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Distrontium lithium beryllium triborate, Sr₂LiBeB₃O₈

Na Yu 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) = 0.005 Å; R factor = 0.026; wR factor = 0.060; data-to-parameter ratio = 11.5.

Single crystals of distrontium lithium beryllium triborate, Sr₂LiBeB₃O₈, were obtained by spontaneous nucleation from a high-temperature melt. In the Sr₂Li[BeB₃O₈] structure, $[BeB_2O_7]^{6-}$ rings, made up from one BeO₄ tetrahedron and two BO_3 triangles, are connected to each other by $[BO_3]$ triangles to form the smallest repeat unit { $[BeB_3O_8]^{8-}$ } and then form chains along the b axis. The Sr^{2+} cations are sevenor eight-coordinated and Li+ cations are tetra-coordinated and lie between the chains.

Related literature

Non-linear optical (NLO) applications of borate crystals with trigonal BO₃ anions have been discussed by Chen et al. (1999). Among this group of compounds, beryllium borates are reported to exhibit the shortest transmission cut-off wavelength (Li, 1989). A review of the geometry of the BO₃ group is given by Zobetz (1982), and a similar configuration of the $[BeB_2O_7]^{6-}$ unit is found in LiB₃O₅ (LBO; Chen *et al.*, 2005) in which $[B_3O_7]^{5-}$ rings are present. The structure of the beryllium borate group $[BeB_2O_7]^{6-}$ is given by Li & Ye (2007).

Experimental

Crystal data

Sr ₂ LiBeB ₃ O ₈	V = 687.4 (7) Å ³
$M_r = 351.62$	Z = 4
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
a = 8.609 (5) Å	$\mu = 15.53 \text{ mm}^{-1}$
b = 6.486 (4) Å	T = 293 K
c = 12.868 (8) Å	$0.20 \times 0.12 \times 0.10$
$\beta = 106.91 \ (1)^{\circ}$	

Data collection

Rigaku Mercury2 diffractometer Absorption correction: multi-scan (CrystalClear; Rigaku, 2007) $T_{\min} = 0.123, T_{\max} = 0.212$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.026$ $wR(F^2) = 0.060$ S = 1.051574 reflections

137 parameters $\Delta \rho_{\rm max} = 0.97 \ {\rm e} \ {\rm \AA}^{-3}$

 $\Delta \rho_{\rm min} = -0.81$ e Å⁻³

5147 measured reflections

 $R_{\rm int} = 0.038$

1574 independent reflections

1429 reflections with $I > 2\sigma(I)$

mm

Data collection: CrystalClear (Rigaku, 2007); 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: SHELXTL (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2197).

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supplementary materials

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Comment

Based on a theoretical study, beryllium borates possess the largest energy gap among all alkaline and alkaline earth borates, and hence the shortest transmission cut-off wavelength (Li, 1989). In addition, borate crystals containing parallelly aligned BO₃ anionic groups are considered to be good candidates for NLO applications (Chen *et al.*, 1999). Therefore, beryllium borates are studied intensively with the purpose of searching for novel compounds with potential applications in the UV region. The title compound, $Sr_2LiBeB_3O_8$, was found from the investigation of the beryllium borate system containing strontium and lithium.

A perspective view of the Sr₂LiBeB₃O₈ structure in the a-c plane is shown in Fig.1. It contains a similar beryllium borate group [BeB₂O₇]⁶⁻ which was found in the structure Na₂BeB₂O₅(Li & Ye, 2007) as the basic group in the Sr₂LiBeB₃O₈ structure. In the structure of non-planar six-ring [BeB₂O₇]⁶⁻, the Be atoms are bonded to four O atoms to form distorted BeO₄ tetrahedral. The B atoms are coordinated to three O atoms to form planar BO₃ triangles and two planar BO₃ groups share one common O1 atom, and each of them also shares a different O atom with a BeO₄ tetrahedral.(Fig.3) This structure of the basic structural unit, [BeB₂O₇]⁶⁻, is similar to that of [B₃O₇]⁵⁻ in LiB₃O₅ (LBO) (Chen *et al.*, 2005), with a BO₄ replaced by BeO₄. In the Sr₂LiBeB₃O₈ structure, the [BeB₂O₇]⁶⁻ rings are linked each other by a bridging BO₃ group(B3 atom) to form the smallest repeat unit {[BeB₃O₈]⁸⁻} (n→∞) one dimensional chains along the b Axis (Fig.2). From the study of LBO, it is known that the [B₃O₇]⁵⁻ group can yield large NLO effects and short UV transmission cutoffs, but spatial arrangement of the endless helices of [B₃O₇](n→∞) chains along the *b* axis may be a good candidate for DUV NLO applications. Unfortunately, in the case of Sr₂LiBeB₃O₈, the direction of [BeB₂O₇]⁶⁻ group along the *b* axis are completely opposite and, therefore, their contributions to the NLO effect cancel out.

Experimental

Single crystals of $Sr_2LiBeB_3O_8$ were grown from a high-temperature solution using $SrO-B_2O_3$ — Li_2CO_3 as a flux. This solution was prepared in a platinum crucible after melting of a mixture of $SrCO_3$, BeO, B_2O_3 and Li_2CO_3 at the ratio of $SrO/BeO/B_2O_3/Li_2CO_3=4:2:3:2$. The mixture (10 g) was heated in a temperature-programmable electric furnace at 1273 K until the melt became transparent and clear. The homogenized melt solution was then cooled rapidly (323 K/h) to the initial crystallization temperature (1073 K). It was further cooled slowly (276 K/h) to the final crystallization temperature (973 K) and then allowed to cool to room temperature after the furnace was turned off. The flux attached to the crystal was readily dissolved in water.

Computing details

Data collection: *CrystalClear* (Rigaku, 2007); cell refinement: *CrystalClear* (Rigaku, 2007); data reduction: *CrystalClear* (Rigaku, 2007); 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: *SHELXTL* (Sheldrick, 2008).



Figure 1

The crystal structure of $Sr_2Li[BeB_3O_8]$, viewed along the *b* axis, and drawn with anisotropic displacement paremeters at the 50% probability level. Sr—O bonds and Li—O bonds were omitted for clarity.



Figure 2

The parallel arrangement of the smallest repeat unit $\{[BeB_3O_8]^{8-}\}$ $(n \rightarrow \infty)$ along b axis which forms a one-dimensional infinite chain.



Figure 3

 $[BeB_2O_7]^{6-}$ building unit in the title compound.

Distrontium lithium beryllium triborate

Crystal data

Sr₂LiBeB₃O₈ $M_r = 351.62$ Monoclinic, $P2_1/c$ Hall symbol: -P 2ybc a = 8.609 (5) Å b = 6.486 (4) Å c = 12.868 (8) Å $\beta = 106.91$ (1)° V = 687.4 (7) Å³ Z = 4

Data collection

Rigaku Mercury2 diffractometer Radiation source: fine-focus sealed tube Graphite monochromator Detector resolution: 13.6612 pixels mm⁻¹ CCD_Profile_fitting scans Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2007) $T_{min} = 0.123, T_{max} = 0.212$ F(000) = 648 $D_x = 3.397 \text{ Mg m}^{-3}$ Mo K α radiation, $\lambda = 0.71073 \text{ Å}$ Cell parameters from 764 reflections $\theta = 4.1-27.5^{\circ}$ $\mu = 15.53 \text{ mm}^{-1}$ T = 293 KPrism, colorless $0.20 \times 0.12 \times 0.10 \text{ mm}$

5147 measured reflections 1574 independent reflections 1429 reflections with $I > 2\sigma(I)$ $R_{int} = 0.038$ $\theta_{max} = 27.5^{\circ}, \ \theta_{min} = 2.5^{\circ}$ $h = -11 \rightarrow 9$ $k = -7 \rightarrow 8$ $l = -16 \rightarrow 16$ Refinement

Refinement on F^2	Secondary atom site location: difference Fourier
Least-squares matrix: full	map
$R[F^2 > 2\sigma(F^2)] = 0.026$	$w = 1/[\sigma^2(F_o^2) + (0.0325P)^2]$
$wR(F^2) = 0.060$	where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{\rm max} < 0.001$
1574 reflections	$\Delta \rho_{\rm max} = 0.97 \text{ e } \text{\AA}^{-3}$
137 parameters	$\Delta \rho_{\rm min} = -0.81 \text{ e} \text{ Å}^{-3}$
0 restraints	Extinction correction: SHELXL97 (Sheldrick,
Primary atom site location: structure-invariant	2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/sin(2\theta)]^{-1/4}$
direct methods	Extinction coefficient: 0.0525 (14)

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 (A^2)

	x	у	Ζ	$U_{ m iso}$ */ $U_{ m eq}$
Sr1	0.35975 (4)	0.24425 (5)	0.42862 (2)	0.00870 (12)
Sr2	0.96530 (4)	0.89027 (5)	0.34184 (2)	0.01077 (12)
B1	0.7378 (5)	0.2697 (6)	0.4861 (3)	0.0081 (7)
B2	0.9374 (5)	0.3471 (6)	0.3805 (3)	0.0086 (7)
B3	0.4005 (5)	0.4529 (6)	0.2060 (3)	0.0089 (7)
Be1	0.6756 (5)	0.5709 (7)	0.3439 (3)	0.0087 (9)
Li1	0.3681 (9)	0.7734 (10)	0.3261 (5)	0.0212 (15)
01	0.8842 (3)	0.2319 (4)	0.4584 (2)	0.0115 (5)
O2	0.6391 (3)	0.4284 (4)	0.43886 (18)	0.0108 (5)
O3	0.7074 (3)	0.1423 (4)	0.56005 (19)	0.0135 (5)
O4	0.8589 (3)	0.5215 (4)	0.3371 (2)	0.0143 (5)
O5	1.0594 (3)	0.2620 (4)	0.3497 (2)	0.0118 (5)
O6	0.5555 (3)	0.5273 (4)	0.22195 (18)	0.0105 (5)
O7	0.6566 (3)	0.8100 (4)	0.37736 (19)	0.0132 (5)
08	0.3055 (3)	0.5106 (4)	0.26900 (19)	0.0114 (5)

Atomic displacement parameters $(Å^2)$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.01050 (19)	0.0059 (2)	0.01079 (19)	0.00014 (11)	0.00487 (13)	0.00049 (11)
Sr2	0.01267 (19)	0.00595 (19)	0.01254 (19)	-0.00039 (12)	0.00184 (13)	0.00046 (12)
B1	0.0104 (19)	0.0045 (19)	0.0099 (18)	-0.0021 (14)	0.0039 (14)	-0.0027 (14)
B2	0.0091 (18)	0.008 (2)	0.0102 (17)	-0.0036 (14)	0.0042 (14)	-0.0019 (15)
B3	0.0151 (19)	0.0043 (19)	0.0073 (17)	0.0016 (15)	0.0032 (14)	0.0022 (14)
Be1	0.012 (2)	0.005 (2)	0.010 (2)	-0.0002 (16)	0.0055 (16)	0.0020 (16)
Li1	0.039 (4)	0.010 (4)	0.021 (3)	-0.007 (3)	0.019 (3)	-0.005 (3)

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01	0.0113 (13)	0.0102 (14)	0.0147 (12)	0.0034 (9)	0.0063 (9)	0.0045 (10)
O2	0.0117 (12)	0.0087 (13)	0.0136 (12)	0.0004 (9)	0.0062 (9)	0.0027 (10)
O3	0.0227 (14)	0.0057 (13)	0.0154 (12)	0.0011 (10)	0.0109 (10)	0.0022 (10)
O4	0.0122 (13)	0.0085 (13)	0.0248 (13)	0.0011 (10)	0.0093 (10)	0.0070 (11)
05	0.0127 (13)	0.0097 (14)	0.0148 (12)	0.0001 (9)	0.0069 (10)	-0.0013 (10)
O6	0.0123 (12)	0.0091 (13)	0.0112 (12)	-0.0013 (9)	0.0050 (9)	-0.0012 (10)
O7	0.0253 (14)	0.0039 (13)	0.0091 (11)	0.0031 (10)	0.0029 (10)	0.0009 (10)
08	0.0126 (12)	0.0103 (14)	0.0125 (12)	-0.0018 (10)	0.0054 (9)	-0.0019 (10)

Geometric parameters (Å, °)

Sr1—O5 ⁱ	2.491 (3)	B1—O3	1.342 (4)
Sr1—O7 ⁱⁱ	2.565 (3)	B1—O2	1.360 (5)
Sr1—O3 ⁱⁱⁱ	2.586 (3)	B1—O1	1.428 (5)
Sr1-08	2.620(3)	B2—O5	1.344 (4)
Sr102	2.654 (3)	B2—O4	1.352 (5)
Sr1—O6 ^{iv}	2.663 (3)	B2—O1	1.428 (4)
Sr1—O2 ⁱⁱ	2.722 (3)	B3—O8	1.361 (5)
Sr1—O3	3.051 (3)	B3—O6	1.377 (5)
Sr2—O8 ^v	2.478 (3)	$B3-07^{iv}$	1.395 (5)
Sr2—O5 ^{vi}	2.536 (3)	Be1—O7	1.630 (5)
Sr2—O5 ^{vii}	2.551 (3)	Be1—O6	1.634 (5)
Sr2—O4	2.556 (3)	Be1—O2	1.634 (5)
Sr2—O1 ^{viii}	2.642 (3)	Be1—O4	1.638 (5)
Sr2—O3 ^{viii}	2.740 (3)	Li1—O3 ⁱⁱ	1.849 (7)
Sr2—07	2.872 (3)	Li1—O8	1.872 (7)
Sr2—O1 ^{vi}	2.873 (3)	Li1—O6 ^v	1.940 (7)
Sr2—O4 ^{vii}	3.217 (3)	Li1—O7	2.389 (8)
$O5^{i}$ — $Sr1$ — $O7^{ii}$	93.38 (9)	O8 ^v —Sr2—O7	52.40 (8)
O5 ⁱ —Sr1—O3 ⁱⁱⁱ	81.09 (8)	O5 ^{vi} —Sr2—O7	117.75 (8)
O7 ⁱⁱ —Sr1—O3 ⁱⁱⁱ	74.69 (8)	O5 ^{vii} —Sr2—O7	105.89 (8)
O5 ⁱ —Sr1—O8	73.89 (8)	O4—Sr2—O7	59.49 (8)
O7 ⁱⁱ —Sr1—O8	143.67 (8)	O1 ^{viii} —Sr2—O7	90.30 (8)
O3 ⁱⁱⁱ —Sr1—O8	133.75 (8)	O3 ^{viii} —Sr2—O7	141.98 (7)
O5 ⁱ —Sr1—O2	144.86 (8)	$O8^v$ — $Sr2$ — $O1^{vi}$	74.15 (8)
O7 ⁱⁱ —Sr1—O2	108.59 (8)	$O5^{vi}$ — $Sr2$ — $O1^{vi}$	50.90 (8)
O3 ⁱⁱⁱ —Sr1—O2	130.36 (8)	$O5^{vii}$ — $Sr2$ — $O1^{vi}$	142.30 (8)
O8—Sr1—O2	72.22 (8)	$O4$ — $Sr2$ — $O1^{vi}$	126.47 (8)
$O5^{i}$ — $Sr1$ — $O6^{iv}$	101.50 (8)	O1 ^{viii} —Sr2—O1 ^{vi}	81.27 (9)
$O7^{ii}$ —Sr1—O6 ^{iv}	137.73 (9)	O3 ^{viii} —Sr2—O1 ^{vi}	101.09 (8)
$O3^{iii}$ —Sr1—O6 ^{iv}	69.01 (8)	$O7$ — $Sr2$ — $O1^{vi}$	71.36 (8)
$O8$ — $Sr1$ — $O6^{iv}$	78.59 (9)	$O8^v$ — $Sr2$ — $O4^{vii}$	93.68 (8)
$O2$ — $Sr1$ — $O6^{iv}$	80.66 (8)	$O5^{vi}$ — $Sr2$ — $O4^{vii}$	64.26 (7)
$O5^{i}$ — $Sr1$ — $O2^{ii}$	91.93 (8)	O5 ^{vii} —Sr2—O4 ^{vii}	47.06 (8)
O7 ⁱⁱ —Sr1—O2 ⁱⁱ	59.23 (8)	O4—Sr2—O4 ^{vii}	118.07 (7)
O3 ⁱⁱⁱ —Sr1—O2 ⁱⁱ	132.93 (8)	O1 ^{viii} —Sr2—O4 ^{vii}	125.21 (8)
O8—Sr1—O2 ⁱⁱ	86.79 (9)	O3 ^{viii} —Sr2—O4 ^{vii}	73.47 (8)
O2—Sr1—O2 ⁱⁱ	77.27 (8)	O7—Sr2—O4 ^{vii}	144.26 (7)
$O6^{iv}$ —Sr1—O2 ⁱⁱ	156.42 (7)	O1 ^{vi} —Sr2—O4 ^{vii}	113.95 (7)

O5 ⁱ —Sr1—O3	166.09 (8)	O3—B1—O2	123.9 (3)
O7 ⁱⁱ —Sr1—O3	75.73 (8)	O3—B1—O1	116.1 (3)
O3 ⁱⁱⁱ —Sr1—O3	87.60 (8)	O2—B1—O1	120.0 (3)
O8—Sr1—O3	120.00 (7)	O5—B2—O4	124.2 (3)
O2—Sr1—O3	48.81 (8)	O5—B2—O1	115.4 (3)
O6 ^{iv} —Sr1—O3	81.75 (7)	O4—B2—O1	120.2 (3)
O2 ⁱⁱ —Sr1—O3	89.86 (7)	O8—B3—O6	122.7 (3)
O8 ^v —Sr2—O5 ^{vi}	87.68 (9)	O8—B3—O7 ^{iv}	120.2 (3)
O8 ^v —Sr2—O5 ^{vii}	75.33 (8)	O6—B3—O7 ^{iv}	117.2 (3)
$O5^{vi}$ — $Sr2$ — $O5^{vii}$	106.52 (6)	O7—Be1—O6	109.5 (3)
O8 ^v —Sr2—O4	90.61 (9)	O7—Be1—O2	106.6 (3)
O5 ^{vi} —Sr2—O4	177.22 (8)	O6—Be1—O2	114.5 (3)
O5 ^{vii} —Sr2—O4	75.13 (8)	O7—Be1—O4	111.9 (3)
O8 ^v —Sr2—O1 ^{viii}	140.12 (7)	O6—Be1—O4	105.4 (3)
$O5^{vi}$ —Sr2—O1 ^{viii}	100.72 (8)	O2—Be1—O4	109.1 (3)
O5 ^{vii} —Sr2—O1 ^{viii}	136.21 (8)	O3 ⁱⁱ —Li1—O8	116.9 (3)
O4—Sr2—O1 ^{viii}	79.23 (8)	O3 ⁱⁱ —Li1—O6 ^v	103.4 (3)
O8 ^v —Sr2—O3 ^{viii}	163.40 (8)	O8—Li1—O6 ^v	137.1 (4)
$O5^{vi}$ —Sr2—O3 ^{viii}	77.37 (8)	O3 ⁱⁱ —Li1—O7	109.2 (3)
O5 ^{vii} —Sr2—O3 ^{viii}	101.86 (8)	O8—Li1—O7	110.9 (3)
O4—Sr2—O3 ^{viii}	104.60 (8)	O6 ^v —Li1—O7	65.3 (2)
O1 ^{viii} —Sr2—O3 ^{viii}	51.76 (7)		

Symmetry codes: (i) *x*-1, *y*, *z*; (ii) -*x*+1, -*y*+1, -*z*+1; (iii) -*x*+1, -*y*, -*z*+1; (iv) -*x*+1, *y*-1/2, -*z*+1/2; (v) -*x*+1, *y*+1/2, -*z*+1/2; (vi) *x*, *y*+1, *z*; (vii) -*x*+2, *y*+1/2, -*z*+1/2; (viii) -*x*+2, -*y*+1, -*z*+1.