## Acta Crystallographica Section E

## Structure Reports

Online
ISSN 1600-5368

## Distrontium lithium beryllium triborate, $\mathrm{Sr}_{2} \mathrm{LiBeB}_{3} \mathrm{O}_{8}$

Na Yu and Ning Ye*<br>Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, People's Republic of China<br>Correspondence e-mail: nye@fjirsm.ac.cn

Received 28 March 2012; accepted 6 April 2012

Key indicators: single-crystal X-ray study; $T=293 \mathrm{~K}$; mean $\sigma(\mathrm{O}-\mathrm{B})=0.005 \mathrm{~A}$; $R$ factor $=0.026 ; w R$ factor $=0.060 ;$ data-to-parameter ratio $=11.5$.

## Experimental

Crystal data
$\mathrm{Sr}_{2} \mathrm{LiBeB}_{3} \mathrm{O}_{8}$
$M_{r}=351.62$

$$
Z=4
$$

Monoclinic, $P 2_{1} / c$
$a=8.609$ (5) A
$b=6.486$ (4) A
$c=12.868$ (8) $\AA$
$\beta=106.91(1)^{\circ}$

## Data collection

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

$$
V=687.4(7) \AA^{3}
$$

Mo $K \alpha$ radiation
$\mu=15.53 \mathrm{~mm}^{-1}$
$T=293 \mathrm{~K}$
$0.20 \times 0.12 \times 0.10 \mathrm{~mm}$

5147 measured reflections 1574 independent reflections 1429 reflections with $I>2 \sigma(I)$ $R_{\text {int }}=0.038$

## Refinement

$R\left[F^{2}>2 \sigma\left(F^{2}\right)\right]=0.026 \quad 137$ parameters
$w R\left(F^{2}\right)=0.060$
$S=1.05$
1574 reflections
$\Delta \rho_{\text {max }}=0.97 \mathrm{e}^{-3}$
$\Delta \rho_{\min }=-0.81 \mathrm{e}^{\AA^{-3}}$

Single crystals of distrontium lithium beryllium triborate, $\mathrm{Sr}_{2} \mathrm{LiBeB}_{3} \mathrm{O}_{8}$, were obtained by spontaneous nucleation from a high-temperature melt. In the $\mathrm{Sr}_{2} \mathrm{Li}\left[\mathrm{BeB}_{3} \mathrm{O}_{8}\right]$ structure, $\left[\mathrm{BeB}_{2} \mathrm{O}_{7}\right]^{6-}$ rings, made up from one $\mathrm{BeO}_{4}$ tetrahedron and two $\mathrm{BO}_{3}$ triangles, are connected to each other by $\left[\mathrm{BO}_{3}\right]$ triangles to form the smallest repeat unit $\left\{\left[\mathrm{BeB}_{3} \mathrm{O}_{8}\right]^{8-}\right\}$ and then form chains along the $b$ axis. The $\mathrm{Sr}^{2+}$ cations are sevenor eight-coordinated and $\mathrm{Li}^{+}$cations are tetra-coordinated and lie between the chains.

## Related literature

Non-linear optical (NLO) applications of borate crystals with trigonal $\mathrm{BO}_{3}$ 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 $\mathrm{BO}_{3}$ group is given by Zobetz (1982), and a similar configuration of the $\left[\mathrm{BeB}_{2} \mathrm{O}_{7}\right]^{6-}$ unit is found in $\mathrm{LiB}_{3} \mathrm{O}_{5}(\mathrm{LBO}$; Chen et al., 2005) in which $\left[\mathrm{B}_{3} \mathrm{O}_{7}\right]^{5-}$ rings are present. The structure of the beryllium borate group $\left[\mathrm{BeB}_{2} \mathrm{O}_{7}\right]^{6-}$ is given by $\mathrm{Li} \& \mathrm{Ye}$ (2007).

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).

This work was supported by the National Natural Science Foundation of China (Nos. 50872132 and 90922035) and the Fujian High Technology Research and Development Program of China (No. 2010H0021).

[^0]
## References

Brandenburg, K. (2004). DIAMOND. Crystal Impact GbR, Bonn, Germany. Chen, C. T., Lin, Z. S. \& Wang, Z. Z. (2005). Appl. Phys. B, 80, 1-25.
Chen, C. T., Ye, N., Lin, J., Jiang, J., Zeng, W. R. \& Wu, B. C. (1999). Adv. Mater. 11, 1071-1078.
Li, R. K. (1989). J. Non-Cryst. Solids, 111, 199-204.
Li, W. \& Ye, N. (2007). Acta Cryst. E63, i160.
Rigaku (2007). CrystalClear. Rigaku Corporation, Tokyo, Japan. Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.
Zobetz, E. (1982). Z. Kristallogr. 160, 81-92.

## supplementary materials

Acta Cryst. (2012). E68, i32 [doi:10.1107/S1600536812015164]

## Distrontium lithium beryllium triborate, $\mathrm{Sr}_{2} \mathrm{LiBeB}_{3} \mathrm{O}_{8}$

## Na Yu and Ning Ye

## 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 $\mathrm{BO}_{3}$ 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, $\mathrm{Sr}_{2} \mathrm{LiBeB}_{3} \mathrm{O}_{8}$, was found from the investigation of the beryllium borate system containing strontium and lithium.
A perspective view of the $\mathrm{Sr}_{2} \mathrm{LiBeB}_{3} \mathrm{O}_{8}$ structure in the a-c plane is shown in Fig.1. It contains a similar beryllium borate group $\left[\mathrm{BeB}_{2} \mathrm{O}_{7}\right]^{6-}$ which was found in the structure $\mathrm{Na}_{2} \mathrm{BeB}_{2} \mathrm{O}_{5}(\mathrm{Li} \& \mathrm{Ye}, 2007)$ as the basic group in the $\mathrm{Sr}_{2} \mathrm{LiBeB}_{3} \mathrm{O}_{8}$ structure. In the structure of non-planar six-ring $\left[\mathrm{BeB}_{2} \mathrm{O}_{7}\right]^{6}$, the Be atoms are bonded to four O atoms to form distorted $\mathrm{BeO}_{4}$ tetrahedral. The B atoms are coordinated to three O atoms to form planar $\mathrm{BO}_{3}$ triangles and two planar $\mathrm{BO}_{3}$ groups share one common Ol atom, and each of them also shares a different O atom with a $\mathrm{BeO}_{4}$ tetrahedral.(Fig.3) This structure of the basic structural unit, $\left[\mathrm{BeB}_{2} \mathrm{O}_{7}\right]^{6}$, is similar to that of $\left[\mathrm{B}_{3} \mathrm{O}_{7}\right]^{5-}$ in $\mathrm{LiB}_{3} \mathrm{O}_{5}(\mathrm{LBO})$ (Chen et al., 2005), with a $\mathrm{BO}_{4}$ replaced by $\mathrm{BeO}_{4}$. In the $\mathrm{Sr}_{2} \mathrm{LiBeB}_{3} \mathrm{O}_{8}$ structure, the $\left[\mathrm{BeB}_{2} \mathrm{O}_{7}\right]^{6-}$ rings are linked each other by a bridging $\mathrm{BO}_{3}$ group ( B 3 atom) to form the smallest repeat unit $\left\{\left[\mathrm{BeB}_{3} \mathrm{O}_{8}\right]^{8-}\right\}(\mathrm{n} \rightarrow \infty)$ one dimensional chains along the b Axis (Fig.2). From the study of LBO, it is known that the $\left[\mathrm{B}_{3} \mathrm{O}_{7}\right]^{5-}$ group can yield large NLO effects and short UV transmission cutoffs, but spatial arrangement of the endless helices of $\left[\mathrm{B}_{3} \mathrm{O}_{7}\right](\mathrm{n} \rightarrow \infty)$ chains along the $z$ axis is unfavorable for producing a large birefringence. Therefore, the resulting layer structure of $\left[\mathrm{BeB}_{2} \mathrm{O}_{7}\right](\mathrm{n} \rightarrow \infty)$ along the $b$ axis may be a good candidate for DUV NLO applications. Unfortunately, in the case of $\mathrm{Sr}_{2} \mathrm{LiBeB}_{3} \mathrm{O}_{8}$, the direction of $\left[\mathrm{BeB}_{2} \mathrm{O}_{7}\right]^{6-}$ group along the $b$ axis are completely opposite and, therefore, their contributions to the NLO effect cancel out.

## Experimental

Single crystals of $\mathrm{Sr}_{2} \mathrm{LiBeB}_{3} \mathrm{O}_{8}$ were grown from a high-temperature solution using $\mathrm{SrO}-\mathrm{B}_{2} \mathrm{O}_{3}-\mathrm{Li}_{2} \mathrm{CO}_{3}$ as a flux. This solution was prepared in a platinum crucible after melting of a mixture of $\mathrm{SrCO}_{3}, \mathrm{BeO}, \mathrm{B}_{2} \mathrm{O}_{3}$ and $\mathrm{Li}_{2} \mathrm{CO}_{3}$ at the ratio of $\mathrm{SrO} / \mathrm{BeO} / \mathrm{B}_{2} \mathrm{O}_{3} / \mathrm{Li}_{2} \mathrm{CO}_{3}=4: 2: 3: 2$. The mixture $(10 \mathrm{~g})$ 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 ( $323 \mathrm{~K} / \mathrm{h}$ ) to the initial crystallization temperature ( 1073 K ). It was further cooled slowly ( $276 \mathrm{~K} / \mathrm{h}$ ) to the final crystallization temperature $(973 \mathrm{~K})$ 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 $\mathrm{Sr}_{2} \mathrm{Li}\left[\mathrm{BeB}_{3} \mathrm{O}_{8}\right]$, viewed along the $b$ axis, and drawn with anisotropic displacement paremeters at the $50 \%$ probability level. $\mathrm{Sr}-\mathrm{O}$ bonds and $\mathrm{Li}-\mathrm{O}$ bonds were omitted for clarity.


Figure 2
The parallel arrangement of the smallest repeat unit $\left\{\left[\mathrm{BeB}_{3} \mathrm{O}_{8}\right]^{8-}\right\}(\mathrm{n} \rightarrow \infty)$ along b axis which forms a one-dimensional infinite chain.


## Figure 3

$\left[\mathrm{BeB}_{2} \mathrm{O}_{7}\right]^{6-}$ building unit in the title compound.

## Distrontium lithium beryllium triborate

## Crystal data

$\mathrm{Sr}_{2} \mathrm{LiBeB}_{3} \mathrm{O}_{8}$
$M_{r}=351.62$
Monoclinic, $P 2{ }_{1} / c$
Hall symbol: -P 2ybc
$a=8.609$ (5) $\AA$
$b=6.486$ (4) $\AA$
$c=12.868(8) \AA$
$\beta=106.91(1)^{\circ}$
$V=687.4(7) \AA^{3}$
$Z=4$
Data collection
Rigaku Mercury2
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels $\mathrm{mm}^{-1}$
CCD_Profile_fitting scans
Absorption correction: multi-scan
(CrystalClear; Rigaku, 2007)
$T_{\min }=0.123, T_{\text {max }}=0.212$
$F(000)=648$
$D_{\mathrm{x}}=3.397 \mathrm{Mg} \mathrm{m}^{-3}$
Mo $K \alpha$ radiation, $\lambda=0.71073 \AA$
Cell parameters from 764 reflections
$\theta=4.1-27.5^{\circ}$
$\mu=15.53 \mathrm{~mm}^{-1}$
$T=293 \mathrm{~K}$
Prism, colorless
$0.20 \times 0.12 \times 0.10 \mathrm{~mm}$

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

## Refinement

Refinement on $F^{2}$
Least-squares matrix: full
$R\left[F^{2}>2 \sigma\left(F^{2}\right)\right]=0.026$
$w R\left(F^{2}\right)=0.060$
$S=1.05$
1574 reflections
137 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

## 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 1.s. planes.
Refinement. Refinement of $F^{2}$ against ALL reflections. The weighted $R$-factor $w R$ 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 $F^{2}>\sigma\left(F^{2}\right)$ 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 ( $\AA^{2}$ )

|  | $x$ | $y$ | $z$ | $U_{\text {iso }} * / U_{\text {eq }}$ |
| :--- | :--- | :--- | :--- | :--- |
| 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 | $0.3681(9)$ | $0.7734(10)$ | $0.3261(5)$ | $0.0212(15)$ |
| O1 | $0.8842(3)$ | $0.2319(4)$ | $0.4584(2)$ | $0.0115(5)$ |
| 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 | $0.6566(3)$ | $0.8100(4)$ | $0.37736(19)$ | $0.0132(5)$ |
| O8 | $0.3055(3)$ | $0.5106(4)$ | $0.26900(19)$ | $0.0114(5)$ |

Atomic displacement parameters $\left(\dot{A}^{2}\right)$

|  | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 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 | $0.039(4)$ | $0.010(4)$ | $0.021(3)$ | $-0.007(3)$ | $0.019(3)$ | $-0.005(3)$ |


| O1 | $0.0113(13)$ | $0.0102(14)$ | $0.0147(12)$ | $0.0034(9)$ | $0.0063(9)$ | $0.0045(10)$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 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 | $0.0122(13)$ | $0.0085(13)$ | $0.0248(13)$ | $0.0011(10)$ | $0.0093(10)$ | $0.0070(11)$ |
| O5 | $0.0127(13)$ | $0.0097(14)$ | $0.0148(12)$ | $0.0001(9)$ | $0.0069(10)$ | $-0.0013(10)$ |
| O6 | $0.0123(12)$ | $0.0091(13)$ | $0.0112(12)$ | $-0.0013(9)$ | $0.0050(9)$ | $-0.0012(10)$ |
| O7 | $0.0253(14)$ | $0.0039(13)$ | $0.0091(11)$ | $0.0031(10)$ | $0.0029(10)$ | $0.0009(10)$ |
| O8 | $0.0126(12)$ | $0.0103(14)$ | $0.0125(12)$ | $-0.0018(10)$ | $0.0054(9)$ | $-0.0019(10)$ |

Geometric parameters $\left({ }^{( },{ }^{\circ}\right)$

| Sr1-O5 ${ }^{\text {i }}$ | 2.491 (3) | $\mathrm{B} 1-\mathrm{O} 3$ | 1.342 (4) |
| :---: | :---: | :---: | :---: |
| $\mathrm{Sr} 1-\mathrm{O} 7^{\text {ii }}$ | 2.565 (3) | $\mathrm{B} 1-\mathrm{O} 2$ | 1.360 (5) |
| Sr1-O3 ${ }^{\text {iii }}$ | 2.586 (3) | $\mathrm{B} 1-\mathrm{O} 1$ | 1.428 (5) |
| Sr1-O8 | 2.620 (3) | B2-O5 | 1.344 (4) |
| $\mathrm{Sr} 1-\mathrm{O} 2$ | 2.654 (3) | B2-O4 | 1.352 (5) |
| $\mathrm{Sr} 1-\mathrm{O} 6^{\text {iv }}$ | 2.663 (3) | B2-O1 | 1.428 (4) |
| $\mathrm{Sr} 1-\mathrm{O} 2^{\text {ii }}$ | 2.722 (3) | B3-O8 | 1.361 (5) |
| $\mathrm{Sr} 1-\mathrm{O} 3$ | 3.051 (3) | B3-O6 | 1.377 (5) |
| $\mathrm{Sr} 2-\mathrm{O} 8^{\mathrm{v}}$ | 2.478 (3) | B3-O7 ${ }^{\text {iv }}$ | 1.395 (5) |
| $\mathrm{Sr} 2-\mathrm{O} 5^{\text {vi }}$ | 2.536 (3) | Be1-O7 | 1.630 (5) |
| $\mathrm{Sr} 2-\mathrm{O} 5^{\text {vii }}$ | 2.551 (3) | Be1-O6 | 1.634 (5) |
| Sr2-O4 | 2.556 (3) | Be1-O2 | 1.634 (5) |
| Sr2-O1 ${ }^{\text {viii }}$ | 2.642 (3) | Be1-O4 | 1.638 (5) |
| $\mathrm{Sr} 2-\mathrm{O} 3{ }^{\text {viii }}$ | 2.740 (3) | $\mathrm{Li} 1-\mathrm{O} 3{ }^{\text {ii }}$ | 1.849 (7) |
| $\mathrm{Sr} 2-\mathrm{O} 7$ | 2.872 (3) | Li1-O8 | 1.872 (7) |
| $\mathrm{Sr} 2-\mathrm{O} 1^{\text {vi }}$ | 2.873 (3) | Li1-O6 ${ }^{\text {V }}$ | 1.940 (7) |
| Sr2-O4 $4^{\text {vii }}$ | 3.217 (3) | Lil-O7 | 2.389 (8) |
| $\mathrm{O} 5^{\mathrm{i}}-\mathrm{Sr} 1-\mathrm{O} 7^{\mathrm{ii}}$ | 93.38 (9) | O8- ${ }^{\text {v }} \mathrm{Sr} 2-\mathrm{O} 7$ | 52.40 (8) |
| $\mathrm{O} 5^{\mathrm{i}}-\mathrm{Sr} 1-\mathrm{O} 3{ }^{\text {iii }}$ | 81.09 (8) | O5 ${ }^{\text {vi }}-\mathrm{Sr} 2-\mathrm{O} 7$ | 117.75 (8) |
| O7 ${ }^{\text {ii }}-\mathrm{Sr} 1-\mathrm{O} 3{ }^{\text {iii }}$ | 74.69 (8) | O5 ${ }^{\text {vii }} \mathrm{Sr} 2-\mathrm{O} 7$ | 105.89 (8) |
| O5i-Sr1-O8 | 73.89 (8) | $\mathrm{O} 4-\mathrm{Sr} 2-\mathrm{O} 7$ | 59.49 (8) |
| O7ii-Sr1-08 | 143.67 (8) | $\mathrm{O} 1^{\text {viii- }} \mathrm{Sr} 2-\mathrm{O} 7$ | 90.30 (8) |
| O3iii-Sr1-O8 | 133.75 (8) | O3 ${ }^{\text {viii- }} \mathrm{Sr} 2-\mathrm{O} 7$ | 141.98 (7) |
| $\mathrm{O} 5{ }^{\text {i }}$ - $\mathrm{Sr} 1-\mathrm{O} 2$ | 144.86 (8) | $\mathrm{O} 8^{\mathrm{v}}-\mathrm{Sr} 2-\mathrm{O} 1^{\text {vi }}$ | 74.15 (8) |
| $\mathrm{O} 7^{\mathrm{ii}}-\mathrm{Sr} 1-\mathrm{O} 2$ | 108.59 (8) | $\mathrm{O} 5{ }^{\text {vi }}-\mathrm{Sr} 2-\mathrm{O} 1^{\text {vi }}$ | 50.90 (8) |
| $\mathrm{O} 3 \mathrm{iii}-\mathrm{Sr} 1-\mathrm{O} 2$ | 130.36 (8) | $\mathrm{O} 5^{\text {vii }}$ - $\mathrm{Sr} 2-\mathrm{O} 1^{\text {vi }}$ | 142.30 (8) |
| $\mathrm{O} 8-\mathrm{Sr} 1-\mathrm{O} 2$ | 72.22 (8) | $\mathrm{O} 4-\mathrm{Sr} 2-\mathrm{O} 1^{\text {vi }}$ | 126.47 (8) |
| $\mathrm{O} 5-\mathrm{Sr} 1-\mathrm{O}^{\text {iv }}$ | 101.50 (8) | $\mathrm{O} 1{ }^{\text {viii }}-\mathrm{Sr} 2-\mathrm{O} 1^{\text {vi }}$ | 81.27 (9) |
| $\mathrm{O} 7^{\text {ii- }}$ - Sr1-O6 ${ }^{\text {iv }}$ | 137.73 (9) | $\mathrm{O} 3{ }^{\text {viii }}-\mathrm{Sr} 2-\mathrm{O} 1^{\text {vi }}$ | 101.09 (8) |
| $\mathrm{O} 3{ }^{\text {iii }}-\mathrm{Sr} 1-\mathrm{O}^{\text {iv }}$ | 69.01 (8) | $\mathrm{O} 7-\mathrm{Sr} 2-\mathrm{O} 1^{\text {vi }}$ | 71.36 (8) |
| O8-Sr1-O6 ${ }^{\text {iv }}$ | 78.59 (9) | $\mathrm{O} 8^{\mathrm{v}}-\mathrm{Sr} 2-\mathrm{O} 4{ }^{\text {vii }}$ | 93.68 (8) |
| $\mathrm{O} 2-\mathrm{Sr} 1-\mathrm{O}^{\text {iv }}$ | 80.66 (8) | $\mathrm{O} 5^{\text {vi }}-\mathrm{Sr} 2-\mathrm{O} 4{ }^{\text {vii }}$ | 64.26 (7) |
| $\mathrm{O} 5-\mathrm{Sr} 1-\mathrm{O} 2{ }^{\text {ii }}$ | 91.93 (8) | $\mathrm{O} 5^{\text {vii }}-\mathrm{Sr} 2-\mathrm{O} 4^{\text {vii }}$ | 47.06 (8) |
| $\mathrm{O} 7^{\mathrm{ii}}-\mathrm{Sr} 1-\mathrm{O} 2^{\text {ii }}$ | 59.23 (8) | $\mathrm{O} 4-\mathrm{Sr} 2-\mathrm{O} 4{ }^{\text {vii }}$ | 118.07 (7) |
| $\mathrm{O} 3{ }^{\text {iii }}-\mathrm{Sr} 1-\mathrm{O} 2{ }^{\text {ii }}$ | 132.93 (8) | $\mathrm{O} 1{ }^{\text {viii }}-\mathrm{Sr} 2-\mathrm{O} 4{ }^{\text {vii }}$ | 125.21 (8) |
| $\mathrm{O} 8-\mathrm{Sr} 1-\mathrm{O} 2{ }^{\text {ii }}$ | 86.79 (9) | $\mathrm{O} 3{ }^{\text {viii }}-\mathrm{Sr} 2-\mathrm{O} 4{ }^{\text {vii }}$ | 73.47 (8) |
| $\mathrm{O} 2-\mathrm{Sr} 1-\mathrm{O} 2{ }^{\text {ii }}$ | 77.27 (8) | $\mathrm{O} 7-\mathrm{Sr} 2-\mathrm{O} 4{ }^{\text {vii }}$ | 144.26 (7) |
| $\mathrm{O} 6^{\text {iv }}-\mathrm{Sr} 1-\mathrm{O} 2^{\text {ii }}$ | 156.42 (7) | $\mathrm{O} 1^{\text {vi }}-\mathrm{Sr} 2-\mathrm{O} 4{ }^{\text {vii }}$ | 113.95 (7) |

## supplementary materials

| O 5 - $\mathrm{Sr} 1-\mathrm{O} 3$ | 166.09 (8) | $\mathrm{O} 3-\mathrm{B} 1-\mathrm{O} 2$ | 123.9 (3) |
| :---: | :---: | :---: | :---: |
| O7ii- ${ }^{\text {iid }} 1-\mathrm{O} 3$ | 75.73 (8) | $\mathrm{O} 3-\mathrm{B} 1-\mathrm{O} 1$ | 116.1 (3) |
| $\mathrm{O} 3 \mathrm{iii}-\mathrm{Sr} 1-\mathrm{O} 3$ | 87.60 (8) | $\mathrm{O} 2-\mathrm{B} 1-\mathrm{O} 1$ | 120.0 (3) |
| O8-Sr1-O3 | 120.00 (7) | O5-B2-O4 | 124.2 (3) |
| $\mathrm{O} 2-\mathrm{Sr} 1-\mathrm{O} 3$ | 48.81 (8) | $\mathrm{O} 5-\mathrm{B} 2-\mathrm{O} 1$ | 115.4 (3) |
| $\mathrm{O} 6^{\text {iv }}-\mathrm{Sr} 1-\mathrm{O} 3$ | 81.75 (7) | O4-B2-O1 | 120.2 (3) |
| O2 ${ }^{\text {iii }}$-Sr1-O3 | 89.86 (7) | O8-B3-O6 | 122.7 (3) |
| $\mathrm{O} 8^{\text {v}}-\mathrm{Sr} 2-\mathrm{O} 5^{\text {vi }}$ | 87.68 (9) | O8-B3-O7 ${ }^{\text {iv }}$ | 120.2 (3) |
| $\mathrm{O} 8^{\mathrm{v}}$ - $\mathrm{Sr} 2-\mathrm{O} 5^{\text {vii }}$ | 75.33 (8) | O6-B3-O7 $7^{\text {iv }}$ | 117.2 (3) |
| $\mathrm{O} 5^{\text {vi }}-\mathrm{Sr} 2-\mathrm{O} 5^{\text {vii }}$ | 106.52 (6) | O7-Be1-O6 | 109.5 (3) |
| O8 ${ }^{\text {v }}$ - $\mathrm{Sr} 2-\mathrm{O} 4$ | 90.61 (9) | O7-Be1-O2 | 106.6 (3) |
| O5vi-Sr2-04 | 177.22 (8) | O6-Be1-O2 | 114.5 (3) |
| O5 ${ }^{\text {vii- }} \mathrm{Sr} 2-\mathrm{O} 4$ | 75.13 (8) | O7-Be1-O4 | 111.9 (3) |
| O8 ${ }^{\text {v }}$ - $\mathrm{Sr} 2-\mathrm{O} 1^{\text {viii }}$ | 140.12 (7) | $\mathrm{O} 6-\mathrm{Be} 1-\mathrm{O} 4$ | 105.4 (3) |
| $\mathrm{O} 5^{\text {vi }}-\mathrm{Sr} 2-\mathrm{O} 1^{\text {viii }}$ | 100.72 (8) | $\mathrm{O} 2-\mathrm{Be} 1-\mathrm{O} 4$ | 109.1 (3) |
| $\mathrm{O} 5^{\text {vii }}$ - $\mathrm{Sr} 2-\mathrm{O} 1^{\text {viii }}$ | 136.21 (8) | O3ii-Li1-O8 | 116.9 (3) |
| $\mathrm{O} 4-\mathrm{Sr} 2-\mathrm{O} 1^{\text {viii }}$ | 79.23 (8) | O3ii-Li1- ${ }^{\text {ii }} 6^{\text {v }}$ | 103.4 (3) |
| $\mathrm{O} 8^{v}-\mathrm{Sr} 2-\mathrm{O} 3^{\text {viii }}$ | 163.40 (8) | O8-Li1- $\mathrm{O6}^{\text {v }}$ | 137.1 (4) |
| $\mathrm{O} 5^{\text {vi }}-\mathrm{Sr} 2-\mathrm{O} 3^{\text {viii }}$ | 77.37 (8) | O3ii-Li1-O7 | 109.2 (3) |
| $\mathrm{O} 5^{\text {vii }}$ - $\mathrm{Sr} 2-\mathrm{O} 3^{\text {viii }}$ | 101.86 (8) | O8-Li1-O7 | 110.9 (3) |
| $\mathrm{O} 4-\mathrm{Sr} 2-\mathrm{O} 3{ }^{\text {viii }}$ | 104.60 (8) | O6 ${ }^{\text {- }} \mathrm{Li} 11-\mathrm{O} 7$ | 65.3 (2) |
| O1 ${ }^{\text {viii- }} \mathrm{Sr} 2-\mathrm{O} 3{ }^{\text {viii }}$ | 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) $-x+2,-y+1,-z+1$.


[^0]:    Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2197).

