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Ba₄GaN₃O

Takayuki Hashimoto and Hisanori Yamane*

Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai, 980-8577, Japan

Correspondence e-mail: yamane@tagen.tohoku.ac.jp

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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{Ga-N}) = 0.008$ Å; R factor = 0.043; wR factor = 0.099; data-to-parameter ratio = 22.2.

Red transparent platelet-shaped single crystals of tetrabarium gallium trinitride oxide, Ba₄GaN₃O, were synthesized by the Na flux method. The crystal structure is isotypic with Sr₄GaN₃O, containing isolated triangular [GaN₃]⁶⁻ anionic groups. O²⁻ atoms are inserted between the slabs of [Ba₄GaN₃]²⁺, in which the [GaN₃]⁶⁻ groups are surrounded by Ba²⁺ atoms.

Related literature

For isotypic Sr₄GaN₃O, see: Mallinson *et al.* (2006). For the major phase in the product, Ba₃Ga₂N₄, see: Yamane & DiSalvo (1996). For compounds containing isolated triangular-planar [GaN₃]⁶⁻ nitridogallate anions, see: Park *et al.* (2003); Mallinson *et al.* (2006); Hintze & Schnick (2010). For details of Madelung site potential and energy calculations, see: O'Keeffe (1992); Orhan *et al.* (2002); Paszkowicz *et al.* (2004); Taylor (1984). For details of the synthetic procedure, see: Kowach *et al.* (1998).

Experimental

Crystal data

Ba ₄ GaN ₃ O	$V = 1586.14$ (12) Å ³
$M_r = 677.11$	$Z = 8$
Orthorhombic, <i>Pbca</i>	Mo $K\alpha$ radiation
$a = 7.8130$ (3) Å	$\mu = 22.84$ mm ⁻¹
$b = 25.6453$ (10) Å	$T = 293$ K
$c = 7.9162$ (4) Å	$0.18 \times 0.13 \times 0.07$ mm

Data collection

Rigaku R-AXIS RAPID II diffractometer	14273 measured reflections
Absorption correction: numerical (NUMABS; Higashi, 1999)	1820 independent reflections
$T_{\min} = 0.071$, $T_{\max} = 0.411$	1588 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.133$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$	82 parameters
$wR(F^2) = 0.099$	$\Delta\rho_{\text{max}} = 2.54$ e Å ⁻³
$S = 1.05$	$\Delta\rho_{\text{min}} = -1.72$ e Å ⁻³
1820 reflections	

Table 1

Selected geometric parameters (Å, °).

Ba1—N1 ⁱ	2.675 (8)	Ba3—N3 ⁱ	2.762 (8)
Ba1—N1	2.799 (9)	Ba3—N3	2.764 (7)
Ba1—N2 ⁱⁱ	2.998 (7)	Ba3—N1 ⁱ	2.914 (9)
Ba1—O1 ⁱⁱⁱ	2.999 (8)	Ba3—N3 ⁱⁱ	2.994 (8)
Ba1—O1 ^{iv}	3.054 (9)	Ba4—N3 ⁱⁱ	2.661 (8)
Ba2—N2 ^v	2.683 (9)	Ba4—N2	2.808 (7)
Ba2—N2 ^v	2.687 (8)	Ba4—N2 ^v	2.862 (8)
Ba2—N1 ⁱⁱⁱ	2.991 (9)	Ba4—O1	3.133 (10)
Ba2—N2	3.158 (8)	Ba4—N1 ^{viii}	3.231 (9)
Ba2—O1	3.184 (9)	Ga1—N3	1.876 (8)
Ba2—O1 ^{vi}	3.264 (10)	Ga1—N2	1.908 (8)
Ba3—N3 ^{vii}	2.730 (7)	Ga1—N1 ⁱⁱⁱ	1.924 (8)
N3—Ga1—N2	125.3 (3)	N2—Ga1—N1 ⁱⁱⁱ	114.6 (4)
N3—Ga1—N1 ⁱⁱⁱ	119.8 (3)		

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

Data collection: *RAPID-AUTO* (Rigaku Corporation, 2005); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *VESTA* (Momma & Izumi, 2008); software used to prepare material for publication: *SHELXL97*.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HP2067).

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supporting information

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Ba₄GaN₃O**Takayuki Hashimoto and Hisanori Yamane****S1. Comment**

Ba₄GaN₃O is isostructural with Sr₄GaN₃O (Mallinson *et al.*, 2006) which crystallizes in an orthorhombic cell with the space group *Pbca* (No. 61). The coordination environment around Ga1 site and Ba1–Ba3 sites are shown in Fig. 1. Ga1 atom is bonded to N1, N2 and N3 atoms and form a triangular anionic group of [GaN₃]⁶⁻. Ga–N bond lengths of 1.876 (8)–1.924 (8) Å are comparable with those observed in [GaN₃]⁶⁻ groups of Sr₃GaN₃ and Sr₆GaN₅ (1.938 Å, 1.895 Å, Park *et al.*, 2003), Sr₄GaN₃O (1.880–1.921 Å, Mallinson *et al.*, 2006) and LiBa₅GaN₃F₅ (1.896–1.945 Å, Hintze & Schnick, 2010). Ba1 atom is coordinated by two N1, one N2 and three O1 atoms, and Ba2 atom is by one N1, two N2 and three O1 atoms. N1 and N2 atoms are in seven-fold coordination sites of one Ga and six Ba atoms, and N3 atom is in the six-fold coordination site of one Ga and five Ba atoms. O1 atom is coordinated by seven Ba atoms. As shown in Fig. 2, O1 atoms are situated at the sites between [Ba₄GaN₃] slabs which are composed of triangular [GaN₃] groups and Ba atoms in the *a*–*c* plane.

Mallinson *et al.*, (2006) calculated Madelung site potential and Madelung energy per formula of Sr₄GaN₃O for four models of O and N atom arrangement. They concluded the model with O atom located at the O1 site coordinated by only Sr atoms is the most stable structure because this model showed the smallest deviation of the site potentials in atom sites of the same species and the lowest energy. The site potentials and energy calculated by using *EUTAX* (O'Keeffe, 1992) and *VESTA* (Momma & Izumi, 2008) programs with the data of the present study are -17.12 – -17.87 V for Ba1–Ba4, -36.17 V for Ga1, 28.24 – 29.45 V for N1–N3, 16.86 V for O1, and -26,100 kJ/mol for Ba₄GaN₃O. The values of Ga, N and O sites were consistent with the site potentials reported for Sr₄GaN₃O (Ga: -35.01 V, N: 29.58 – 31.38 V, O: 17.36 V) (Mallinson *et al.*, 2006). The difference between the Madelung energy per formula of Ba₄GaN₃O and the sum of Madelung energies of Ba₃N₂ derived by the theoretical calculation (-12,200 kJ/mol, Orhan *et al.*, 2002), BaO (-3,500 kJ/mol, Taylor, 1984) and GaN (-10,500 kJ/mol, Paszkowicz *et al.*, 2004) calculated from the crystal structure data is 0.4%.

S2. Experimental

Starting materials were pieces of Ba (Sigma-Aldrich, 99.99%), Ga (Rasa Industries, 99.99995%) and Na (Nippon Soda Co. Ltd., 99.95%), and powders of Si (Kojundo Chemical Laboratory, 99.999%) and NaN₃ (Toyo Kasei Kogyo Co. Ltd., 99.9%). In an Ar gas-filled glove box (O₂ < 1 ppm, H₂O < 1 ppm), Ba (1.00 mmol), Ga (0.25 mmol), Na (2.4 mmol), Si (0.50 mmol) and NaN₃ (1.2 mmol) were weighed and placed in a BN crucible (Showa Denko, 99.5%). The crucible was sealed in a stainless-steel tube. The sample was heated to 750°C in an electric furnace with a rate of 6°C min⁻¹. This temperature was maintained for 2 hours and lowered to 550°C with a cooling rate of -2.8°C min⁻¹. After that the sample was cooled to room temperature by shutting off the electric power to the furnace. The stainless-steel tube was cut and opened in the glove box, and the crucible was washed with liquid NH₃ (Japan Fine Products, >99.999%) to dissolve away Na. The details of the Na removing method have been described in the literature (Kowach *et al.*, 1998). The initial

objective was to synthesize a Ba–Ga–Si–N quaternary compound by the Na flux method, but the main product obtained was yellow transparent granular single crystals of $\text{Ba}_3\text{Ga}_2\text{N}_4$ (Yamane & DiSalvo, 1996). A small amount of red transparent platelet single crystals of $\text{Ba}_4\text{GaN}_3\text{O}$ were included in the product.

Semi-quantitative elemental analysis of the red single crystals was carried out with an energy-dispersive X-ray detector (EDX, EDAX, Genesis) attached to a scanning electron microscope (SEM, Hitachi, S-4800). Ba:Ga molar ratio determined by the EDX analysis was 78:22 which was close to the ratio (4:1) of $\text{Ba}_4\text{GaN}_3\text{O}$. The oxygen was probably originated from the surface oxide layers of the starting materials. Since $\text{Ba}_4\text{GaN}_3\text{O}$ is unstable in air, a single crystal was picked up from the product and sealed in glass capillaries in the glove box for XRD data collection.

The peaks of $2.25\text{--}2.54 \text{ e \AA}^{-3}$ in the $F_o\text{--}F_c$ map were observed at $0.88\text{--}0.96 \text{ \AA}$ distant from Ba1–Ba3 atoms. These large differences are probably a result of the cut-off effect of the Fourier synthesis.

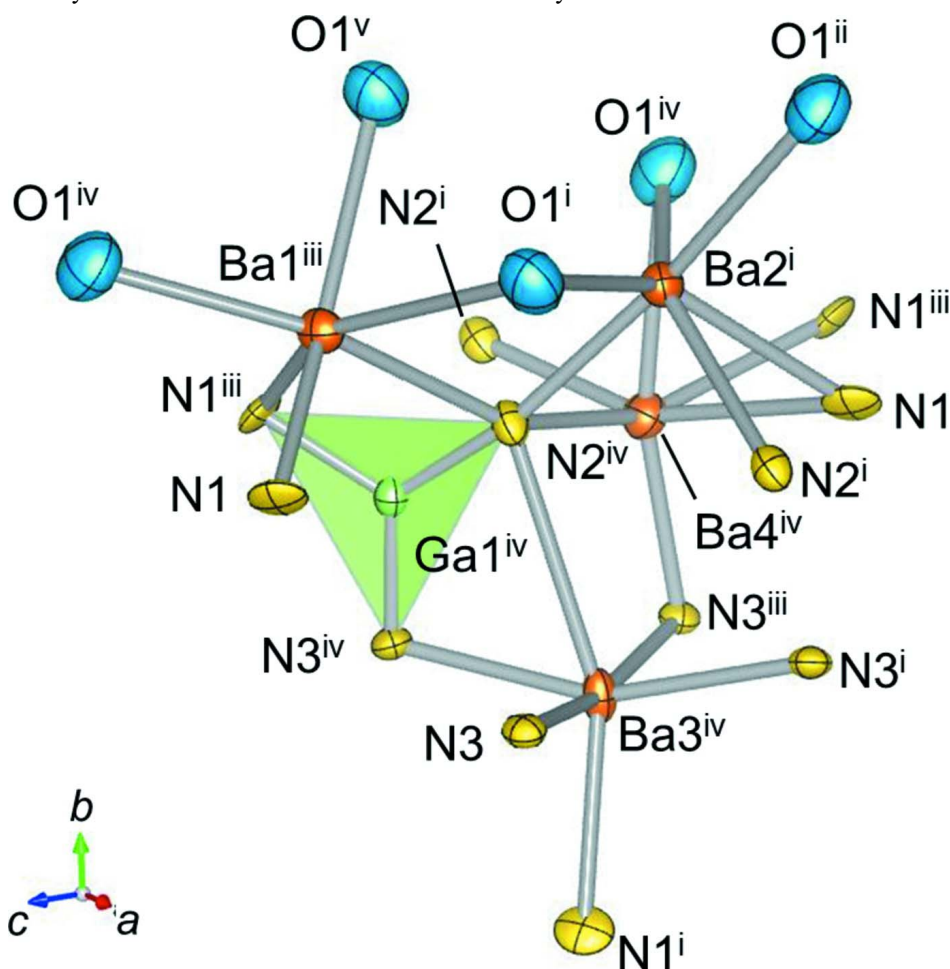


Figure 1

The atomic arrangement around Ba and Ga atoms in the structure of $\text{Ba}_4\text{GaN}_3\text{O}$. Displacement ellipsoids are drawn at 70% probability. Symmetry codes: (i) $x, -y + 1/2, z + 1/2$; (ii) $-x + 1/2, y + 1/2, z$; (iii) $x + 1/2, y, -z + 1/2$; (iv) $x + 1/2, -y + 1/2, -z$; (v) $-x, y + 1/2, -z + 1/2$.

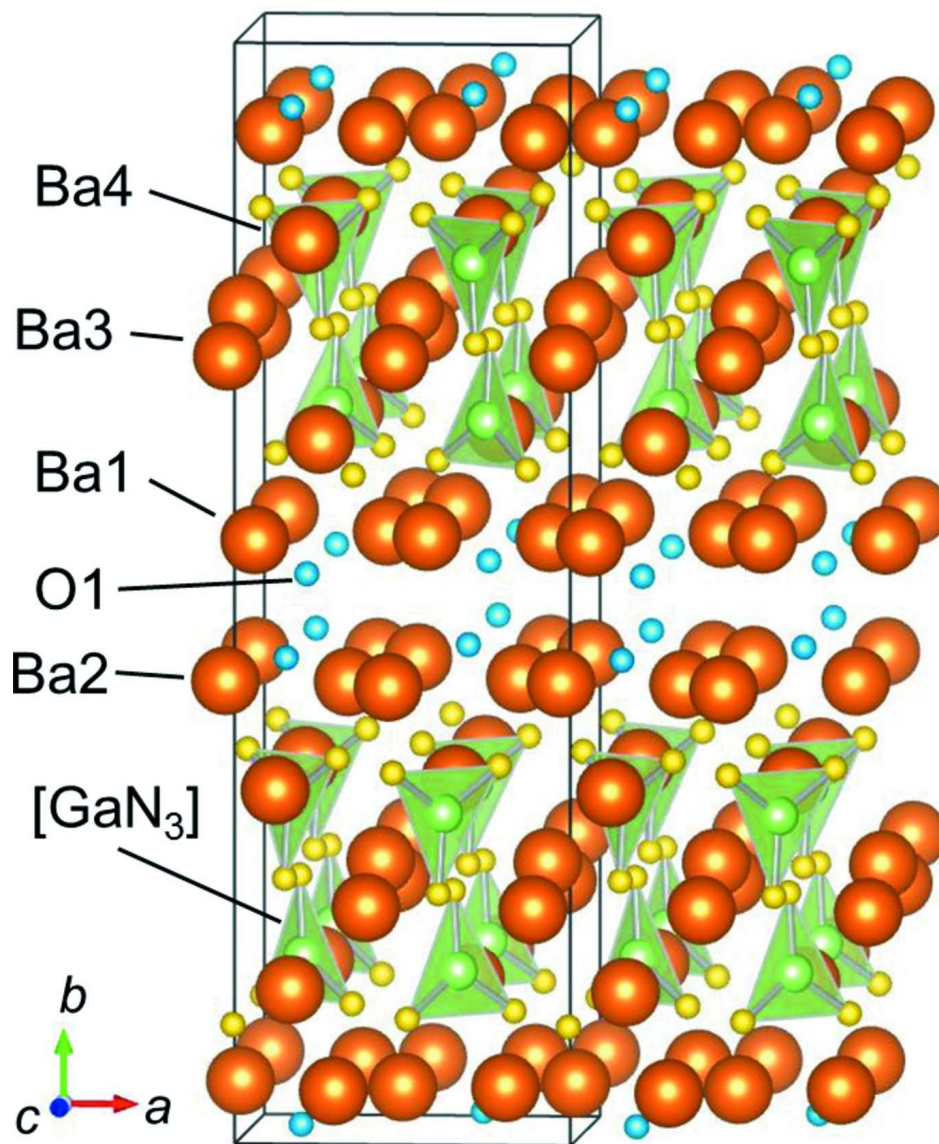


Figure 2

Crystal structure of $\text{Ba}_4\text{GaN}_3\text{O}$ illustrated with Ga-centered N atom triangles.

Tetrabarium gallium trinitride oxide

Crystal data

$\text{Ba}_4\text{GaN}_3\text{O}$

$M_r = 677.11$

Orthorhombic, $Pbca$

Hall symbol: $-P\ 2ac\ 2ab$

$a = 7.8130\ (3)\ \text{\AA}$

$b = 25.6453\ (10)\ \text{\AA}$

$c = 7.9162\ (4)\ \text{\AA}$

$V = 1586.14\ (12)\ \text{\AA}^3$

$Z = 8$

$F(000) = 2272$

$D_x = 5.671\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71075\ \text{\AA}$

Cell parameters from 11112 reflections

$\theta = 3.0\text{--}27.5^\circ$

$\mu = 22.84\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Platelet, red

$0.18 \times 0.13 \times 0.07\ \text{mm}$

Data collection

Rigaku R-AXIS RAPID II diffractometer	14273 measured reflections
Radiation source: fine-focus sealed tube	1820 independent reflections
Graphite monochromator	1588 reflections with $I > 2\sigma(I)$
Detector resolution: 10.0 pixels mm ⁻¹	$R_{\text{int}} = 0.133$
ω scans	$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 3.0^\circ$
Absorption correction: numerical (NUMABS; Higashi, 1999)	$h = -9 \rightarrow 10$
$T_{\text{min}} = 0.071$, $T_{\text{max}} = 0.411$	$k = -33 \rightarrow 33$
	$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.043$	$w = 1/[\sigma^2(F_o^2) + (0.P)^2 + 18.6031P]$
$wR(F^2) = 0.099$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{\text{max}} = 0.001$
1820 reflections	$\Delta\rho_{\text{max}} = 2.54 \text{ e } \text{\AA}^{-3}$
82 parameters	$\Delta\rho_{\text{min}} = -1.72 \text{ e } \text{\AA}^{-3}$
0 restraints	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Ba1	0.36690 (8)	0.42906 (2)	0.32613 (7)	0.02148 (18)
Ba2	0.03129 (8)	0.06166 (2)	0.16149 (7)	0.02055 (18)
Ba3	0.45621 (7)	0.26486 (2)	0.23802 (7)	0.02003 (18)
Ba4	0.20527 (8)	0.15269 (2)	0.46083 (7)	0.02310 (19)
Ga1	0.20637 (12)	0.17178 (4)	0.01682 (12)	0.0157 (2)
N1	0.0710 (11)	0.3685 (3)	0.3614 (11)	0.0246 (19)
N2	0.3630 (10)	0.1319 (3)	0.1492 (9)	0.0187 (17)
N3	0.1943 (10)	0.2448 (3)	0.0124 (9)	0.0169 (17)
O1	0.2416 (12)	0.0314 (4)	0.4918 (11)	0.049 (2)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.0234 (3)	0.0214 (4)	0.0196 (3)	0.0002 (2)	0.0046 (2)	0.0002 (2)
Ba2	0.0211 (3)	0.0211 (4)	0.0194 (3)	-0.0001 (2)	0.0009 (2)	-0.0004 (2)
Ba3	0.0152 (3)	0.0326 (4)	0.0123 (3)	0.0000 (2)	0.0001 (2)	0.0007 (2)
Ba4	0.0258 (3)	0.0226 (4)	0.0209 (3)	0.0000 (2)	0.0001 (2)	-0.0023 (2)

Ga1	0.0158 (5)	0.0183 (6)	0.0132 (5)	-0.0002 (4)	-0.0006 (4)	-0.0001 (4)
N1	0.026 (4)	0.019 (5)	0.029 (5)	0.011 (4)	-0.010 (4)	0.006 (3)
N2	0.022 (4)	0.020 (4)	0.015 (4)	0.006 (3)	-0.002 (3)	0.000 (3)
N3	0.022 (4)	0.011 (4)	0.018 (4)	-0.002 (3)	-0.002 (3)	-0.001 (3)
O1	0.053 (5)	0.052 (6)	0.041 (5)	-0.007 (5)	0.001 (4)	-0.010 (4)

Geometric parameters (Å, °)

Ba1—N1 ⁱ	2.675 (8)	Ba4—N1 ^{viii}	3.231 (9)
Ba1—N1	2.799 (9)	Ga1—N3	1.876 (8)
Ba1—N2 ⁱⁱ	2.998 (7)	Ga1—N2	1.908 (8)
Ba1—O1 ⁱⁱⁱ	2.999 (8)	Ga1—N1 ⁱⁱⁱ	1.924 (8)
Ba1—O1 ^{iv}	3.054 (9)	Ga1—Ba3 ^{ix}	3.2450 (11)
Ba1—Ga1 ⁱⁱ	3.2466 (12)	Ga1—Ba1 ⁱⁱⁱ	3.2467 (12)
Ba2—O1 ^v	2.683 (9)	Ga1—Ba3 ⁱⁱⁱ	3.3648 (11)
Ba2—N2 ^v	2.687 (8)	N1—Ga1 ⁱⁱ	1.924 (8)
Ba2—N1 ⁱⁱⁱ	2.991 (9)	N1—Ba1 ^v	2.675 (8)
Ba2—N2	3.158 (8)	N1—Ba3 ^v	2.914 (9)
Ba2—O1	3.184 (9)	N1—Ba2 ⁱⁱ	2.991 (9)
Ba2—O1 ^{vi}	3.264 (10)	N1—Ba4 ^x	3.231 (9)
Ba2—Ga1	3.3405 (12)	N2—Ba2 ⁱ	2.687 (8)
Ba3—N3 ^{vii}	2.730 (7)	N2—Ba4 ⁱ	2.862 (8)
Ba3—N3 ⁱ	2.762 (8)	N2—Ba1 ⁱⁱⁱ	2.998 (7)
Ba3—N3	2.764 (7)	N3—Ba4 ⁱⁱⁱ	2.661 (8)
Ba3—N1 ⁱ	2.914 (9)	N3—Ba3 ^{ix}	2.730 (7)
Ba3—N3 ⁱⁱ	2.994 (8)	N3—Ba3 ^v	2.762 (8)
Ba3—Ga1 ^{vii}	3.2450 (11)	N3—Ba3 ⁱⁱⁱ	2.994 (8)
Ba3—Ga1 ⁱⁱ	3.3647 (11)	O1—Ba2 ⁱ	2.683 (9)
Ba4—N3 ⁱⁱ	2.661 (8)	O1—Ba1 ⁱⁱ	2.999 (8)
Ba4—N2	2.808 (7)	O1—Ba1 ^{xi}	3.054 (9)
Ba4—N2 ^v	2.862 (8)	O1—Ba2 ^{xii}	3.264 (10)
Ba4—O1	3.133 (10)		
N1 ⁱ —Ba1—N1	103.0 (3)	Ba4 ⁱⁱⁱ —Ba3—Ba4 ^{viii}	109.76 (2)
N1 ⁱ —Ba1—N2 ⁱⁱ	100.2 (2)	Ga1 ⁱ —Ba3—Ba4 ^{viii}	75.61 (2)
N1—Ba1—N2 ⁱⁱ	67.5 (2)	N3 ^{vii} —Ba3—Ba4 ⁱ	44.25 (16)
N1 ⁱ —Ba1—O1 ⁱⁱⁱ	84.3 (3)	N3 ⁱ —Ba3—Ba4 ⁱ	79.12 (16)
N1—Ba1—O1 ⁱⁱⁱ	90.3 (2)	N3—Ba3—Ba4 ⁱ	88.33 (16)
N2 ⁱⁱ —Ba1—O1 ⁱⁱⁱ	157.8 (2)	N1 ⁱ —Ba3—Ba4 ⁱ	114.81 (15)
N1 ⁱ —Ba1—O1 ^{iv}	154.5 (3)	N3 ⁱⁱ —Ba3—Ba4 ⁱ	125.84 (15)
N1—Ba1—O1 ^{iv}	101.8 (3)	Ga1 ^{vii} —Ba3—Ba4 ⁱ	79.26 (2)
N2 ⁱⁱ —Ba1—O1 ^{iv}	94.5 (2)	Ga1 ⁱⁱ —Ba3—Ba4 ⁱ	158.61 (3)
O1 ⁱⁱⁱ —Ba1—O1 ^{iv}	89.88 (12)	Ga1—Ba3—Ba4 ⁱ	64.48 (2)
N1 ⁱ —Ba1—Ga1 ⁱⁱ	91.49 (19)	Ba4 ⁱⁱⁱ —Ba3—Ba4 ⁱ	117.798 (17)
N1—Ba1—Ga1 ⁱⁱ	36.16 (16)	Ga1 ⁱ —Ba3—Ba4 ⁱ	56.77 (2)
N2 ⁱⁱ —Ba1—Ga1 ⁱⁱ	35.30 (15)	Ba4 ^{viii} —Ba3—Ba4 ⁱ	115.14 (2)
O1 ⁱⁱⁱ —Ba1—Ga1 ⁱⁱ	123.61 (19)	N3 ⁱⁱ —Ba4—N2	109.6 (2)
O1 ^{iv} —Ba1—Ga1 ⁱⁱ	112.20 (18)	N3 ⁱⁱ —Ba4—N2 ^v	101.6 (2)

N1 ⁱ —Ba1—Ba2 ^{iv}	102.02 (19)	N2—Ba4—N2 ^v	96.16 (14)
N1—Ba1—Ba2 ^{iv}	135.83 (16)	N3 ⁱⁱ —Ba4—O1	166.3 (2)
N2 ⁱⁱ —Ba1—Ba2 ^{iv}	140.93 (15)	N2—Ba4—O1	80.8 (2)
O1 ⁱⁱⁱ —Ba1—Ba2 ^{iv}	56.82 (19)	N2 ^v —Ba4—O1	85.6 (2)
O1 ^{iv} —Ba1—Ba2 ^{iv}	54.92 (18)	N3 ⁱⁱ —Ba4—N1 ^{viii}	97.3 (2)
Ga1 ⁱⁱ —Ba1—Ba2 ^{iv}	166.34 (3)	N2—Ba4—N1 ^{viii}	87.9 (2)
N1 ⁱ —Ba1—Ba2 ⁱⁱ	148.09 (19)	N2 ^v —Ba4—N1 ^{viii}	158.0 (2)
N1—Ba1—Ba2 ⁱⁱ	52.06 (18)	O1—Ba4—N1 ^{viii}	73.7 (2)
N2 ⁱⁱ —Ba1—Ba2 ⁱⁱ	54.58 (15)	N3 ⁱⁱ —Ba4—Ga1	90.91 (16)
O1 ⁱⁱⁱ —Ba1—Ba2 ⁱⁱ	112.10 (18)	N2—Ba4—Ga1	32.35 (15)
O1 ^{iv} —Ba1—Ba2 ⁱⁱ	56.35 (18)	N2 ^v —Ba4—Ga1	74.12 (15)
Ga1 ⁱⁱ —Ba1—Ba2 ⁱⁱ	56.61 (2)	O1—Ba4—Ga1	102.37 (15)
Ba2 ^{iv} —Ba1—Ba2 ⁱⁱ	109.870 (18)	N1 ^{viii} —Ba4—Ga1	116.90 (14)
N1 ⁱ —Ba1—Ba4 ^{viii}	60.51 (19)	N3 ⁱⁱ —Ba4—Ba2 ⁱ	134.97 (17)
N1—Ba1—Ba4 ^{viii}	103.06 (16)	N2—Ba4—Ba2 ⁱ	47.79 (16)
N2 ⁱⁱ —Ba1—Ba4 ^{viii}	48.37 (15)	N2 ^v —Ba4—Ba2 ⁱ	117.38 (16)
O1 ⁱⁱⁱ —Ba1—Ba4 ^{viii}	144.23 (18)	O1—Ba4—Ba2 ⁱ	46.44 (17)
O1 ^{iv} —Ba1—Ba4 ^{viii}	118.70 (17)	N1 ^{viii} —Ba4—Ba2 ⁱ	51.70 (15)
Ga1 ⁱⁱ —Ba1—Ba4 ^{viii}	67.67 (2)	Ga1—Ba4—Ba2 ⁱ	79.68 (2)
Ba2 ^{iv} —Ba1—Ba4 ^{viii}	120.92 (2)	N3 ⁱⁱ —Ba4—Ba2	136.94 (16)
Ba2 ⁱⁱ —Ba1—Ba4 ^{viii}	102.089 (19)	N2—Ba4—Ba2	57.57 (17)
N1 ⁱ —Ba1—Ba4 ⁱⁱⁱ	56.90 (19)	N2 ^v —Ba4—Ba2	47.55 (15)
N1—Ba1—Ba4 ⁱⁱⁱ	59.59 (18)	O1—Ba4—Ba2	56.00 (16)
N2 ⁱⁱ —Ba1—Ba4 ⁱⁱⁱ	111.04 (15)	N1 ^{viii} —Ba4—Ba2	120.82 (16)
O1 ⁱⁱⁱ —Ba1—Ba4 ⁱⁱⁱ	53.45 (19)	Ga1—Ba4—Ba2	55.77 (2)
O1 ^{iv} —Ba1—Ba4 ⁱⁱⁱ	135.30 (17)	Ba2 ⁱ —Ba4—Ba2	70.604 (15)
Ga1 ⁱⁱ —Ba1—Ba4 ⁱⁱⁱ	77.60 (2)	N3 ⁱⁱ —Ba4—Ba3 ⁱⁱ	49.31 (16)
Ba2 ^{iv} —Ba1—Ba4 ⁱⁱⁱ	108.003 (19)	N2—Ba4—Ba3 ⁱⁱ	113.90 (17)
Ba2 ⁱⁱ —Ba1—Ba4 ⁱⁱⁱ	110.09 (2)	N2 ^v —Ba4—Ba3 ⁱⁱ	142.97 (15)
Ba4 ^{viii} —Ba1—Ba4 ⁱⁱⁱ	105.50 (2)	O1—Ba4—Ba3 ⁱⁱ	118.88 (16)
N1 ⁱ —Ba1—Ba2 ^{vii}	47.19 (19)	N1 ^{viii} —Ba4—Ba3 ⁱⁱ	49.91 (15)
N1—Ba1—Ba2 ^{vii}	112.78 (17)	Ga1—Ba4—Ba3 ⁱⁱ	121.19 (3)
N2 ⁱⁱ —Ba1—Ba2 ^{vii}	147.32 (16)	Ba2 ⁱ —Ba4—Ba3 ⁱⁱ	99.15 (2)
O1 ⁱⁱⁱ —Ba1—Ba2 ^{vii}	41.16 (18)	Ba2—Ba4—Ba3 ⁱⁱ	169.46 (2)
O1 ^{iv} —Ba1—Ba2 ^{vii}	116.36 (17)	N3 ⁱⁱ —Ba4—Ba3 ^x	47.62 (16)
Ga1 ⁱⁱ —Ba1—Ba2 ^{vii}	127.49 (3)	N2—Ba4—Ba3 ^x	153.75 (16)
Ba2 ^{iv} —Ba1—Ba2 ^{vii}	63.146 (17)	N2 ^v —Ba4—Ba3 ^x	79.21 (15)
Ba2 ⁱⁱ —Ba1—Ba2 ^{vii}	152.86 (2)	O1—Ba4—Ba3 ^x	124.02 (16)
Ba4 ^{viii} —Ba1—Ba2 ^{vii}	103.594 (19)	N1 ^{viii} —Ba4—Ba3 ^x	106.15 (15)
Ba4 ⁱⁱⁱ —Ba1—Ba2 ^{vii}	54.148 (15)	Ga1—Ba4—Ba3 ^x	123.74 (2)
N1 ⁱ —Ba1—Ba1 ⁱ	42.85 (19)	Ba2 ⁱ —Ba4—Ba3 ^x	155.60 (2)
N1—Ba1—Ba1 ⁱ	144.95 (17)	Ba2—Ba4—Ba3 ^x	126.28 (2)
N2 ⁱⁱ —Ba1—Ba1 ⁱ	105.14 (15)	Ba3 ⁱⁱ —Ba4—Ba3 ^x	64.206 (12)
O1 ⁱⁱⁱ —Ba1—Ba1 ⁱ	92.97 (19)	N3 ⁱⁱ —Ba4—Ba1 ^x	117.25 (17)
O1 ^{iv} —Ba1—Ba1 ⁱ	113.06 (19)	N2—Ba4—Ba1 ^x	126.50 (17)
Ga1 ⁱⁱ —Ba1—Ba1 ⁱ	120.41 (2)	N2 ^v —Ba4—Ba1 ^x	51.53 (15)
Ba2 ^{iv} —Ba1—Ba1 ⁱ	72.121 (14)	O1—Ba4—Ba1 ^x	58.44 (17)
Ba2 ⁱⁱ —Ba1—Ba1 ⁱ	151.58 (2)	N1 ^{viii} —Ba4—Ba1 ^x	109.36 (14)

Ba4 ^{viii} —Ba1—Ba1 ⁱ	57.460 (13)	Ga1—Ba4—Ba1 ^x	121.41 (2)
Ba4 ⁱⁱⁱ —Ba1—Ba1 ⁱ	95.36 (2)	Ba2 ⁱ —Ba4—Ba1 ^x	104.86 (2)
Ba2 ^{vii} —Ba1—Ba1 ⁱ	54.518 (17)	Ba2—Ba4—Ba1 ^x	70.646 (17)
O1 ^v —Ba2—N2 ^v	91.9 (3)	Ba3 ⁱⁱ —Ba4—Ba1 ^x	115.65 (2)
O1 ^v —Ba2—N1 ⁱⁱⁱ	84.3 (2)	Ba3 ^x —Ba4—Ba1 ^x	70.370 (17)
N2 ^v —Ba2—N1 ⁱⁱⁱ	95.3 (2)	N3 ⁱⁱ —Ba4—Ba1 ⁱⁱ	116.11 (16)
O1 ^v —Ba2—N2	147.5 (2)	N2—Ba4—Ba1 ⁱⁱ	114.79 (16)
N2 ^v —Ba2—N2	92.1 (2)	N2 ^v —Ba4—Ba1 ⁱⁱ	116.15 (16)
N1 ⁱⁱⁱ —Ba2—N2	63.2 (2)	O1—Ba4—Ba1 ⁱⁱ	50.26 (16)
O1 ^v —Ba2—O1	137.4 (3)	N1 ^{viii} —Ba4—Ba1 ⁱⁱ	43.92 (14)
N2 ^v —Ba2—O1	87.6 (2)	Ga1—Ba4—Ba1 ⁱⁱ	146.26 (3)
N1 ⁱⁱⁱ —Ba2—O1	138.1 (2)	Ba2 ⁱ —Ba4—Ba1 ⁱⁱ	67.004 (17)
N2—Ba2—O1	75.0 (2)	Ba2—Ba4—Ba1 ⁱⁱ	105.66 (2)
O1 ^v —Ba2—O1 ^{vi}	93.5 (3)	Ba3 ⁱⁱ —Ba4—Ba1 ⁱⁱ	71.359 (18)
N2 ^v —Ba2—O1 ^{vi}	170.4 (2)	Ba3 ^x —Ba4—Ba1 ⁱⁱ	89.987 (19)
N1 ⁱⁱⁱ —Ba2—O1 ^{vi}	93.1 (2)	Ba1 ^x —Ba4—Ba1 ⁱⁱ	65.465 (13)
N2—Ba2—O1 ^{vi}	87.6 (2)	N3—Ga1—N2	125.3 (3)
O1—Ba2—O1 ^{vi}	83.07 (11)	N3—Ga1—N1 ⁱⁱⁱ	119.8 (3)
O1 ^v —Ba2—Ga1	115.78 (19)	N2—Ga1—N1 ⁱⁱⁱ	114.6 (4)
N2 ^v —Ba2—Ga1	79.89 (17)	N3—Ga1—Ba3 ^{ix}	57.2 (2)
N1 ⁱⁱⁱ —Ba2—Ga1	34.82 (15)	N2—Ga1—Ba3 ^{ix}	174.9 (2)
N2—Ba2—Ga1	34.00 (14)	N1 ⁱⁱⁱ —Ga1—Ba3 ^{ix}	62.6 (3)
O1—Ba2—Ga1	106.04 (17)	N3—Ga1—Ba1 ⁱⁱⁱ	143.7 (2)
O1 ^{vi} —Ba2—Ga1	104.74 (16)	N2—Ga1—Ba1 ⁱⁱⁱ	65.2 (2)
O1 ^v —Ba2—Ba4 ^v	57.8 (2)	N1 ⁱⁱⁱ —Ga1—Ba1 ⁱⁱⁱ	59.1 (3)
N2 ^v —Ba2—Ba4 ^v	50.72 (16)	Ba3 ^{ix} —Ga1—Ba1 ⁱⁱⁱ	110.03 (3)
N1 ⁱⁱⁱ —Ba2—Ba4 ^v	57.98 (17)	N3—Ga1—Ba2	146.1 (2)
N2—Ba2—Ba4 ^v	101.71 (14)	N2—Ga1—Ba2	67.8 (2)
O1—Ba2—Ba4 ^v	138.28 (17)	N1 ⁱⁱⁱ —Ga1—Ba2	62.6 (3)
O1 ^{vi} —Ba2—Ba4 ^v	138.65 (15)	Ba3 ^{ix} —Ga1—Ba2	112.94 (3)
Ga1—Ba2—Ba4 ^v	69.40 (2)	Ba1 ⁱⁱⁱ —Ga1—Ba2	69.15 (3)
O1 ^v —Ba2—Ba4	143.6 (2)	N3—Ga1—Ba3 ⁱⁱⁱ	62.3 (2)
N2 ^v —Ba2—Ba4	51.81 (17)	N2—Ga1—Ba3 ⁱⁱⁱ	104.3 (2)
N1 ⁱⁱⁱ —Ba2—Ba4	95.48 (15)	N1 ⁱⁱⁱ —Ga1—Ba3 ⁱⁱⁱ	99.1 (3)
N2—Ba2—Ba4	48.63 (13)	Ba3 ^{ix} —Ga1—Ba3 ⁱⁱⁱ	72.53 (2)
O1—Ba2—Ba4	54.66 (17)	Ba1 ⁱⁱⁱ —Ga1—Ba3 ⁱⁱⁱ	81.70 (3)
O1 ^{vi} —Ba2—Ba4	122.74 (17)	Ba2—Ga1—Ba3 ⁱⁱⁱ	150.54 (4)
Ga1—Ba2—Ba4	61.44 (2)	N3—Ga1—Ba3	50.6 (2)
Ba4 ^v —Ba2—Ba4	91.37 (2)	N2—Ga1—Ba3	74.7 (2)
O1 ^v —Ba2—Ba1 ^{xi}	94.3 (2)	N1 ⁱⁱⁱ —Ga1—Ba3	168.6 (3)
N2 ^v —Ba2—Ba1 ^{xi}	121.42 (16)	Ba3 ^{ix} —Ga1—Ba3	107.55 (3)
N1 ⁱⁱⁱ —Ba2—Ba1 ^{xi}	143.29 (17)	Ba1 ⁱⁱⁱ —Ga1—Ba3	123.58 (3)
N2—Ba2—Ba1 ^{xi}	110.87 (14)	Ba2—Ga1—Ba3	128.70 (3)
O1—Ba2—Ba1 ^{xi}	51.72 (17)	Ba3 ⁱⁱⁱ —Ga1—Ba3	71.31 (2)
O1 ^{vi} —Ba2—Ba1 ^{xi}	50.26 (15)	N3—Ga1—Ba4	99.0 (2)
Ga1—Ba2—Ba1 ^{xi}	143.49 (3)	N2—Ga1—Ba4	51.9 (2)
Ba4 ^v —Ba2—Ba1 ^{xi}	147.07 (2)	N1 ⁱⁱⁱ —Ga1—Ba4	123.9 (3)
Ba4—Ba2—Ba1 ^{xi}	106.34 (2)	Ba3 ^{ix} —Ga1—Ba4	133.11 (3)

O1 ^v —Ba2—Ba1 ⁱⁱⁱ	106.80 (19)	Ba1 ⁱⁱⁱ —Ga1—Ba4	110.58 (3)
N2 ^v —Ba2—Ba1 ⁱⁱⁱ	134.13 (17)	Ba2—Ga1—Ba4	62.79 (2)
N1 ⁱⁱⁱ —Ba2—Ba1 ⁱⁱⁱ	47.56 (17)	Ba3 ⁱⁱⁱ —Ga1—Ba4	135.86 (3)
N2—Ba2—Ba1 ⁱⁱⁱ	50.68 (13)	Ba3—Ga1—Ba4	66.74 (2)
O1—Ba2—Ba1 ⁱⁱⁱ	103.69 (17)	N3—Ga1—Ba3 ^v	47.9 (2)
O1 ^{vi} —Ba2—Ba1 ⁱⁱⁱ	51.16 (15)	N2—Ga1—Ba3 ^v	113.7 (2)
Ga1—Ba2—Ba1 ⁱⁱⁱ	54.24 (2)	N1 ⁱⁱⁱ —Ga1—Ba3 ^v	113.4 (3)
Ba4 ^v —Ba2—Ba1 ⁱⁱⁱ	105.36 (2)	Ba3 ^{ix} —Ga1—Ba3 ^v	71.35 (2)
Ba4—Ba2—Ba1 ⁱⁱⁱ	99.30 (2)	Ba1 ⁱⁱⁱ —Ga1—Ba3 ^v	167.54 (4)
Ba1 ^{xi} —Ba2—Ba1 ⁱⁱⁱ	99.012 (17)	Ba2—Ga1—Ba3 ^v	98.71 (3)
O1 ^v —Ba2—Ba1 ^{ix}	47.36 (18)	Ba3 ⁱⁱⁱ —Ga1—Ba3 ^v	110.13 (3)
N2 ^v —Ba2—Ba1 ^{ix}	109.56 (16)	Ba3—Ga1—Ba3 ^v	65.886 (19)
N1 ⁱⁱⁱ —Ba2—Ba1 ^{ix}	41.01 (14)	Ba4—Ga1—Ba3 ^v	64.00 (2)
N2—Ba2—Ba1 ^{ix}	101.32 (13)	Ga1 ⁱⁱ —N1—Ba1 ^v	173.9 (5)
O1—Ba2—Ba1 ^{ix}	162.69 (17)	Ga1 ⁱⁱ —N1—Ba1	84.7 (3)
O1 ^{vi} —Ba2—Ba1 ^{ix}	79.87 (15)	Ba1 ^v —N1—Ba1	96.6 (3)
Ga1—Ba2—Ba1 ^{ix}	75.82 (2)	Ga1 ⁱⁱ —N1—Ba3 ^v	81.5 (3)
Ba4 ^v —Ba2—Ba1 ^{ix}	58.845 (16)	Ba1 ^v —N1—Ba3 ^v	101.3 (3)
Ba4—Ba2—Ba1 ^{ix}	134.90 (2)	Ba1—N1—Ba3 ^v	137.2 (3)
Ba1 ^{xi} —Ba2—Ba1 ^{ix}	116.853 (17)	Ga1 ⁱⁱ —N1—Ba2 ⁱⁱ	82.6 (3)
Ba1 ⁱⁱⁱ —Ba2—Ba1 ^{ix}	62.918 (10)	Ba1 ^v —N1—Ba2 ⁱⁱ	91.8 (2)
N3 ^{vii} —Ba3—N3 ⁱ	92.5 (2)	Ba1—N1—Ba2 ⁱⁱ	80.4 (2)
N3 ^{vii} —Ba3—N3	91.05 (3)	Ba3 ^v —N1—Ba2 ⁱⁱ	136.8 (3)
N3 ⁱ —Ba3—N3	157.9 (3)	Ga1 ⁱⁱ —N1—Ba4 ^x	96.7 (3)
N3 ^{vii} —Ba3—N1 ⁱ	71.2 (2)	Ba1 ^v —N1—Ba4 ^x	79.2 (2)
N3 ⁱ —Ba3—N1 ⁱ	98.9 (2)	Ba1—N1—Ba4 ^x	150.1 (3)
N3—Ba3—N1 ⁱ	102.9 (2)	Ba3 ^v —N1—Ba4 ^x	72.1 (2)
N3 ^{vii} —Ba3—N3 ⁱⁱ	170.0 (3)	Ba2 ⁱⁱ —N1—Ba4 ^x	70.32 (19)
N3 ⁱ —Ba3—N3 ⁱⁱ	85.75 (3)	Ga1—N2—Ba2 ⁱ	168.3 (4)
N3—Ba3—N3 ⁱⁱ	87.0 (2)	Ga1—N2—Ba4	95.7 (3)
N1 ⁱ —Ba3—N3 ⁱⁱ	118.8 (2)	Ba2 ⁱ —N2—Ba4	81.5 (2)
N3 ^{vii} —Ba3—Ga1 ^{vii}	35.28 (16)	Ga1—N2—Ba4 ⁱ	109.4 (3)
N3 ⁱ —Ba3—Ga1 ^{vii}	97.59 (15)	Ba2 ⁱ —N2—Ba4 ⁱ	80.6 (2)
N3—Ba3—Ga1 ^{vii}	97.89 (16)	Ba4—N2—Ba4 ⁱ	130.0 (3)
N1 ⁱ —Ba3—Ga1 ^{vii}	35.89 (15)	Ga1—N2—Ba1 ⁱⁱⁱ	79.5 (2)
N3 ⁱⁱ —Ba3—Ga1 ^{vii}	154.71 (15)	Ba2 ⁱ —N2—Ba1 ⁱⁱⁱ	96.9 (2)
N3 ^{vii} —Ba3—Ga1 ⁱⁱ	156.30 (16)	Ba4—N2—Ba1 ⁱⁱⁱ	148.5 (3)
N3 ⁱ —Ba3—Ga1 ⁱⁱ	90.65 (16)	Ba4 ⁱ —N2—Ba1 ⁱⁱⁱ	80.09 (19)
N3—Ba3—Ga1 ⁱⁱ	94.83 (16)	Ga1—N2—Ba2	78.2 (3)
N1 ⁱ —Ba3—Ga1 ⁱⁱ	85.14 (15)	Ba2 ⁱ —N2—Ba2	90.1 (2)
N3 ⁱⁱ —Ba3—Ga1 ⁱⁱ	33.68 (15)	Ba4—N2—Ba2	73.80 (18)
Ga1 ^{vii} —Ba3—Ga1 ⁱⁱ	121.03 (4)	Ba4 ⁱ —N2—Ba2	151.9 (3)
N3 ^{vii} —Ba3—Ga1	87.43 (16)	Ba1 ⁱⁱⁱ —N2—Ba2	74.74 (18)
N3 ⁱ —Ba3—Ga1	126.79 (16)	Ga1—N3—Ba4 ⁱⁱⁱ	170.9 (4)
N3—Ba3—Ga1	31.61 (16)	Ga1—N3—Ba3 ^{ix}	87.5 (3)
N1 ⁱ —Ba3—Ga1	130.55 (17)	Ba4 ⁱⁱⁱ —N3—Ba3 ^{ix}	90.0 (2)
N3 ⁱⁱ —Ba3—Ga1	85.77 (15)	Ga1—N3—Ba3 ^v	101.9 (3)
Ga1 ^{vii} —Ba3—Ga1	111.20 (2)	Ba4 ⁱⁱⁱ —N3—Ba3 ^v	87.0 (2)

Ga1 ⁱⁱ —Ba3—Ga1	109.24 (3)	Ba3 ^{ix} —N3—Ba3 ^v	94.4 (2)
N3 ^{vii} —Ba3—Ba4 ⁱⁱⁱ	88.97 (16)	Ga1—N3—Ba3	97.8 (3)
N3 ⁱ —Ba3—Ba4 ⁱⁱⁱ	154.98 (16)	Ba4 ⁱⁱⁱ —N3—Ba3	83.8 (2)
N3—Ba3—Ba4 ⁱⁱⁱ	46.89 (16)	Ba3 ^{ix} —N3—Ba3	172.1 (3)
N1 ⁱ —Ba3—Ba4 ⁱⁱⁱ	58.03 (17)	Ba3 ^v —N3—Ba3	90.1 (2)
N3 ⁱⁱ —Ba3—Ba4 ⁱⁱⁱ	96.78 (14)	Ga1—N3—Ba3 ⁱⁱⁱ	84.1 (3)
Ga1 ^{vii} —Ba3—Ba4 ⁱⁱⁱ	69.95 (2)	Ba4 ⁱⁱⁱ —N3—Ba3 ⁱⁱⁱ	87.1 (2)
Ga1 ⁱⁱ —Ba3—Ba4 ⁱⁱⁱ	78.55 (2)	Ba3 ^{ix} —N3—Ba3 ⁱⁱⁱ	86.1 (2)
Ga1—Ba3—Ba4 ⁱⁱⁱ	78.22 (2)	Ba3 ^v —N3—Ba3 ⁱⁱⁱ	174.0 (3)
N3 ^{vii} —Ba3—Ga1 ⁱ	87.80 (16)	Ba3—N3—Ba3 ⁱⁱⁱ	88.8 (2)
N3 ⁱ —Ba3—Ga1 ⁱ	30.24 (16)	Ba2 ⁱ —O1—Ba1 ⁱⁱ	91.5 (3)
N3—Ba3—Ga1 ⁱ	128.27 (16)	Ba2 ⁱ —O1—Ba1 ^{xi}	106.8 (3)
N1 ⁱ —Ba3—Ga1 ⁱ	125.19 (17)	Ba1 ⁱⁱ —O1—Ba1 ^{xi}	139.5 (3)
N3 ⁱⁱ —Ba3—Ga1 ⁱ	85.74 (14)	Ba2 ⁱ —O1—Ba4	75.8 (2)
Ga1 ^{vii} —Ba3—Ga1 ⁱ	109.63 (3)	Ba1 ⁱⁱ —O1—Ba4	76.3 (2)
Ga1 ⁱⁱ —Ba3—Ga1 ⁱ	106.15 (2)	Ba1 ^{xi} —O1—Ba4	142.6 (3)
Ga1—Ba3—Ga1 ⁱ	96.74 (3)	Ba2 ⁱ —O1—Ba2	89.6 (2)
Ba4 ⁱⁱⁱ —Ba3—Ga1 ⁱ	174.14 (3)	Ba1 ⁱⁱ —O1—Ba2	144.2 (3)
N3 ^{vii} —Ba3—Ba4 ^{viii}	99.21 (16)	Ba1 ^{xi} —O1—Ba2	73.36 (19)
N3 ⁱ —Ba3—Ba4 ^{viii}	45.37 (16)	Ba4—O1—Ba2	69.3 (2)
N3—Ba3—Ba4 ^{viii}	154.63 (16)	Ba2 ⁱ —O1—Ba2 ^{xii}	86.5 (3)
N1 ⁱ —Ba3—Ba4 ^{viii}	59.70 (17)	Ba1 ⁱⁱ —O1—Ba2 ^{xii}	72.9 (2)
N3 ⁱⁱ —Ba3—Ba4 ^{viii}	86.56 (15)	Ba1 ^{xi} —O1—Ba2 ^{xii}	72.5 (2)
Ga1 ^{vii} —Ba3—Ba4 ^{viii}	78.43 (2)	Ba4—O1—Ba2 ^{xii}	143.9 (3)
Ga1 ⁱⁱ —Ba3—Ba4 ^{viii}	67.05 (2)	Ba2—O1—Ba2 ^{xii}	142.8 (3)
Ga1—Ba3—Ba4 ^{viii}	169.55 (3)		

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