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$Ba_{11}La_4Br_{34}$: a new barium lanthanum bromide

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Key indicators: single-crystal X-ray study; T = 150 K; mean σ(La–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 \=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 $BaBr_8$ square prisms and $BaBr_{10}$ 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

$Ba_{11}La_4Br_{34}$	Z = 2
M_r = 4783.10	Mo $K\alpha$ radiation
Tetragonal, $I4/m$	μ = 30.05 mm^{-1}
a = 11.909 (3) Å	T = 150 K
c = 22.888 (5) Å	0.25 × 0.15 × 0.1 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_{int} = 0.168

Refinement

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

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

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S1. 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, $Ba_{11}La_4Br_{34}$, 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).

$Ba_{11}La_4Br_{34}$ 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 $[M_6ZX_{36}]$ polyhedral clusters (Meyer & Wickleder 2000). There is some confusion about whether the interstitial atom, *Z*, is a halide or an oxide.

In $Ba_{11}La_4Br_{34}$, n = 15 following the $M_{15}X_{35}$ = MZX_{34} 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, $[M_6ZX_{36}]$ polyhedral clusters consist of six corner sharing MX_8 square antiprisms whose metals are arranged in an octahedral geometry and the *Z* atom occupies the octahedral site. In the case of $Ba_{11}La_4Br_{34}$, the clusters consist of four edge sharing Ba(3)/La(1)Br_{10} groups and capped by two La(2)Br_8 square antiprisms having a $[(Ba(3)/La(1))_4La(2)_2Br_{16}Br_{40/2}]$ 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.

S2. Experimental

Small crystals of $Ba_{11}La_4Br_{34}$ 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.

S3. Refinement

(type here to add refinement details)

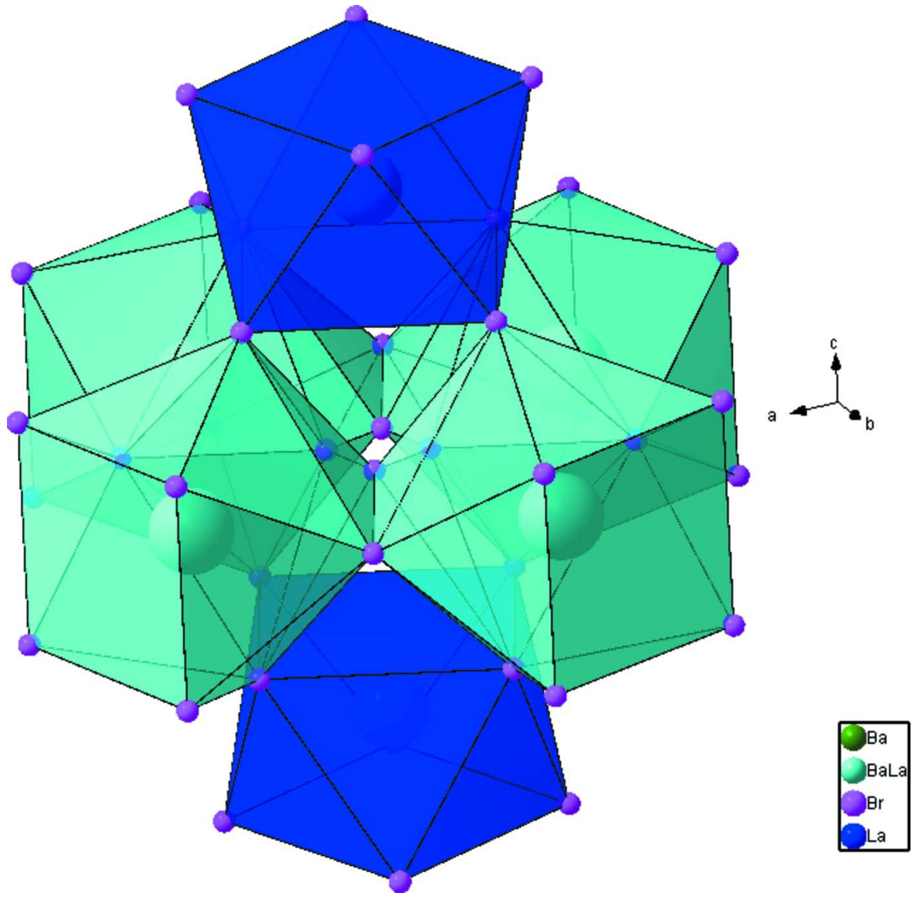

Figure 1

Representation of [{(Ba/La)6La4Br36}] polyhedral cluster

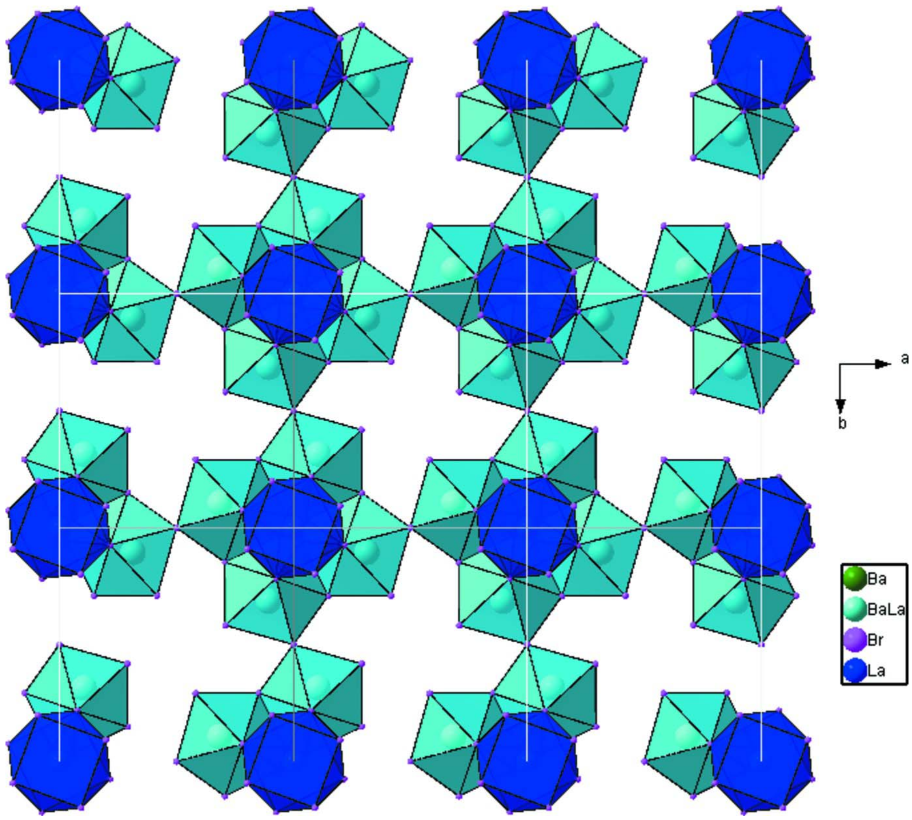

Figure 2

Connectivity of [{(Ba/La)6La4Br36}] polyhedral cluster along a-b plane

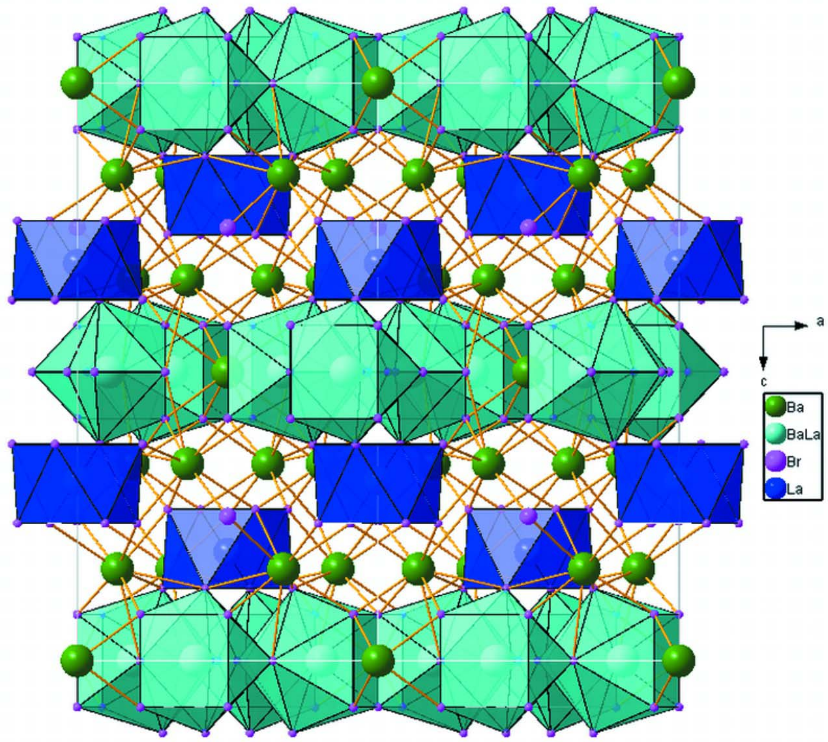

Figure 3

Structure of Ba11La4Br34viewing along (010) axis

undecabarium tetralanthanum tetratricontabromide

Crystal data

$Ba_{11}La_4Br_{34}$
$M_r = 4783.10$
Tetragonal, $I4/m$
$a = 11.909$ (3) Å
$c = 22.888$ (5) Å
$V = 3246.2$ (10) Å^3
$Z = 2$
$F(000) = 4068$
$D_x = 4.894$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 119 reflections
$\theta = 12.9$–37.1°
$\mu = 30.05$ mm^{-1}
$T = 150$ K
Block, colorless
0.25 × 0.15 × 0.1 mm

Data collection

Bruker SMART1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.141$, $T_{max} = 0.403$
12169 measured reflections
1687 independent reflections
1193 reflections with $I > 2\sigma(I)$
$R_{int} = 0.168$
$\theta_{max} = 26.4°$, $\theta_{min} = 1.9°$
$h = -14 \rightarrow 14$
$k = -14 \rightarrow 14$
$l = -28 \rightarrow 28$

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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.100$
$\Delta\rho_{max} = 5.72$ e Å^{-3}
$\Delta\rho_{min} = -3.31$ e Å^{-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 (Å^2)

	x	y	z	U_{iso}*/U_{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
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 (Å^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 (Å, º)

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)
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)
Br1^{ii}—Ba2—Br5^{ix}	125.90 (4)
Br1—Ba2—Br5^{ix}	63.14 (3)
Br2—Ba2—Br5^{ix}	130.45 (3)
Br4—Ba2—Br5^{ix}	144.17 (4)
Br3—Ba2—Br5^{x}	63.25 (3)
Br4^{viii}—Ba2—Br5^{x}	64.40 (3)
Br4^{iii}—Ba2—Br5^{x}	132.90 (4)
Br1^{ii}—Ba2—Br5^{x}	125.20 (4)
Br1—Ba2—Br5^{x}	116.55 (4)
Br2—Ba2—Br5^{x}	79.13 (3)
Br4—Ba2—Br5^{x}	144.49 (4)
Br5^{ix}—Ba2—Br5^{x}	64.33 (5)
Br3—Ba2—Br6A^{xi}	60.17 (4)
Br4^{viii}—Ba2—Br6A^{xi}	120.71 (6)
Br4^{iii}—Ba2—Br6A^{xi}	124.53 (5)
Br1^{ii}—Ba2—Br6A^{xi}	73.22 (5)
Br1—Ba2—Br6A^{xi}	61.85 (4)
Br2—Ba2—Br6A^{xi}	128.40 (4)
Br4—Ba2—Br6A^{xi}	136.16 (5)
Br5^{ix}—Ba2—Br6A^{xi}	64.89 (5)
Br5^{x}—Ba2—Br6A^{xi}	65.31 (5)
Br6A^{xii}—Ba3—Br6A	133.19 (11)
Br6A^{xii}—Ba3—Br5^{xiii}	80.78 (4)
Br6A—Ba3—Br5^{xiii}	81.22 (4)
Br6A^{xii}—Ba3—Br5^{xiv}	80.78 (4)
Br6A—Ba3—Br5^{xiv}	81.22 (4)
Br5^{xiii}—Ba3—Br5^{xiv}	133.61 (7)
Br6A^{xii}—Ba3—Br1^{ii}	74.74 (6)
Br6A—Ba3—Br1^{ii}	137.40 (4)
Br5^{xiii}—Ba3—Br1^{ii}	140.84 (5)
Br5^{xiv}—Ba3—Br1^{ii}	71.89 (4)
Br6A^{xii}—Ba3—Br1^{i}	74.74 (6)
Br6A—Ba3—Br1^{i}	137.40 (4)
Br5^{xiii}—Ba3—Br1^{i}	71.89 (4)
Br5^{xiv}—Ba3—Br1^{i}	140.84 (5)
Br1^{ii}—Ba3—Br1^{i}	72.44 (5)
Br6A^{xii}—Ba3—Br3	140.27 (4)
Br6A—Ba3—Br3	70.23 (5)
Br5^{xiii}—Ba3—Br3	138.90 (5)
Br5^{xiv}—Ba3—Br3	71.25 (4)
Br1^{ii}—Ba3—Br3	70.13 (3)
Br1^{i}—Ba3—Br3	110.56 (5)
Br6A^{xii}—Ba3—Br3^{xi}	140.27 (4)
Br6A—Ba3—Br3^{xi}	70.23 (5)
Br5^{xiii}—Ba3—Br3^{xi}	71.25 (4)
Br5^{xiv}—Ba3—Br3^{xi}	138.90 (5)
Br1^{ii}—Ba3—Br3^{xi}	110.56 (5)
Ba3^{xviii}—Br5—Ba2^{x}	96.46 (4)
Ba2^{xix}—Br5—Ba2^{x}	145.74 (5)
La1^{xv}—Br6A—Ba3^{xv}	0.00 (5)
La1^{xv}—Br6A—Ba3	136.81 (11)
Ba3^{xv}—Br6A—Ba3	136.81 (11)
La1^{xv}—Br6A—Ba2^{xvi}	95.61 (4)
Ba3^{xv}—Br6A—Ba2^{xvi}	95.61 (4)
Ba3—Br6A—Ba2^{xvi}	95.48 (4)
La1^{xv}—Br6A—Ba2^{xi}	95.61 (4)
Ba3^{xv}—Br6A—Ba2^{xi}	95.61 (4)
Ba3—Br6A—Ba2^{xi}	95.48 (4)
Ba2^{xvi}—Br6A—Ba2^{xi}	149.57 (9)
Br6B^{xii}—Br6B—Br6B^{xv}	90.000 (7)
Br6B^{xii}—Br6B—Br6B^{xx}	45.000 (3)
Br6B^{xv}—Br6B—Br6B^{xx}	45.000 (9)
Br6B^{xii}—Br6B—Ba3	174.7 (13)
Br6B^{xv}—Br6B—Ba3	84.7 (13)
Br6B^{xx}—Br6B—Ba3	129.7 (13)
Br6B^{xii}—Br6B—La1^{xii}	76.8 (13)
Br6B^{xv}—Br6B—La1^{xii}	166.8 (13)
Br6B^{xx}—Br6B—La1^{xii}	121.8 (13)
Ba3—Br6B—La1^{xii}	108.5 (3)
Br6B^{xii}—Br6B—Ba3^{xii}	76.8 (13)
Br6B^{xv}—Br6B—Ba3^{xii}	166.8 (13)
Br6B^{xx}—Br6B—Ba3^{xii}	121.8 (13)
Ba3—Br6B—Ba3^{xii}	108.5 (3)
La1^{xii}—Br6B—Ba3^{xii}	0.00 (3)
Br5—La2—Br5^{vi}	124.10 (7)
Br5—La2—Br5^{ii}	77.31 (3)
Br5^{vi}—La2—Br5^{ii}	77.31 (3)
Br5—La2—Br5^{iii}	77.31 (3)
Br5^{vi}—La2—Br5^{iii}	77.31 (3)
Br5^{ii}—La2—Br5^{iii}	124.10 (7)
Br5—La2—Br4	140.14 (3)
Br5^{vi}—La2—Br4	75.01 (4)
Br5^{ii}—La2—Br4	73.67 (4)
Br5^{iii}—La2—Br4	142.20 (4)
Br5—La2—Br4^{iii}	73.67 (4)
Br5^{vi}—La2—Br4^{iii}	142.20 (3)
Br5^{ii}—La2—Br4^{iii}	75.01 (4)
Br5^{iii}—La2—Br4^{iii}	140.14 (4)
Br4—La2—Br4^{iii}	72.85 (3)
Br5—La2—Br4^{ii}	142.20 (3)
Br5^{vi}—La2—Br4^{ii}	73.67 (4)
Br5^{ii}—La2—Br4^{ii}	140.14 (4)
Br5^{iii}—La2—Br4^{ii}	75.01 (4)
Br4—La2—Br4^{ii}	72.85 (3)
Br4^{iii}—La2—Br4^{ii}	114.21 (6)

Br1^{i}—Ba3—Br3^{xi}	70.13 (3)
Br3—Ba3—Br3^{xi}	71.57 (6)
Br6A^{xii}—Ba3—Br6B	58.0 (2)
Br6A—Ba3—Br6B	75.1 (2)
Br5^{xiii}—Ba3—Br6B	67.04 (4)
Br5^{xiv}—Ba3—Br6B	67.04 (4)
Br1^{ii}—Ba3—Br6B	120.51 (17)
Br1^{i}—Ba3—Br6B	120.51 (17)
Br5—La2—Br4^{vi}	75.01 (4)
Br5^{vi}—La2—Br4^{vi}	140.14 (3)
Br5^{ii}—La2—Br4^{vi}	142.20 (4)
Br5^{iii}—La2—Br4^{vi}	73.67 (4)
Br4—La2—Br4^{vi}	114.21 (6)
Br4^{iii}—La2—Br4^{vi}	72.85 (3)
Br4^{ii}—La2—Br4^{vi}	72.85 (3)

Br1^{i}—Ba1—Br1—La1^{iii}	53.75 (5)
Br1^{ii}—Ba1—Br1—La1^{iii}	113.02 (6)
Br1^{iii}—Ba1—Br1—La1^{iii}	−126.25 (5)
Br1^{iv}—Ba1—Br1—La1^{iii}	−41 (100)
Br1^{v}—Ba1—Br1—La1^{iii}	−6.61 (5)
Br1^{vi}—Ba1—Br1—La1^{iii}	173.39 (5)
Br1^{vii}—Ba1—Br1—La1^{iii}	−66.98 (6)
Br1^{i}—Ba1—Br1—Ba3^{iii}	53.75 (5)
Br1^{ii}—Ba1—Br1—Ba3^{iii}	113.02 (6)
Br1^{iii}—Ba1—Br1—Ba3^{iii}	−126.25 (5)
Br1^{iv}—Ba1—Br1—Ba3^{iii}	−41 (100)
Br1^{v}—Ba1—Br1—Ba3^{iii}	−6.61 (5)
Br1^{vi}—Ba1—Br1—Ba3^{iii}	173.39 (5)
Br1^{vii}—Ba1—Br1—Ba3^{iii}	−66.98 (6)
Br1^{i}—Ba1—Br1—Ba2^{iii}	175.49 (4)
Br1^{ii}—Ba1—Br1—Ba2^{iii}	−125.24 (2)
Br1^{iii}—Ba1—Br1—Ba2^{iii}	−4.51 (4)
Br1^{iv}—Ba1—Br1—Ba2^{iii}	81 (100)
Br1^{v}—Ba1—Br1—Ba2^{iii}	115.12 (3)
Br1^{vi}—Ba1—Br1—Ba2^{iii}	−64.88 (3)
Br1^{vii}—Ba1—Br1—Ba2^{iii}	54.76 (2)
Br1^{i}—Ba1—Br1—Ba2	−54.85 (2)
Br1^{ii}—Ba1—Br1—Ba2	4.42 (4)
Br1^{iii}—Ba1—Br1—Ba2	125.15 (2)
Br1^{iv}—Ba1—Br1—Ba2	−150 (100)
Br1^{v}—Ba1—Br1—Ba2	−115.21 (3)
Br1^{vi}—Ba1—Br1—Ba2	64.79 (3)
Br1^{vii}—Ba1—Br1—Ba2	−175.58 (4)
Br3—Ba2—Br1—La1^{iii}	−69.57 (4)
Br4^{viii}—Ba2—Br1—La1^{iii}	74.96 (5)
Br4^{iii}—Ba2—Br1—La1^{iii}	128.07 (4)
Br1^{ii}—Ba2—Br1—La1^{iii}	−118.64 (4)
Br2—Ba2—Br1—La1^{iii}	−170.37 (10)
Br4—Ba2—Br1—La1^{iii}	−174.58 (4)
Br5^{ix}—Ba2—Br1—La1^{iii}	38.07 (4)
Br5^{x}—Ba2—Br1—La1^{iii}	0.80 (5)
Br6A^{xi}—Ba2—Br1—La1^{iii}	−36.35 (5)
Br3—Ba2—Br1—Ba3^{iii}	−69.57 (4)
Br4^{viii}—Ba2—Br1—Ba3^{iii}	74.96 (5)
Br5^{ix}—Ba2—Br3—Ba2^{xvi}	126.62 (4)
Br5^{x}—Ba2—Br3—Ba2^{xvi}	87.13 (3)
Br6A^{xi}—Ba2—Br3—Ba2^{xvi}	162.64 (5)
Br3—Ba2—Br4—La2	−174.93 (4)
Br4^{viii}—Ba2—Br4—La2	63.28 (6)
Br4^{iii}—Ba2—Br4—La2	−2.80 (5)
Br1^{ii}—Ba2—Br4—La2	−119.13 (5)
Br1—Ba2—Br4—La2	−59.75 (5)
Br2—Ba2—Br4—La2	121.51 (4)
Br5^{ix}—Ba2—Br4—La2	−4.45 (8)
Br5^{x}—Ba2—Br4—La2	127.37 (6)
Br6A^{xi}—Ba2—Br4—La2	−117.74 (7)
Br3—Ba2—Br4—Ba2^{xvii}	74.12 (5)
Br4^{viii}—Ba2—Br4—Ba2^{xvii}	−47.66 (4)
Br4^{iii}—Ba2—Br4—Ba2^{xvii}	−113.75 (4)
Br1^{ii}—Ba2—Br4—Ba2^{xvii}	129.92 (5)
Br1—Ba2—Br4—Ba2^{xvii}	−170.70 (4)
Br2—Ba2—Br4—Ba2^{xvii}	10.56 (3)
Br5^{ix}—Ba2—Br4—Ba2^{xvii}	−115.39 (6)
Br5^{x}—Ba2—Br4—Ba2^{xvii}	16.43 (8)
Br6A^{xi}—Ba2—Br4—Ba2^{xvii}	131.31 (6)
Br3—Ba2—Br4—Ba2^{ii}	−46.75 (5)
Br4^{viii}—Ba2—Br4—Ba2^{ii}	−168.54 (4)
Br4^{iii}—Ba2—Br4—Ba2^{ii}	125.38 (3)
Br1^{ii}—Ba2—Br4—Ba2^{ii}	9.05 (4)
Br1—Ba2—Br4—Ba2^{ii}	68.43 (4)
Br2—Ba2—Br4—Ba2^{ii}	−110.31 (4)
Br5^{ix}—Ba2—Br4—Ba2^{ii}	123.73 (5)
Br5^{x}—Ba2—Br4—Ba2^{ii}	−104.45 (7)
Br6A^{xi}—Ba2—Br4—Ba2^{ii}	10.44 (8)
Br6A^{xii}—Ba3—Br6A—La1^{xv}	0.0
Br5^{xiii}—Ba3—Br6A—La1^{xv}	−68.45 (3)
Br5^{xiv}—Ba3—Br6A—La1^{xv}	68.45 (3)
Br1^{ii}—Ba3—Br6A—La1^{xv}	119.19 (8)
Br1^{i}—Ba3—Br6A—La1^{xv}	−119.19 (8)
Br3—Ba3—Br6A—La1^{xv}	141.58 (3)
Br3^{xi}—Ba3—Br6A—La1^{xv}	−141.58 (3)
Br6B—Ba3—Br6A—La1^{xv}	0.0
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)
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*.