

Strontium magnesium borate, Sr₂Mg(BO₃)₂

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Key indicators: single-crystal X-ray study; $T = 113$ K; mean $\sigma(\text{O}-\text{B}) = 0.024$ Å; R factor = 0.065; wR factor = 0.153; data-to-parameter ratio = 9.7.

The title compound contains layers built up from isolated BO₃ triangles and MgO₆ octahedra, interleaved with SrO₉ polyhedra to form a three-dimensional framework. The Sr atom is nine-coordinate in a distorted tricapped trigonal prismatic geometry. Sr, B and one O atom have m point symmetry and Mg $2/m$ point symmetry.

Related literature

For related literature, see: Akella & Keszler (1995); Diaz & Keszler (1997); Versteegen (1974).

Experimental

Crystal data

Sr₂Mg(BO₃)₂

$M_r = 317.17$

Monoclinic, $C2/m$

$a = 9.046$ (4) Å

$b = 5.1579$ (18) Å

$c = 6.103$ (3) Å

$\beta = 118.691$ (12)°

$V = 249.81$ (19) Å³

$Z = 2$

Mo $K\alpha$ radiation

$\mu = 21.44$ mm⁻¹

$T = 113$ (2) K

0.34 × 0.22 × 0.20 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: numerical
(NUMABS; Rigaku, 2005)
 $T_{\min} = 0.052$, $T_{\max} = 0.100$

1180 measured reflections
329 independent reflections
239 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.124$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.065$

$wR(F^2) = 0.153$

$S = 1.14$

329 reflections

34 parameters

6 restraints

$\Delta\rho_{\max} = 1.93$ e Å⁻³

$\Delta\rho_{\min} = -2.76$ e Å⁻³

Table 1

Selected bond lengths (Å).

Sr1—O1 ⁱ	2.585 (8)	Mg1—O1 ⁱⁱ	2.067 (8)
Sr1—O1 ⁱⁱ	2.649 (8)	Mg1—O2 ^v	2.145 (12)
Sr1—O1 ⁱⁱⁱ	2.654 (9)	O1—B1	1.411 (14)
Sr1—O2 ^{iv}	2.716 (4)	O2—B1	1.34 (2)
Sr1—O2	2.730 (13)		

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *CrystalStructure* (Rigaku/MS, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: MG2030).

References

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supplementary materials

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Strontium magnesium borate, $\text{Sr}_2\text{Mg}(\text{BO}_3)_2$

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Comment

$\text{Sr}_2\text{Mg}(\text{BO}_3)_2$ has been examined as a luminescent host material (Verstegen, 1974; Diaz & Keszler, 1997). Although Diaz & Keszler (1997) alluded to its structure determination and provided cell parameters ($a = 9.035 \text{ \AA}$, $b = 5.146 \text{ \AA}$, $c = 6.099 \text{ \AA}$, $\beta = 118.59^\circ$), a full structure report had not appeared to date, to our knowledge. The structure determined here confirms that it is isostructural to $\text{Ba}_2\text{Mg}(\text{BO}_3)_2$, which has been previously described in detail (Akella & Keszler, 1995). Briefly, MgO_6 octahedra and BO_3 triangles are connected to form calcite-like layers which are alternately stacked with double layers of Sr atoms (Fig. 1). Each Sr atom is nine-coordinate, in a distorted tricapped trigonal prismatic geometry.

Experimental

A mixture of 0.3 mol SrCO_3 , 0.6 mol MgO , 0.6 mol, H_3BO_3 , 0.1 mol SrF_2 , and 0.7 mol LiF was heated until molten. A Pt thread was dipped into the melt, and the temperature was decreased from 1173 K to 1123 K at 5 K/day, during which time crystals grew on the Pt thread. Upon cooling to room temperature at 20 K/h, block-shaped colourless crystals with dimensions up to $25 \times 15 \times 13 \text{ mm}^3$ were obtained. The crystal used for the data collection was a fragment of the larger crystal.

Refinement

The maximum peak and deepest hole are located 1.40 \AA and 1.23 \AA , respectively, from Sr.

Figures

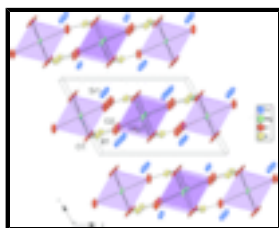


Fig. 1. $\text{Sr}_2\text{Mg}(\text{BO}_3)_2$ viewed down the [010] direction. Displacement ellipsoids are drawn at the 80% probability level.

Distrontium magnesium diborate

Crystal data

$\text{Sr}_2\text{Mg}(\text{BO}_3)_2$

$M_r = 317.17$

Monoclinic, $C2/m$

Hall symbol: $-C 2y$

$F_{000} = 292$

$D_x = 4.217 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71070 \text{ \AA}$

Cell parameters from 345 reflections

supplementary materials

$a = 9.046 (4) \text{ \AA}$	$\theta = 3.8\text{--}29.8^\circ$
$b = 5.1579 (18) \text{ \AA}$	$\mu = 21.44 \text{ mm}^{-1}$
$c = 6.103 (3) \text{ \AA}$	$T = 113 (2) \text{ K}$
$\beta = 118.691 (12)^\circ$	Prism, colourless
$V = 249.81 (19) \text{ \AA}^3$	$0.34 \times 0.22 \times 0.20 \text{ mm}$
$Z = 2$	

Data collection

Rigaku Saturn diffractometer	329 independent reflections
Radiation source: rotating anode	239 reflections with $I > 2\sigma(I)$
Monochromator: confocal	$R_{\text{int}} = 0.124$
$T = 113(2) \text{ K}$	$\theta_{\text{max}} = 27.9^\circ$
ω scans	$\theta_{\text{min}} = 3.8^\circ$
Absorption correction: numerical (NUMABS; Rigaku, 2005)	$h = -11 \rightarrow 11$
$T_{\text{min}} = 0.052$, $T_{\text{max}} = 0.100$	$k = -6 \rightarrow 6$
1180 measured reflections	$l = -8 \rightarrow 8$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.065$	$w = 1/[\sigma^2(F_o^2) + (0.0588P)^2]$
$wR(F^2) = 0.153$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.14$	$(\Delta/\sigma)_{\text{max}} < 0.001$
329 reflections	$\Delta\rho_{\text{max}} = 1.93 \text{ e \AA}^{-3}$
34 parameters	$\Delta\rho_{\text{min}} = -2.76 \text{ e \AA}^{-3}$
6 restraints	Extinction correction: SHELXL97, $F_c^* = kF_c[1 + 0.001 \times F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.015 (3)

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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Sr1	0.2895 (2)	0.0000	0.8170 (3)	0.0101 (9)
Mg1	0.5000	0.0000	0.5000	0.0100 (19)
O1	-0.0227 (11)	-0.2346 (16)	0.2319 (14)	0.013 (2)
O2	0.2305 (15)	0.0000	0.334 (2)	0.014 (3)
B1	0.065 (3)	0.0000	0.262 (4)	0.015 (5)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.0114 (11)	0.0111 (13)	0.0122 (11)	0.000	0.0092 (8)	0.000
Mg1	0.008 (5)	0.013 (5)	0.014 (4)	0.000	0.009 (4)	0.000
O1	0.017 (5)	0.016 (5)	0.016 (4)	0.004 (4)	0.015 (4)	0.001 (4)
O2	0.012 (7)	0.009 (8)	0.025 (7)	0.000	0.012 (6)	0.000
B1	0.015 (13)	0.018 (14)	0.014 (11)	0.000	0.009 (10)	0.000

Geometric parameters (\AA , $^\circ$)

Sr1—O1 ⁱ	2.585 (8)	Mg1—Sr1 ^x	3.302 (2)
Sr1—O1 ⁱⁱ	2.585 (8)	Mg1—Sr1 ^{viii}	3.5196 (16)
Sr1—O1 ⁱⁱⁱ	2.649 (8)	Mg1—Sr1 ^{xi}	3.5197 (16)
Sr1—O1 ^{iv}	2.649 (8)	Mg1—Sr1 ^{vii}	3.5197 (16)
Sr1—O1 ^v	2.654 (9)	Mg1—Sr1 ^{iv}	3.5197 (16)
Sr1—O1 ^{vi}	2.654 (8)	O1—B1	1.411 (14)
Sr1—O2 ^{vii}	2.716 (4)	O1—Mg1 ^{xii}	2.067 (8)
Sr1—O2 ^{iv}	2.716 (4)	O1—Sr1 ⁱ	2.585 (8)
Sr1—O2	2.730 (13)	O1—Sr1 ^{iv}	2.649 (8)
Sr1—B1	3.00 (2)	O1—Sr1 ^{xiii}	2.654 (8)
Sr1—B1 ⁱ	3.01 (2)	O2—B1	1.34 (2)
Sr1—B1 ^{vii}	3.036 (12)	O2—Sr1 ^{vii}	2.716 (4)
Mg1—O1 ⁱⁱⁱ	2.067 (8)	O2—Sr1 ^{iv}	2.716 (4)
Mg1—O1 ^{viii}	2.067 (8)	B1—O1 ^{xiv}	1.411 (14)
Mg1—O1 ^{iv}	2.067 (8)	B1—Sr1 ⁱ	3.01 (2)
Mg1—O1 ^{ix}	2.067 (8)	B1—Sr1 ^{vii}	3.036 (12)
Mg1—O2 ^x	2.145 (12)	B1—Sr1 ^{iv}	3.036 (12)
Mg1—O2	2.145 (12)		
O1 ⁱ —Sr1—O1 ⁱⁱ	55.8 (4)	O1 ⁱⁱⁱ —Mg1—Sr1	53.3 (2)
O1 ⁱ —Sr1—O1 ⁱⁱⁱ	119.65 (7)	O1 ^{viii} —Mg1—Sr1	126.7 (2)
O1 ⁱⁱ —Sr1—O1 ⁱⁱⁱ	168.1 (3)	O1 ^{iv} —Mg1—Sr1	53.3 (2)
O1 ⁱ —Sr1—O1 ^{iv}	168.1 (3)	O1 ^{ix} —Mg1—Sr1	126.7 (2)
O1 ⁱⁱ —Sr1—O1 ^{iv}	119.65 (7)	O2 ^x —Mg1—Sr1	124.6 (4)

supplementary materials

O1 ⁱⁱⁱ —Sr1—O1 ^{iv}	62.2 (4)	O2—Mg1—Sr1	55.4 (4)
O1 ⁱ —Sr1—O1 ^v	90.2 (3)	Sr1 ^x —Mg1—Sr1	180.0
O1 ⁱⁱ —Sr1—O1 ^v	119.07 (18)	O1 ⁱⁱⁱ —Mg1—Sr1 ^{viii}	46.7 (2)
O1 ⁱⁱⁱ —Sr1—O1 ^v	70.2 (3)	O1 ^{viii} —Mg1—Sr1 ^{viii}	73.4 (2)
O1 ^{iv} —Sr1—O1 ^v	101.2 (2)	O1 ^{iv} —Mg1—Sr1 ^{viii}	106.6 (2)
O1 ⁱ —Sr1—O1 ^{vi}	119.07 (18)	O1 ^{ix} —Mg1—Sr1 ^{viii}	133.3 (2)
O1 ⁱⁱ —Sr1—O1 ^{vi}	90.2 (3)	O2 ^x —Mg1—Sr1 ^{viii}	50.46 (11)
O1 ⁱⁱⁱ —Sr1—O1 ^{vi}	101.2 (2)	O2—Mg1—Sr1 ^{viii}	129.54 (11)
O1 ^{iv} —Sr1—O1 ^{vi}	70.2 (3)	Sr1 ^x —Mg1—Sr1 ^{viii}	80.56 (5)
O1 ^v —Sr1—O1 ^{vi}	62.1 (4)	Sr1—Mg1—Sr1 ^{viii}	99.44 (5)
O1 ⁱ —Sr1—O2 ^{vii}	67.1 (3)	O1 ⁱⁱⁱ —Mg1—Sr1 ^{xi}	106.6 (2)
O1 ⁱⁱ —Sr1—O2 ^{vii}	119.9 (3)	O1 ^{viii} —Mg1—Sr1 ^{xi}	133.3 (2)
O1 ⁱⁱⁱ —Sr1—O2 ^{vii}	53.0 (3)	O1 ^{iv} —Mg1—Sr1 ^{xi}	46.7 (2)
O1 ^{iv} —Sr1—O2 ^{vii}	112.3 (3)	O1 ^{ix} —Mg1—Sr1 ^{xi}	73.4 (2)
O1 ^v —Sr1—O2 ^{vii}	75.1 (3)	O2 ^x —Mg1—Sr1 ^{xi}	50.46 (11)
O1 ^{vi} —Sr1—O2 ^{vii}	136.2 (3)	O2—Mg1—Sr1 ^{xi}	129.54 (11)
O1 ⁱ —Sr1—O2 ^{iv}	119.9 (3)	Sr1 ^x —Mg1—Sr1 ^{xi}	80.56 (5)
O1 ⁱⁱ —Sr1—O2 ^{iv}	67.1 (3)	Sr1—Mg1—Sr1 ^{xi}	99.44 (5)
O1 ⁱⁱⁱ —Sr1—O2 ^{iv}	112.3 (3)	Sr1 ^{viii} —Mg1—Sr1 ^{xi}	94.23 (5)
O1 ^{iv} —Sr1—O2 ^{iv}	53.0 (3)	O1 ⁱⁱⁱ —Mg1—Sr1 ^{vii}	73.4 (2)
O1 ^v —Sr1—O2 ^{iv}	136.2 (3)	O1 ^{viii} —Mg1—Sr1 ^{vii}	46.7 (2)
O1 ^{vi} —Sr1—O2 ^{iv}	75.1 (3)	O1 ^{iv} —Mg1—Sr1 ^{vii}	133.3 (2)
O2 ^{vii} —Sr1—O2 ^{iv}	143.5 (5)	O1 ^{ix} —Mg1—Sr1 ^{vii}	106.6 (2)
O1 ⁱ —Sr1—O2	100.8 (3)	O2 ^x —Mg1—Sr1 ^{vii}	129.55 (11)
O1 ⁱⁱ —Sr1—O2	100.8 (3)	O2—Mg1—Sr1 ^{vii}	50.46 (11)
O1 ⁱⁱⁱ —Sr1—O2	68.4 (3)	Sr1 ^x —Mg1—Sr1 ^{vii}	99.44 (5)
O1 ^{iv} —Sr1—O2	68.4 (3)	Sr1—Mg1—Sr1 ^{vii}	80.56 (5)
O1 ^v —Sr1—O2	137.2 (3)	Sr1 ^{viii} —Mg1—Sr1 ^{vii}	85.77 (5)
O1 ^{vi} —Sr1—O2	137.2 (3)	Sr1 ^{xi} —Mg1—Sr1 ^{vii}	180.0
O2 ^{vii} —Sr1—O2	71.7 (3)	O1 ⁱⁱⁱ —Mg1—Sr1 ^{iv}	133.3 (2)
O2 ^{iv} —Sr1—O2	71.7 (3)	O1 ^{viii} —Mg1—Sr1 ^{iv}	106.6 (2)
O1 ⁱ —Sr1—B1	77.4 (4)	O1 ^{iv} —Mg1—Sr1 ^{iv}	73.4 (2)
O1 ⁱⁱ —Sr1—B1	77.4 (4)	O1 ^{ix} —Mg1—Sr1 ^{iv}	46.7 (2)
O1 ⁱⁱⁱ —Sr1—B1	90.9 (4)	O2 ^x —Mg1—Sr1 ^{iv}	129.54 (11)
O1 ^{iv} —Sr1—B1	90.9 (4)	O2—Mg1—Sr1 ^{iv}	50.46 (11)
O1 ^v —Sr1—B1	148.65 (19)	Sr1 ^x —Mg1—Sr1 ^{iv}	99.44 (5)
O1 ^{vi} —Sr1—B1	148.65 (19)	Sr1—Mg1—Sr1 ^{iv}	80.56 (5)
O2 ^{vii} —Sr1—B1	73.6 (3)	Sr1 ^{viii} —Mg1—Sr1 ^{iv}	180.0
O2 ^{iv} —Sr1—B1	73.6 (3)	Sr1 ^{xi} —Mg1—Sr1 ^{iv}	85.77 (5)
O2—Sr1—B1	26.5 (5)	Sr1 ^{vii} —Mg1—Sr1 ^{iv}	94.23 (5)
O1 ⁱ —Sr1—B1 ⁱ	27.94 (19)	B1—O1—Mg1 ^{xii}	128.9 (10)

O1 ⁱⁱ —Sr1—B1 ⁱ	27.94 (19)	B1—O1—Sr1 ⁱ	92.9 (9)
O1 ⁱⁱⁱ —Sr1—B1 ⁱ	145.9 (2)	Mg1 ^{xii} —O1—Sr1 ⁱ	97.7 (3)
O1 ^{iv} —Sr1—B1 ⁱ	145.9 (2)	B1—O1—Sr1 ^{iv}	91.6 (9)
O1 ^v —Sr1—B1 ⁱ	107.4 (4)	Mg1 ^{xii} —O1—Sr1 ^{iv}	88.0 (3)
O1 ^{vi} —Sr1—B1 ⁱ	107.4 (4)	Sr1 ⁱ —O1—Sr1 ^{iv}	168.1 (3)
O2 ^{vii} —Sr1—B1 ⁱ	93.1 (3)	B1—O1—Sr1 ^{xiii}	129.1 (10)
O2 ^{iv} —Sr1—B1 ⁱ	93.1 (3)	Mg1 ^{xii} —O1—Sr1 ^{xiii}	100.9 (3)
O2—Sr1—B1 ⁱ	100.7 (5)	Sr1 ⁱ —O1—Sr1 ^{xiii}	89.8 (3)
B1—Sr1—B1 ⁱ	74.2 (7)	Sr1 ^{iv} —O1—Sr1 ^{xiii}	78.8 (2)
O1 ⁱ —Sr1—B1 ^{vii}	92.0 (4)	B1—O2—Mg1	172.3 (13)
O1 ⁱⁱ —Sr1—B1 ^{vii}	146.1 (4)	B1—O2—Sr1 ^{vii}	90.4 (4)
O1 ⁱⁱⁱ —Sr1—B1 ^{vii}	27.7 (4)	Mg1—O2—Sr1 ^{vii}	92.0 (3)
O1 ^{iv} —Sr1—B1 ^{vii}	89.6 (4)	B1—O2—Sr1 ^{iv}	90.4 (4)
O1 ^v —Sr1—B1 ^{vii}	65.6 (4)	Mg1—O2—Sr1 ^{iv}	92.0 (3)
O1 ^{vi} —Sr1—B1 ^{vii}	117.6 (5)	Sr1 ^{vii} —O2—Sr1 ^{iv}	143.5 (5)
O2 ^{vii} —Sr1—B1 ^{vii}	26.2 (4)	B1—O2—Sr1	87.9 (11)
O2 ^{iv} —Sr1—B1 ^{vii}	135.7 (4)	Mg1—O2—Sr1	84.4 (4)
O2—Sr1—B1 ^{vii}	72.7 (4)	Sr1 ^{vii} —O2—Sr1	108.3 (3)
B1—Sr1—B1 ^{vii}	86.0 (5)	Sr1 ^{iv} —O2—Sr1	108.3 (3)
B1 ⁱ —Sr1—B1 ^{vii}	118.9 (4)	O2—B1—O1 ^{xiv}	120.9 (9)
O1 ⁱⁱⁱ —Mg1—O1 ^{viii}	97.0 (4)	O2—B1—O1	120.9 (9)
O1 ⁱⁱⁱ —Mg1—O1 ^{iv}	83.0 (4)	O1 ^{xiv} —B1—O1	118.0 (17)
O1 ^{viii} —Mg1—O1 ^{iv}	179.998 (1)	O2—B1—Sr1	65.6 (10)
O1 ⁱⁱⁱ —Mg1—O1 ^{ix}	180.0	O1 ^{xiv} —B1—Sr1	100.5 (9)
O1 ^{viii} —Mg1—O1 ^{ix}	83.0 (4)	O1—B1—Sr1	100.5 (9)
O1 ^{iv} —Mg1—O1 ^{ix}	97.0 (4)	O2—B1—Sr1 ⁱ	171.4 (14)
O1 ⁱⁱⁱ —Mg1—O2 ^x	88.2 (4)	O1 ^{xiv} —B1—Sr1 ⁱ	59.1 (9)
O1 ^{viii} —Mg1—O2 ^x	91.8 (4)	O1—B1—Sr1 ⁱ	59.1 (9)
O1 ^{iv} —Mg1—O2 ^x	88.2 (4)	Sr1—B1—Sr1 ⁱ	105.8 (7)
O1 ^{ix} —Mg1—O2 ^x	91.8 (4)	O2—B1—Sr1 ^{vii}	63.4 (5)
O1 ⁱⁱⁱ —Mg1—O2	91.8 (4)	O1 ^{xiv} —B1—Sr1 ^{vii}	60.7 (6)
O1 ^{viii} —Mg1—O2	88.2 (4)	O1—B1—Sr1 ^{vii}	165.3 (13)
O1 ^{iv} —Mg1—O2	91.8 (4)	Sr1—B1—Sr1 ^{vii}	94.0 (5)
O1 ^{ix} —Mg1—O2	88.2 (4)	Sr1 ⁱ —B1—Sr1 ^{vii}	118.9 (4)
O2 ^x —Mg1—O2	180.0	O2—B1—Sr1 ^{iv}	63.4 (5)
O1 ⁱⁱⁱ —Mg1—Sr1 ^x	126.7 (2)	O1 ^{xiv} —B1—Sr1 ^{iv}	165.3 (13)
O1 ^{viii} —Mg1—Sr1 ^x	53.3 (2)	O1—B1—Sr1 ^{iv}	60.7 (6)
O1 ^{iv} —Mg1—Sr1 ^x	126.7 (2)	Sr1—B1—Sr1 ^{iv}	94.0 (5)
O1 ^{ix} —Mg1—Sr1 ^x	53.3 (2)	Sr1 ⁱ —B1—Sr1 ^{iv}	118.9 (4)
O2 ^x —Mg1—Sr1 ^x	55.4 (4)	Sr1 ^{vii} —B1—Sr1 ^{iv}	116.3 (7)
O2—Mg1—Sr1 ^x	124.6 (4)		

supplementary materials

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

Fig. 1

