Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993).

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$LaAl_{2.03}(B_4O_{10})O_{0.54}$

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Abstract

The title compound, lanthanum aluminium borate, has been found to be isostructural with hexagonal $NdAl_{2.07}(B_4O_{10})O_{0.6}$. Each La ion is coordinated by six O atoms to form a trigonal prism, while each Al is coordinated by five O atoms to form a pyramid.

Comment

The structure determination of the title compound was carried out as part of a sequence of research on MAl$_3$(BO$_3$)$_4$ (M = La, Sm, Gd, Nd) materials. The compound is non-stoichiometric. The structure is different from the rhombohedral structure of the $NdAl_3(BO_3)_4$ family (Hong & Dwight, 1974), but similar to that of $NdAl_{2.07}(B_4O_{10})O_{0.6}$ (Pushcharovskii *et al.*, 1978). The La, Al and B atoms are surrounded by O atoms in trigonal prismatic, pyramidal and tetrahedral arrangements, respectively. The BO_4 tetrahedra distinguish this structure from that of the $NdAl_3(BO_3)_4$ family, where the BO_3 units are planar. BO_4 tetrahedra share corners to form a net parallel to the *ab* plane; the other polyhedra share corners and edges.

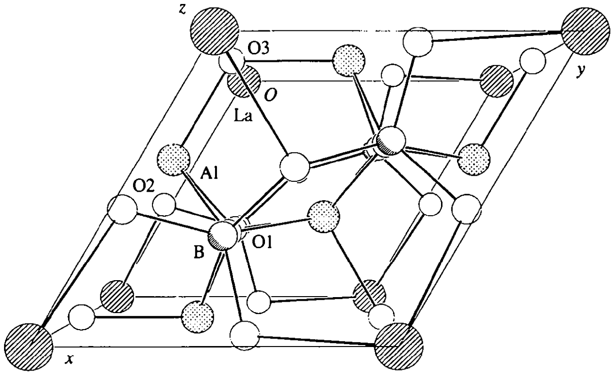

Fig. 1. Projection of the structure of the title compound on the *ab* plane.

Experimental

The title compound was prepared by heating a mixture of La_2O_3 and Al_2O_3 over B_2O_3, with PbF_2 and PbO as stabilizers, in a platinum crucible at 1323 K for 12 h (Wei, Jiang & Liu, 1993). The crucible was cooled slowly to room temperature, yielding single crystals.

Crystal data

$LaAl_{2.03}B_4O_{10.54}$
M_r = 405.55
Hexagonal
$P\bar{6}2m$
a = 4.606 (1) Å
c = 9.348 (2) Å
V = 171.75 (6) Å^3
Z = 1
D_x = 3.921 Mg m^{-3}
D_m = 3.94 (1) Mg m^{-3}
D_m measured by flotation in H_2O

Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 25 reflections
θ = 3–13°
μ = 6.547 mm^{-1}
T = 295 K
Prism
0.20 × 0.10 × 0.06 mm
Colourless

Data collection

Nicolet *R*3*m*/*E* diffractometer
$\theta/2\theta$ scans

407 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.021

Absorption correction:
XEMP in *SHELXTL*
(Sheldrick, 1985) using
ψ-scan data
$T_{min} = 0.375$, $T_{max} = 0.675$
753 measured reflections
421 independent reflections

$\theta_{max} = 25.6°$
$h = -8 \rightarrow 0$
$k = -8 \rightarrow 0$
$l = -20 \rightarrow 0$
2 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.119$
$S = 1.091$
407 reflections
23 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0443P)^2$
$+ 0.138P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 2.89$ e Å^{-3}
$\Delta\rho_{min} = -2.09$ e Å^{-3}

Extinction correction:
*SHELXL*93 (Sheldrick,
1993)
Extinction coefficient:
0.00 (17)
Scattering factors from
International Tables for
Crystallography (Vol. C)
Absolute configuration:
Flack (1983)
Flack parameter = 0.38 (4)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U^{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
La	0	0	0	0.00705 (7)
Al†	0.3885 (4)	0	1/2	0.0043 (3)
B	2/3	1/3	0.2208 (3)	0.0064 (3)
O1	2/3	1/3	0.3751 (2)	0.0054 (2)
O2	0.5718 (5)	0	0.1608 (2)	0.0081 (2)
O3‡	0	0	1/2	0.0018 (9)

† Site occupancy = 0.676 (6). ‡ Site occupancy = 0.54 (3).

Table 2. *Selected geometric parameters (Å, °)*

La—O2^{i}	2.479 (2)	Al—O1^{viii}	1.8425 (12)
La—O2^{ii}	2.479 (2)	Al—O1^{ix}	1.8425 (12)
La—O2^{iii}	2.479 (2)	Al—O1	1.8425 (12)
La—O2^{iv}	2.479 (2)	B—O1	1.444 (3)
La—O2^{v}	2.479 (2)	B—O2	1.4804 (13)
La—O2^{vi}	2.479 (2)	B—O2^{x}	1.4804 (13)
Al—O3	1.789 (2)	B—O2^{i}	1.4804 (13)
Al—O1^{vii}	1.8425 (12)		
O2^{i}—La—O2^{ii}	133.13 (4)	O1^{vii}—Al—O1^{ix}	147.59 (12)
O2^{ii}—La—O2^{iii}	87.08 (8)	O1^{viii}—Al—O1^{ix}	92.38 (7)
O2^{i}—La—O2^{iv}	74.61 (11)	O1—B—O2	112.23 (11)
O3—Al—O1^{vii}	106.20 (6)	O2—B—O2^{x}	106.57 (12)
O1^{vii}—Al—O1^{viii}	78.62 (8)		

Symmetry codes: (i) $1 - x + y, 1 - x, z$; (ii) $-y, x - y - 1, -z$; (iii) $x - 1, y, -z$; (iv) $1 - x + y, 1 - x, -z$; (v) $x - 1, y, z$; (vi) $-y, x - y - 1, z$; (vii) $y, x - 1, z$; (viii) $y, x - 1, 1 - z$; (ix) $x, y, 1 - z$; (x) $1 - y, x - y, z$.

The formula of the compound was obtained by refinement of the occupancies of Al and O3, and the agreement that this gave between the calculated and measured densities. The largest peak in the difference map (2.89 e Å^{-3}) is at 0,0,0.3402 and the largest hole (−2.09 e Å^{-3}) is at 0.5684,0.1638,0. A chiral twin or positional disorder was indicated by refinement of the Flack (1983) parameter [$\chi = 0.38\,(4)$].

Data collection: Nicolet *P*3 software (Nicolet, 1985). Cell refinement: Nicolet *P*3 software. Data reduction: *SHELXTL* (Sheldrick, 1985). Program(s) used to solve structure: *SHELXTL*. Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *SHELXTL*. Software used to prepare material for publication: *SHELXL*93.

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