁱ	2.48 (2)
B1—O1 ⁱⁱ	1.461 (3)	Li2—O1 ^{xiii}	2.65 (2)
O3—P1—O4	115.28 (12)	Li2 ⁱⁱⁱ —O6—Li2 ^{vii}	116.4 (10)
O3—P1—O1 ⁱ	111.30 (11)	Li2—O6—Li1 ^{xi}	75.9 (9)

O4—P1—O1 ⁱ	105.63 (11)	Li2 ⁱⁱⁱ —O6—Li1 ^{xi}	69.1 (7)
O3—P1—O2 ⁱⁱ	106.09 (10)	Li2 ^{vii} —O6—Li1 ^{xi}	114.4 (7)
O4—P1—O2 ⁱⁱ	111.75 (10)	Li2—O6—Li2 ^{xiii}	117.5 (12)
O1 ⁱ —P1—O2 ⁱⁱ	106.53 (10)	Li2 ⁱⁱⁱ —O6—Li2 ^{xiii}	64.5 (10)
O3—P1—Li2 ⁱⁱⁱ	134.1 (4)	Li2 ^{vii} —O6—Li2 ^{xiii}	142.5 (11)
O1 ⁱ —P1—Li2 ⁱⁱⁱ	63.9 (4)	Li1 ^{xi} —O6—Li2 ^{xiii}	101.1 (6)
O2 ⁱⁱ —P1—Li2 ⁱⁱⁱ	119.2 (4)	O3 ^x —Li1—O3	109.7 (9)
O4 ⁱ —Mg1—O4 ^{iv}	95.33 (13)	O3 ^x —Li1—O5 ^x	80.9 (3)
O4 ⁱ —Mg1—O3 ^v	91.45 (8)	O3—Li1—O5 ^x	97.7 (4)
O4 ^{iv} —Mg1—O3 ^v	99.96 (8)	O3 ^x —Li1—O5	97.7 (4)
O4 ⁱ —Mg1—O3	99.96 (8)	O3—Li1—O5	80.9 (3)
O4 ^{iv} —Mg1—O3	91.45 (8)	O5 ^x —Li1—O5	177.4 (11)
O3 ^v —Mg1—O3	163.06 (13)	O3 ^x —Li1—O6 ^{vi}	125.3 (5)
O4 ⁱ —Mg1—O5	178.78 (8)	O3—Li1—O6 ^{vi}	124.4 (5)
O4 ^{iv} —Mg1—O5	85.31 (9)	O5 ^x —Li1—O6 ^{vi}	98.0 (6)
O3 ^v —Mg1—O5	87.42 (8)	O5—Li1—O6 ^{vi}	84.6 (5)
O3—Mg1—O5	81.04 (8)	O3 ^x —Li1—O6 ^{iv}	124.4 (5)
O4 ⁱ —Mg1—O5 ^v	85.31 (9)	O3—Li1—O6 ^{iv}	125.3 (5)
O4 ^{iv} —Mg1—O5 ^v	178.78 (8)	O5 ^x —Li1—O6 ^{iv}	84.6 (5)
O3 ^v —Mg1—O5 ^v	81.04 (8)	O5—Li1—O6 ^{iv}	98.0 (6)
O3—Mg1—O5 ^v	87.42 (8)	O6 ^{vi} —Li1—O6 ^{iv}	13.5 (4)
O5—Mg1—O5 ^v	94.06 (13)	O6—Li2—O6 ⁱⁱⁱ	10.0 (7)
B1 ^{xiii} —O1—P1 ^{xiii}	128.00 (16)	O6—Li2—O4 ⁱⁱⁱ	121.6 (14)
B1 ^{xiii} —O1—Li2 ^{xii}	147.5 (5)	O6 ⁱⁱⁱ —Li2—O4 ⁱⁱⁱ	112.3 (11)
P1 ^{xiii} —O1—Li2 ^{xii}	84.3 (5)	O6—Li2—O6 ^{vii}	92.9 (11)
B1—O2—P1 ⁱⁱ	130.40 (17)	O6 ⁱⁱⁱ —Li2—O6 ^{vii}	102.9 (10)
P1—O3—Mg1	130.05 (11)	O4 ⁱⁱⁱ —Li2—O6 ^{vii}	134.3 (10)
P1—O3—Li1	127.6 (4)	O6—Li2—O5 ^{xi}	121.0 (13)
Mg1—O3—Li1	97.1 (2)	O6 ⁱⁱⁱ —Li2—O5 ^{xi}	119.2 (11)
P1—O4—Mg1 ^{xiii}	141.40 (12)	O4 ⁱⁱⁱ —Li2—O5 ^{xi}	86.5 (8)
P1—O4—Li2 ⁱⁱⁱ	109.2 (6)	O6 ^{vii} —Li2—O5 ^{xi}	101.1 (9)
Mg1 ^{xiii} —O4—Li2 ⁱⁱⁱ	96.3 (6)	O6—Li2—O6 ⁱ	102.1 (12)
Li2 ^{vi} —O5—Li1	69.3 (8)	O6 ⁱⁱⁱ —Li2—O6 ⁱ	112.0 (10)
Li2 ^{vi} —O5—Mg1	91.8 (6)	O4 ⁱⁱⁱ —Li2—O6 ⁱ	125.2 (9)
Li1—O5—Mg1	92.95 (17)	O6 ^{vii} —Li2—O6 ⁱ	9.6 (4)
O1 ⁱⁱ —B1—O1 ⁱ	102.5 (3)	O5 ^{xi} —Li2—O6 ⁱ	98.5 (8)
O1 ⁱⁱ —B1—O2	112.10 (10)	O6—Li2—O1 ^{xii}	99.7 (11)
O1 ⁱ —B1—O2	114.14 (10)	O6 ⁱⁱⁱ —Li2—O1 ^{xii}	98.7 (9)
O1 ⁱⁱ —B1—O2 ^{ix}	114.14 (10)	O4 ⁱⁱⁱ —Li2—O1 ^{xii}	60.6 (6)
O1 ⁱ —B1—O2 ^{ix}	112.10 (10)	O6 ^{vii} —Li2—O1 ^{xii}	86.7 (7)
O2—B1—O2 ^{ix}	102.2 (3)	O5 ^{xi} —Li2—O1 ^{xii}	137.7 (9)

supplementary materials

Li2—O6—Li2ⁱⁱⁱ 144.4 (15) O6ⁱ—Li2—O1^{xii} 82.4 (6)

Li2—O6—Li2^{vii} 84.1 (12)

Symmetry codes: (i) $y, -x+y+1, z+1/6$; (ii) $x-y+1, -y+2, -z$; (iii) $-x+y+1, y, -z+1/2$; (iv) $-x+1, -x+y+1, -z+1/3$; (v) $-x+y, y, -z+1/2$; (vi) $x-y, x, z-1/6$; (vii) $y, x, -z+2/3$; (viii) $-x+y, -x+1, z+1/3$; (ix) $-y+2, -x+2, -z+1/6$; (x) $-y+1, -x+1, -z+1/6$; (xi) $y, -x+y, z+1/6$; (xii) $-x+2, -x+y+1, -z+1/3$; (xiii) $x-y+1, x, z-1/6$.

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O5—H1 \cdots O4 ^v	0.862	2.085	2.852 (3)	147.93
O5—H2 \cdots O2 ^{xiv}	0.875	1.979	2.779 (3)	151.43
O5—H2 \cdots O3 ^x	0.875	2.463	3.198 (3)	141.96

Symmetry codes: (v) $-x+y, y, -z+1/2$; (xiv) $y-1, -x+y, z+1/6$; (x) $-y+1, -x+1, -z+1/6$.

Fig. 1

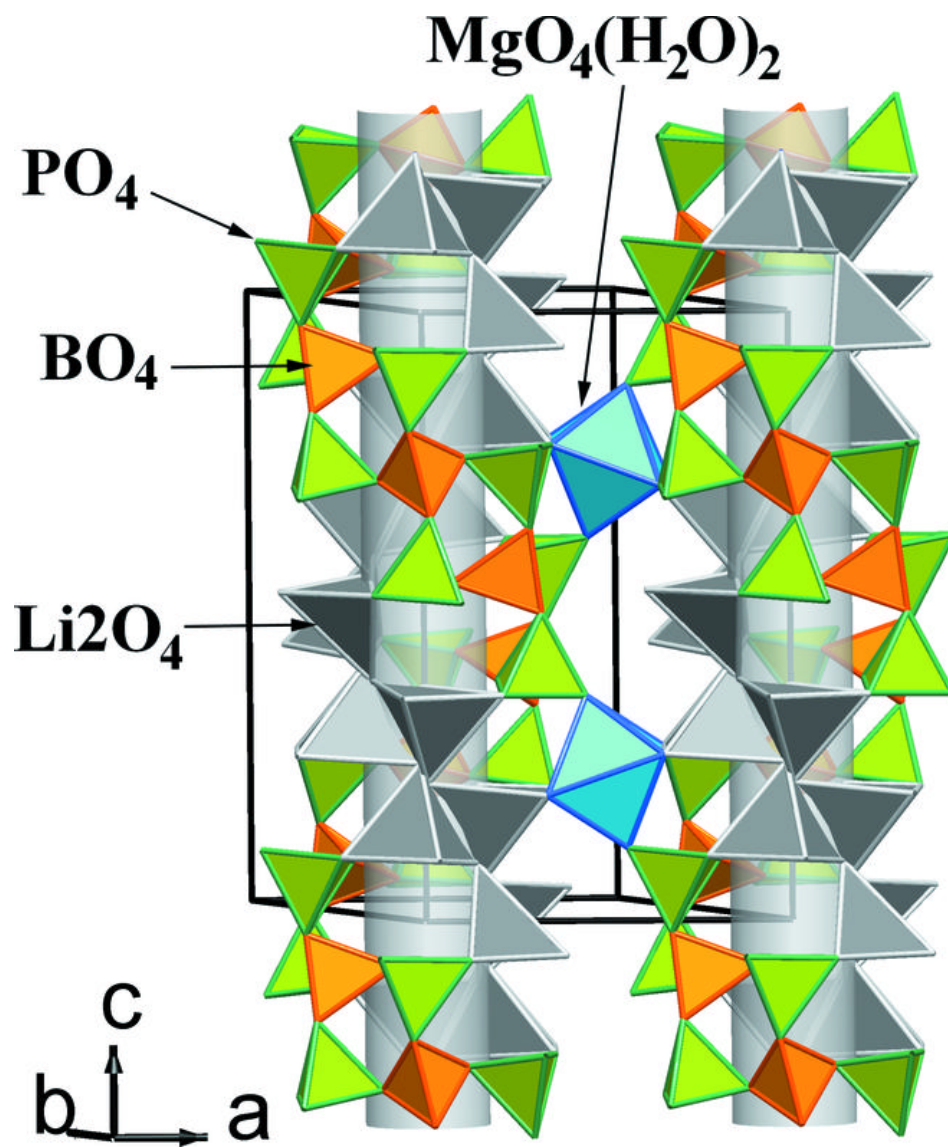


Fig. 2

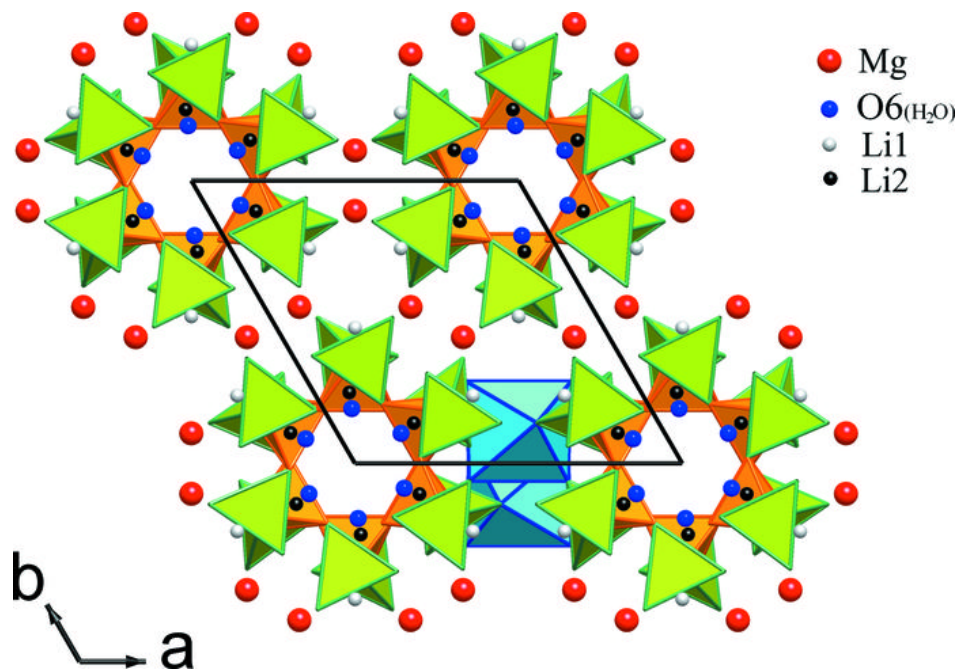


Fig. 3

