

Ba₁₁La₄Br₃₄: a new barium lanthanum bromideYetta Eagleman,^{a*} Guang Wu,^b Gautam Gundiah,^a Edith Bourret-Courchesne^a and Stephen Derenzo^a^aLawrence Berkeley National Laboratory, One Cyclotron Rd, Berkeley, CA 94720, USA, and ^bDepartment of Chemistry and Biochemistry, University of California Santa Barbara, Santa Barbara, CA 93106, USA

Correspondence e-mail: ydeagleman@lbl.gov

Received 25 June 2011; accepted 13 September 2011

Key indicators: single-crystal X-ray study; $T = 150$ K; mean $\sigma(\text{La}-\text{Br}) = 0.002$ Å; disorder in main residue; R factor = 0.049; wR factor = 0.118; data-to-parameter ratio = 26.8.

The structure of the title compound, barium lanthanum bromide (11/4/34), can be derived from the fluorite structure. The asymmetric unit contains two Ba sites (one with site symmetry $4/m..$), one La site (site symmetry $4..$), one mixed-occupied Ba and La site (ratio 1:1, site symmetry $m..$) and six Br sites (one with site symmetry $\backslash=4..$, one with $2..$, one with $m..$, the latter being disordered over two positions with a 0.86:0.14 ratio). The fundamental building units of the structure are edge-sharing polyhedral clusters made up of Ba and La bromide clusters interconnected to BaBr₈ square prisms and BaBr₁₀ groups.

Related literature

Alkaline earth halides (Cherepy *et al.*, 2008), rare earth halides (van Loef *et al.*, 2002; Glodo *et al.*, 2008), and compounds based on such binaries (Bourret-Courchesne *et al.*, 2009, 2010) are efficient scintillators when doped with divalent europium or trivalent cerium. For a detailed study of the luminescence properties of the title compound, see: Eagleman *et al.* (2011). Similar structure types to that of the title compound have been observed in ternary alkaline earth and rare earth fluorides (Bevan *et al.*, 1980, 1982; Burns *et al.*, 1968), chlorides (Liu & Eick, 1988, 1999; Löchner & Blachnik, 2011; Meyer & Masselmann, 1998), and bromides (Masselmann & Meyer, 1999; Liu & Eick, 1989) and in mixed valent rare earth halides (Druding & Corbett 1961; Liu & Eick, 1991). For structural details of simple and complex halides, see: Meyer & Wickleder (2000). For structural details of these types of superstructures, see: Meyer & Masselmann (1998).

Experimental*Crystal data*

Ba ₁₁ La ₄ Br ₃₄	$Z = 2$
$M_r = 4783.10$	Mo $K\alpha$ radiation
Tetragonal, $I4/m$	$\mu = 30.05 \text{ mm}^{-1}$
$a = 11.909$ (3) Å	$T = 150$ K
$c = 22.888$ (5) Å	$0.25 \times 0.15 \times 0.1 \text{ mm}$
$V = 3246.2$ (10) Å ³	

Data collection

Bruker SMART1000 CCD area-detector diffractometer	12169 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1687 independent reflections
$T_{\min} = 0.141$, $T_{\max} = 0.403$	1193 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.168$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.049$	63 parameters
$wR(F^2) = 0.118$	$(\Delta/\sigma)_{\text{max}} = 0.100$
$S = 1.00$	$\Delta\rho_{\text{max}} = 5.72 \text{ e } \text{Å}^{-3}$
1687 reflections	$\Delta\rho_{\text{min}} = -3.31 \text{ e } \text{Å}^{-3}$

Data collection: SMART (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg, 2005); software used to prepare material for publication: publCIF (Westrip, 2010).

This work was supported by the US Department of Homeland Security and carried out at the Lawrence Berkeley National Laboratory under U.S. Department of Energy Contract No. AC02-05CH11231.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RU2009).

References

- Bevan, D. J. M., Greis, O. & Strähle, J. (1980). *Acta Cryst.* **A36**, 889–890.
 Bevan, D. J. M., Strähle, J. & Greis, O. (1982). *J. Solid State Chem.* **44**, 75–81.
 Bourret-Courchesne, E., Bizarri, G., Borade, R., Yan, Z., Hanrahan, S. M., Gundiah, G., Chaudhry, A., Canning, A. & Derenzo, S. E. (2009). *Nucl. Instrum. Methods Phys. Res. Sect. A*, **612**, 138–142.
 Bourret-Courchesne, E., Bizarri, G., Hanrahan, S. M., Yan, Z. & Derenzo, S. E. (2010). *Nucl. Instrum. Methods Phys. Res. Sect. A*, **613**, 95–97.
 Brandenburg, K. (2005). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
 Bruker (2007). *SMART* and *SAINTE*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Burns, J. H., Ellison, R. D. & Levy, H. A. (1968). *Acta Cryst.* **B24**, 230–237.
 Cherepy, N. J., *et al.* (2008). *Appl. Phys. Lett.* **92**, 083508.
 Druding, L. F. & Corbett, J. D. (1961). *J. Am. Chem. Soc.* **83**, 2462–2467.
 Eagleman, Y., Bourret-Courchesne, E. & Derenzo, S. E. (2011). In preparation.
 Glodo, J., van Loef, E. V. D., Higgins, W. M. & Shah, K. S. (2008). *IEEE Trans. Nucl. Sci.* **55**, 1496–1500.
 Liu, G. & Eick, H. A. (1988). *Inorg. Chem.* **27**, 2161–2163.
 Liu, G. & Eick, H. A. (1989). *J. Less Common Met.* **149**, 47–53.
 Liu, G. & Eick, H. A. (1991). *J. Solid State Chem.* **95**, 99–110.
 Liu, G. & Eick, H. A. (1999). *J. Solid State Chem.* **146**, 124–128.
 Löchner, U. & Blachnik, R. (2011). *Z. Kristallogr.* **183**, 207–212.
 Loef, E. V. D. van, Dorenbos, P., van Eijk, C. W. E., Kramer, K. W. & Gudiel, H. U. (2002). *Nucl. Instrum. Methods Phys. Res. Sect. A*, **486**, 254–258.
 Masselmann, S. & Meyer, G. (1999). *Z. Anorg. Allg. Chem.* **625**, 1–2.
 Meyer, G. & Masselmann, S. (1998). *Chem. Mater.* **10**, 2994–3004.

Meyer, G. & Wickleder, M. S. (2000). *Simple and Complex Halides*, pp. 53–129. Amsterdam: Elsevier.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supplementary materials

Acta Cryst. (2011). E67, i53-i54 [doi:10.1107/S1600536811037354]

Ba₁₁La₄Br₃₄: a new barium lanthanum bromide

Y. Eagleman, G. Wu, G. Gundiah, E. Bourret-Courchesne and S. Derenzo

Comment

Alkaline earth halides (Cherepy *et al.* 2008), rare earth halides (van Loef *et al.* 2002; Glodo *et al.* 2008), and compounds based on such binaries (Bourret-Courchesne *et al.* 2010; Bourret-Courchesne *et al.* 2009) are efficient scintillators when doped with divalent europium or trivalent cerium. In an effort to discover new scintillators, a new mixed alkaline earth – rare earth bromide, Ba₁₁La₄Br₃₄, has been obtained. When doped with either aforementioned activator this material displays high luminosities making them attractive as a promising scintillators. A detailed study of the luminescence properties will be presented in a future publication (Eagleman *et al.* 2011).

Ba₁₁La₄Br₃₄ has a three dimensional tetragonal superstructure which can be derived from the fluorite structure. Similar structure types have been observed in ternary alkaline earth and rare earth fluorides (Bevan *et al.* 1980; Bevan *et al.* 1982; Burns *et al.* 1968), chlorides (Liu & Eick 1988; Liu & Eick 1999; Löchner & Blachnik 2011; Meyer & Masselmann 1998), and bromides (Masselmann & Meyer 1999; Liu & Eick 1989) and in mixed valent rare earth halides (Druding & Corbett 1961; Liu & Eick 1991). These superstructures follow the general formula of M_nX_{2n+5} forming either a rhombohedral (n = 14) or tetragonal (n = 15) structure and consists of [M₆ZX₃₆] polyhedral clusters (Meyer & Wickleder 2000). There is some confusion about whether the interstitial atom, Z, is a halide or an oxide.

In Ba₁₁La₄Br₃₄, n = 15 following the M₁₅X₃₅ = MZX₃₄ general formula. There are six bromine sites, two barium sites (Ba1 & Ba2), one site that is occupied by Ba(3) and La(1) atoms, and one lanthanum site (La2). Each Ba1 is coordinated to 8 bromines in square prism arrangements and have 4/m site symmetry and Ba—Br distances of 3.2521 (12) Å. Each Ba(2) is coordinated to 10 bromines and have 1 symmetry and Ba—Br bond distances ranging from 3.2632 (12) – 3.7696 (13) Å. The Ba(3) and La(1) cations occupy the same site at 50% occupancy each. They are coordinated to 10 bromines and have m symmetry and bond distances ranging from 2.9708 (3) – 3.4805 (14) Å. Each La(2) is coordinated to 8 bromines in square antiprism arrangement and have 4 symmetry and La—Br distances of 3.0833 (15) Å (4x) and 3.1052 (15) Å (4x).

Typically, [M₆ZX₃₆] polyhedral clusters consist of six corner sharing MX₈ square antiprisms whose metals are arranged in an octahedral geometry and the Z atom occupies the octahedral site. In the case of Ba₁₁La₄Br₃₄, the clusters consist of four edge sharing Ba(3)/La(1)Br₁₀ groups and capped by two La(2)Br₈ square antiprisms having a [(Ba(3)/La(1))₄La(2)₂Br₁₆Br_{40/2}] formulation, shown in Figure 1. The interstitial atom, Z, is not present. The clusters are connected *via* four outer edges parallel to the (100) and (010) axis, Figure 2. The overall structure is made three dimensional by the interconnectivity of the clusters to Ba(1) and Ba(2) cations, Figure 3.

Experimental

Small crystals of Ba₁₁La₄Br₃₄ were formed from solid state reaction of a stoichiometric mixture of barium bromide and lanthanum bromide. The reactants were sealed in an evacuated quartz ampoule, heated at 1000 °C for 10 hr, and then slow cooled to room temperature at a rate of 0.5 °C/hr.

Refinement

(type here to add refinement details)

Figures

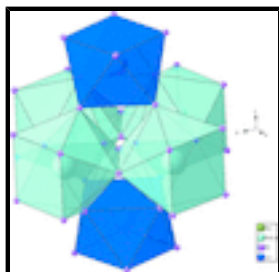


Fig. 1. Representation of $[\{(Ba/La)_6La_4Br_{36}\}]$ polyhedral cluster

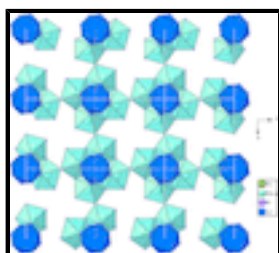


Fig. 2. Connectivity of $[\{(Ba/La)_6La_4Br_{36}\}]$ polyhedral cluster along a-b plane

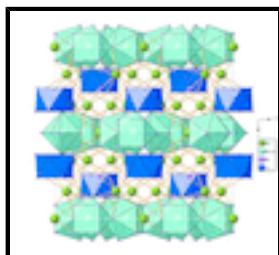


Fig. 3. Structure of $Ba_{11}La_4Br_{34}$ viewing along (010) axis

undecabarium tetralanthanum tetratricontabromide

Crystal data

$Ba_{11}La_4Br_{34}$

$M_r = 4783.10$

Tetragonal, $I4/m$

$a = 11.909(3) \text{ \AA}$

$c = 22.888(5) \text{ \AA}$

$V = 3246.2(10) \text{ \AA}^3$

$Z = 2$

$F(000) = 4068$

$D_x = 4.894 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 119 reflections

$\theta = 12.9\text{--}37.1^\circ$

$\mu = 30.05 \text{ mm}^{-1}$

$T = 150 \text{ K}$

Block, colorless

$0.25 \times 0.15 \times 0.1 \text{ mm}$

Data collection

Bruker SMART1000 CCD area-detector
diffractometer

1687 independent reflections

Radiation source: fine-focus sealed tube
 graphite
 ω scans
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.141$, $T_{\max} = 0.403$
 12169 measured reflections

1193 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.168$
 $\theta_{\max} = 26.4^\circ$, $\theta_{\min} = 1.9^\circ$
 $h = -14 \rightarrow 14$
 $k = -14 \rightarrow 14$
 $l = -28 \rightarrow 28$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.049$
 $wR(F^2) = 0.118$
 $S = 1.00$
 1687 reflections
 63 parameters

0 restraints
 Primary atom site location: structure-invariant direct methods
 Secondary atom site location: difference Fourier map
 $w = 1/[\sigma^2(F_o^2) + (0.0501P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.100$
 $\Delta\rho_{\max} = 5.72 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -3.31 \text{ e } \text{\AA}^{-3}$

Special details

Experimental. Disclaimer: This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor The Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or The Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or The Regents of the University of California.

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Ba1	1.0000	1.0000	0.0000	0.0070 (5)	
Ba2	1.13364 (7)	0.68518 (6)	0.15892 (3)	0.0095 (2)	
Ba3	0.81444 (11)	0.60582 (10)	0.0000	0.0184 (3)	0.50

supplementary materials

Br1	1.20905 (10)	0.91792 (11)	0.08083 (5)	0.0103 (3)	
Br2	1.0000	0.5000	0.2500	0.0113 (6)	
Br3	1.0000	0.5000	0.08013 (7)	0.0086 (4)	
Br4	0.90821 (10)	0.80123 (10)	0.23802 (5)	0.0100 (3)	
Br5	1.21627 (12)	1.07440 (11)	0.37484 (6)	0.0190 (4)	
Br6A	0.7919 (2)	0.3517 (2)	0.0000	0.0264 (6)	0.86
Br6B	0.5329 (13)	0.5572 (11)	0.0000	0.0190 (4)	0.14
La1	0.81444 (11)	0.60582 (10)	0.0000	0.0184 (3)	0.50
La2	1.0000	1.0000	0.31170 (6)	0.0063 (3)	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.0081 (7)	0.0081 (7)	0.0046 (10)	0.000	0.000	0.000
Ba2	0.0103 (4)	0.0073 (4)	0.0110 (4)	-0.0016 (3)	-0.0052 (3)	-0.0002 (3)
Ba3	0.0373 (8)	0.0135 (6)	0.0045 (6)	0.0125 (6)	0.000	0.000
Br1	0.0110 (6)	0.0108 (7)	0.0092 (7)	-0.0022 (5)	-0.0023 (5)	-0.0005 (5)
Br2	0.0113 (8)	0.0113 (8)	0.0114 (13)	0.000	0.000	0.000
Br3	0.0119 (9)	0.0056 (8)	0.0084 (9)	-0.0004 (7)	0.000	0.000
Br4	0.0084 (6)	0.0114 (7)	0.0101 (7)	0.0008 (5)	-0.0016 (5)	0.0013 (5)
Br5	0.0190 (7)	0.0145 (7)	0.0237 (8)	-0.0003 (6)	-0.0103 (6)	-0.0024 (6)
Br6A	0.0470 (16)	0.0229 (13)	0.0092 (12)	-0.0234 (12)	0.000	0.000
Br6B	0.0190 (7)	0.0145 (7)	0.0237 (8)	-0.0003 (6)	-0.0103 (6)	-0.0024 (6)
La1	0.0373 (8)	0.0135 (6)	0.0045 (6)	0.0125 (6)	0.000	0.000
La2	0.0048 (5)	0.0048 (5)	0.0093 (8)	0.000	0.000	0.000

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

Ba1—Br1 ⁱ	3.2521 (12)	Br1—Ba2 ⁱⁱⁱ	3.3737 (14)
Ba1—Br1 ⁱⁱ	3.2521 (12)	Br2—Ba2 ^{xvi}	3.4266 (8)
Ba1—Br1 ⁱⁱⁱ	3.2521 (12)	Br2—Ba2 ^{viii}	3.4266 (9)
Ba1—Br1	3.2521 (13)	Br2—Ba2 ^{xvii}	3.4266 (9)
Ba1—Br1 ^{iv}	3.2521 (13)	Br3—La1 ^{xi}	3.1361 (14)
Ba1—Br1 ^v	3.2521 (13)	Br3—Ba3 ^{xi}	3.1361 (14)
Ba1—Br1 ^{vi}	3.2521 (13)	Br3—Ba2 ^{xvi}	3.2633 (12)
Ba1—Br1 ^{vii}	3.2521 (12)	Br4—La2	3.1052 (14)
Ba2—Br3	3.2633 (12)	Br4—Ba2 ^{xvii}	3.2839 (15)
Ba2—Br4 ^{viii}	3.2839 (15)	Br4—Ba2 ⁱⁱ	3.3067 (15)
Ba2—Br4 ⁱⁱⁱ	3.3067 (14)	Br5—La2	3.0833 (15)
Ba2—Br1 ⁱⁱ	3.3737 (15)	Br5—La1 ^{xviii}	3.1167 (16)
Ba2—Br1	3.4182 (15)	Br5—Ba3 ^{xviii}	3.1167 (16)
Ba2—Br2	3.4266 (8)	Br5—Ba2 ^{xix}	3.5810 (16)
Ba2—Br4	3.5207 (15)	Br5—Ba2 ^x	3.6536 (16)
Ba2—Br5 ^{ix}	3.5810 (17)	Br6A—La1 ^{xv}	2.971 (3)
Ba2—Br5 ^x	3.6536 (16)	Br6A—Ba3 ^{xv}	2.971 (3)

Ba2—Br6A ^{xi}	3.7696 (13)	Br6A—Ba2 ^{xvi}	3.7696 (13)
Ba3—Br6A ^{xii}	2.971 (3)	Br6A—Ba2 ^{xi}	3.7696 (13)
Ba3—Br6A	3.038 (3)	Br6B—Br6B ^{xii}	1.111 (18)
Ba3—Br5 ^{xiii}	3.1167 (16)	Br6B—Br6B ^{xv}	1.111 (18)
Ba3—Br5 ^{xiv}	3.1167 (16)	Br6B—Br6B ^{xx}	1.57 (3)
Ba3—Br1 ⁱⁱ	3.1308 (16)	Br6B—La1 ^{xii}	3.480 (14)
Ba3—Br1 ⁱ	3.1308 (16)	Br6B—Ba3 ^{xii}	3.480 (14)
Ba3—Br3	3.1361 (14)	La2—Br5 ^{vi}	3.0833 (15)
Ba3—Br3 ^{xi}	3.1361 (14)	La2—Br5 ⁱⁱ	3.0833 (15)
Ba3—Br6B	3.402 (15)	La2—Br5 ⁱⁱⁱ	3.0833 (15)
Ba3—Br6B ^{xv}	3.480 (14)	La2—Br4 ⁱⁱⁱ	3.1052 (15)
Br1—La1 ⁱⁱⁱ	3.1308 (16)	La2—Br4 ⁱⁱ	3.1052 (15)
Br1—Ba3 ⁱⁱⁱ	3.1308 (16)	La2—Br4 ^{vi}	3.1052 (15)
Br1 ⁱ —Ba1—Br1 ⁱⁱ	69.34 (5)	Br3—Ba3—Br6B	128.76 (15)
Br1 ⁱ —Ba1—Br1 ⁱⁱⁱ	180.00 (4)	Br3 ^{xi} —Ba3—Br6B	128.76 (15)
Br1 ⁱⁱ —Ba1—Br1 ⁱⁱⁱ	110.66 (5)	Br6A ^{xii} —Ba3—Br6B ^{xv}	76.6 (2)
Br1 ⁱ —Ba1—Br1	108.88 (2)	Br6A—Ba3—Br6B ^{xv}	56.6 (2)
Br1 ⁱⁱ —Ba1—Br1	71.12 (2)	Br5 ^{xiii} —Ba3—Br6B ^{xv}	67.22 (4)
Br1 ⁱⁱⁱ —Ba1—Br1	71.12 (2)	Br5 ^{xiv} —Ba3—Br6B ^{xv}	67.22 (4)
Br1 ⁱ —Ba1—Br1 ^{iv}	71.12 (2)	Br1 ⁱⁱ —Ba3—Br6B ^{xv}	132.90 (14)
Br1 ⁱⁱ —Ba1—Br1 ^{iv}	108.88 (2)	Br1 ⁱ —Ba3—Br6B ^{xv}	132.90 (14)
Br1 ⁱⁱⁱ —Ba1—Br1 ^{iv}	108.88 (2)	Br3—Ba3—Br6B ^{xv}	115.43 (18)
Br1—Ba1—Br1 ^{iv}	180.0	Br3 ^{xi} —Ba3—Br6B ^{xv}	115.43 (18)
Br1 ⁱ —Ba1—Br1 ^v	71.12 (2)	Br6B—Ba3—Br6B ^{xv}	18.5 (3)
Br1 ⁱⁱ —Ba1—Br1 ^v	108.88 (2)	La1 ⁱⁱⁱ —Br1—Ba3 ⁱⁱⁱ	0.00 (4)
Br1 ⁱⁱⁱ —Ba1—Br1 ^v	108.88 (2)	La1 ⁱⁱⁱ —Br1—Ba1	108.74 (4)
Br1—Ba1—Br1 ^v	69.34 (5)	Ba3 ⁱⁱⁱ —Br1—Ba1	108.74 (4)
Br1 ^{iv} —Ba1—Br1 ^v	110.66 (5)	La1 ⁱⁱⁱ —Br1—Ba2 ⁱⁱⁱ	110.48 (4)
Br1 ⁱ —Ba1—Br1 ^{vi}	108.88 (2)	Ba3 ⁱⁱⁱ —Br1—Ba2 ⁱⁱⁱ	110.48 (4)
Br1 ⁱⁱ —Ba1—Br1 ^{vi}	71.12 (2)	Ba1—Br1—Ba2 ⁱⁱⁱ	111.00 (4)
Br1 ⁱⁱⁱ —Ba1—Br1 ^{vi}	71.12 (2)	La1 ⁱⁱⁱ —Br1—Ba2	100.07 (4)
Br1—Ba1—Br1 ^{vi}	110.66 (5)	Ba3 ⁱⁱⁱ —Br1—Ba2	100.07 (4)
Br1 ^{iv} —Ba1—Br1 ^{vi}	69.34 (5)	Ba1—Br1—Ba2	109.88 (4)
Br1 ^v —Ba1—Br1 ^{vi}	180.0	Ba2 ⁱⁱⁱ —Br1—Ba2	116.01 (4)
Br1 ⁱ —Ba1—Br1 ^{vii}	110.66 (5)	Ba2 ^{xvi} —Br2—Ba2 ^{viii}	111.721 (15)
Br1 ⁱⁱ —Ba1—Br1 ^{vii}	180.00 (4)	Ba2 ^{xvi} —Br2—Ba2	105.06 (3)
Br1 ⁱⁱⁱ —Ba1—Br1 ^{vii}	69.34 (5)	Ba2 ^{viii} —Br2—Ba2	111.721 (18)
Br1—Ba1—Br1 ^{vii}	108.88 (2)	Ba2 ^{xvi} —Br2—Ba2 ^{xvii}	111.721 (18)
Br1 ^{iv} —Ba1—Br1 ^{vii}	71.12 (2)	Ba2 ^{viii} —Br2—Ba2 ^{xvii}	105.06 (3)
Br1 ^v —Ba1—Br1 ^{vii}	71.12 (2)	Ba2—Br2—Ba2 ^{xvii}	111.721 (15)

supplementary materials

Br1 ^{vi} —Ba1—Br1 ^{vii}	108.88 (2)	Ba3—Br3—La1 ^{xi}	108.43 (6)
Br3—Ba2—Br4 ^{viii}	117.68 (4)	Ba3—Br3—Ba3 ^{xi}	108.43 (6)
Br3—Ba2—Br4 ⁱⁱⁱ	163.70 (4)	La1 ^{xi} —Br3—Ba3 ^{xi}	0.00 (4)
Br4 ^{viii} —Ba2—Br4 ⁱⁱⁱ	74.71 (4)	Ba3—Br3—Ba2	113.28 (2)
Br3—Ba2—Br1 ⁱⁱ	65.68 (3)	La1 ^{xi} —Br3—Ba2	104.54 (3)
Br4 ^{viii} —Ba2—Br1 ⁱⁱ	165.89 (4)	Ba3 ^{xi} —Br3—Ba2	104.54 (3)
Br4 ⁱⁱⁱ —Ba2—Br1 ⁱⁱ	99.72 (4)	Ba3—Br3—Ba2 ^{xvi}	104.54 (3)
Br3—Ba2—Br1	112.77 (4)	La1 ^{xi} —Br3—Ba2 ^{xvi}	113.28 (2)
Br4 ^{viii} —Ba2—Br1	119.38 (4)	Ba3 ^{xi} —Br3—Ba2 ^{xvi}	113.28 (2)
Br4 ⁱⁱⁱ —Ba2—Br1	64.74 (4)	Ba2—Br3—Ba2 ^{xvi}	112.90 (6)
Br1 ⁱⁱ —Ba2—Br1	67.68 (4)	La2—Br4—Ba2 ^{xvii}	101.10 (4)
Br3—Ba2—Br2	71.02 (3)	La2—Br4—Ba2 ⁱⁱ	113.66 (4)
Br4 ^{viii} —Ba2—Br2	68.12 (3)	Ba2 ^{xvii} —Br4—Ba2 ⁱⁱ	105.29 (4)
Br4 ⁱⁱⁱ —Ba2—Br2	107.03 (3)	La2—Br4—Ba2	108.06 (4)
Br1 ⁱⁱ —Ba2—Br2	102.06 (3)	Ba2 ^{xvii} —Br4—Ba2	112.89 (4)
Br1—Ba2—Br2	164.16 (3)	Ba2 ⁱⁱ —Br4—Ba2	115.03 (4)
Br3—Ba2—Br4	100.23 (3)	La2—Br5—La1 ^{xviii}	141.14 (6)
Br4 ^{viii} —Ba2—Br4	103.12 (3)	La2—Br5—Ba3 ^{xviii}	141.14 (6)
Br4 ⁱⁱⁱ —Ba2—Br4	65.29 (4)	La1 ^{xviii} —Br5—Ba3 ^{xviii}	0.0
Br1 ⁱⁱ —Ba2—Br4	62.95 (4)	La2—Br5—Ba2 ^{xix}	95.25 (4)
Br1—Ba2—Br4	98.68 (4)	La1 ^{xviii} —Br5—Ba2 ^{xix}	96.92 (4)
Br2—Ba2—Br4	65.52 (3)	Ba3 ^{xviii} —Br5—Ba2 ^{xix}	96.92 (4)
Br3—Ba2—Br5 ^{ix}	115.10 (4)	La2—Br5—Ba2 ^x	93.81 (4)
Br4 ^{viii} —Ba2—Br5 ^{ix}	66.41 (4)	La1 ^{xviii} —Br5—Ba2 ^x	96.46 (4)
Br4 ⁱⁱⁱ —Ba2—Br5 ^{ix}	78.89 (4)	Ba3 ^{xviii} —Br5—Ba2 ^x	96.46 (4)
Br1 ⁱⁱ —Ba2—Br5 ^{ix}	125.90 (4)	Ba2 ^{xix} —Br5—Ba2 ^x	145.74 (5)
Br1—Ba2—Br5 ^{ix}	63.14 (3)	La1 ^{xv} —Br6A—Ba3 ^{xv}	0.00 (5)
Br2—Ba2—Br5 ^{ix}	130.45 (3)	La1 ^{xv} —Br6A—Ba3	136.81 (11)
Br4—Ba2—Br5 ^{ix}	144.17 (4)	Ba3 ^{xv} —Br6A—Ba3	136.81 (11)
Br3—Ba2—Br5 ^x	63.25 (3)	La1 ^{xv} —Br6A—Ba2 ^{xvi}	95.61 (4)
Br4 ^{viii} —Ba2—Br5 ^x	64.40 (3)	Ba3 ^{xv} —Br6A—Ba2 ^{xvi}	95.61 (4)
Br4 ⁱⁱⁱ —Ba2—Br5 ^x	132.90 (4)	Ba3—Br6A—Ba2 ^{xvi}	95.48 (4)
Br1 ⁱⁱ —Ba2—Br5 ^x	125.20 (4)	La1 ^{xv} —Br6A—Ba2 ^{xi}	95.61 (4)
Br1—Ba2—Br5 ^x	116.55 (4)	Ba3 ^{xv} —Br6A—Ba2 ^{xi}	95.61 (4)
Br2—Ba2—Br5 ^x	79.13 (3)	Ba3—Br6A—Ba2 ^{xi}	95.48 (4)
Br4—Ba2—Br5 ^x	144.49 (4)	Ba2 ^{xvi} —Br6A—Ba2 ^{xi}	149.57 (9)
Br5 ^{ix} —Ba2—Br5 ^x	64.33 (5)	Br6B ^{xii} —Br6B—Br6B ^{xv}	90.000 (7)
Br3—Ba2—Br6A ^{xi}	60.17 (4)	Br6B ^{xii} —Br6B—Br6B ^{xx}	45.000 (3)
Br4 ^{viii} —Ba2—Br6A ^{xi}	120.71 (6)	Br6B ^{xv} —Br6B—Br6B ^{xx}	45.000 (9)
Br4 ⁱⁱⁱ —Ba2—Br6A ^{xi}	124.53 (5)	Br6B ^{xii} —Br6B—Ba3	174.7 (13)
Br1 ⁱⁱ —Ba2—Br6A ^{xi}	73.22 (5)	Br6B ^{xv} —Br6B—Ba3	84.7 (13)

Br1—Ba2—Br6A ^{xi}	61.85 (4)	Br6B ^{xx} —Br6B—Ba3	129.7 (13)
Br2—Ba2—Br6A ^{xi}	128.40 (4)	Br6B ^{xii} —Br6B—La1 ^{xii}	76.8 (13)
Br4—Ba2—Br6A ^{xi}	136.16 (5)	Br6B ^{xv} —Br6B—La1 ^{xii}	166.8 (13)
Br5 ^{ix} —Ba2—Br6A ^{xi}	64.89 (5)	Br6B ^{xx} —Br6B—La1 ^{xii}	121.8 (13)
Br5 ^x —Ba2—Br6A ^{xi}	65.31 (5)	Ba3—Br6B—La1 ^{xii}	108.5 (3)
Br6A ^{xii} —Ba3—Br6A	133.19 (11)	Br6B ^{xii} —Br6B—Ba3 ^{xii}	76.8 (13)
Br6A ^{xii} —Ba3—Br5 ^{xiii}	80.78 (4)	Br6B ^{xv} —Br6B—Ba3 ^{xii}	166.8 (13)
Br6A—Ba3—Br5 ^{xiii}	81.22 (4)	Br6B ^{xx} —Br6B—Ba3 ^{xii}	121.8 (13)
Br6A ^{xii} —Ba3—Br5 ^{xiv}	80.78 (4)	Ba3—Br6B—Ba3 ^{xii}	108.5 (3)
Br6A—Ba3—Br5 ^{xiv}	81.22 (4)	La1 ^{xii} —Br6B—Ba3 ^{xii}	0.00 (3)
Br5 ^{xiii} —Ba3—Br5 ^{xiv}	133.61 (7)	Br5—La2—Br5 ^{vi}	124.10 (7)
Br6A ^{xii} —Ba3—Br1 ⁱⁱ	74.74 (6)	Br5—La2—Br5 ⁱⁱ	77.31 (3)
Br6A—Ba3—Br1 ⁱⁱ	137.40 (4)	Br5 ^{vi} —La2—Br5 ⁱⁱ	77.31 (3)
Br5 ^{xiii} —Ba3—Br1 ⁱⁱ	140.84 (5)	Br5—La2—Br5 ⁱⁱⁱ	77.31 (3)
Br5 ^{xiv} —Ba3—Br1 ⁱⁱ	71.89 (4)	Br5 ^{vi} —La2—Br5 ⁱⁱⁱ	77.31 (3)
Br6A ^{xii} —Ba3—Br1 ⁱ	74.74 (6)	Br5 ⁱⁱ —La2—Br5 ⁱⁱⁱ	124.10 (7)
Br6A—Ba3—Br1 ⁱ	137.40 (4)	Br5—La2—Br4	140.14 (3)
Br5 ^{xiii} —Ba3—Br1 ⁱ	71.89 (4)	Br5 ^{vi} —La2—Br4	75.01 (4)
Br5 ^{xiv} —Ba3—Br1 ⁱ	140.84 (5)	Br5 ⁱⁱ —La2—Br4	73.67 (4)
Br1 ⁱⁱ —Ba3—Br1 ⁱ	72.44 (5)	Br5 ⁱⁱⁱ —La2—Br4	142.20 (4)
Br6A ^{xii} —Ba3—Br3	140.27 (4)	Br5—La2—Br4 ⁱⁱⁱ	73.67 (4)
Br6A—Ba3—Br3	70.23 (5)	Br5 ^{vi} —La2—Br4 ⁱⁱⁱ	142.20 (3)
Br5 ^{xiii} —Ba3—Br3	138.90 (5)	Br5 ⁱⁱ —La2—Br4 ⁱⁱⁱ	75.01 (4)
Br5 ^{xiv} —Ba3—Br3	71.25 (4)	Br5 ⁱⁱⁱ —La2—Br4 ⁱⁱⁱ	140.14 (4)
Br1 ⁱⁱ —Ba3—Br3	70.13 (3)	Br4—La2—Br4 ⁱⁱⁱ	72.85 (3)
Br1 ⁱ —Ba3—Br3	110.56 (5)	Br5—La2—Br4 ⁱⁱ	142.20 (3)
Br6A ^{xii} —Ba3—Br3 ^{xi}	140.27 (4)	Br5 ^{vi} —La2—Br4 ⁱⁱ	73.67 (4)
Br6A—Ba3—Br3 ^{xi}	70.23 (5)	Br5 ⁱⁱ —La2—Br4 ⁱⁱ	140.14 (4)
Br5 ^{xiii} —Ba3—Br3 ^{xi}	71.25 (4)	Br5 ⁱⁱⁱ —La2—Br4 ⁱⁱ	75.01 (4)
Br5 ^{xiv} —Ba3—Br3 ^{xi}	138.90 (5)	Br4—La2—Br4 ⁱⁱ	72.85 (3)
Br1 ⁱⁱ —Ba3—Br3 ^{xi}	110.56 (5)	Br4 ⁱⁱⁱ —La2—Br4 ⁱⁱ	114.21 (6)
Br1 ⁱ —Ba3—Br3 ^{xi}	70.13 (3)	Br5—La2—Br4 ^{vi}	75.01 (4)
Br3—Ba3—Br3 ^{xi}	71.57 (6)	Br5 ^{vi} —La2—Br4 ^{vi}	140.14 (3)
Br6A ^{xii} —Ba3—Br6B	58.0 (2)	Br5 ⁱⁱ —La2—Br4 ^{vi}	142.20 (4)
Br6A—Ba3—Br6B	75.1 (2)	Br5 ⁱⁱⁱ —La2—Br4 ^{vi}	73.67 (4)
Br5 ^{xiii} —Ba3—Br6B	67.04 (4)	Br4—La2—Br4 ^{vi}	114.21 (6)
Br5 ^{xiv} —Ba3—Br6B	67.04 (4)	Br4 ⁱⁱⁱ —La2—Br4 ^{vi}	72.85 (3)
Br1 ⁱⁱ —Ba3—Br6B	120.51 (17)	Br4 ⁱⁱ —La2—Br4 ^{vi}	72.85 (3)
Br1 ⁱ —Ba3—Br6B	120.51 (17)		
Br1 ⁱ —Ba1—Br1—La1 ⁱⁱⁱ	53.75 (5)	Br5 ^{ix} —Ba2—Br3—Ba2 ^{xvi}	126.62 (4)

supplementary materials

Br1 ⁱⁱ —Ba1—Br1—La1 ⁱⁱⁱ	113.02 (6)	Br5 ^x —Ba2—Br3—Ba2 ^{xvi}	87.13 (3)
Br1 ⁱⁱⁱ —Ba1—Br1—La1 ⁱⁱⁱ	-126.25 (5)	Br6A ^{xi} —Ba2—Br3—Ba2 ^{xvi}	162.64 (5)
Br1 ^{iv} —Ba1—Br1—La1 ⁱⁱⁱ	-41 (100)	Br3—Ba2—Br4—La2	-174.93 (4)
Br1 ^v —Ba1—Br1—La1 ⁱⁱⁱ	-6.61 (5)	Br4 ^{viii} —Ba2—Br4—La2	63.28 (6)
Br1 ^{vi} —Ba1—Br1—La1 ⁱⁱⁱ	173.39 (5)	Br4 ⁱⁱⁱ —Ba2—Br4—La2	-2.80 (5)
Br1 ^{vii} —Ba1—Br1—La1 ⁱⁱⁱ	-66.98 (6)	Br1 ⁱⁱ —Ba2—Br4—La2	-119.13 (5)
Br1 ⁱ —Ba1—Br1—Ba3 ⁱⁱⁱ	53.75 (5)	Br1—Ba2—Br4—La2	-59.75 (5)
Br1 ⁱⁱ —Ba1—Br1—Ba3 ⁱⁱⁱ	113.02 (6)	Br2—Ba2—Br4—La2	121.51 (4)
Br1 ⁱⁱⁱ —Ba1—Br1—Ba3 ⁱⁱⁱ	-126.25 (5)	Br5 ^{ix} —Ba2—Br4—La2	-4.45 (8)
Br1 ^{iv} —Ba1—Br1—Ba3 ⁱⁱⁱ	-41 (100)	Br5 ^x —Ba2—Br4—La2	127.37 (6)
Br1 ^v —Ba1—Br1—Ba3 ⁱⁱⁱ	-6.61 (5)	Br6A ^{xi} —Ba2—Br4—La2	-117.74 (7)
Br1 ^{vi} —Ba1—Br1—Ba3 ⁱⁱⁱ	173.39 (5)	Br3—Ba2—Br4—Ba2 ^{xvii}	74.12 (5)
Br1 ^{vii} —Ba1—Br1—Ba3 ⁱⁱⁱ	-66.98 (6)	Br4 ^{viii} —Ba2—Br4—Ba2 ^{xvii}	-47.66 (4)
Br1 ⁱ —Ba1—Br1—Ba2 ⁱⁱⁱ	175.49 (4)	Br4 ⁱⁱⁱ —Ba2—Br4—Ba2 ^{xvii}	-113.75 (4)
Br1 ⁱⁱ —Ba1—Br1—Ba2 ⁱⁱⁱ	-125.24 (2)	Br1 ⁱⁱ —Ba2—Br4—Ba2 ^{xvii}	129.92 (5)
Br1 ⁱⁱⁱ —Ba1—Br1—Ba2 ⁱⁱⁱ	-4.51 (4)	Br1—Ba2—Br4—Ba2 ^{xvii}	-170.70 (4)
Br1 ^{iv} —Ba1—Br1—Ba2 ⁱⁱⁱ	81 (100)	Br2—Ba2—Br4—Ba2 ^{xvii}	10.56 (3)
Br1 ^v —Ba1—Br1—Ba2 ⁱⁱⁱ	115.12 (3)	Br5 ^{ix} —Ba2—Br4—Ba2 ^{xvii}	-115.39 (6)
Br1 ^{vi} —Ba1—Br1—Ba2 ⁱⁱⁱ	-64.88 (3)	Br5 ^x —Ba2—Br4—Ba2 ^{xvii}	16.43 (8)
Br1 ^{vii} —Ba1—Br1—Ba2 ⁱⁱⁱ	54.76 (2)	Br6A ^{xi} —Ba2—Br4—Ba2 ^{xvii}	131.31 (6)
Br1 ⁱ —Ba1—Br1—Ba2	-54.85 (2)	Br3—Ba2—Br4—Ba2 ⁱⁱ	-46.75 (5)
Br1 ⁱⁱ —Ba1—Br1—Ba2	4.42 (4)	Br4 ^{viii} —Ba2—Br4—Ba2 ⁱⁱ	-168.54 (4)
Br1 ⁱⁱⁱ —Ba1—Br1—Ba2	125.15 (2)	Br4 ⁱⁱⁱ —Ba2—Br4—Ba2 ⁱⁱ	125.38 (3)
Br1 ^{iv} —Ba1—Br1—Ba2	-150 (100)	Br1 ⁱⁱ —Ba2—Br4—Ba2 ⁱⁱ	9.05 (4)
Br1 ^v —Ba1—Br1—Ba2	-115.21 (3)	Br1—Ba2—Br4—Ba2 ⁱⁱ	68.43 (4)
Br1 ^{vi} —Ba1—Br1—Ba2	64.79 (3)	Br2—Ba2—Br4—Ba2 ⁱⁱ	-110.31 (4)
Br1 ^{vii} —Ba1—Br1—Ba2	-175.58 (4)	Br5 ^{ix} —Ba2—Br4—Ba2 ⁱⁱ	123.73 (5)
Br3—Ba2—Br1—La1 ⁱⁱⁱ	-69.57 (4)	Br5 ^x —Ba2—Br4—Ba2 ⁱⁱ	-104.45 (7)
Br4 ^{viii} —Ba2—Br1—La1 ⁱⁱⁱ	74.96 (5)	Br6A ^{xi} —Ba2—Br4—Ba2 ⁱⁱ	10.44 (8)
Br4 ⁱⁱⁱ —Ba2—Br1—La1 ⁱⁱⁱ	128.07 (4)	Br6A ^{xii} —Ba3—Br6A—La1 ^{xv}	0.0
Br1 ⁱⁱ —Ba2—Br1—La1 ⁱⁱⁱ	-118.64 (4)	Br5 ^{xiii} —Ba3—Br6A—La1 ^{xv}	-68.45 (3)
Br2—Ba2—Br1—La1 ⁱⁱⁱ	-170.37 (10)	Br5 ^{xiv} —Ba3—Br6A—La1 ^{xv}	68.45 (3)
Br4—Ba2—Br1—La1 ⁱⁱⁱ	-174.58 (4)	Br1 ⁱⁱ —Ba3—Br6A—La1 ^{xv}	119.19 (8)
Br5 ^{ix} —Ba2—Br1—La1 ⁱⁱⁱ	38.07 (4)	Br1 ⁱ —Ba3—Br6A—La1 ^{xv}	-119.19 (8)
Br5 ^x —Ba2—Br1—La1 ⁱⁱⁱ	0.80 (5)	Br3—Ba3—Br6A—La1 ^{xv}	141.58 (3)
Br6A ^{xi} —Ba2—Br1—La1 ⁱⁱⁱ	-36.35 (5)	Br3 ^{xi} —Ba3—Br6A—La1 ^{xv}	-141.58 (3)
Br3—Ba2—Br1—Ba3 ⁱⁱⁱ	-69.57 (4)	Br6B—Ba3—Br6A—La1 ^{xv}	0.0
Br4 ^{viii} —Ba2—Br1—Ba3 ⁱⁱⁱ	74.96 (5)	Br6B ^{xv} —Ba3—Br6A—La1 ^{xv}	0.0
Br4 ⁱⁱⁱ —Ba2—Br1—Ba3 ⁱⁱⁱ	128.07 (4)	Br6A ^{xii} —Ba3—Br6A—Ba3 ^{xv}	0.0
Br1 ⁱⁱ —Ba2—Br1—Ba3 ⁱⁱⁱ	-118.64 (4)	Br5 ^{xiii} —Ba3—Br6A—Ba3 ^{xv}	-68.45 (3)
Br2—Ba2—Br1—Ba3 ⁱⁱⁱ	-170.37 (10)	Br5 ^{xiv} —Ba3—Br6A—Ba3 ^{xv}	68.45 (3)

Br4—Ba2—Br1—Ba3 ⁱⁱⁱ	-174.58 (4)	Br1 ⁱⁱ —Ba3—Br6A—Ba3 ^{xv}	119.19 (8)
Br5 ^{ix} —Ba2—Br1—Ba3 ⁱⁱⁱ	38.07 (4)	Br1 ⁱ —Ba3—Br6A—Ba3 ^{xv}	-119.19 (8)
Br5 ^x —Ba2—Br1—Ba3 ⁱⁱⁱ	0.80 (5)	Br3—Ba3—Br6A—Ba3 ^{xv}	141.58 (3)
Br6A ^{xi} —Ba2—Br1—Ba3 ⁱⁱⁱ	-36.35 (5)	Br3 ^{xi} —Ba3—Br6A—Ba3 ^{xv}	-141.58 (3)
Br3—Ba2—Br1—Ba1	44.70 (5)	Br6B—Ba3—Br6A—Ba3 ^{xv}	0.0
Br4 ^{viii} —Ba2—Br1—Ba1	-170.76 (4)	Br6B ^{xv} —Ba3—Br6A—Ba3 ^{xv}	0.0
Br4 ⁱⁱⁱ —Ba2—Br1—Ba1	-117.65 (4)	Br6A ^{xii} —Ba3—Br6A—Ba2 ^{xvi}	-104.22 (5)
Br1 ⁱⁱ —Ba2—Br1—Ba1	-4.36 (4)	Br5 ^{xiii} —Ba3—Br6A—Ba2 ^{xvi}	-172.66 (6)
Br2—Ba2—Br1—Ba1	-56.10 (13)	Br5 ^{xiv} —Ba3—Br6A—Ba2 ^{xvi}	-35.77 (5)
Br4—Ba2—Br1—Ba1	-60.30 (4)	Br1 ⁱⁱ —Ba3—Br6A—Ba2 ^{xvi}	14.97 (12)
Br5 ^{ix} —Ba2—Br1—Ba1	152.34 (5)	Br1 ⁱ —Ba3—Br6A—Ba2 ^{xvi}	136.60 (6)
Br5 ^x —Ba2—Br1—Ba1	115.08 (4)	Br3—Ba3—Br6A—Ba2 ^{xvi}	37.37 (5)
Br6A ^{xi} —Ba2—Br1—Ba1	77.92 (6)	Br3 ^{xi} —Ba3—Br6A—Ba2 ^{xvi}	114.20 (7)
Br3—Ba2—Br1—Ba2 ⁱⁱⁱ	171.61 (3)	Br6B—Ba3—Br6A—Ba2 ^{xvi}	-104.22 (5)
Br4 ^{viii} —Ba2—Br1—Ba2 ⁱⁱⁱ	-43.86 (6)	Br6B ^{xv} —Ba3—Br6A—Ba2 ^{xvi}	-104.22 (5)
Br4 ⁱⁱⁱ —Ba2—Br1—Ba2 ⁱⁱⁱ	9.25 (4)	Br6A ^{xii} —Ba3—Br6A—Ba2 ^{xi}	104.22 (5)
Br1 ⁱⁱ —Ba2—Br1—Ba2 ⁱⁱⁱ	122.54 (3)	Br5 ^{xiii} —Ba3—Br6A—Ba2 ^{xi}	35.77 (5)
Br2—Ba2—Br1—Ba2 ⁱⁱⁱ	70.81 (12)	Br5 ^{xiv} —Ba3—Br6A—Ba2 ^{xi}	172.66 (6)
Br4—Ba2—Br1—Ba2 ⁱⁱⁱ	66.60 (4)	Br1 ⁱⁱ —Ba3—Br6A—Ba2 ^{xi}	-136.60 (6)
Br5 ^{ix} —Ba2—Br1—Ba2 ⁱⁱⁱ	-80.75 (5)	Br1 ⁱ —Ba3—Br6A—Ba2 ^{xi}	-14.97 (12)
Br5 ^x —Ba2—Br1—Ba2 ⁱⁱⁱ	-118.02 (5)	Br3—Ba3—Br6A—Ba2 ^{xi}	-114.20 (7)
Br6A ^{xi} —Ba2—Br1—Ba2 ⁱⁱⁱ	-155.17 (7)	Br3 ^{xi} —Ba3—Br6A—Ba2 ^{xi}	-37.37 (5)
Br3—Ba2—Br2—Ba2 ^{xvi}	0.0	Br6B—Ba3—Br6A—Ba2 ^{xi}	104.22 (5)
Br4 ^{viii} —Ba2—Br2—Ba2 ^{xvi}	-131.87 (3)	Br6B ^{xv} —Ba3—Br6A—Ba2 ^{xi}	104.22 (5)
Br4 ⁱⁱⁱ —Ba2—Br2—Ba2 ^{xvi}	162.98 (4)	Br6A ^{xii} —Ba3—Br6B—Br6B ^{xii}	180.0
Br1 ⁱⁱ —Ba2—Br2—Ba2 ^{xvi}	58.74 (3)	Br6A—Ba3—Br6B—Br6B ^{xii}	0.0
Br1—Ba2—Br2—Ba2 ^{xvi}	106.71 (12)	Br5 ^{xiii} —Ba3—Br6B—Br6B ^{xii}	86.61 (10)
Br4—Ba2—Br2—Ba2 ^{xvi}	111.28 (3)	Br5 ^{xiv} —Ba3—Br6B—Br6B ^{xii}	-86.61 (10)
Br5 ^{ix} —Ba2—Br2—Ba2 ^{xvi}	-107.23 (4)	Br1 ⁱⁱ —Ba3—Br6B—Br6B ^{xii}	-136.69 (10)
Br5 ^x —Ba2—Br2—Ba2 ^{xvi}	-65.25 (3)	Br1 ⁱ —Ba3—Br6B—Br6B ^{xii}	136.69 (10)
Br6A ^{xi} —Ba2—Br2—Ba2 ^{xvi}	-19.29 (6)	Br3—Ba3—Br6B—Br6B ^{xii}	-48.58 (14)
Br3—Ba2—Br2—Ba2 ^{viii}	121.314 (8)	Br3 ^{xi} —Ba3—Br6B—Br6B ^{xii}	48.58 (14)
Br4 ^{viii} —Ba2—Br2—Ba2 ^{viii}	-10.56 (3)	Br6B ^{xv} —Ba3—Br6B—Br6B ^{xii}	0.0
Br4 ⁱⁱⁱ —Ba2—Br2—Ba2 ^{viii}	-75.71 (4)	Br6A ^{xii} —Ba3—Br6B—Br6B ^{xv}	180.0
Br1 ⁱⁱ —Ba2—Br2—Ba2 ^{viii}	-179.94 (3)	Br6A—Ba3—Br6B—Br6B ^{xv}	0.0
Br1—Ba2—Br2—Ba2 ^{viii}	-131.98 (12)	Br5 ^{xiii} —Ba3—Br6B—Br6B ^{xv}	86.61 (10)
Br4—Ba2—Br2—Ba2 ^{viii}	-127.41 (3)	Br5 ^{xiv} —Ba3—Br6B—Br6B ^{xv}	-86.61 (10)
Br5 ^{ix} —Ba2—Br2—Ba2 ^{viii}	14.08 (4)	Br1 ⁱⁱ —Ba3—Br6B—Br6B ^{xv}	-136.69 (10)
Br5 ^x —Ba2—Br2—Ba2 ^{viii}	56.06 (2)	Br1 ⁱ —Ba3—Br6B—Br6B ^{xv}	136.69 (10)
Br6A ^{xi} —Ba2—Br2—Ba2 ^{viii}	102.03 (6)	Br3—Ba3—Br6B—Br6B ^{xv}	-48.58 (14)
Br3—Ba2—Br2—Ba2 ^{xvii}	-121.314 (12)	Br3 ^{xi} —Ba3—Br6B—Br6B ^{xv}	48.58 (14)

supplementary materials

Br4 ^{viii} —Ba2—Br2—Ba2 ^{xvii}	106.82 (3)	Br6A ^{xii} —Ba3—Br6B—Br6B ^{xx}	180.0
Br4 ⁱⁱⁱ —Ba2—Br2—Ba2 ^{xvii}	41.67 (4)	Br6A—Ba3—Br6B—Br6B ^{xx}	0.0
Br1 ⁱⁱ —Ba2—Br2—Ba2 ^{xvii}	-62.57 (2)	Br5 ^{xiii} —Ba3—Br6B—Br6B ^{xx}	86.61 (10)
Br1—Ba2—Br2—Ba2 ^{xvii}	-14.60 (11)	Br5 ^{xiv} —Ba3—Br6B—Br6B ^{xx}	-86.61 (10)
Br4—Ba2—Br2—Ba2 ^{xvii}	-10.03 (3)	Br1 ⁱⁱ —Ba3—Br6B—Br6B ^{xx}	-136.69 (10)
Br5 ^{ix} —Ba2—Br2—Ba2 ^{xvii}	131.46 (5)	Br1 ⁱ —Ba3—Br6B—Br6B ^{xx}	136.69 (10)
Br5 ^x —Ba2—Br2—Ba2 ^{xvii}	173.43 (3)	Br3—Ba3—Br6B—Br6B ^{xx}	-48.58 (14)
Br6A ^{xi} —Ba2—Br2—Ba2 ^{xvii}	-140.60 (6)	Br3 ^{xi} —Ba3—Br6B—Br6B ^{xx}	48.58 (14)
Br6A ^{xii} —Ba3—Br3—La1 ^{xi}	-150.15 (11)	Br6B ^{xv} —Ba3—Br6B—Br6B ^{xx}	0.0
Br6A—Ba3—Br3—La1 ^{xi}	74.99 (4)	Br6A ^{xii} —Ba3—Br6B—La1 ^{xii}	0.0
Br5 ^{xiii} —Ba3—Br3—La1 ^{xi}	26.19 (6)	Br6A—Ba3—Br6B—La1 ^{xii}	180.0
Br5 ^{xiv} —Ba3—Br3—La1 ^{xi}	162.16 (4)	Br5 ^{xiii} —Ba3—Br6B—La1 ^{xii}	-93.39 (10)
Br1 ⁱⁱ —Ba3—Br3—La1 ^{xi}	-120.93 (4)	Br5 ^{xiv} —Ba3—Br6B—La1 ^{xii}	93.39 (10)
Br1 ⁱ —Ba3—Br3—La1 ^{xi}	-59.49 (3)	Br1 ⁱⁱ —Ba3—Br6B—La1 ^{xii}	43.31 (10)
Br3 ^{xi} —Ba3—Br3—La1 ^{xi}	0.0	Br1 ⁱ —Ba3—Br6B—La1 ^{xii}	-43.31 (10)
Br6B—Ba3—Br3—La1 ^{xi}	125.4 (2)	Br3—Ba3—Br6B—La1 ^{xii}	131.42 (14)
Br6B ^{xv} —Ba3—Br3—La1 ^{xi}	110.05 (17)	Br3 ^{xi} —Ba3—Br6B—La1 ^{xii}	-131.42 (14)
Br6A ^{xii} —Ba3—Br3—Ba3 ^{xi}	-150.15 (11)	Br6B ^{xv} —Ba3—Br6B—La1 ^{xii}	180.0
Br6A—Ba3—Br3—Ba3 ^{xi}	74.99 (4)	Br6A ^{xii} —Ba3—Br6B—Ba3 ^{xii}	0.0
Br5 ^{xiii} —Ba3—Br3—Ba3 ^{xi}	26.19 (6)	Br6A—Ba3—Br6B—Ba3 ^{xii}	180.0
Br5 ^{xiv} —Ba3—Br3—Ba3 ^{xi}	162.16 (4)	Br5 ^{xiii} —Ba3—Br6B—Ba3 ^{xii}	-93.39 (10)
Br1 ⁱⁱ —Ba3—Br3—Ba3 ^{xi}	-120.93 (4)	Br5 ^{xiv} —Ba3—Br6B—Ba3 ^{xii}	93.39 (10)
Br1 ⁱ —Ba3—Br3—Ba3 ^{xi}	-59.49 (3)	Br1 ⁱⁱ —Ba3—Br6B—Ba3 ^{xii}	43.31 (10)
Br3 ^{xi} —Ba3—Br3—Ba3 ^{xi}	0.0	Br1 ⁱ —Ba3—Br6B—Ba3 ^{xii}	-43.31 (10)
Br6B—Ba3—Br3—Ba3 ^{xi}	125.4 (2)	Br3—Ba3—Br6B—Ba3 ^{xii}	131.42 (14)
Br6B ^{xv} —Ba3—Br3—Ba3 ^{xi}	110.05 (17)	Br3 ^{xi} —Ba3—Br6B—Ba3 ^{xii}	-131.42 (14)
Br6A ^{xii} —Ba3—Br3—Ba2	-34.59 (12)	Br6B ^{xv} —Ba3—Br6B—Ba3 ^{xii}	180.0
Br6A—Ba3—Br3—Ba2	-169.45 (6)	La1 ^{xviii} —Br5—La2—Br5 ^{vi}	0.77 (6)
Br5 ^{xiii} —Ba3—Br3—Ba2	141.75 (7)	Ba3 ^{xviii} —Br5—La2—Br5 ^{vi}	0.77 (6)
Br5 ^{xiv} —Ba3—Br3—Ba2	-82.28 (5)	Ba2 ^{xix} —Br5—La2—Br5 ^{vi}	-107.10 (4)
Br1 ⁱⁱ —Ba3—Br3—Ba2	-5.37 (4)	Ba2 ^x —Br5—La2—Br5 ^{vi}	105.98 (3)
Br1 ⁱ —Ba3—Br3—Ba2	56.07 (6)	La1 ^{xviii} —Br5—La2—Br5 ⁱⁱ	-64.11 (7)
Br3 ^{xi} —Ba3—Br3—Ba2	115.56 (4)	Ba3 ^{xviii} —Br5—La2—Br5 ⁱⁱ	-64.11 (7)
Br6B—Ba3—Br3—Ba2	-119.1 (2)	Ba2 ^{xix} —Br5—La2—Br5 ⁱⁱ	-171.99 (3)
Br6B ^{xv} —Ba3—Br3—Ba2	-134.39 (17)	Ba2 ^x —Br5—La2—Br5 ⁱⁱ	41.09 (5)
Br6A ^{xii} —Ba3—Br3—Ba2 ^{xvi}	88.72 (10)	La1 ^{xviii} —Br5—La2—Br5 ⁱⁱⁱ	65.66 (7)
Br6A—Ba3—Br3—Ba2 ^{xvi}	-46.14 (4)	Ba3 ^{xviii} —Br5—La2—Br5 ⁱⁱⁱ	65.66 (7)
Br5 ^{xiii} —Ba3—Br3—Ba2 ^{xvi}	-94.93 (8)	Ba2 ^{xix} —Br5—La2—Br5 ⁱⁱⁱ	-42.21 (6)
Br5 ^{xiv} —Ba3—Br3—Ba2 ^{xvi}	41.04 (4)	Ba2 ^x —Br5—La2—Br5 ⁱⁱⁱ	170.87 (3)
Br1 ⁱⁱ —Ba3—Br3—Ba2 ^{xvi}	117.95 (5)	La1 ^{xviii} —Br5—La2—Br4	-108.12 (10)
Br1 ⁱ —Ba3—Br3—Ba2 ^{xvi}	179.38 (4)	Ba3 ^{xviii} —Br5—La2—Br4	-108.12 (10)

Br3 ^{xi} —Ba3—Br3—Ba2 ^{xvi}	-121.12 (3)	Ba2 ^{xix} —Br5—La2—Br4	144.01 (7)
Br6B—Ba3—Br3—Ba2 ^{xvi}	4.2 (2)	Ba2 ^x —Br5—La2—Br4	-2.91 (9)
Br6B ^{xv} —Ba3—Br3—Ba2 ^{xvi}	-11.07 (17)	La1 ^{xviii} —Br5—La2—Br4 ⁱⁱⁱ	-141.98 (8)
Br4 ^{viii} —Ba2—Br3—Ba3	169.88 (4)	Ba3 ^{xviii} —Br5—La2—Br4 ⁱⁱⁱ	-141.98 (8)
Br4 ⁱⁱⁱ —Ba2—Br3—Ba3	32.77 (17)	Ba2 ^{xix} —Br5—La2—Br4 ⁱⁱⁱ	110.15 (4)
Br1 ⁱⁱ —Ba2—Br3—Ba3	5.14 (4)	Ba2 ^x —Br5—La2—Br4 ⁱⁱⁱ	-36.77 (4)
Br1—Ba2—Br3—Ba3	-44.94 (5)	La1 ^{xviii} —Br5—La2—Br4 ⁱⁱ	109.38 (11)
Br2—Ba2—Br3—Ba3	118.59 (4)	Ba3 ^{xviii} —Br5—La2—Br4 ⁱⁱ	109.38 (11)
Br4—Ba2—Br3—Ba3	59.07 (5)	Ba2 ^{xix} —Br5—La2—Br4 ⁱⁱ	1.51 (10)
Br5 ^{ix} —Ba2—Br3—Ba3	-114.79 (4)	Ba2 ^x —Br5—La2—Br4 ⁱⁱ	-145.42 (8)
Br5 ^x —Ba2—Br3—Ba3	-154.28 (6)	La1 ^{xviii} —Br5—La2—Br4 ^{vi}	141.89 (9)
Br6A ^{xi} —Ba2—Br3—Ba3	-78.77 (7)	Ba3 ^{xviii} —Br5—La2—Br4 ^{vi}	141.89 (9)
Br4 ^{viii} —Ba2—Br3—La1 ^{xi}	-72.27 (6)	Ba2 ^{xix} —Br5—La2—Br4 ^{vi}	34.02 (4)
Br4 ⁱⁱⁱ —Ba2—Br3—La1 ^{xi}	150.61 (13)	Ba2 ^x —Br5—La2—Br4 ^{vi}	-112.90 (4)
Br1 ⁱⁱ —Ba2—Br3—La1 ^{xi}	122.99 (5)	Ba2 ^{xvii} —Br4—La2—Br5	87.56 (9)
Br1—Ba2—Br3—La1 ^{xi}	72.91 (4)	Ba2 ⁱⁱ —Br4—La2—Br5	-160.15 (7)
Br2—Ba2—Br3—La1 ^{xi}	-123.56 (3)	Ba2—Br4—La2—Br5	-31.19 (10)
Br4—Ba2—Br3—La1 ^{xi}	176.92 (4)	Ba2 ^{xvii} —Br4—La2—Br5 ^{vi}	-38.25 (4)
Br5 ^{ix} —Ba2—Br3—La1 ^{xi}	3.06 (5)	Ba2 ⁱⁱ —Br4—La2—Br5 ^{vi}	74.05 (5)
Br5 ^x —Ba2—Br3—La1 ^{xi}	-36.43 (3)	Ba2—Br4—La2—Br5 ^{vi}	-157.00 (5)
Br6A ^{xi} —Ba2—Br3—La1 ^{xi}	39.07 (6)	Ba2 ^{xvii} —Br4—La2—Br5 ⁱⁱ	42.63 (4)
Br4 ^{viii} —Ba2—Br3—Ba3 ^{xi}	-72.27 (6)	Ba2 ⁱⁱ —Br4—La2—Br5 ⁱⁱ	154.93 (5)
Br4 ⁱⁱⁱ —Ba2—Br3—Ba3 ^{xi}	150.61 (13)	Ba2—Br4—La2—Br5 ⁱⁱ	-76.12 (4)
Br1 ⁱⁱ —Ba2—Br3—Ba3 ^{xi}	122.99 (5)	Ba2 ^{xvii} —Br4—La2—Br5 ⁱⁱⁱ	-82.52 (9)
Br1—Ba2—Br3—Ba3 ^{xi}	72.91 (4)	Ba2 ⁱⁱ —Br4—La2—Br5 ⁱⁱⁱ	29.78 (11)
Br2—Ba2—Br3—Ba3 ^{xi}	-123.56 (3)	Ba2—Br4—La2—Br5 ⁱⁱⁱ	158.74 (8)
Br4—Ba2—Br3—Ba3 ^{xi}	176.92 (4)	Ba2 ^{xvii} —Br4—La2—Br4 ⁱⁱⁱ	121.58 (5)
Br5 ^{ix} —Ba2—Br3—Ba3 ^{xi}	3.06 (5)	Ba2 ⁱⁱ —Br4—La2—Br4 ⁱⁱⁱ	-126.12 (2)
Br5 ^x —Ba2—Br3—Ba3 ^{xi}	-36.43 (3)	Ba2—Br4—La2—Br4 ⁱⁱⁱ	2.83 (5)
Br6A ^{xi} —Ba2—Br3—Ba3 ^{xi}	39.07 (6)	Ba2 ^{xvii} —Br4—La2—Br4 ⁱⁱ	-115.43 (5)
Br4 ^{viii} —Ba2—Br3—Ba2 ^{xvi}	51.29 (3)	Ba2 ⁱⁱ —Br4—La2—Br4 ⁱⁱ	-3.13 (5)
Br4 ⁱⁱⁱ —Ba2—Br3—Ba2 ^{xvi}	-85.82 (14)	Ba2—Br4—La2—Br4 ⁱⁱ	125.82 (2)
Br1 ⁱⁱ —Ba2—Br3—Ba2 ^{xvi}	-113.45 (3)	Ba2 ^{xvii} —Br4—La2—Br4 ^{vi}	-176.92 (4)
Br1—Ba2—Br3—Ba2 ^{xvi}	-163.52 (4)	Ba2 ⁱⁱ —Br4—La2—Br4 ^{vi}	-64.63 (4)
Br2—Ba2—Br3—Ba2 ^{xvi}	0.0	Ba2—Br4—La2—Br4 ^{vi}	64.33 (3)
Br4—Ba2—Br3—Ba2 ^{xvi}	-59.51 (2)		

Symmetry codes: (i) $y, -x+2, -z$; (ii) $y, -x+2, z$; (iii) $-y+2, x, z$; (iv) $-x+2, -y+2, -z$; (v) $x, y, -z$; (vi) $-x+2, -y+2, z$; (vii) $-y+2, x, -z$; (viii) $y+1/2, -x+3/2, -z+1/2$; (ix) $-y+5/2, x-1/2, -z+1/2$; (x) $-x+5/2, -y+3/2, -z+1/2$; (xi) $-x+2, -y+1, -z$; (xii) $-y+1, x, z$; (xiii) $x-1/2, y-1/2, z-1/2$; (xiv) $x-1/2, y-1/2, -z+1/2$; (xv) $y, -x+1, -z$; (xvi) $-x+2, -y+1, z$; (xvii) $-y+3/2, x-1/2, -z+1/2$; (xviii) $x+1/2, y+1/2, z+1/2$; (xix) $y+1/2, -x+5/2, -z+1/2$; (xx) $-x+1, -y+1, -z$.

Table 1

supplementary materials

Observed and calculated structure factors of $Ba11La4Br34$

h	k	l	F _o	F _c	s	h	k	l	F _o	F _c	s	h	k	l	F _o	F _c	s	h	k	l	F _o	F _c	s	h	k	l	F _o	F _c	s
1	1	0	76	74	4	2	3	1	272	273	7	4	4	2	77	68	7	-2	5	3	309	311	5	0	6	4	131	127	6
0	2	0	99	89	7	-3	4	1	158	138	4	-3	5	2	155	165	4	0	5	3	109	110	25	2	6	4	105	113	7
2	2	0	115	85	8	1	4	1	717	693	24	-1	5	2	69	69	7	2	5	3	515	524	10	4	6	4	203	185	4
1	3	0	26	10	25	3	4	1	49	46	11	1	5	2	322	306	8	4	5	3	380	368	7	6	6	4	291	281	6
3	3	0	917	852	22	-4	5	1	44	29	15	3	5	2	130	150	5	-5	6	3	259	255	7	-5	7	4	49	80	22
0	4	0	43	54	16	-2	5	1	203	194	4	5	5	2	269	266	5	-3	6	3	36	21	24	-3	7	4	55	64	14
4	4	0	283	285	5	0	5	1	150	141	4	-4	6	2	196	188	5	-1	6	3	78	81	10	-1	7	4	416	406	12
-3	5	0	523	504	10	2	5	1	81	70	7	-2	6	2	253	240	5	1	6	3	185	186	6	1	7	4	93	105	8
-1	5	0	29	10	28	4	5	1	82	93	8	0	6	2	59	94	13	3	6	3	894	862	10	3	7	4	106	109	8
1	5	0	163	160	8	-5	6	1	106	110	7	2	6	2	150	159	5	5	6	3	591	538	9	5	7	4	287	288	9
3	5	0	250	231	7	-3	6	1	520	505	9	4	6	2	117	115	7	-6	7	3	365	358	7	7	7	4	198	202	7
5	5	0	401	391	9	-1	6	1	87	97	7	6	6	2	62	56	14	-4	7	3	597	573	9	-6	8	4	331	347	9
-4	6	0	321	333	5	1	6	1	81	93	7	-5	7	2	99	89	9	-2	7	3	629	619	15	-4	8	4	356	345	7
-2	6	0	1526	1646	40	3	6	1	283	267	4	-3	7	2	241	242	5	0	7	3	506	470	8	-2	8	4	57	58	20
0	6	0	414	387	11	5	6	1	84	114	9	-1	7	2	140	149	6	2	7	3	345	331	5	0	8	4	124	134	10
2	6	0	208	199	9	-6	7	1	210	209	6	1	7	2	281	276	5	4	7	3	34	5	34	2	8	4	239	232	6
4	6	0	190	191	7	-4	7	1	218	202	5	3	7	2	156	141	5	-7	8	3	350	333	10	6	8	4	120	119	10
6	6	0	488	474	5	-2	7	1	67	70	10	5	7	2	33	5	33	-5	8	3	320	306	9	8	8	4	184	191	12
-5	7	0	29	13	29	0	7	1	48	15	19	7	7	2	0	42	1	-3	8	3	227	218	7	-7	9	4	70	80	26
-3	7	0	252	260	9	2	7	1	21	16	21	-6	8	2	83	69	13	-1	8	3	595	558	10	-5	9	4	399	398	8
-1	7	0	879	818	18	4	7	1	67	74	13	-4	8	2	237	228	6	1	8	3	647	648	11	-3	9	4	131	135	9
1	7	0	326	335	11	6	7	1	39	47	39	-2	8	2	118	117	9	3	8	3	435	424	4	-1	9	4	322	304	6
3	7	0	555	523	11	-7	8	1	189	184	10	0	8	2	0	3	1	5	8	3	37	7	37	1	9	4	101	96	11
5	7	0	840	771	18	-5	8	1	56	69	20	2	8	2	126	119	9	7	8	3	406	380	17	3	9	4	189	193	8
7	7	0	829	775	35	-3	8	1	358	351	9	4	8	2	26	16	25	-8	9	3	235	230	14	5	9	4	62	68	26
-6	8	0	1008	980	27	-1	8	1	235	214	5	6	8	2	62	50	23	-6	9	3	170	185	9	7	9	4	36	40	36
-4	8	0	437	446	18	1	8	1	299	301	6	8	8	2	72	76	22	-4	9	3	228	229	7	9	9	4	236	211	14
-2	8	0	464	468	24	5	8	1	82	86	14	-7	9	2	366	353	11	-2	9	3	293	278	6	-8	10	4	182	173	12
0	8	0	74	87	20	7	8	1	291	267	14	-5	9	2	26	17	25	0	9	3	47	73	28	-6	10	4	328	319	7
2	8	0	152	178	12	-8	9	1	170	154	11	-3	9	2	313	310	7	2	9	3	543	537	9	-4	10	4	140	146	11
4	8	0	1162	1078	3	-6	9	1	0	15	1	-1	9	2	344	314	6	4	9	3	314	296	7	-2	10	4	93	102	16
6	8	0	616	559	42	-4	9	1	180	189	8	1	9	2	104	113	12	6	9	3	207	204	14	0	10	4	274	284	7
8	8	0	39	25	38	-2	9	1	61	80	23	3	9	2	90	90	14	8	9	3	50	15	49	2	10	4	285	298	8
-7	9	0	126	147	18	0	9	1	77	82	16	5	9	2	329	300	11	-9	10	3	472	431	25	4	10	4	215	218	8
-5	9	0	807	778	12	2	9	1	60	45	23	7	9	2	216	214	15	-7	10	3	246	248	10	6	10	4	55	8	55
-3	9	0	95	106	21	4	9	1	165	162	9	9	9	2	16	6	15	-5	10	3	45	50	44	8	10	4	45	74	44
-1	9	0	613	594	16	6	9	1	45	15	45	-8	10	2	131	109	19	-3	10	3	706	652	9	10	10	4	308	278	33
1	9	0	116	125	15	8	9	1	0	2	1	-6	10	2	79	92	23	-1	10	3	112	120	14	-9	11	4	0	12	1
3	9	0	78	122	25	-7	10	1	49	45	48	-4	10	2	42	49	41	1	10	3	144	161	10	-7	11	4	59	79	58
5	9	0	72	77	32	-5	10	1	308	312	7	-2	10	2	34	18	33	3	10	3	174	164	9	-5	11	4	181	186	11
7	9	0	387	335	42	-3	10	1	187	198	9	0	10	2	74	81	19	5	10	3	358	326	13	-3	11	4	99	107	17
9	9	0	0	46	1	-1	10	1	473	459	9	2	10	2	81	84	17	7	10	3	425	363	28	-1	11	4	426	418	9
-8	10	0	149	176	26	1	10	1	159	168	9	4	10	2	45	18	45	9	10	3	351	309	22	1	11	4	102	94	15
-6	10	0	254	237	12	3	10	1	106	111	13	6	10	2	0	23	1	-6	11	3	347	322	14	3	11	4	48	31	48
-4	10	0	168	189	14	5	10	1	78	89	20	8	10	2	40	49	40	-4	11	3	141	160	13	5	11	4	155	148	12
-2	10	0	48	13	48	7	10	1	42	47	41	10	10	2	99	83	39	-2	11	3	80	44	20	7	11	4	114	111	20

0	10	0	106310382	9	10	1	293	271	31	-9	11	2	0	5	1	0	11	3	561	557	14	9	11	4	115	127	26			
2	10	0	906	848	31	-10	11	1	79	52	79	-7	11	2	284	278	17	2	11	3	88	87	18	-8	12	4	306	287	15	
4	10	0	53	44	53	-8	11	1	225	231	17	-5	11	2	210	214	10	4	11	3	106	76	16	-6	12	4	0	13	1	
6	10	0	88	18	34	-6	11	1	0	48	1	-3	11	2	47	31	46	6	11	3	338	314	22	-4	12	4	292	301	9	
8	10	0	426	391	54	-4	11	1	97	111	18	-1	11	2	0	32	1	8	11	3	165	163	21	-2	12	4	122	135	18	
10	10	0	552	457	57	-2	11	1	329	328	7	1	11	2	302	290	7	-7	12	3	311	312	13	0	12	4	108	111	16	
-9	11	0	233	221	24	0	11	1	44	85	44	3	11	2	199	210	9	-5	12	3	226	233	10	2	12	4	290	288	8	
-7	11	0	341	305	25	2	11	1	154	153	10	5	11	2	54	53	54	-3	12	3	178	189	12	4	12	4	228	219	9	
-5	11	0	510	501	9	4	11	1	134	118	12	7	11	2	19	15	18	-1	12	3	156	160	11	6	12	4	227	208	13	
-3	11	0	128	131	20	6	11	1	482	413	30	9	11	2	0	13	1	1	12	3	256	264	8	8	12	4	42	10	41	
-1	11	0	28	28	28	8	11	1	244	241	22	-8	12	2	0	47	1	3	12	3	372	365	8	-5	13	4	0	24	1	
1	11	0	310	301	16	10	11	1	237	159	48	-6	12	2	48	47	47	5	12	3	76	57	29	-3	13	4	0	5	1	
3	11	0	317	310	10	-7	12	1	86	104	37	-4	12	2	29	47	29	7	12	3	82	50	32	-1	13	4	0	15	1	
5	11	0	678	613	43	-5	12	1	145	158	15	-2	12	2	219	215	11	-6	13	3	47	55	46	1	13	4	175	185	13	
7	11	0	455	418	62	-3	12	1	60	97	43	0	12	2	0	13	1	-4	13	3	428	442	8	3	13	4	287	264	10	
9	11	0	260	222	31	-1	12	1	54	47	54	2	12	2	125	136	14	-2	13	3	215	216	12	5	13	4	209	180	26	
-8	12	0	538	476	34	1	12	1	153	142	11	4	12	2	89	85	21	0	13	3	88	95	22	-4	14	4	0	24	1	
-6	12	0	94	106	37	3	12	1	123	129	14	6	12	2	55	43	54	2	13	3	64	27	39	-2	14	4	48	62	48	
-4	12	0	791	758	11	5	12	1	206	208	14	8	12	2	52	16	51	4	13	3	183	189	12	0	14	4	221	224	12	
-2	12	0	345	331	17	7	12	1	97	70	26	-7	13	2	0	15	1	6	13	3	292	230	21	2	14	4	253	257	11	
0	12	0	200	208	14	-6	13	1	209	214	14	-5	13	2	115	153	22	-3	14	3	68	34	67	4	14	4	119	105	33	
2	12	0	251	255	13	-4	13	1	307	290	9	-3	13	2	150	165	15	-1	14	3	535	550	10	-1	2	5	182	167	8	
4	12	0	406	388	26	-2	13	1	75	99	32	-1	13	2	228	239	10	1	14	3	120	100	19	1	2	5	242	227	3	
6	12	0	918	788	86	0	13	1	60	42	41	1	13	2	177	184	11	3	14	3	107	103	23	-2	3	5	144	150	3	
8	12	0	423	369	51	2	13	1	61	19	43	3	13	2	99	69	20	1	1	4	94	84	3	0	3	5	186	175	5	
-7	13	0	76	79	76	4	13	1	179	185	12	5	13	2	25	21	24	0	2	4	168	170	9	2	3	5	594	578	12	
-5	13	0	354	337	19	6	13	1	82	53	34	7	13	2	298	241	25	2	2	4	299	279	6	-3	4	5	202	191	3	
-3	13	0	371	380	12	-5	14	1	39	74	38	-4	14	2	7	21	6	-1	3	4	423	417	9	-1	4	5	36	14	17	
-1	13	0	247	275	13	-3	14	1	209	228	14	-2	14	2	71	94	43	1	3	4	652	633	12	1	4	5	270	287	6	
1	13	0	520	541	13	-1	14	1	236	240	10	0	14	2	48	10	47	3	3	4	276	284	4	3	4	5	44	64	12	
3	13	0	295	297	12	1	14	1	120	142	17	2	14	2	122	109	19	-2	4	4	280	293	4	-4	5	5	527	493	10	
5	13	0	29	26	29	3	14	1	119	118	19	4	14	2	78	20	78	0	4	4	30	8	21	-2	5	5	76	82	6	
7	13	0	33	55	33	5	14	1	72	119	71	0	1	3	168	181	6	2	4	4	412	397	8	0	5	5	182	173	7	
-4	14	0	324	328	26	1	1	2	168	172	4	-1	2	3	55	73	4	4	4	4	52	70	11	2	5	5	108	108	6	
-2	14	0	0	7	1	0	2	2	46	38	5	-2	3	3	228	221	3	-3	5	4	0	14	1	4	5	5	182	173	5	
0	14	0	485	483	12	2	2	2	0	11	1	0	3	3	114	108	3	-1	5	4	98	95	6	-5	6	5	341	321	9	
2	14	0	473	467	19	-1	3	2	296	263	4	-3	4	3	113	111	16	18	1	5	4	103	97	5	-3	6	5	223	230	4
4	14	0	554	546	24	1	3	2	59	40	6	-1	4	3	600	593	12	3	5	4	81	107	8	-1	6	5	138	145	8	
0	1	1	33	5	5	-2	4	2	105	79	6	1	4	3	377	386	8	5	5	4	131	134	6	1	6	5	139	140	5	
-1	2	1	21	8	20	0	4	2	19	24	18	3	4	3	411	380	6	-4	6	4	616	589	13	3	6	5	226	233	5	
0	3	1	149	133	5	2	4	2	131	124	4	-4	5	3	179	157	4	-2	6	4	174	197	4	5	6	5	172	149	6	
-6	7	5	85	94	13	7	7	6	158	154	8	-3	8	7	194	219	7	4	8	8	18	5	18	-2	9	9	53	52	31	
-4	7	5	159	149	6	-6	8	6	364	337	12	-1	8	7	332	325	5	6	8	8	46	33	46	0	9	9	122	137	11	
-2	7	5	96	102	8	-4	8	6	494	488	9	1	8	7	78	96	13	8	8	8	99	100	20	2	9	9	221	231	7	
0	7	5	183	169	5	-2	8	6	147	142	9	3	8	7	137	136	8	-7	9	8	97	123	22	4	9	9	634	605	13	
2	7	5	32	12	31	0	8	6	157	156	8	5	8	7	89	90	13	-5	9	8	152	159	12	6	9	9	312	310	17	
4	7	5	266	248	6	2	8	6	433	421	6	7	8	7	291	263	16	-3	9	8	188	190	9	8	9	9	0	27	1	
6	7	5	109	117	10	4	8	6	127	142	9	-8	9	7	396	378	22	-1	9	8	228	209	7	-9	10	9	274	276	15	
-7	8	5	47	2	47	6	8	6	197	200	11	-6	9	7	73	80	27	1	9	8	211	209	7	-7	10	9	284	289	19	

supplementary materials

-5 8 5 0 23 1 8 8 6 654 583 31 -4 9 7 510 513 8 3 9 8 145 158 10 -5 10 9 169 193 12
-3 8 5 82 105 13 -7 9 6 345 335 16 -2 9 7 0 5 1 5 9 8 117 115 13 -3 10 9 367 361 9
-1 8 5 122 108 8 -5 9 6 22 23 21 0 9 7 0 14 1 7 9 8 125 107 14 -1 10 9 99 103 16
1 8 5 121 126 9 -3 9 6 1009 61 17 2 9 7 21 11 21 9 9 8 61 31 60 1 10 9 108 121 13
3 8 5 233 235 6 -1 9 6 392 402 5 4 9 7 186 189 8 -8 10 8 28 7 27 3 10 9 26 12 26
5 8 5 170 172 7 1 9 6 101 111 12 6 9 7 760 653 43 -6 10 8 132 171 15 5 10 9 177 168 12
7 8 5 200 180 9 3 9 6 76 94 17 8 9 7 141 139 15 -4 10 8 255 256 8 7 10 9 225 224 15
-8 9 5 204 182 10 5 9 6 461 419 18 -9 10 7 100 128 27 -2 10 8 367 356 6 9 10 9 102 107 33
-6 9 5 249 245 7 7 9 6 792 725 41 -7 10 7 387 383 14 0 10 8 162 178 9 -8 11 9 113 100 24
-4 9 5 173 175 8 9 9 6 379 376 17 -5 10 7 353 371 10 2 10 8 131 123 11 -6 11 9 254 259 16
-2 9 5 68 73 17 -8 10 6 326 328 17 -3 10 7 22 15 22 4 10 8 133 135 13 -4 11 9 191 212 10
0 9 5 74 83 16 -6 10 6 52 58 51 -1 10 7 27 26 27 6 10 8 28 17 28 -2 11 9 251 258 8
2 9 5 85 86 14 -4 10 6 111 126 14 1 10 7 0 20 1 8 10 8 388 378 30 0 11 9 595 596 6
4 9 5 328 305 6 -2 10 6 599 581 7 3 10 7 42 32 42 10 10 8 27 65 27 2 11 9 241 255 9
6 9 5 199 174 10 0 10 6 333 327 6 5 10 7 139 153 13 -9 11 8 58 101 57 4 11 9 87 97 22
8 9 5 294 276 18 2 10 6 578 551 9 7 10 7 402 339 32 -7 11 8 23 8 22 6 11 9 0 42 1
-9 10 5 15 18 14 4 10 6 529 494 15 9 10 7 71 60 71 -5 11 8 180 172 14 8 11 9 179 173 20
-7 10 5 0 19 1 6 10 6 188 182 12 -8 11 7 217 215 14 -3 11 8 0 64 1 -7 12 9 105 143 52
-5 10 5 64 80 26 8 10 6 224 191 16 -6 11 7 63 67 62 -1 11 8 108 134 19 -5 12 9 105 123 26
-3 10 5 81 103 18 10 10 6 316 292 34 -4 11 7 28 11 28 1 11 8 0 20 1 -3 12 9 126 127 17
-1 10 5 212 219 9 -9 11 6 126 116 51 -2 11 7 376 373 7 3 11 8 114 99 16 -1 12 9 110 118 19
1 10 5 117 138 12 -7 11 6 493 485 14 0 11 7 288 272 8 5 11 8 206 208 11 1 12 9 217 211 10
3 10 5 130 130 12 -5 11 6 223 232 12 2 11 7 542 539 9 7 11 8 72 69 47 3 12 9 333 338 14
5 10 5 115 116 14 -3 11 6 225 233 10 4 11 7 257 235 13 9 11 8 0 47 1 5 12 9 155 156 17
7 10 5 0 13 1 -1 11 6 75 74 29 6 11 7 357 306 21 -6 12 8 202 209 15 -4 13 9 234 262 13
9 10 5 293 225 21 1 11 6 152 173 12 8 11 7 109 135 49 -4 12 8 338 339 9 -2 13 9 50 52 49
-8 11 5 132 129 24 3 11 6 789 753 16 -7 12 7 0 22 1 -2 12 8 199 223 13 0 13 9 126 159 18
-6 11 5 202 213 13 5 11 6 584 537 35 -5 12 7 193 206 14 0 12 8 79 68 26 2 13 9 105 103 22
-4 11 5 82 86 24 7 11 6 0 12 1 -3 12 7 98 105 22 2 12 8 167 180 12 4 13 9 139 166 17
-2 11 5 70 78 28 9 11 6 97 64 78 -1 12 7 166 182 12 4 12 8 318 314 13 -1 14 9 212 201 27
0 11 5 111 122 14 -8 12 6 211 220 33 1 12 7 368 361 8 6 12 8 254 212 22 1 14 9 117 43 117
2 11 5 106 123 15 -6 12 6 484 498 12 3 12 7 112 98 18 -5 13 8 143 110 28 0 0 10 20 3 19
4 11 5 28 3 27 -4 12 6 317 319 9 5 12 7 100 93 23 -3 13 8 42 17 42 1 1 10 244 243 4
6 11 5 100 86 21 -2 12 6 495 503 10 7 12 7 203 176 20 -1 13 8 41 12 41 0 2 10 269 276 3
8 11 5 118 91 23 0 12 6 178 191 12 -6 13 7 374 380 21 1 13 8 76 54 32 2 2 10 155 156 5
-7 12 5 128 149 22 2 12 6 71 76 30 -4 13 7 330 313 14 3 13 8 166 140 19 -1 3 10 218 216 5
-5 12 5 0 1 1 4 12 6 135 137 15 -2 13 7 432 438 9 5 13 8 96 42 50 1 3 10 279 281 6
-3 12 5 48 53 47 6 12 6 176 165 18 0 13 7 69 58 37 -2 14 8 139 139 39 3 3 10 328 357 8
-1 12 5 194 192 11 8 12 6 82 88 82 2 13 7 63 12 55 0 14 8 85 62 51 -2 4 10 228 241 7
1 12 5 150 159 13 -5 13 6 229 215 14 4 13 7 71 74 40 2 14 8 63 34 63 0 4 10 295 307 8
3 12 5 271 277 9 -3 13 6 142 150 16 6 13 7 70 68 70 0 1 9 115 105 4 2 4 10 53 76 12
5 12 5 33 34 33 -1 13 6 477 491 8 -3 14 7 382 388 18 -1 2 9 226 248 5 4 4 10 86 106 8
7 12 5 58 23 57 1 13 6 443 461 18 -1 14 7 140 151 24 1 2 9 1059 1121 4 -3 5 10 4 7 4
-6 13 5 86 91 47 3 13 6 192 185 13 1 14 7 216 205 14 -2 3 9 189 200 7 -1 5 10 432 432 8
-4 13 5 49 30 49 5 13 6 287 261 19 3 14 7 279 282 18 0 3 9 25 23 25 1 5 10 0 11 1
-2 13 5 99 132 26 -4 14 6 95 31 94 0 0 8 938 904 66 2 3 9 0 45 1 3 5 10 151 157 6
0 13 5 23 17 23 -2 14 6 81 79 42 1 1 8 20 28 19 -3 4 9 799 795 25 5 5 10 346 341 15
2 13 5 227 223 11 0 14 6 263 276 11 0 2 8 340 334 7 -1 4 9 232 220 6 -4 6 10 504 507 15
4 13 5 131 82 17 2 14 6 262 264 12 2 2 8 301 329 4 1 4 9 49 48 13 -2 6 10 91 103 9

6	13	5	95	83	47	4	14	6	302	335	33	-1	3	8	251	250	8	3	4	9	292	304	6	0	6	10	0	29	1
-3	14	5	31	56	31	0	1	7	467	439	7	1	3	8	281	301	7	-4	5	9	36	52	31	2	6	10	482	493	10
-1	14	5	106	107	23	-1	2	7	803	845	24	3	3	8	202	205	6	-2	5	9	467	475	13	4	6	10	40	32	40
1	14	5	105	95	22	-2	3	7	522	547	14	-2	4	8	147	151	4	0	5	9	811	809	19	6	6	10	12	12	11
3	14	5	72	63	71	0	3	7	391	406	14	0	4	8	231	238	8	2	5	9	221	241	5	-5	7	10	89	125	17
1	1	6	65	51	5	2	3	7	26	31	26	2	4	8	166	171	4	4	5	9	547	545	14	-3	7	10	0	7	1
0	2	6	419	413	12	-3	4	7	140	140	4	4	4	8	221	215	7	-5	6	9	245	246	9	-1	7	10	236	244	8
2	2	6	256	259	5	-1	4	7	157	137	5	-3	5	8	176	191	4	-3	6	9	242	251	7	1	7	10	338	348	8
1	3	6	492	467	10	1	4	7	110	118	5	-1	5	8	205	204	5	-1	6	9	218	221	8	3	7	10	0	2	1
3	3	6	259	245	6	3	4	7	148	165	4	1	5	8	204	199	6	1	6	9	243	250	6	5	7	10	395	409	16
-2	4	6	72	65	6	-4	5	7	196	211	5	3	5	8	290	295	5	3	6	9	305	319	4	7	7	10	97	103	18
0	4	6	552	549	12	-2	5	7	72	96	7	5	5	8	151	161	6	5	6	9	283	272	11	-6	8	10	115	136	15
4	4	6	38	45	18	0	5	7	129	137	5	-4	6	8	400	399	12	-6	7	9	482	474	23	-4	8	10	178	181	8
-3	5	6	323	319	6	2	5	7	555	548	11	-2	6	8	64	72	9	-4	7	9	516	508	16	-2	8	10	317	317	9
-1	5	6	145	143	7	4	5	7	800	765	21	0	6	8	245	258	6	-2	7	9	545	535	13	0	8	10	125	143	9
1	5	6	45	20	12	-5	6	7	144	145	6	2	6	8	89	103	8	0	7	9	198	192	8	2	8	10	43	27	43
3	5	6	268	267	7	-3	6	7	54	64	12	4	6	8	63	63	14	2	7	9	43	47	27	4	8	10	159	164	8
5	5	6	1458	1444	47	-1	6	7	66	76	11	6	6	8	201	191	13	4	7	9	79	88	13	6	8	10	0	30	1
-4	6	6	689	679	12	1	6	7	390	388	7	-5	7	8	88	82	13	6	7	9	228	203	11	8	8	10	361	352	29
-2	6	6	321	308	7	3	6	7	78	86	10	-3	7	8	27	25	26	-7	8	9	267	252	14	-7	9	10	195	217	13
0	6	6	555	543	11	5	6	7	551	515	19	-1	7	8	246	238	8	-5	8	9	303	302	10	-5	9	10	328	340	17
2	6	6	562	568	9	-6	7	7	57	72	23	1	7	8	103	116	8	-3	8	9	692	672	14	-3	9	10	471	463	9
4	6	6	275	278	8	-4	7	7	321	313	7	3	7	8	0	23	1	-1	8	9	509	511	14	-1	9	10	266	257	8
6	6	6	56	62	20	-2	7	7	351	351	9	5	7	8	126	118	8	1	8	9	362	370	8	1	9	10	413	417	7
-5	7	6	292	303	7	0	7	7	855	866	18	7	7	8	207	191	13	3	8	9	124	146	9	3	9	10	143	159	10
-3	7	6	185	190	6	2	7	7	268	255	4	-6	8	8	120	143	14	5	8	9	225	217	10	5	9	10	128	140	13
-1	7	6	10	19	10	4	7	7	62	70	16	-4	8	8	39	36	39	7	8	9	51	48	50	7	9	10	376	360	29
1	7	6	1413	146	20	6	7	7	32	12	32	-2	8	8	127	148	10	-8	9	9	213	204	14	9	9	10	162	159	21
3	7	6	509	504	9	-7	8	7	205	203	14	0	8	8	286	291	6	-6	9	9	408	412	21	-8	10	10	60	39	60
5	7	6	197	181	10	-5	8	7	58	51	23	2	8	8	390	376	7	-4	9	9	44	57	44	-6	10	10	202	200	11
-4	10	10	0	28	1	0	11	11	92	93	19	1	13	12	260	259	16	-4	6	14	52	48	39	-6	9	15	73	88	34
-2	10	10	227	233	8	2	11	11	137	139	14	3	13	12	90	88	47	-2	6	14	142	153	7	-4	9	15	105	115	22
0	10	10	91	114	17	4	11	11	82	68	27	0	1	13	677	677	5	0	6	14	52	33	22	-2	9	15	23	17	22
2	10	10	86	84	18	6	11	11	121	116	22	-1	2	13	118	122	5	2	6	14	74	80	14	0	9	15	279	296	12
4	10	10	264	271	8	-5	12	11	68	96	67	1	2	13	226	213	4	4	6	14	124	123	9	2	9	15	112	115	15
6	10	10	153	177	16	-3	12	11	75	97	34	-2	3	13	100	111	8	6	6	14	24	58	24	4	9	15	137	156	13
8	10	10	72	81	72	-1	12	11	196	192	12	0	3	13	124	129	6	-5	7	14	14	49	14	6	9	15	152	178	15
-7	11	10	428	449	25	1	12	11	61	50	51	2	3	13	188	205	5	-3	7	14	103	102	12	8	9	15	103	99	26
-5	11	10	146	162	17	3	12	11	102	96	22	-3	4	13	223	229	5	-1	7	14	294	289	9	-7	10	15	244	235	19
-3	11	10	154	168	13	5	12	11	54	37	54	-1	4	13	234	226	6	1	7	14	140	145	9	-5	10	15	165	159	14
-1	11	10	209	208	9	-4	13	11	0	86	1	1	4	13	831	837	17	3	7	14	0	27	1	-3	10	15	409	395	24
1	11	10	37	34	37	-2	13	11	40	10	39	3	4	13	352	366	5	5	7	14	257	266	9	-1	10	15	119	131	15
3	11	10	325	339	10	0	13	11	104	92	23	-4	5	13	273	274	8	7	7	14	92	98	22	1	10	15	263	275	12
5	11	10	21	34	21	2	13	11	191	211	13	-2	5	13	826	829	25	-6	8	14	58	75	58	3	10	15	45	10	44
7	11	10	272	265	26	4	13	11	72	70	72	0	5	13	216	215	7	-4	8	14	93	82	23	5	10	15	0	17	1
-6	12	10	124	130	25	0	0	12	154	162	21	2	5	13	479	483	11	-2	8	14	59	49	26	7	10	15	408	340	44
-4	12	10	262	275	12	1	1	12	351	361	4	4	5	13	160	171	7	0	8	14	0	42	1	-6	11	15	181	195	22
-2	12	10	232	232	12	0	2	12	50	49	16	-5	6	13	329	328	18	2	8	14	83	84	17	-4	11	15	347	335	22
0	12	10	131	146	16	2	2	12	312	315	4	-3	6	13	646	662	29	4	8	14	228	229	10	-2	11	15	133	145	17

supplementary materials

2	12	10	323	327	9	-1	3	12	175	192	5	-1	6	13	229	235	8	6	8	14	30	33	29	0	11	15	164	189	13
4	12	10	51	51	51	1	3	12	434	426	7	1	6	13	23	12	23	8	8	14	69	88	45	2	11	15	79	86	30
6	12	10	127	118	23	3	3	12	649	680	10	3	6	13	199	204	6	-7	9	14	149	151	17	4	11	15	0	19	1
-5	13	10	55	12	55	-2	4	12	126	141	6	5	6	13	151	170	8	-5	9	14	246	248	26	6	11	15	81	123	81
-3	13	10	63	63	62	0	4	12	161	170	5	-6	7	13	778	748	51	-3	9	14	82	80	21	-3	12	15	37	65	37
-1	13	10	380	392	13	2	4	12	1417	508	25	-4	7	13	261	256	15	-1	9	14	0	8	1	-1	12	15	112	131	22
1	13	10	146	153	18	4	4	12	200	222	7	-2	7	13	167	174	8	1	9	14	22	51	21	1	12	15	128	130	20
3	13	10	261	250	11	-3	5	12	302	325	10	0	7	13	282	287	9	3	9	14	50	44	50	3	12	15	385	413	22
5	13	10	214	241	25	-1	5	12	455	452	11	2	7	13	151	155	7	5	9	14	123	140	15	0	0	16	525	498	10
0	1	11	48	35	11	1	5	12	112	113	7	4	7	13	44	58	43	7	9	14	28	26	27	1	1	16	259	259	5
-1	2	11	76	96	7	3	5	12	440	457	10	6	7	13	369	371	14	9	9	14	0	5	1	0	2	16	261	267	6
1	2	11	36	19	20	5	5	12	35	38	35	-7	8	13	592	561	48	-8	10	14	110	65	35	2	2	16	63	57	15
-2	3	11	66	65	11	-4	6	12	115	121	10	-5	8	13	42	57	41	-6	10	14	93	110	37	-1	3	16	66	69	14
0	3	11	136	146	5	-2	6	12	1002	1048	5	-3	8	13	192	190	8	-4	10	14	34	27	33	1	3	16	21	45	21
2	3	11	482	477	8	0	6	12	529	523	17	-1	8	13	210	210	8	-2	10	14	72	71	26	3	3	16	311	319	5
-3	4	11	298	298	9	2	6	12	274	278	5	1	8	13	400	409	10	0	10	14	75	81	24	-2	4	16	470	455	7
-1	4	11	27	36	27	4	6	12	100	99	11	3	8	13	780	776	21	2	10	14	74	87	27	0	4	16	360	360	6
1	4	11	111	130	7	6	6	12	123	142	12	5	8	13	138	132	12	4	10	14	81	84	25	2	4	16	110	121	9
3	4	11	32	44	31	-5	7	12	71	82	23	7	8	13	44	46	43	6	10	14	92	77	32	4	4	16	100	115	12
-4	5	11	344	348	11	-3	7	12	112	123	11	-8	9	13	317	288	30	8	10	14	161	119	55	-3	5	16	117	118	10
-2	5	11	59	74	13	-1	7	12	444	452	13	-6	9	13	49	58	49	-5	11	14	103	41	24	-1	5	16	509	495	15
0	5	11	279	279	9	1	7	12	47	51	28	-4	9	13	81	85	26	-3	11	14	60	48	59	1	5	16	0	7	1
2	5	11	32	55	31	3	7	12	159	180	7	-2	9	13	160	172	10	-1	11	14	32	20	32	3	5	16	381	383	7
4	5	11	177	184	6	5	7	12	667	653	22	0	9	13	404	401	8	1	11	14	303	306	12	5	5	16	16	31	15
-5	6	11	130	127	13	7	7	12	55	60	55	2	9	13	332	334	11	3	11	14	55	45	55	-4	6	16	315	320	18
-3	6	11	45	53	24	-6	8	12	649	626	43	4	9	13	99	93	17	5	11	14	52	85	52	-2	6	16	122	133	10
-1	6	11	212	219	7	-4	8	12	48	54	48	6	9	13	126	152	17	-4	12	14	41	73	41	0	6	16	105	118	12
1	6	11	215	215	7	-2	8	12	17	5	16	8	9	13	99	97	26	-2	12	14	31	11	30	2	6	16	678	666	15
3	6	11	181	193	6	0	8	12	86	103	13	-7	10	13	41	46	40	0	12	14	0	9	1	4	6	16	147	161	9
5	6	11	79	87	14	2	8	12	48	8	35	-5	10	13	252	243	20	2	12	14	15	58	14	6	6	16	14	49	13
-6	7	11	39	46	39	4	8	12	1145	1134	30	-3	10	13	238	238	12	4	12	14	57	31	56	-5	7	16	61	91	44
-4	7	11	133	133	10	6	8	12	233	242	17	-1	10	13	618	618	18	0	1	15	405	393	4	-3	7	16	96	102	16
-2	7	11	0	11	1	8	8	12	78	98	31	1	10	13	347	359	9	-1	2	15	52	64	18	-1	7	16	151	159	12
0	7	11	456	441	16	-7	9	12	27	34	26	3	10	13	33	14	33	1	2	15	709	708	5	1	7	16	17	9	16
2	7	11	92	96	10	-5	9	12	466	463	29	5	10	13	105	116	21	-2	3	15	0	20	1	3	7	16	40	30	39
4	7	11	278	277	7	-3	9	12	439	426	16	7	10	13	127	156	24	0	3	15	66	73	12	5	7	16	360	376	10
6	7	11	231	235	14	-1	9	12	287	287	11	-6	11	13	51	11	51	2	3	15	241	239	5	7	7	16	222	223	11
-7	8	11	76	73	28	1	9	12	499	511	10	-4	11	13	426	414	23	-3	4	15	547	547	12	-6	8	16	350	334	24
-5	8	11	114	126	14	3	9	12	67	87	24	-2	11	13	232	235	10	-1	4	15	82	72	11	-4	8	16	0	18	1
-3	8	11	94	104	15	5	9	12	45	48	44	0	11	13	35	19	35	1	4	15	285	300	5	-2	8	16	523	498	23
-1	8	11	109	123	12	7	9	12	263	218	33	2	11	13	14	32	14	3	4	15	69	83	15	0	8	16	93	86	16
1	8	11	5	30	5	9	9	12	86	88	33	4	11	13	309	290	10	-4	5	15	79	91	15	2	8	16	44	39	44
3	8	11	103	125	12	-8	10	12	94	87	28	6	11	13	113	104	32	-2	5	15	566	564	13	4	8	16	152	159	11
5	8	11	247	249	12	-6	10	12	442	423	34	-5	12	13	535	534	21	0	5	15	543	538	11	6	8	16	116	119	18
7	8	11	31	13	30	-4	10	12	87	123	22	-3	12	13	95	98	33	2	5	15	180	179	7	8	8	16	408	379	32
-8	9	11	28	31	28	-2	10	12	53	70	53	-1	12	13	66	59	46	4	5	15	301	317	8	-7	9	16	175	176	15
-6	9	11	276	261	21	0	10	12	588	600	14	1	12	13	249	238	13	-5	6	15	261	255	15	-5	9	16	248	239	21
-4	9	11	33	20	32	2	10	12	305	294	7	3	12	13	380	384	15	-3	6	15	83	87	16	-3	9	16	396	370	33
-2	9	11	73	70	20	4	10	12	87	81	21	5	12	13	632	613	54	-1	6	15	58	63	18	-1	9	16	298	282	24

0 9 11 61 80 27 6 10 12 205 195 16 -2 13 13 107 106 42 1 6 15 131 140 9 1 9 16 500 519 18
2 9 11 191 203 8 8 10 12 521 515 26 0 13 13 352 319 15 3 6 15 140 158 9 3 9 16 87 87 22
4 9 11 187 182 9 -7 11 12 362 326 47 2 13 13 77 39 77 5 6 15 343 359 12 5 9 16 124 122 17
6 9 11 74 91 26 -5 11 12 266 269 15 0 0 14 688 648 16 -6 7 15 583 570 34 7 9 16 95 122 28
8 9 11 179 162 20 -3 11 12 141 155 13 1 1 14 166 175 5 -4 7 15 299 303 18 -6 10 16 139 112 21
-9 10 11 90 83 58 -1 11 12 238 230 9 0 2 14 158 163 5 -2 7 15 68 71 21 -4 10 16 64 7 49
-7 10 11 145 151 16 1 11 12 497 503 10 2 2 14 14 22 14 0 7 15 22 26 21 -2 10 16 132 139 17
-5 10 11 44 49 44 3 11 12 198 203 12 -1 3 14 240 232 5 2 7 15 120 135 11 0 10 16 321 340 13
-3 10 11 76 97 22 5 11 12 90 84 29 1 3 14 86 91 8 4 7 15 112 118 11 2 10 16 77 76 27
-1 10 11 66 74 29 7 11 12 420 431 27 3 3 14 325 336 5 6 7 15 117 123 15 4 10 16 311 335 9
1 10 11 72 49 23 -6 12 12 0 23 1 -2 4 14 18 16 18 -7 8 15 32 57 31 6 10 16 292 291 15
3 10 11 54 46 46 -4 12 12 236 250 17 0 4 14 114 116 7 -5 8 15 48 56 47 -5 11 16 192 188 20
5 10 11 56 12 56 -2 12 12 342 345 10 2 4 14 394 393 6 -3 8 15 533 506 36 -3 11 16 97 124 25
7 10 11 76 25 51 0 12 12 91 81 24 4 4 14 50 50 23 -1 8 15 348 336 12 -1 11 16 66 71 46
9 10 11 149 153 35 2 12 12 30 5 29 -3 5 14 46 43 32 1 8 15 375 388 10 1 11 16 47 88 46
-8 11 11 88 82 46 4 12 12 241 251 11 -1 5 14 66 87 13 3 8 15 296 304 7 3 11 16 85 108 29
-6 11 11 6 40 6 6 12 12 372 394 23 1 5 14 153 155 6 5 8 15 42 52 41 5 11 16 145 149 31
-4 11 11 85 62 24 -3 13 12 487 482 38 3 5 14 108 121 10 7 8 15 7 41 7 -2 12 16 237 233 27
-2 11 11 70 71 27 -1 13 12 368 355 13 5 5 14 117 135 10 -8 9 15 77 85 39 0 12 16 206 224 18
2 12 16 245 228 18 -5 7 18 42 84 42 1 10 19 220 219 13 -3 8 21 318 298 28 3 8 23 0 57 1
0 1 17 134 141 9 -3 7 18 34 9 34 3 10 19 99 93 25 -1 8 21 168 164 15 0 0 24 930 911 29
-1 2 17 50 67 33 -1 7 18 93 97 18 0 11 19 335 334 14 1 8 21 0 46 1 1 1 24 238 243 11
1 2 17 447 456 5 1 7 18 705 700 23 0 0 20 197 185 17 3 8 21 170 195 13 0 2 24 61 82 44
-2 3 17 102 108 10 3 7 18 217 230 8 1 1 20 81 89 18 5 8 21 64 38 63 2 2 24 15 53 14
0 3 17 66 61 17 5 7 18 167 173 12 0 2 20 82 93 20 -4 9 21 103 86 102 -1 3 24 71 44 44
2 3 17 37 10 37 7 7 18 0 26 1 2 2 20 249 245 9 -2 9 21 90 68 34 1 3 24 234 216 11
-3 4 17 340 337 5 -6 8 18 219 204 14 -1 3 20 594 568 8 0 9 21 139 135 24 3 3 24 431 439 9
-1 4 17 277 267 7 -4 8 18 89 85 24 1 3 20 336 330 8 2 9 21 125 147 20 -2 4 24 151 173 15
1 4 17 22 18 21 -2 8 18 248 229 23 3 3 20 160 157 11 4 9 21 93 115 56 0 4 24 53 34 53
3 4 17 119 127 10 0 8 18 116 116 15 -2 4 20 121 119 14 -1 10 21 34 50 34 2 4 24 519 519 7
-4 5 17 59 60 27 2 8 18 482 482 18 0 4 20 249 235 8 1 10 21 109 75 37 4 4 24 0 21 1
-2 5 17 273 280 11 4 8 18 78 84 23 2 4 20 260 245 8 0 0 22 64 92 63 -3 5 24 113 89 25
0 5 17 339 345 10 6 8 18 17 28 17 4 4 20 79 85 25 1 1 22 214 214 9 -1 5 24 118 123 23
2 5 17 4 15 4 8 8 18 508 439 42 -3 5 20 92 115 18 0 2 22 110 113 16 1 5 24 218 204 11
4 5 17 209 206 7 -7 9 18 37 106 36 -1 5 20 92 95 18 2 2 22 0 8 1 3 5 24 159 137 15
-5 6 17 43 37 42 -5 9 18 51 55 50 1 5 20 109 111 17 -1 3 22 25 13 24 5 5 24 144 142 21
-3 6 17 97 100 15 -3 9 18 514 491 38 3 5 20 68 70 29 1 3 22 221 222 11 -4 6 24 129 144 24
-1 6 17 106 110 13 -1 9 18 97 116 22 5 5 20 558 539 23 3 3 22 318 311 10 -2 6 24 402 380 16
1 6 17 146 146 9 1 9 18 0 21 1 -4 6 20 85 68 25 -2 4 22 72 68 30 0 6 24 68 19 51
3 6 17 72 73 18 3 9 18 100 108 20 -2 6 20 0 45 1 0 4 22 155 155 12 2 6 24 86 76 28
5 6 17 126 136 12 5 9 18 86 118 29 0 6 20 372 374 11 2 4 22 89 66 21 4 6 24 18 4 18
-6 7 17 267 265 15 7 9 18 388 360 15 2 6 20 282 281 7 4 4 22 19 6 18 -3 7 24 131 141 45
-4 7 17 280 269 16 -4 10 18 81 97 38 4 6 20 17 59 17 -3 5 22 0 15 1 -1 7 24 554 488 45
-2 7 17 226 221 12 -2 10 18 527 489 55 6 6 20 42 46 41 -1 5 22 325 323 13 1 7 24 137 123 20
0 7 17 23 23 23 0 10 18 208 206 13 -5 7 20 63 75 62 1 5 22 73 68 29 3 7 24 60 25 60
2 7 17 52 50 40 2 10 18 165 174 14 -3 7 20 39 19 39 3 5 22 196 194 12 0 8 24 110 63 53
4 7 17 43 15 42 4 10 18 434 440 16 -1 7 20 7 57 6 5 5 22 103 103 27 0 1 25 222 233 11
6 7 17 56 29 55 -3 11 18 85 48 84 1 7 20 560 534 16 -4 6 22 363 346 19 -1 2 25 0 19 1
-7 8 17 74 77 38 -1 11 18 72 38 45 3 7 20 105 125 17 -2 6 22 0 16 1 1 2 25 33 36 33

supplementary materials

-5 8 17 166 157 16 1 11 18 48 26 47 5 7 20 122 117 18 0 6 22 134 136 16 -2 3 25 198 197 13
-3 8 17 390 368 29 3 11 18 353 363 16 7 7 20 95 108 33 2 6 22 348 320 12 0 3 25 87 93 27
-1 8 17 289 275 18 0 1 19 94 87 14 -6 8 20 23 11 23 4 6 22 80 84 31 2 3 25 283 279 10
1 8 17 74 87 21 -1 2 19 737 707 8 -4 8 20 136 135 18 6 6 22 91 62 34 -3 4 25 68 47 54
3 8 17 29 68 28 1 2 19 187 184 9 -2 8 20 96 88 33 -5 7 22 149 146 20 -1 4 25 421 416 16
5 8 17 129 125 16 -2 3 19 642 631 8 0 8 20 131 130 15 -3 7 22 99 95 29 1 4 25 624 588 12
7 8 17 147 134 17 0 3 19 320 325 7 2 8 20 216 220 10 -1 7 22 266 248 20 3 4 25 150 167 18
-6 9 17 200 197 24 2 3 19 225 229 8 4 8 20 294 293 16 1 7 22 112 103 24 -4 5 25 59 71 59
-4 9 17 0 24 1 -3 4 19 118 129 13 6 8 20 79 60 43 3 7 22 0 17 1 -2 5 25 383 358 10
-2 9 17 146 155 16 -1 4 19 336 334 6 -5 9 20 89 62 88 5 7 22 384 339 22 0 5 25 72 51 50
0 9 17 90 71 22 1 4 19 3 26 2 -3 9 20 208 172 18 -4 8 22 224 226 22 2 5 25 158 149 16
2 9 17 40 49 39 3 4 19 77 78 22 -1 9 20 81 70 31 -2 8 22 240 226 20 4 5 25 72 27 59
4 9 17 269 275 11 -4 5 19 2 35 2 1 9 20 100 95 24 0 8 22 24 39 23 -3 6 25 455 467 17
6 9 17 31 69 30 -2 5 19 124 135 12 3 9 20 35 39 34 2 8 22 51 32 50 -1 6 25 160 152 22
-5 10 17 111 104 22 0 5 19 107 112 13 5 9 20 204 210 15 4 8 22 151 183 18 1 6 25 67 36 66
-3 10 17 35 55 35 2 5 19 229 228 8 -2 10 20 190 178 25 -1 9 22 159 172 39 3 6 25 103 112 30
-1 10 17 51 32 50 4 5 19 803 785 24 0 10 20 0 12 1 1 9 22 383 368 21 0 7 25 122 44 46
1 10 17 74 91 33 -5 6 19 57 45 56 2 10 20 155 157 17 3 9 22 193 196 24 0 0 26 971 926 12
3 10 17 64 54 42 -3 6 19 163 178 12 0 1 21 24 27 23 0 1 23 108 115 16 1 1 26 0 14 1
5 10 17 87 103 35 -1 6 19 52 48 51 -1 2 21 254 240 8 -1 2 23 0 32 1 0 2 26 53 58 53
-4 11 17 129 105 31 1 6 19 341 340 7 1 2 21 230 238 10 1 2 23 555 536 7 2 2 26 103 78 24
-2 11 17 125 153 22 3 6 19 198 201 9 -2 3 21 198 178 10 -2 3 23 41 34 41 -1 3 26 211 200 14
0 11 17 247 254 16 5 6 19 489 486 19 0 3 21 254 246 8 0 3 23 109 126 17 1 3 26 228 235 12
2 11 17 82 93 29 -6 7 19 167 165 17 2 3 21 316 289 8 2 3 23 20 49 19 3 3 26 207 220 15
4 11 17 92 101 45 -4 7 19 263 247 13 -3 4 21 357 363 10 -3 4 23 459 446 15 -2 4 26 78 73 40
0 0 18 113 111 23 -2 7 19 287 263 22 -1 4 21 109 104 16 -1 4 23 21 20 20 0 4 26 63 63 63
1 1 18 40 57 39 0 7 19 532 519 21 1 4 21 161 162 13 1 4 23 44 50 44 4 4 26 95 93 49
0 2 18 393 400 6 2 7 19 325 316 10 3 4 21 94 109 21 3 4 23 27 51 27 -3 5 26 309 304 21
2 2 18 41 80 41 4 7 19 146 146 12 -4 5 21 352 353 13 -4 5 23 156 149 18 -1 5 26 0 20 1
-1 3 18 100 98 12 6 7 19 228 219 12 -2 5 21 143 159 14 -2 5 23 239 232 14 1 5 26 78 84 38
1 3 18 163 168 8 -7 8 19 115 114 27 0 5 21 359 359 13 0 5 23 461 445 18 3 5 26 0 24 1
3 3 18 205 212 7 -5 8 19 18 6 18 2 5 21 173 175 11 2 5 23 40 13 40 0 6 26 252 212 40
-2 4 18 167 174 9 -3 8 19 628 572 49 4 5 21 335 328 9 4 5 23 146 157 16 0 1 27 70 104 56
0 4 18 531 503 10 -1 8 19 245 236 12 -5 6 21 218 208 11 -5 6 23 256 240 13 -1 2 27 53 27 53
2 4 18 98 96 15 1 8 19 131 138 14 -3 6 21 0 16 1 -3 6 23 89 84 33 1 2 27 105 123 25
4 4 18 141 151 10 3 8 19 20 25 19 -1 6 21 8 9 7 -1 6 23 24 44 23 -2 3 27 0 23 1
-3 5 18 92 99 15 5 8 19 55 62 54 1 6 21 333 312 11 1 6 23 55 5 55 0 3 27 27 36 27
-1 5 18 33 38 32 7 8 19 118 81 28 3 6 21 306 295 12 3 6 23 185 169 13 2 3 27 301 291 11
1 5 18 118 115 11 -6 9 19 279 272 14 5 6 21 14 10 13 5 6 23 307 281 13 -1 4 27 49 51 49
3 5 18 57 54 25 -4 9 19 616 544 53 -6 7 21 228 220 16 -4 7 23 307 267 26 1 4 27 142 146 23
5 5 18 685 686 24 -2 9 19 164 166 31 -4 7 21 201 207 23 -2 7 23 145 146 21 0 0 28 205 162 35
-4 6 18 547 531 26 0 9 19 97 90 23 -2 7 21 222 208 16 0 7 23 34 9 33 1 1 28 0 52 1
-2 6 18 226 226 12 2 9 19 187 179 14 0 7 21 451 437 20 2 7 23 177 177 16 0 2 28 122 153 37
0 6 18 124 117 12 4 9 19 363 389 11 2 7 21 85 67 24 4 7 23 54 16 53 2 2 28 168 158 25
2 6 18 449 444 13 6 9 19 737 664 32 4 7 21 98 109 23 -3 8 23 238 267 45
4 6 18 22 29 22 -3 10 19 75 30 71 6 7 21 146 158 22 -1 8 23 328 281 25
6 6 18 231 222 11 -1 10 19 147 152 16 -5 8 21 87 78 35 1 8 23 340 310 19

Fig. 1

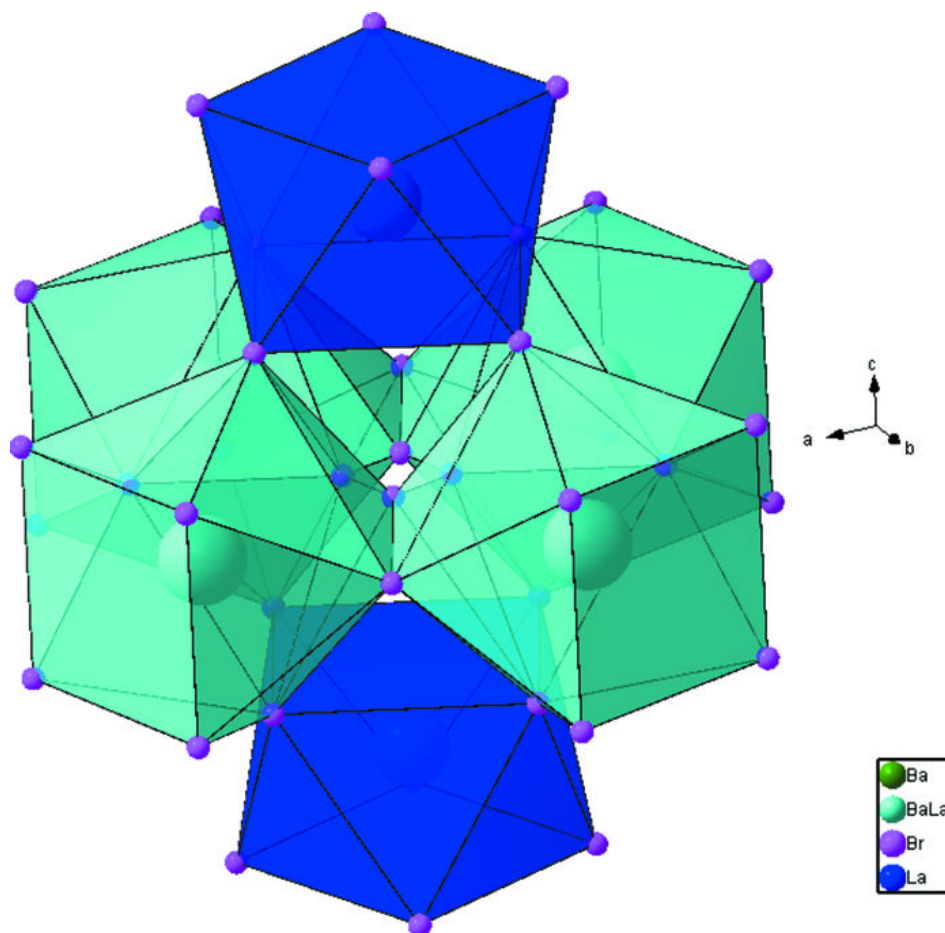


Fig. 2

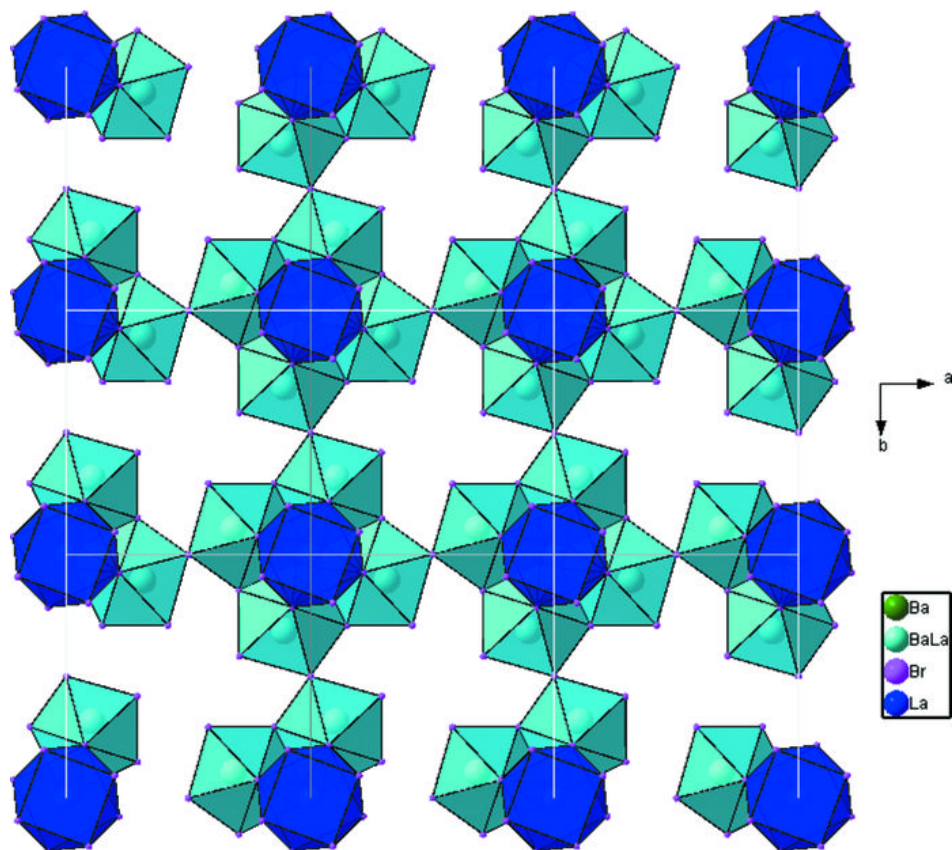


Fig. 3

