

# 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) Å<sup>3</sup>

$Z = 6$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.67$  mm<sup>-1</sup>  
 $T = 173$  (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<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.55$  e Å<sup>-3</sup>  
 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 <sup>iv</sup>	1.469 (3)
P1—O4	1.5033 (19)	Li1—O3 <sup>v</sup>	2.113 (12)
P1—O1 <sup>i</sup>	1.558 (2)	Li1—O5 <sup>v</sup>	2.135 (2)
P1—O2 <sup>ii</sup>	1.5632 (17)	Li1—O6 <sup>vi</sup>	2.35 (2)
Mg1—O4 <sup>i</sup>	2.042 (2)	Li2—O6 <sup>vii</sup>	1.82 (2)
Mg1—O3 <sup>iii</sup>	2.0590 (17)	Li2—O4 <sup>vii</sup>	2.08 (2)
Mg1—O5	2.179 (2)	Li2—O6 <sup>viii</sup>	2.08 (2)
B1—O1 <sup>ii</sup>	1.461 (3)	Li2—O5 <sup>ix</sup>	2.10 (2)
B1 <sup>x</sup> —O1—P1 <sup>x</sup>	128.00 (16)	P1—O3—Mg1	130.05 (11)
B1—O2—P1 <sup>ii</sup>	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 <sup>iii</sup>	0.86	2.09	2.852 (3)	148
O5—H2 $\cdots$ O2 <sup>ii</sup>	0.88	1.98	2.779 (3)	151
O5—H2 $\cdots$ O3 <sup>v</sup>	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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## supporting information

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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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### S1. 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,  $\text{LiMg}(\text{H}_2\text{O})_2[\text{BP}_2\text{O}_8]\cdot\text{H}_2\text{O}$ .

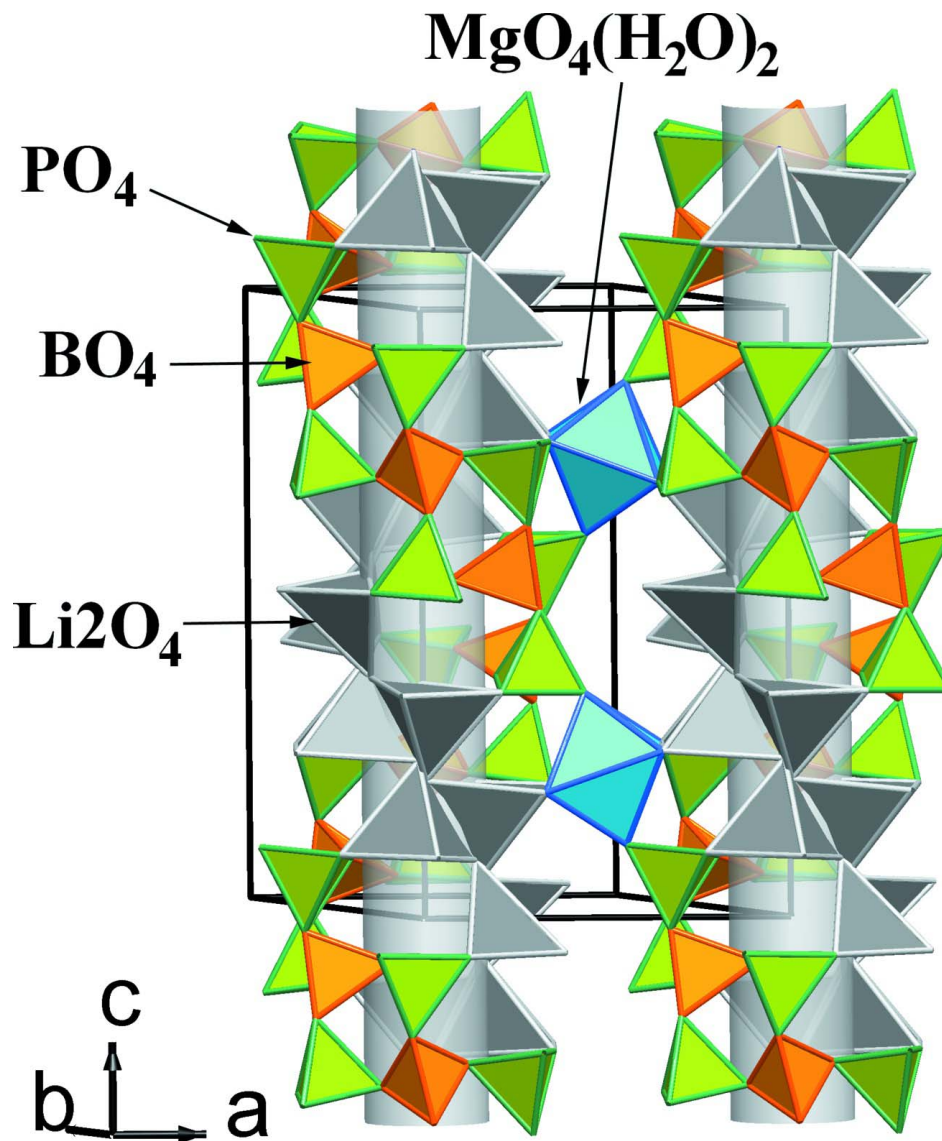
The crystal structure of the title compound contains infinite one-dimensional helical borophosphate ribbons  $\infty^1\{[\text{BP}_2\text{O}_8]^{3-}\}$ , arranged around  $6_5$  screw axes, which are built up from four-membered rings of corner-sharing  $\text{PO}_4$  and  $\text{BO}_4$  tetrahedra (Fig. 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.

### S2. 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),  $\text{H}_3\text{BO}_3$  (1.568 g) and 10 ml (85%)  $\text{H}_3\text{PO}_4$  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 ( $\text{pH} = 1.5$ ) 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.

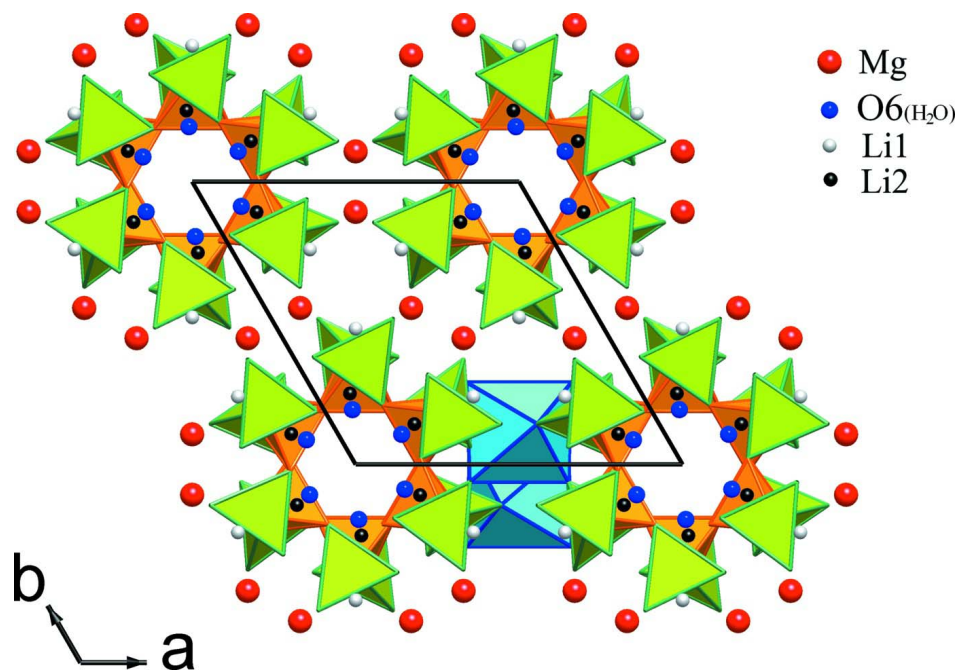
### S3. Refinement

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%.



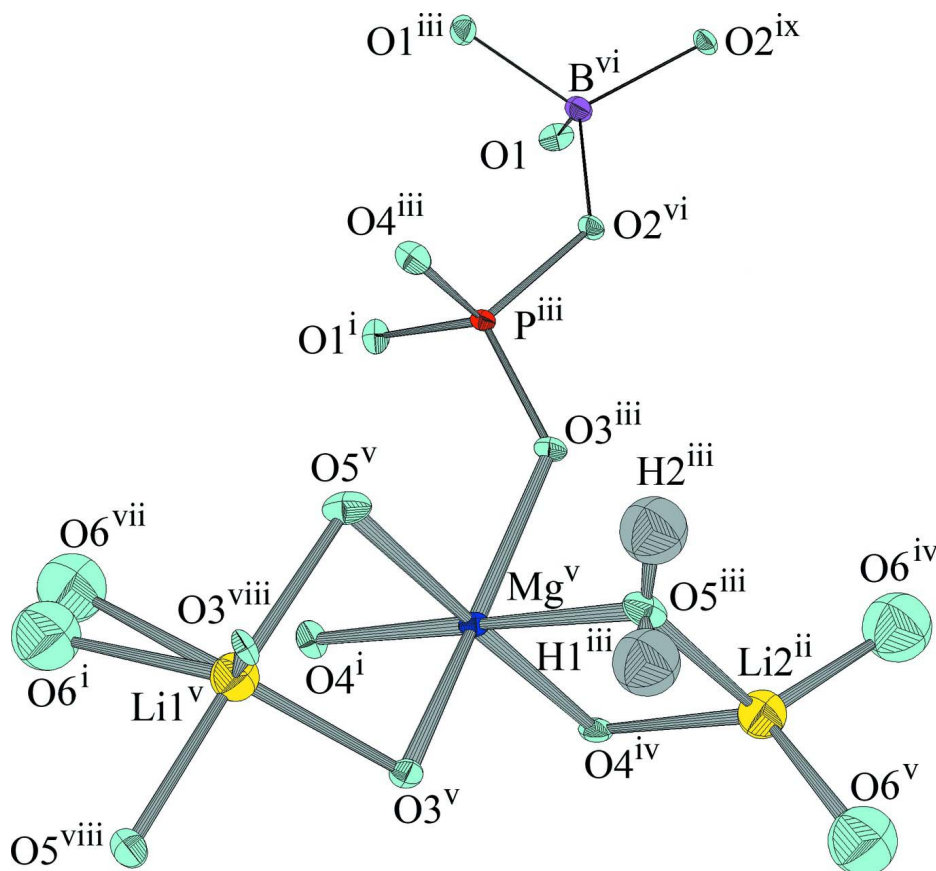
**Figure 1**

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:  $\text{PO}_4$ , Orange tetrahedra:  $\text{BO}_4$ , grey tetrahedra:  $\text{Li}_2\text{O}_4$ .



**Figure 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  $[001]$



**Figure 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,  $P6_322$

Hall symbol: P 65 2 (0 0 1)

$a = 9.4139 (1) \text{ \AA}$

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

$V = 1205.82 (3) \text{ \AA}^3$

$Z = 6$

$F(000) = 864$

#### Data collection

Oxford Diffraction CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

326 images,  $\Delta\omega = 1^\circ$ , Exp time: 40 s. scans

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

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 3404 reflections

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

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

$T = 173 \text{ K}$

Hexagonal bipyramidal, colourless

$0.16 \times 0.07 \times 0.07 \text{ mm}$

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  $I > 2\sigma(I)$

$R_{\text{int}} = 0.033$   
 $\theta_{\text{max}} = 32.6^\circ$ ,  $\theta_{\text{min}} = 2.8^\circ$   
 $h = -7 \rightarrow 14$

$k = -13 \rightarrow 14$   
 $l = -22 \rightarrow 8$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.037$   
 $wR(F^2) = 0.092$   
 $S = 1.06$   
 1343 reflections  
 75 parameters  
 0 restraints  
 Primary atom site location: structure-invariant  
 direct methods  
 Secondary atom site location: difference Fourier  
 map

Hydrogen site location: inferred from  
 neighbouring sites  
 H-atom parameters not refined  
 $w = 1/[\sigma^2(F_o^2) + (0.0493P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.74 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.55 \text{ e } \text{\AA}^{-3}$   
 Absolute structure: Flack (1983), 410 Friedel  
 pairs  
 Absolute structure 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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
P1	0.61413 (8)	0.82894 (8)	0.08573 (4)	0.00616 (14)	
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 ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
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 (Å, °)*

P1—O3	1.501 (2)	B1—O1 <sup>i</sup>	1.461 (3)
P1—O4	1.5033 (19)	B1—O2 <sup>ix</sup>	1.469 (3)
P1—O1 <sup>i</sup>	1.558 (2)	B1—O2	1.469 (3)
P1—O2 <sup>ii</sup>	1.5632 (17)	O6—O6 <sup>iii</sup>	0.549 (14)
P1—Li2 <sup>iii</sup>	2.94 (2)	Li1—O3 <sup>x</sup>	2.113 (12)
Mg1—O4 <sup>i</sup>	2.042 (2)	Li1—O5 <sup>x</sup>	2.135 (2)
Mg1—O4 <sup>iv</sup>	2.042 (2)	Li1—O6 <sup>vi</sup>	2.35 (2)
Mg1—O3 <sup>v</sup>	2.0590 (17)	Li1—O6 <sup>iv</sup>	2.35 (2)
Mg1—O3	2.0590 (17)	Li1—Li2 <sup>iv</sup>	2.40 (3)
Mg1—O5	2.179 (2)	Li2—O6 <sup>iii</sup>	1.82 (2)
Mg1—O5 <sup>v</sup>	2.179 (2)	Li2—O4 <sup>iii</sup>	2.08 (2)
Mg1—Li2 <sup>vi</sup>	3.07 (2)	Li2—O6 <sup>vii</sup>	2.08 (2)
Mg1—Li2 <sup>vii</sup>	3.07 (2)	Li2—O5 <sup>xi</sup>	2.10 (2)
Mg1—Li1 <sup>viii</sup>	3.128 (4)	Li2—Li2 <sup>vii</sup>	2.36 (4)
Mg1—Li1	3.128 (4)	Li2—O6 <sup>i</sup>	2.48 (2)
B1—O1 <sup>ii</sup>	1.461 (3)	Li2—O1 <sup>xii</sup>	2.65 (2)
O3—P1—O4	115.28 (12)	Li2 <sup>iii</sup> —O6—Li2 <sup>vii</sup>	116.4 (10)
O3—P1—O1 <sup>i</sup>	111.30 (11)	Li2—O6—Li1 <sup>xi</sup>	75.9 (9)
O4—P1—O1 <sup>i</sup>	105.63 (11)	Li2 <sup>iii</sup> —O6—Li1 <sup>xi</sup>	69.1 (7)
O3—P1—O2 <sup>ii</sup>	106.09 (10)	Li2 <sup>vii</sup> —O6—Li1 <sup>xi</sup>	114.4 (7)
O4—P1—O2 <sup>ii</sup>	111.75 (10)	Li2—O6—Li2 <sup>xiii</sup>	117.5 (12)
O1 <sup>i</sup> —P1—O2 <sup>ii</sup>	106.53 (10)	Li2 <sup>iii</sup> —O6—Li2 <sup>xiii</sup>	64.5 (10)
O3—P1—Li2 <sup>iii</sup>	134.1 (4)	Li2 <sup>vii</sup> —O6—Li2 <sup>xiii</sup>	142.5 (11)
O1 <sup>i</sup> —P1—Li2 <sup>iii</sup>	63.9 (4)	Li1 <sup>xi</sup> —O6—Li2 <sup>xiii</sup>	101.1 (6)
O2 <sup>ii</sup> —P1—Li2 <sup>iii</sup>	119.2 (4)	O3 <sup>x</sup> —Li1—O3	109.7 (9)
O4 <sup>i</sup> —Mg1—O4 <sup>iv</sup>	95.33 (13)	O3 <sup>x</sup> —Li1—O5 <sup>x</sup>	80.9 (3)
O4 <sup>i</sup> —Mg1—O3 <sup>v</sup>	91.45 (8)	O3—Li1—O5 <sup>x</sup>	97.7 (4)
O4 <sup>iv</sup> —Mg1—O3 <sup>v</sup>	99.96 (8)	O3 <sup>x</sup> —Li1—O5	97.7 (4)
O4 <sup>i</sup> —Mg1—O3	99.96 (8)	O3—Li1—O5	80.9 (3)
O4 <sup>iv</sup> —Mg1—O3	91.45 (8)	O5 <sup>x</sup> —Li1—O5	177.4 (11)
O3 <sup>v</sup> —Mg1—O3	163.06 (13)	O3 <sup>x</sup> —Li1—O6 <sup>vi</sup>	125.3 (5)
O4 <sup>i</sup> —Mg1—O5	178.78 (8)	O3—Li1—O6 <sup>vi</sup>	124.4 (5)
O4 <sup>iv</sup> —Mg1—O5	85.31 (9)	O5 <sup>x</sup> —Li1—O6 <sup>vi</sup>	98.0 (6)
O3 <sup>v</sup> —Mg1—O5	87.42 (8)	O5—Li1—O6 <sup>vi</sup>	84.6 (5)
O3—Mg1—O5	81.04 (8)	O3 <sup>x</sup> —Li1—O6 <sup>iv</sup>	124.4 (5)
O4 <sup>i</sup> —Mg1—O5 <sup>v</sup>	85.31 (9)	O3—Li1—O6 <sup>iv</sup>	125.3 (5)
O4 <sup>iv</sup> —Mg1—O5 <sup>v</sup>	178.78 (8)	O5 <sup>x</sup> —Li1—O6 <sup>iv</sup>	84.6 (5)
O3 <sup>v</sup> —Mg1—O5 <sup>v</sup>	81.04 (8)	O5—Li1—O6 <sup>iv</sup>	98.0 (6)
O3—Mg1—O5 <sup>v</sup>	87.42 (8)	O6 <sup>vi</sup> —Li1—O6 <sup>iv</sup>	13.5 (4)



O5—Mg1—O5 <sup>v</sup>	94.06 (13)	O6—Li2—O6 <sup>iii</sup>	10.0 (7)
B1 <sup>xiii</sup> —O1—P1 <sup>xiii</sup>	128.00 (16)	O6—Li2—O4 <sup>iii</sup>	121.6 (14)
B1 <sup>xiii</sup> —O1—Li2 <sup>xii</sup>	147.5 (5)	O6 <sup>iii</sup> —Li2—O4 <sup>iii</sup>	112.3 (11)
P1 <sup>xiii</sup> —O1—Li2 <sup>xii</sup>	84.3 (5)	O6—Li2—O6 <sup>vii</sup>	92.9 (11)
B1—O2—P1 <sup>ii</sup>	130.40 (17)	O6 <sup>iii</sup> —Li2—O6 <sup>vii</sup>	102.9 (10)
P1—O3—Mg1	130.05 (11)	O4 <sup>iii</sup> —Li2—O6 <sup>vii</sup>	134.3 (10)
P1—O3—Li1	127.6 (4)	O6—Li2—O5 <sup>xi</sup>	121.0 (13)
Mg1—O3—Li1	97.1 (2)	O6 <sup>iii</sup> —Li2—O5 <sup>xi</sup>	119.2 (11)
P1—O4—Mg1 <sup>xiii</sup>	141.40 (12)	O4 <sup>iii</sup> —Li2—O5 <sup>xi</sup>	86.5 (8)
P1—O4—Li2 <sup>iii</sup>	109.2 (6)	O6 <sup>vii</sup> —Li2—O5 <sup>xi</sup>	101.1 (9)
Mg1 <sup>xiii</sup> —O4—Li2 <sup>iii</sup>	96.3 (6)	O6—Li2—O6 <sup>i</sup>	102.1 (12)
Li2 <sup>vi</sup> —O5—Li1	69.3 (8)	O6 <sup>iii</sup> —Li2—O6 <sup>i</sup>	112.0 (10)
Li2 <sup>vi</sup> —O5—Mg1	91.8 (6)	O4 <sup>iii</sup> —Li2—O6 <sup>i</sup>	125.2 (9)
Li1—O5—Mg1	92.95 (17)	O6 <sup>vii</sup> —Li2—O6 <sup>i</sup>	9.6 (4)
O1 <sup>ii</sup> —B1—O1 <sup>i</sup>	102.5 (3)	O5 <sup>xi</sup> —Li2—O6 <sup>i</sup>	98.5 (8)
O1 <sup>ii</sup> —B1—O2	112.10 (10)	O6—Li2—O1 <sup>xii</sup>	99.7 (11)
O1 <sup>i</sup> —B1—O2	114.14 (10)	O6 <sup>iii</sup> —Li2—O1 <sup>xii</sup>	98.7 (9)
O1 <sup>ii</sup> —B1—O2 <sup>ix</sup>	114.14 (10)	O4 <sup>iii</sup> —Li2—O1 <sup>xii</sup>	60.6 (6)
O1 <sup>i</sup> —B1—O2 <sup>ix</sup>	112.10 (10)	O6 <sup>vii</sup> —Li2—O1 <sup>xii</sup>	86.7 (7)
O2—B1—O2 <sup>ix</sup>	102.2 (3)	O5 <sup>xi</sup> —Li2—O1 <sup>xii</sup>	137.7 (9)
Li2—O6—Li2 <sup>iii</sup>	144.4 (15)	O6 <sup>i</sup> —Li2—O1 <sup>xii</sup>	82.4 (6)
Li2—O6—Li2 <sup>vii</sup>	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 <sup>v</sup>	0.862	2.085	2.852 (3)	147.93
O5—H2 $\cdots$ O2 <sup>xiv</sup>	0.875	1.979	2.779 (3)	151.43
O5—H2 $\cdots$ O3 <sup>x</sup>	0.875	2.463	3.198 (3)	141.96

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