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Trilithium scandium bis(orthoborate)

Lizhong Mao, Tianyong Zhou and Ning Ye*

Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, People's Republic of China
Correspondence e-mail: nye@fjirsm.ac.cn

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Key indicators: single-crystal X-ray study; T = 293 K; mean σ(O–B) = 0.002 Å; R factor = 0.017; wR factor = 0.059; data-to-parameter ratio = 9.2.

Single crystals of the title compound, $Li_3Sc(BO_3)_2$, have been obtained by spontaneous nucleation from a high-temperature melt. The title compound adopts a framework structure and is composed of distorted [ScO_6] octahedra, [LiO_4] tetrahedra, [LiO_4] rectangles and isolated [BO_3] triangles. Except for the Sc and one Li atom (both on inversion centres), all atoms are in general positions.

Related literature

For a review of structural data of BO_3 groups, see: Zobetz (1982). For sodium scandium borates, see: Becker & Held (2001); Zhang *et al.* (2006).

Experimental

Crystal data

$Li_3Sc(BO_3)_2$
M_r = 183.4
Monoclinic, $P2_1/n$
a = 4.7831 (17) Å
b = 5.954 (2) Å
c = 8.163 (3) Å
β = 90.702 (9)°
V = 232.44 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.53 mm^{-1}
T = 293 (2) K
0.12 × 0.10 × 0.10 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2000)
T_{min} = 0.833, T_{max} = 0.858
1734 measured reflections
534 independent reflections
518 reflections with $I > 2\sigma(I)$
R_{int} = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.017
$wR(F^2)$ = 0.058
S = 1.10
534 reflections
58 parameters
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sc—O1	2.0854 (12)	Li2—O2	1.946 (3)
Sc—O2^{i}	2.1101 (12)	Li2—O3^{iv}	1.983 (3)
Sc—O3^{i}	2.1197 (13)	Li2—O3^{i}	2.137 (3)
Li1—O2	2.0107 (12)	B—O2	1.376 (2)
Li1—O1^{ii}	2.1173 (12)	B—O3^{v}	1.384 (2)
Li2—O1^{iii}	1.896 (3)	B—O1^{vi}	1.385 (2)
O2—B—O3^{v}	122.09 (14)	O3^{v}—B—O1^{vi}	118.72 (14)
O2—B—O1^{vi}	119.13 (14)		

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

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2004); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2180).

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supplementary materials

Acta Cryst. (2008). E**64**, i38 [**doi:10.1107/S1600536808014797**]

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Comment

$Li_3Sc(BO_3)_2$, (I), was found from analysis of phase equilibria in the system Li_2O—Sc_2O_3—B_2O_3, in which it is the first characterized pseudo-ternary phase. For the heavier Na homologue, two phases are already known, viz. $Na_3Sc_2(BO_3)_3$ (Zhang *et al.*, 2006) and $NaScB_2O_5$ (Becker & Held, 2001).

The framework structure of (I) is made up of distorted [ScO_6] octahedra, [LiO_4] tetrahedra, [LiO_4] rectangles and [BO_3] triangles as single building units. The [ScO_6] octahedra are linked via [LiO_4] rectangles by sharing edges to form columns parallel to [010]. The columns are linked to each other through [LiO_4] tetrahedra and [BO_3] triangles by sharing edges and corners (Figs 1 and 2).

The B atom is coordinated to three oxygen atoms forming nearly trigonal planar $[BO_3]^{3-}$ anions. The B—O bond lengths range from 1.376 (2) to 1.385 (2) Å, and the O—B—O angles are close to 120° (Table 1), values that are typical for BO_3 groups (Zobetz, 1982). The Sc^{3+} cation is coordinated by six oxygen atoms to form a distorted [ScO_6] ocahedron with Sc—O bond lengths ranging from 2.0854 (12) to 2.1197 (13) Å. There are two crystallographically different Li atoms. One is situated on an inversion centre ($\bar{1}$ symmetry) and is coordinated to four oxygen atoms forming a nearly planar [LiO_4] rectangle with Li1—O bond lengths ranging from 2.0107 (12) to 2.1173 (12) Å. The other Li atom is also coordinated to four O atoms, but is in the centre of a distorted tetrahedron with Li2—O bond lengths from 1.896 (3) to 2.137 (3) Å (Table 1). The average Li—O bond length of the [$Li1O_4$] rectangle (2.064 Å) is slightly longer than that of the [$Li2O_4$] tetrahedron (1.991 Å).

Experimental

Single crystals of compound (I) were grown using a $LiBO_2$-containing flux. The composition of the mixture for crystal growth was 4:1:4 of Li_2CO_3 (Sinopharm Reagents, 99.99%), Sc_2O_3 (Sinopharm Reagents, 4 N), and B_2O_3 (Sinopharm Reagents, 99%). This mixture was heated in a platinum crucible to 1373 K, held at this temperature for several hours, and then cooled at a rate of 10 K/h from 1373 to 873 K. The remaining flux attached to the crystals was readily dissolved in water. Crystals with an average size of 0.5 mm and mostly block shaped habit were obtained.

Figures

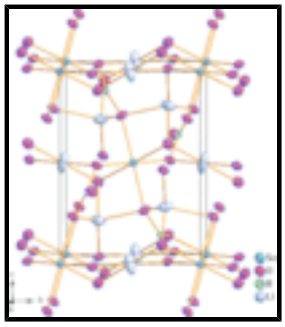

Fig. 1. The structure of (I) in a projection approximatly along the [001] direction with displacement ellipsoids drawn at the 85% probability level.

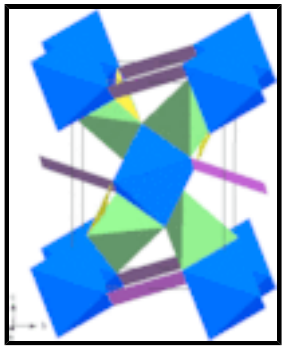

Fig. 2. The structure of (I) given in the polyhedral description. [ScO_6] octahedra are blue, [LiO_4] tetrahedra are green, [LiO_4] rectangles are purple, and [BO_3] units are yellow.

trilithium scandium bis(orthoborate)

Crystal data

$Li_3Sc(BO_3)_2$	F_{000} = 176
M_r = 183.4	D_x = 2.62 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 623 reflections
a = 4.7831 (17) Å	θ = 4.2–23.6º
b = 5.954 (2) Å	μ = 1.53 mm^{-1}
c = 8.163 (3) Å	T = 293 (2) K
β = 90.702 (9)º	Block, colourless
V = 232.44 (15) Å^3	0.12 × 0.10 × 0.10 mm
Z = 2	

Data collection

Rigaku Mercury CCD diffractometer	534 independent reflections
Radiation source: Sealed Tube	518 reflections with $I > 2\sigma(I)$
Monochromator: Graphite Monochromator	R_{int} = 0.015
Detector resolution: 14.6306 pixels mm^{-1}	θ_{max} = 27.5º
T = 293(1) K	θ_{min} = 4.2º
CCD_Profile_fitting scans	h = −6→4

Absorption correction: multi-scan (CrystalClear; Rigaku, 2000)	$k = -7 \rightarrow 7$
$T_{min} = 0.833$, $T_{max} = 0.858$	$l = -10 \rightarrow 10$
1734 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0318P)^2 + 0.216P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.017$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.058$	$\Delta\rho_{max} = 0.28$ e Å^{-3}
$S = 1.10$	$\Delta\rho_{min} = -0.23$ e Å^{-3}
534 reflections	Extinction correction: SHELXL97 (Sheldrick, 2008)
58 parameters	Extinction coefficient: ?

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.

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

	x	y	z	U_{iso}*/U_{eq}
Sc	0	0	0	0.00510 (15)
Li1	0	−0.5	0	0.0209 (10)
Li2	−0.0144 (6)	−0.2513 (5)	0.2977 (4)	0.0133 (6)
B	0.5149 (4)	−0.3045 (3)	0.1254 (2)	0.0061 (3)
O1	0.3101 (2)	0.24622 (18)	0.00179 (14)	0.0077 (2)
O2	0.2330 (2)	−0.26155 (19)	0.11029 (14)	0.0086 (3)
O3	0.1280 (2)	−0.08686 (19)	−0.23947 (13)	0.0086 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sc	0.0050 (2)	0.0054 (2)	0.0049 (2)	−0.00002 (13)	0.00011 (14)	0.00009 (12)
Li1	0.015 (2)	0.012 (2)	0.035 (3)	0.0000 (15)	−0.008 (2)	−0.0062 (17)
Li2	0.0119 (13)	0.0182 (15)	0.0098 (13)	−0.0025 (11)	−0.0018 (10)	0.0015 (10)
B	0.0074 (7)	0.0042 (7)	0.0067 (7)	−0.0009 (6)	0.0000 (6)	−0.0014 (6)
O1	0.0065 (5)	0.0095 (5)	0.0070 (5)	−0.0013 (4)	0.0004 (4)	0.0005 (4)
O2	0.0060 (5)	0.0099 (5)	0.0099 (6)	0.0013 (4)	0.0000 (4)	0.0012 (4)
O3	0.0084 (5)	0.0102 (6)	0.0071 (5)	0.0006 (4)	−0.0009 (4)	−0.0023 (4)

Geometric parameters (Å, °)

Sc—O1	2.0854 (12)	Li2—O1^{x}	1.896 (3)
Sc—O1^{i}	2.0854 (12)	Li2—O2	1.946 (3)
Sc—O2^{i}	2.1101 (12)	Li2—O3^{xi}	1.983 (3)
Sc—O2	2.1101 (12)	Li2—O3^{i}	2.137 (3)
Sc—O3^{i}	2.1197 (13)	Li2—B^{viii}	2.659 (3)
Sc—O3	2.1197 (13)	Li2—B^{xi}	2.697 (3)
Sc—Li2^{i}	2.855 (3)	Li2—B^{xii}	2.733 (4)
Sc—Li2	2.855 (3)	Li2—Sc^{ix}	3.226 (3)
Sc—Li1^{ii}	2.9768 (11)	Li2—Li1^{iii}	3.234 (3)
Sc—Li1	2.9768 (11)	Li2—Sc^{x}	3.297 (3)
Sc—Li2^{iii}	3.226 (3)	B—O2	1.376 (2)
Sc—Li2^{iv}	3.226 (3)	B—O3^{xiii}	1.384 (2)
Li1—O2	2.0107 (12)	B—O1^{xiv}	1.385 (2)
Li1—O2^{v}	2.0107 (12)	B—Li2^{xv}	2.659 (3)
Li1—O1^{vi}	2.1173 (12)	B—Li2^{iv}	2.697 (3)
Li1—O1^{i}	2.1173 (12)	B—Li2^{x}	2.733 (4)
Li1—B^{vii}	2.8008 (18)	B—Li1^{xv}	2.8008 (18)
Li1—B^{viii}	2.8008 (18)	O1—B^{xiv}	1.385 (2)
Li1—Li2^{v}	2.847 (3)	O1—Li2^{xii}	1.896 (3)
Li1—Li2	2.847 (3)	O1—Li1^{ii}	2.1173 (12)
Li1—Sc^{vi}	2.9768 (11)	O3—B^{xvi}	1.384 (2)
Li1—Li2^{ix}	3.234 (3)	O3—Li2^{iv}	1.983 (3)
Li1—Li2^{iv}	3.234 (3)	O3—Li2^{i}	2.137 (3)
O1—Sc—O1^{i}	180.00 (4)	O1^{x}—Li2—O3^{i}	109.04 (14)
O1—Sc—O2^{i}	81.73 (5)	O2—Li2—O3^{i}	90.58 (12)
O1^{i}—Sc—O2^{i}	98.27 (5)	O3^{xi}—Li2—O3^{i}	101.95 (13)
O1—Sc—O2	98.27 (5)	O2—B—O3^{xiii}	122.09 (14)
O1^{i}—Sc—O2	81.73 (5)	O2—B—O1^{xiv}	119.13 (14)
O2^{i}—Sc—O2	180.00 (8)	O3^{xiii}—B—O1^{xiv}	118.72 (14)
O1—Sc—O3^{i}	92.04 (4)	B^{xiv}—O1—Li2^{xii}	109.58 (13)
O1^{i}—Sc—O3^{i}	87.96 (4)	B^{xiv}—O1—Sc	127.37 (10)
O2^{i}—Sc—O3^{i}	93.23 (5)	Li2^{xii}—O1—Sc	111.74 (11)
O2—Sc—O3^{i}	86.77 (5)	B^{xiv}—O1—Li1^{ii}	104.23 (9)
O1—Sc—O3	87.96 (4)	Li2^{xii}—O1—Li1^{ii}	110.73 (10)
O1^{i}—Sc—O3	92.04 (4)	Sc—O1—Li1^{ii}	90.19 (5)
O2^{i}—Sc—O3	86.77 (5)	B—O2—Li2	122.67 (13)
O2—Sc—O3	93.23 (5)	B—O2—Li1	116.47 (10)
O3^{i}—Sc—O3	180.00 (5)	Li2—O2—Li1	92.02 (10)

O2—Li1—O2^{v}	180.00 (6)	B—O2—Sc	133.37 (10)
O2—Li1—O1^{vi}	96.68 (5)	Li2—O2—Sc	89.39 (10)
O2^{v}—Li1—O1^{vi}	83.32 (5)	Li1—O2—Sc	92.47 (5)
O2—Li1—O1^{i}	83.32 (5)	B^{xvi}—O3—Li2^{iv}	102.89 (13)
O2^{v}—Li1—O1^{i}	96.68 (5)	B^{xvi}—O3—Sc	137.30 (10)
O1^{vi}—Li1—O1^{i}	180	Li2^{iv}—O3—Sc	103.64 (10)
O1^{x}—Li2—O2	111.51 (16)	B^{xvi}—O3—Li2^{i}	99.62 (12)
O1^{x}—Li2—O3^{xi}	124.23 (16)	Li2^{iv}—O3—Li2^{i}	135.08 (11)
O2—Li2—O3^{xi}	113.33 (15)	Sc—O3—Li2^{i}	84.24 (9)

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

Fig. 1

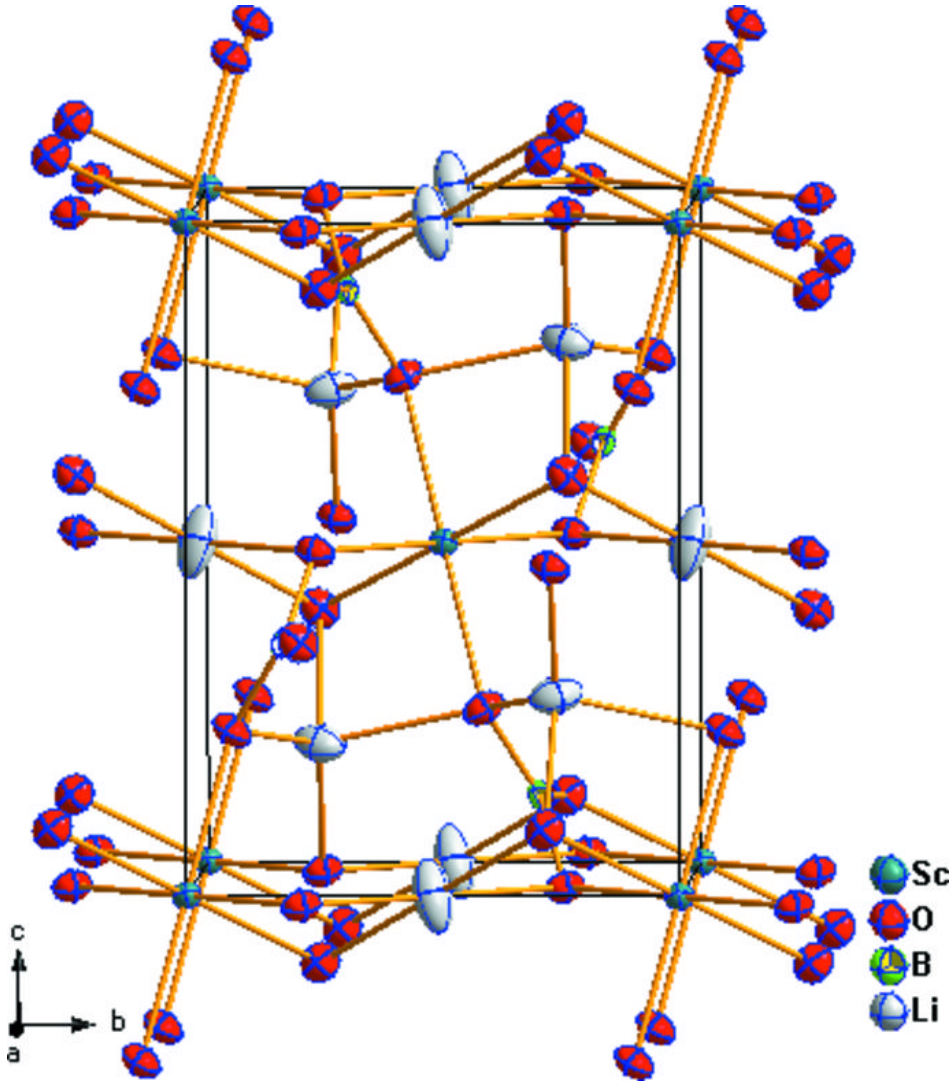

Fig. 2