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$Li_2AlB_5O_{10}$

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A new compound, dilithium aluminium pentaborate, $Li_2AlB_5O_{10}$, has been synthesized by solid-state reaction and its structure determined by single-crystal X-ray diffraction. This compound is composed of $[B_5O_{10}]^{5-}$ groups linked by AlO_4 tetrahedra. The $[B_5O_{10}]^{5-}$ group consists of two hexagonal B–O rings perpendicular to each other connected by tetracoordinated boron. All the B–O rings in this structure can be divided into two groups, with one group approximately parallel and the other perpendicular to the *c* axis.

Comment

The present work is part of a series of studies aimed at exploring new optical materials. Up to now, many optical materials have been found in borates. According to previous work (Cheng & Lu, 1997), the excellent optical properties of LiB_3O_5, one of the most important non-linear optical crystals, mainly come from its anionic groups, $[B_3O_7]^{5-}$. The $[B_3O_7]^{5-}$ group consists of two BO_3 triangles and one BO_4 tetrahedron and forms a hexagonal B–O ring. Hoping to synthesize a new optical material, we have tried to introduce aluminium into alkali metal borates. Recently, a new compound, $LiAlB_2O_5$ (He *et al.*, 2001), has been reported and its structure determined from powder diffraction data. In this structure, Al substitutes the tetracoordinated boron in $[B_3O_7]^{5-}$ rings and a new anionic group, $[AlB_2O_7]^{5-}$, is formed. When the Li:(Al+B):O ratio of 1:3:5 was maintained but the Al:B ratio lowered from 1:2 to 1:5, the title compound was found to exist. This new compound crystallizes in monoclinic space group $P2_1/c$ and its structure can be characterized as a three-dimensional network of $[B_5O_{10}]^{5-}$ groups and AlO_4 tetrahedra. The $[B_5O_{10}]^{5-}$ group consists of two planar hexagonal B–O rings linked by a tetracoordinated B atom and these two rings are perpendicular to each other. Moreover, all the B–O rings in this structure can be divided into two groups, with one group approximately parallel and the other perpendicular to the *c* axis (shown in Fig. 1). The unique configuration of planar B–O rings in this structure suggests that the title compound may be an excellent birefringent material. Unlike the Al atoms in $LiAlB_2O_5$, where Al atoms act much like tetracoordinated boron, Al atoms in the title compound only connect to four different $[B_5O_{10}]^{5-}$ groups through O atoms and are not part of the B–O rings. In other words, $[B_5O_{10}]^{5-}$ groups are completely separated from each other by AlO_4 tetrahedra. The Li^+ cations are tetracoordinated, with Li—O distances ranging from 1.932 (2) to 2.063 (2) Å. The displacement ellipsoids of the asymmetric unit are shown in Fig. 2.

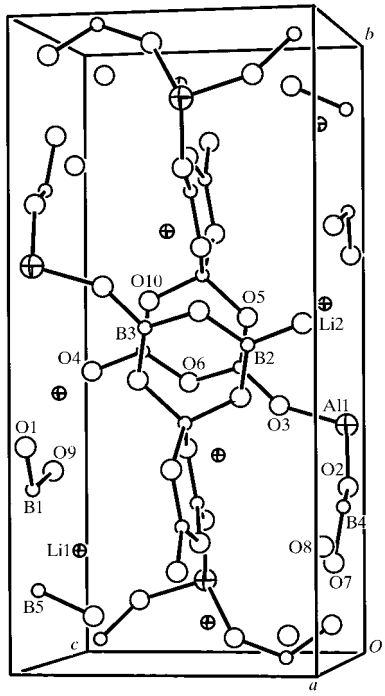

Figure 1
The unit cell of $Li_2AlB_5O_{10}$ viewed along [100]; large circles with crosses represent Al atoms and small circles with crosses Li atoms, while large open circles depict O atoms and small open circles B atoms.

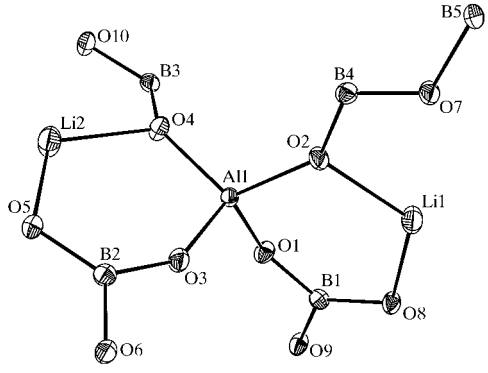

Figure 2
The asymmetric unit of $Li_2AlB_5O_{10}$. Displacement ellipsoids are drawn at the 50% probability level.

Experimental

A powder mixture of Li_2CO_3 (0.7388 g, 10 mmol), Al_2O_3 (0.5098 g, 5 mmol) and H_3BO_3 (3.7098 g, 60 mmol), all obtained from the Beijing Chemical Company, p.a., was melted at 1173 K in a Pt crucible. The melt was kept at 1173 K for 3 h to homogenise and then

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cooled to 1123 K at a rate of 10 K h^{-1} and to 1023 K at 2 K h^{-1}. Finally, the sample was cooled to 673 K at a rate of 20 K h^{-1} and the furnace was switched off. The crucible was removed from the furnace after it had cooled to room temperature. It was found that the title compound crystallized as transparent irregular grains. The X-ray powder diffraction pattern of the sample can be indexed with a unit cell that is given by the single-crystal data and shows some very weak additional reflections of LiB_3O_5.

Crystal data

$Li_2AlB_5O_{10}$	D_x = 2.286 Mg m^{-3}
M_r = 254.91	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 7060 reflections
a = 7.0402 (4) Å	θ = 2.7–33.3°
b = 14.9404 (8) Å	μ = 0.32 mm^{-1}
c = 7.0433 (4) Å	T = 295 (2) K
β = 90.7020 (10)°	Prism, colourless
V = 740.78 (7) $Å^3$	0.20 × 0.15 × 0.10 mm
Z = 4	

Data collection

Bruker APEX CCD area-detector diffractometer	R_{int} = 0.042
φ and ω scans	θ_{max} = 33.3°
6930 measured reflections	$h = -10 \rightarrow 9$
2728 independent reflections	$k = -23 \rightarrow 18$
	$l = -10 \rightarrow 10$

Table 1
Selected bond lengths (Å).

Al1—O3	1.7357 (7)	B4—O2	1.3536 (12)
Al1—O2	1.7405 (7)	B4—O9^{ii}	1.3931 (12)
Al1—O1	1.7414 (7)	B5—O7	1.4421 (12)
Al1—O4	1.7491 (7)	B5—O10^{iii}	1.4586 (13)
B1—O1	1.3502 (12)	B5—O5^{iv}	1.4885 (12)
B1—O8	1.3591 (12)	B5—O8^{ii}	1.5124 (12)
B1—O9	1.3976 (12)	Li1—O2	1.964 (2)
B2—O3	1.3495 (11)	Li2—O4	1.988 (2)
B2—O5	1.3556 (12)	Li2—O5	1.952 (2)
B2—O6	1.4013 (12)	Li1—O8	1.932 (2)
B3—O10	1.3447 (12)	Li1—O6^{v}	1.955 (2)
B3—O4	1.3644 (12)	Li1—O3^{v}	2.030 (2)
B3—O6^{i}	1.3917 (12)	Li2—O9^{vi}	1.970 (2)
B4—O7	1.3469 (12)	Li2—O1^{vi}	2.063 (2)

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

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.034	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.107	$\Delta\rho_{max}$ = 0.48 e $Å^{-3}$
S = 0.87	$\Delta\rho_{min}$ = −0.52 e $Å^{-3}$
2728 reflections	
163 parameters	

Data collection: *SMART* (Bruker, 2000); cell refinement: *SMART*; data reduction: *SHELXTL* (Bruker, 2000); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1999); software used to prepare material for publication: *SHELXL*97.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: BR1324). Services for accessing these data are described at the back of the journal.

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