



Lu-atom-ordered oxonitridoaluminosilicate

 $\text{Ba}_{0.9}\text{Ce}_{0.1}\text{LuAl}_{0.2}\text{Si}_{3.8}\text{N}_{6.9}\text{O}_{0.1}$

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A single crystal of $\text{Ba}_{0.9}\text{Ce}_{0.1}\text{LuAl}_{0.2}\text{Si}_{3.8}\text{N}_{6.9}\text{O}_{0.1}$ (barium cerium lutetium aluminosilicate nitride oxide) was obtained by heating a mixed powder of Ba_3N_2 , Si_3N_4 , Al, Lu_2O_3 , and CeO_2 at 2173 K for 1 h under N_2 gas at 0.85 MPa. X-ray single-crystal structure analysis revealed that the title oxynitride is hexagonal (lattice constants: $a = 6.0378(5) \text{ \AA}$, $c = 9.8133(9) \text{ \AA}$; space group: $P6_3mc$) and isostructural with $\text{BaYbSi}_4\text{N}_7$. (Ba,Ce) and Lu atoms occupy twelfold and sixfold coordination sites, respectively.

1. Chemical context

Huppertz & Schnick (1997*b*) determined the hexagonal crystal structures of two isotypic nitrides, $\text{SrYbSi}_4\text{N}_7$ [$a = 5.9880(3) \text{ \AA}$, $c = 9.7499(9) \text{ \AA}$] and $\text{BaYbSi}_4\text{N}_7$ [$a = 6.0307(2) \text{ \AA}$, $c = 9.8198(4) \text{ \AA}$] with space group $P6_3mc$ ($Z = 2$), by single-crystal X-ray diffraction (XRD). In the crystal structure of $\text{BaYbSi}_4\text{N}_7$, the Ba, Yb, and Si atoms are coordinated by twelve, six, and four N atoms of an anticuboctahedron, octahedron, and a tetrahedron, respectively. A three-dimensional framework of SiN_4 tetrahedra is formed by sharing vertex N atoms, and the interspaces of the framework are occupied by Ba and Yb atoms. N atoms at the N1 and N2 sites bond to two Si atoms, and N atoms at the N3 site are surrounded by four Si atoms. Such a high coordination number for the N3 site is characteristic of the crystal structures of $\text{SrYbSi}_4\text{N}_7$ and $\text{BaYbSi}_4\text{N}_7$ (Huppertz & Schnick, 1997*b*).

Other nitrides having the same structure type have been synthesized by substitution of Ca and/or other rare-earth (R) atoms for Sr, Ba, and Yb atoms. The crystal structure of SrYSi_4N_7 ($a = 6.0160(1) \text{ \AA}$, $c = 9.7894(1) \text{ \AA}$) was clarified by powder X-ray diffraction (pXRD) (Li, Fang, *et al.*, 2004). Some nitrides doped with Eu^{2+} , such as $\text{Ba}_{0.99}\text{Eu}_{0.01}\text{YSi}_4\text{N}_7$ [$a = 6.0275(6) \text{ \AA}$, $c = 9.880(1) \text{ \AA}$], $\text{Sr}_{0.99}\text{Eu}_{0.01}\text{YSi}_4\text{N}_7$ [$a = 6.0269(7) \text{ \AA}$, $c = 9.878(1) \text{ \AA}$], and $\text{Ca}_{0.99}\text{Eu}_{0.01}\text{YSi}_4\text{N}_7$ [$a = 5.9866(5) \text{ \AA}$, $c = 9.800(1) \text{ \AA}$] (Li, Fang, *et al.*, 2004; Porob *et al.*, 2012), have also been reported. Oxynitrides $\text{SrR}(\text{Si,Al})_4(\text{N,O})_7$ and $\text{BaR}(\text{Si,Al})_4(\text{N,O})_7$ ($R = \text{Ho, Er, Tm, Yb}$; Lieb *et al.*, 2007), in which the Si and N atoms are partly replaced by Al and O atoms, have also been synthesized. The crystal structures of the aforementioned compounds were found to be isotypic with $\text{SrYbSi}_4\text{N}_7$ and $\text{BaYbSi}_4\text{N}_7$. The alkaline-earth (A) atoms of Ca, Sr, or Ba are ordered at the anticuboctahedral (*a*) site of twelfold coordination of N or O atoms, and the R atoms are located at the octahedral (*o*) site of sixfold coordination of N or O atoms. However, the crystal

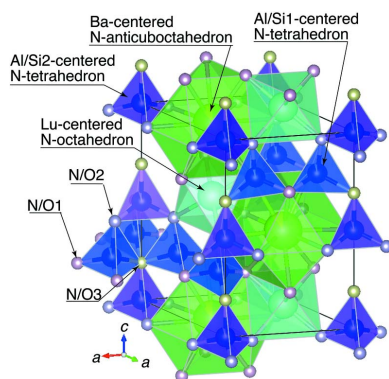


Table 1
Experimental details.

Crystal data	
Chemical formula	Ba _{0.9} Ce _{0.1} LuAl _{0.2} Si _{3.8} N _{6.9} O _{0.1}
M_r	1045.99
Crystal system, space group	Hexagonal, $P6_3mc$
Temperature (K)	301
a, c (Å)	6.0378 (5), 9.8133 (9)
V (Å ³)	309.82 (6)
Z	1
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	22.95
Crystal size (μm)	0.13 \times 0.07 \times 0.02
Data collection	
Diffractionmeter	Bruker D8 QUEST
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2018)
$T_{\text{min}}, T_{\text{max}}$	0.37, 0.68
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	2818, 395, 381
R_{int}	0.059
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.713
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.022, 0.055, 1.04
No. of reflections	395
No. of parameters	33
No. of restraints	1
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	1.70, -1.40
Absolute structure	Refined as an inversion twin
Absolute structure parameter	0.10 (3)

Computer programs: Instrument Service (Bruker, 2018), *APEX3* (Bruker, 2018), *SAINT* (Bruker, 2018), *SHELXT2014/5* (Sheldrick, 2015a), *SHELXL2014/7* (Sheldrick, 2015b), *VESTA* (Momma & Izumi, 2011), pubCIF (Westrip, 2010).

structures of BaLuSi₄N₇ [$a = 6.02185$ (2) Å, $c = 9.81219$ (7) Å] and SrLuSi₄N₇ [$a = 6.02113$ (2) Å, $c = 9.80105$ (7) Å] were analyzed by the Rietveld method for pXRD patterns using a disordered model in which both Ba/Sr and Lu atoms were statistically located at the a and o sites with the same occupancy of 0.5 (Park *et al.*, 2012).

During our materials survey of novel Ce-doped phosphors in the Ba–Lu–Si–N system, small numbers of needle-like single crystals of 10 μm in diameter and 60 μm in length (at maximum) were grown at the contact surface between the BN crucible and an aggregate of fine particles consisting of amorphous and crystalline materials. The powder XRD pattern of the crystalline materials were indexed by the similar lattice constants as that of the needle-like crystals. Electron-probe microanalysis (EPMA) performed at 12 points on one of the needle-like single crystals gave a composition of Ce:Ba:Lu:Si:Al:N:O = 0.8 (2):7.6 (5):7.6 (6):29.6 (20):1.6 (4):49 (3):4(1) in weight percent (total mass was normalized to 100 mass%). The lower precision of the N and O contents was due to the lower energy of the characteristic X-rays of these light elements. The molar ratio obtained from the composition was Ce:Ba:Lu:Si:Al:N:O = 0.1 (3):0.99 (7):0.99 (8):3.9 (3):0.21 (5):6.4 (4):0.5 (2) (total sum 13), and the composition of the single crystal was regarded to be Ce_{0.1}Ba_{0.9}Lu_{1.0}Si_{3.8}Al_{0.2}N_{6.9}O_{0.1} by assuming Ce atoms situated at the a site with Ba atoms. The XRD spots from the crystal were indexed with hexagonal lattice constants of $a = 6.0378$ (5) Å and $c = 9.8133$ (9) Å (Table 1), which were approximately the same as those

Table 2
Disordered model (Ce_{0.1}Ba_{0.4}Lu_{0.5})(Ba_{0.5}Lu_{0.5})(Al_{0.05}Si_{0.95})₄(N_{0.99}O_{0.01})₇.

Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.042, 0.115, 1.32
No. of reflections	395
No. of parameters	39
No. of restraints	1
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	5.52, -3.46
Absolute structure	Refined as an inversion twin
Absolute structure parameter	0.12 (9)

reported for BaLuSi₄N₇ (Park *et al.*, 2012) within differences of 0.1 and 0.2%, respectively. Initially, a structure refinement of Ce_{0.1}Ba_{0.9}Lu_{1.0}Si_{3.8}Al_{0.2}N_{6.9}O_{0.1} was carried out with a disordered model of (Ce_{0.1}Ba_{0.4}Lu_{0.5})(Ba_{0.5}Lu_{0.5})Al_{0.05}Si_{0.95})₄(N_{0.99}O_{0.01})₇, in which the Ce, Ba, and Lu atoms were at the a site with a ratio of 0.1:0.4:0.5 and Ba and Lu atoms were at the o site with a 0.5:0.5 ratio, in accordance with the structure model of BaLuSi₄N₇ (Park *et al.*, 2012). The R value of refinement was 4.2%, and residual electron densities of 5.52 and -3.46 e Å⁻³ were observed at 0.89 and 1.67 Å, respectively, from the a site and the N/O site (Table 2). Refinement using the ordered model of (Ce_{0.1}Ba_{0.9})(Lu)(Al_{0.05}Si_{0.95})₄(N_{0.99}O_{0.01})₇, in which the Ba and Ce atoms are at the a site with a ratio of 0.9:0.1 and Lu atoms fully occupy the o site, yielded an R value of 2.2% with residual electron densities of 1.70 and -1.40 e Å⁻³ (Table 1). As a consequence, the Ba and Lu atoms in Ba_{0.9}Ce_{0.1}LuAl_{0.2}Si_{3.8}N_{6.9}O_{0.1} were clarified to be ordered at the a and o sites, respectively (Fig. 1).

2. Structural commentary

The interatomic distances of Ba/Ce–N/O for Ba_{0.9}Ce_{0.1}LuAl_{0.2}Si_{3.8}N_{6.9}O_{0.1} are 2.975 (10) Å \times 3, 3.0236 (5) Å \times 4, 3.0236 (5) Å \times 2, and 3.052 (10) Å \times 3, which are comparable with the Ba/Lu–N distances for the a site of BaLuSi₄N₇ (2.975 Å \times 3, 3.0372 Å \times 3, 3.038 Å \times 3, 3.0783 Å \times 3) reported by Park *et al.* (2012). Lu–N/O distances in the title compound are 2.271 (10) Å \times 3 and 2.312 (9) Å \times 3, which are 0.139 Å shorter than the Ba/Lu–N distances (2.414 Å \times 3, 2.451 Å \times 3) for the o site of BaLuSi₄N₇.

The Al/Si1–N/O distances are 1.701 (9) Å \times 3 and 1.85 (2) Å, and the Al/Si2–N/O distances are 1.738 (9) Å, 1.743 (6) Å \times 2, and 1.954 (7) Å. These distances are consistent with those of Si–N (1.705 Å \times 3, 1.887 Å and 1.724 Å, 1.721 Å \times 2, 1.962 Å) for BaYbSi₄N₇ (Huppertz & Schnick, 1997b) but 0.07–0.2 Å longer than those of Si1–N (1.478 Å \times 3, 1.776 Å) and Si2–N (1.671, 1.673, 1.889, 1.937 Å) reported for BaLuSi₄N₇ by Park *et al.* (2012), although the lattice constants of Ba_{0.9}Ce_{0.1}LuAl_{0.2}Si_{3.8}N_{6.9}O_{0.1} and BaLuSi₄N₇ are similar, as previously mentioned. The average distances of Al/Si2–N/O and Si2–O of 1.792 and 1.782 Å, respectively, are slightly longer than those of Al/Si1–N/O (1.741 Å) and Si1–N (1.750 Å). The ^{IV}Si⁴⁺–^{IV}N³⁻ and ^{IV}Al³⁺–^{IV}N³⁻ distances calculated with the effective ionic radius for nitrides (^{IV}Si⁴⁺ = 0.29, ^{IV}Al³⁺ = 0.41 Å, ^{IV}N³⁻ = 1.46 Å; Baur, 1987) are 1.75 and

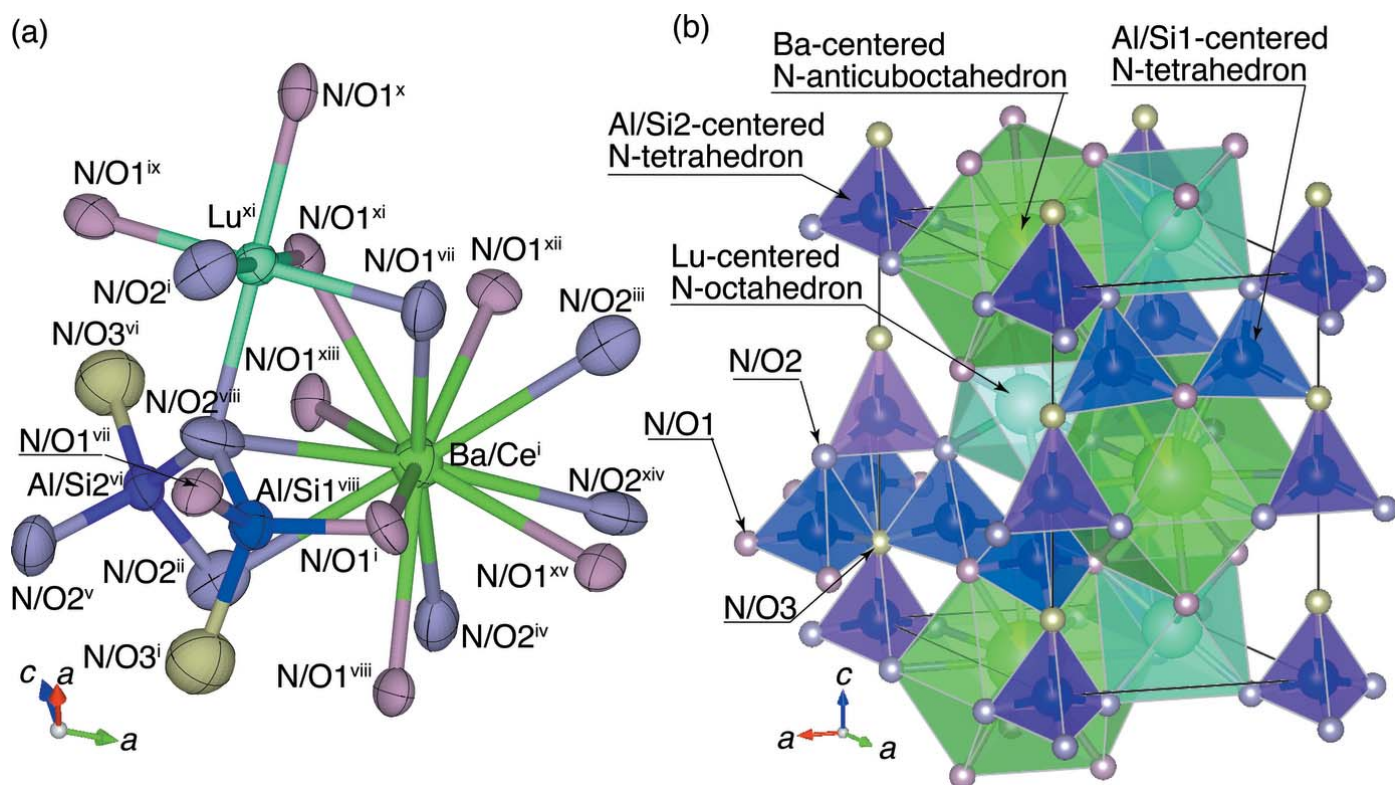


Figure 1

(a) Arrangement of cation-centered N/O atoms and (b) the crystal structure illustrated with cation-centered N/O-coordinated polyhedra for $\text{Ba}_{0.90}\text{Ce}_{0.10}\text{LuSi}_{3.80}\text{Al}_{0.20}\text{N}_{6.90}\text{O}_{0.10}$. Symmetry codes: (i) x, y, z ; (ii) $x - 1, y, z$; (iii) $x, y + 1, z$; (iv) $-y, x - y, z$; (v) $-y, x - y - 1, z$; (vi) $-x, -y, z + \frac{1}{2}$; (vii) $-y + 1, x - y, z$; (viii) $-x + y + 1, -x + 1, z$; (ix) $y, -x + y, z + \frac{1}{2}$; (x) $x - y + 1, x, z + \frac{1}{2}$; (xi) $-x + 1, -y + 1, z + \frac{1}{2}$; (xii) $y, -x + y + 1, z + \frac{1}{2}$; (xiii) $x - y, x, z + \frac{1}{2}$; (xiv) $-x + y + 1, -x + 2, z$; (xv) $-y + 1, x - y + 1, z$.

1.87 Å, respectively, which are similar to the Si–N and Al/Si–N/O distances of $\text{BaYbSi}_4\text{N}_7$ and $\text{Ba}_{0.9}\text{Ce}_{0.1}\text{LuAl}_{0.2}\text{Si}_{3.8}\text{N}_{6.9}\text{O}_{0.1}$. The bond-valence sum (BVS) (Brown & Altermatt, 1985) for the Lu site of $\text{Ba}_{0.9}\text{Ce}_{0.1}\text{LuAl}_{0.2}\text{Si}_{3.8}\text{N}_{6.9}\text{O}_{0.1}$ was calculated to be 3.07 with a bond-valence parameter of Lu–N ($r_0 = 2.046, b = 0.37$) reported by Brese & O’Keeffe (1991), in good agreement with the valence of Lu^{3+} . The BVS with a parameter of Ba–N [$r_0 = 2.47$; Brese and O’Keeffe (1991)] is 2.73, which is greater than the valence of Ba^{2+} . The BVSs of Al/Si1 and Al/Si2 with the parameter of Si–N ($r_0 = 1.77, b = 0.37$) are 4.39 and 3.87, respectively.

3. Database survey

The Inorganic Crystal Structure Database (ICSD) includes some records of $\text{BaYbSi}_4\text{N}_7$ -type nitrides and oxynitrides that include alkaline-earth and rare-earth elements: $\text{BaYbSi}_4\text{N}_7$ and $\text{SrYbSi}_4\text{N}_7$ by Huppertz & Schnick (1997b) and SrYSi_4N_7 by Li, Fang *et al.* (2004). $\text{EuYbSi}_4\text{N}_7$ and EuYSi_4N_7 (Huppertz & Schnick, 1997a; Li, Fang *et al.*, 2004) are isostructural with $\text{BaYbSi}_4\text{N}_7$ but do not include an alkaline-earth metal element.

Oxynitrides in which Si and N atoms were partly replaced with Al and O atoms, respectively, have also been reported: $\text{BaYb}(\text{Si},\text{Al})_4(\text{O},\text{N})_7$ (Vinograd *et al.*, 2007), $\text{BaEr}(\text{Si},\text{Al})_4(\text{O},\text{N})_7$, $\text{BaHo}(\text{Si},\text{Al})_4(\text{O},\text{N})_7$, $\text{BaTm}(\text{Si},\text{Al})_4(\text{O},\text{N})_7$, $\text{BaYb}(\text{Si},\text{Al})_4(\text{O},\text{N})_7$, $\text{SrEr}(\text{Si},\text{Al})_4(\text{O},\text{N})_7$, $\text{SrHo}(\text{Si},\text{Al})_4(\text{O},\text{N})_7$,

$\text{SrTm}(\text{Si},\text{Al})_4(\text{O},\text{N})_7$, $\text{SrYb}(\text{Si},\text{Al})_4(\text{O},\text{N})_7$, $\text{EuEr}(\text{Si},\text{Al})_4(\text{O},\text{N})_7$, $\text{EuHo}(\text{Si},\text{Al})_4(\text{O},\text{N})_7$, $\text{EuTm}(\text{Si},\text{Al})_4(\text{O},\text{N})_7$, and $\text{EuYb}(\text{Si},\text{Al})_4(\text{O},\text{N})_7$ (Lieb *et al.*, 2007).

First-principles calculations of the electronic structures of SrYSi_4N_7 and BaYSi_4N_7 have been reported (Fang *et al.*, 2003). Moreover, numerous researchers have investigated the luminescence of oxynitrides and nitrides doped with Ce and Eu, including Ce^{3+} - BaYSi_4N_7 , Eu^{2+} - BaYSi_4N_7 (Li, deWith *et al.*, 2004), Ce^{3+} - SrYSi_4N_7 , Eu^{2+} - SrYSi_4N_7 (Li, Fang *et al.*, 2004), Eu^{2+} -(Ca, Sr, or Ba) YSi_4N_7 , Eu^{2+} -(Ca, Sr, or Ba) $\text{Y}(\text{Si},\text{Al})_4(\text{N},\text{O})_7$ (Kurushima *et al.*, 2010), Eu^{2+} -(Ca, Sr, or Ba)(Sc, Y, or La) Si_4N_7 (Horikawa *et al.*, 2012), Eu^{2+} -(Ca, Sr, or Ba) $\text{Y}(\text{Y}, \text{La}, \text{or Lu})\text{Si}_4\text{N}_7$ (Park *et al.*, 2012), and Eu^{2+} - $\text{SrScSi}_4(\text{N},\text{O})_7$ (Porob *et al.*, 2012).

4. Synthesis and crystallization

Powdered Si_3N_4 (Ube Industries Ltd., UBE-SN-E10, 95+%), Ba_3N_2 (Materion Corp., ~20 mesh 99.7%), Al (Rare Metallic, ~200 mesh, 99.9%), Lu_2O_3 (Nippon Yttrium Co. Ltd., 99.999%), CeO_2 (Shin-Etsu Chemical Co. Ltd., 99.99%) were weighed out in an Si:Ba:Lu:Al:Ce molar ratio of 3.25:1:1:0.25:0.04 in an Ar-filled glove box (MBRAUN; $[\text{O}_2]$ and $[\text{H}_2\text{O}] < 1$ ppm). The weighed powders were mixed in an agate mortar, and a disk-shaped pellet with a diameter of 10 mm was formed with a die in an Ar gas-filled glove box. The pellet was placed in a BN crucible (Showa Denko, K. K.,

99.5%) with an 18 mm inner diameter and 20 mm height, and a BN lid was placed on it. The BN crucible was heated to 1200°C for 1 h under vacuum using a carbon furnace (VESTA, Shimadzu Industrial Systems Co., Ltd.), and the temperature was maintained at 1200 °C for 1 h. N₂ gas (Taiyo Nippon Sanso Corp., 99.9995+%) was introduced into the furnace to a pressure of 0.85 MPa, and the furnace was then heated to 1900°C for 25 min. After the temperature and the N₂ gas pressure were maintained for 1 h, the sample was cooled to 1200°C for 25 min. The heater power was then cut off. After the furnace reached room temperature, the crucible was removed from the furnace. The chemical composition of the single crystal was analyzed by EPMA (JEOL JXA-8200).

5. Refinement

Crystal data and the data collection details are summarized in Table 1, and the structural refinement details are reported in Table 2. Ordered and disordered models were investigated, and the best result was obtained using an ordered model in which the Ce/Ba mixed site and Lu site are located at the *a* site and *o* site, respectively. Because the *R* and *S* values were not affected by refinement with ordered models of Al and Si atoms and N and O atoms, the occupancies of the Al/Si and N/O sites were fixed at 0.05/0.95 and 0.99/0.01, respectively. Final refinement was carried out with anisotropic displacement parameters.

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supporting information

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Lu-atom-ordered oxonitridoaluminosilicate Ba_{0.9}Ce_{0.1}LuAl_{0.2}Si_{3.8}N_{6.9}O_{0.1}

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Computing details

Data collection: Instrument Service (Bruker, 2018); cell refinement: *APEX3* (Bruker, 2018); data reduction: *S SAINT* (Bruker, 2018); program(s) used to solve structure: *SHELXT2014/5* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014/7* (Sheldrick, 2015b); molecular graphics: *VESTA* (Momma & Izumi, 2011); software used to prepare material for publication: pubCIF (Westrip, 2010).

Barium cerium lutetium aluminosilicate nitride oxide

Crystal data

Ba_{0.9}Ce_{0.1}LuAl_{0.2}Si_{3.8}N_{6.9}O_{0.1}

$M_r = 1045.99$

Hexagonal, *P6₃mc*

$a = 6.0378$ (5) Å

$c = 9.8133$ (9) Å

$V = 309.82$ (6) Å³

$Z = 1$

$F(000) = 464$

$D_x = 5.606$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 127 reflections

$\theta = 4.2\text{--}30.8^\circ$

$\mu = 22.95$ mm⁻¹

$T = 301$ K

Block, colorless

$0.13 \times 0.07 \times 0.02$ mm

Data collection

Bruker D8 QUEST

diffractometer

Detector resolution: 7.3910 pixels mm⁻¹

ω and σ cans

Absorption correction: multi-scan

(SADABS; Bruker, 2018)

$T_{\min} = 0.37$, $T_{\max} = 0.68$

2818 measured reflections

395 independent reflections

381 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.059$

$\theta_{\max} = 30.5^\circ$, $\theta_{\min} = 3.9^\circ$

$h = -7 \rightarrow 8$

$k = -8 \rightarrow 8$

$l = -14 \rightarrow 14$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.022$

$wR(F^2) = 0.055$

$S = 1.04$

395 reflections

33 parameters

1 restraint

$w = 1/[\sigma^2(F_o^2) + (0.0313P)^2 + 0.7267P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 1.70$ e Å⁻³

$\Delta\rho_{\min} = -1.40$ e Å⁻³

Extinction correction: SHELXL-2014/7

(Sheldrick 2015b),

$F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0052 (16)

Absolute structure: Refined as an inversion twin.

Absolute structure parameter: 0.10 (3)

Special details

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

Refinement. Refined as a two-component inversion twin

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)
Lu1	0.3333	0.6667	0.07616 (4)	0.0074 (2)	
Ba2	0.3333	0.6667	0.44902 (10)	0.0099 (3)	0.9
Ce2	0.3333	0.6667	0.44902 (10)	0.0099 (3)	0.1
Si1	0.8275 (2)	0.1725 (2)	0.2646 (5)	0.0084 (5)	0.95
Al1	0.8275 (2)	0.1725 (2)	0.2646 (5)	0.0084 (5)	0.05
Si2	0.0000	0.0000	0.0006 (7)	0.0071 (9)	0.95
Al2	0.0000	0.0000	0.0006 (7)	0.0071 (9)	0.05
N1	0.5097 (8)	0.4903 (8)	0.2112 (11)	0.0087 (14)	0.9857
O1	0.5097 (8)	0.4903 (8)	0.2112 (11)	0.0087 (14)	0.0143
N2	0.8474 (8)	0.1526 (8)	0.4404 (9)	0.0123 (19)	0.9857
O2	0.8474 (8)	0.1526 (8)	0.4404 (9)	0.0123 (19)	0.0143
N3	0.0000	0.0000	0.1880 (18)	0.016 (3)	0.9857
O3	0.0000	0.0000	0.1880 (18)	0.016 (3)	0.0143

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Lu1	0.0075 (3)	0.0075 (3)	0.0072 (4)	0.00374 (13)	0.000	0.000
Ba2	0.0098 (4)	0.0098 (4)	0.0101 (6)	0.00489 (18)	0.000	0.000
Ce2	0.0098 (4)	0.0098 (4)	0.0101 (6)	0.00489 (18)	0.000	0.000
Si1	0.0076 (8)	0.0076 (8)	0.0097 (10)	0.0035 (9)	-0.0002 (6)	0.0002 (6)
Al1	0.0076 (8)	0.0076 (8)	0.0097 (10)	0.0035 (9)	-0.0002 (6)	0.0002 (6)
Si2	0.0061 (10)	0.0061 (10)	0.009 (3)	0.0031 (5)	0.000	0.000
Al2	0.0061 (10)	0.0061 (10)	0.009 (3)	0.0031 (5)	0.000	0.000
N1	0.007 (2)	0.007 (2)	0.010 (3)	0.002 (2)	0.0010 (16)	-0.0010 (16)
O1	0.007 (2)	0.007 (2)	0.010 (3)	0.002 (2)	0.0010 (16)	-0.0010 (16)
N2	0.015 (3)	0.015 (3)	0.011 (5)	0.011 (4)	0.0010 (14)	-0.0010 (14)
O2	0.015 (3)	0.015 (3)	0.011 (5)	0.011 (4)	0.0010 (14)	-0.0010 (14)
N3	0.018 (5)	0.018 (5)	0.013 (8)	0.009 (3)	0.000	0.000
O3	0.018 (5)	0.018 (5)	0.013 (8)	0.009 (3)	0.000	0.000

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

Lu1—O1 ⁱ	2.271 (10)	Si1—Ba2 ^{ix}	3.521 (2)
Lu1—N1 ⁱ	2.271 (10)	Si1—Ba2 ^x	3.521 (2)
Lu1—O1 ⁱⁱ	2.271 (10)	Si2—O2 ^{xi}	1.701 (9)
Lu1—N1 ⁱⁱ	2.271 (10)	Si2—N2 ^{xi}	1.701 (9)
Lu1—N1	2.271 (10)	Si2—O2 ^{iv}	1.701 (9)

Lu1—O2 ⁱⁱⁱ	2.312 (9)	Si2—N2 ^{iv}	1.701 (9)
Lu1—N2 ⁱⁱⁱ	2.312 (9)	Si2—O2 ^{xii}	1.701 (9)
Lu1—O2 ^{iv}	2.312 (9)	Si2—N2 ^{xii}	1.701 (9)
Lu1—N2 ^{iv}	2.312 (9)	Si2—N3	1.839 (19)
Lu1—O2 ^v	2.312 (9)	Si2—Ba2 ^{xiii}	3.5225 (11)
Lu1—N2 ^v	2.312 (9)	Si2—Ba2 ^{xiv}	3.5225 (11)
Ba2—N1	2.975 (10)	Si2—Ba2 ^v	3.5226 (11)
Ba2—O1 ⁱⁱ	2.975 (10)	N1—Al1 ^{vii}	1.743 (6)
Ba2—N1 ⁱⁱ	2.975 (10)	N1—Si1 ^{vii}	1.743 (6)
Ba2—O1 ⁱ	2.975 (10)	N1—Al1 ^{vi}	1.743 (6)
Ba2—N1 ⁱ	2.975 (10)	N1—Si1 ^{vi}	1.743 (6)
Ba2—O2 ^{vi}	3.0236 (5)	N1—Ba2 ^{xiv}	3.052 (10)
Ba2—N2 ^{vi}	3.0236 (5)	N2—Al2 ^{xv}	1.701 (9)
Ba2—O2 ^{vii}	3.0236 (5)	N2—Si2 ^{xv}	1.701 (9)
Ba2—N2 ^{vii}	3.0236 (5)	N2—Lu1 ^{xv}	2.313 (9)
Ba2—O2 ^{viii}	3.0237 (6)	N2—Ba2 ^{ix}	3.0237 (6)
Ba2—N2 ^{viii}	3.0237 (6)	N2—Ce2 ^{ix}	3.0237 (6)
Si1—N2	1.738 (9)	N2—Ce2 ^x	3.0237 (6)
Si1—O1 ^{vi}	1.743 (6)	N2—Ba2 ^x	3.0237 (6)
Si1—N1 ^{vi}	1.743 (6)	N3—Al1 ^{vi}	1.954 (7)
Si1—O1 ^{vii}	1.743 (6)	N3—Si1 ^{vi}	1.954 (7)
Si1—N1 ^{vii}	1.743 (6)	N3—Al1 ^{xvi}	1.954 (7)
Si1—O3 ^{ix}	1.954 (7)	N3—Si1 ^{xvi}	1.954 (7)
Si1—N3 ^{ix}	1.954 (7)	N3—Si1 ^{viii}	1.954 (7)
Si1—Al1 ^{vii}	2.914 (4)	N3—Al1 ^{viii}	1.954 (7)
Si1—Al1 ^{vi}	2.914 (4)		
O1 ⁱ —Lu1—N1 ⁱ	0.0	N1 ^{vi} —Si1—Al1 ^{vi}	88.8 (2)
O1 ⁱ —Lu1—O1 ⁱⁱ	89.4 (3)	O1 ^{vii} —Si1—Al1 ^{vi}	33.3 (3)
N1 ⁱ —Lu1—O1 ⁱⁱ	89.4 (3)	N1 ^{vii} —Si1—Al1 ^{vi}	33.3 (3)
O1 ⁱ —Lu1—N1 ⁱⁱ	89.4	O3 ^{ix} —Si1—Al1 ^{vi}	143.1 (3)
N1 ⁱ —Lu1—N1 ⁱⁱ	89.4 (3)	N3 ^{ix} —Si1—Al1 ^{vi}	143.1 (3)
O1 ⁱⁱ —Lu1—N1 ⁱⁱ	0.0	Al1 ^{vii} —Si1—Al1 ^{vi}	60.0
O1 ⁱ —Lu1—N1	89.4	N2—Si1—Ba2 ^{ix}	59.17 (6)
N1 ⁱ —Lu1—N1	89.4 (3)	O1 ^{vi} —Si1—Ba2 ^{ix}	57.6 (3)
O1 ⁱⁱ —Lu1—N1	89.4	N1 ^{vi} —Si1—Ba2 ^{ix}	57.6 (3)
N1 ⁱⁱ —Lu1—N1	89.4 (3)	O1 ^{vii} —Si1—Ba2 ^{ix}	149.6 (3)
O1 ⁱ —Lu1—O2 ⁱⁱⁱ	90.2 (2)	N1 ^{vii} —Si1—Ba2 ^{ix}	149.6 (3)
N1 ⁱ —Lu1—O2 ⁱⁱⁱ	90.2 (2)	O3 ^{ix} —Si1—Ba2 ^{ix}	100.5 (2)
O1 ⁱⁱ —Lu1—O2 ⁱⁱⁱ	90.2 (2)	N3 ^{ix} —Si1—Ba2 ^{ix}	100.5 (2)
N1 ⁱⁱ —Lu1—O2 ⁱⁱⁱ	90.2 (2)	Al1 ^{vii} —Si1—Ba2 ^{ix}	65.56 (4)
N1—Lu1—O2 ⁱⁱⁱ	179.5 (3)	Al1 ^{vi} —Si1—Ba2 ^{ix}	116.34 (4)
O1 ⁱ —Lu1—N2 ⁱⁱⁱ	90.2 (2)	N2—Si1—Ba2 ^x	59.17 (6)
N1 ⁱ —Lu1—N2 ⁱⁱⁱ	90.2 (2)	O1 ^{vi} —Si1—Ba2 ^x	149.6 (3)
O1 ⁱⁱ —Lu1—N2 ⁱⁱⁱ	90.2 (2)	N1 ^{vi} —Si1—Ba2 ^x	149.6 (3)
N1 ⁱⁱ —Lu1—N2 ⁱⁱⁱ	90.2 (2)	O1 ^{vii} —Si1—Ba2 ^x	57.6 (3)
N1—Lu1—N2 ⁱⁱⁱ	179.5 (3)	N1 ^{vii} —Si1—Ba2 ^x	57.6 (3)
O2 ⁱⁱⁱ —Lu1—N2 ⁱⁱⁱ	0.0	O3 ^{ix} —Si1—Ba2 ^x	100.5 (2)

O1 ⁱ —Lu1—O2 ^{iv}	179.5 (3)	N3 ^{ix} —Si1—Ba2 ^x	100.5 (2)
N1 ⁱ —Lu1—O2 ^{iv}	179.5 (3)	All ^{vii} —Si1—Ba2 ^x	116.34 (4)
O1 ⁱⁱ —Lu1—O2 ^{iv}	90.2 (2)	All ^{vi} —Si1—Ba2 ^x	65.56 (4)
N1 ⁱⁱ —Lu1—O2 ^{iv}	90.2 (2)	Ba2 ^{ix} —Si1—Ba2 ^x	118.08 (12)
N1—Lu1—O2 ^{iv}	90.2 (2)	O2 ^{xi} —Si2—N2 ^{xi}	0.0
O2 ⁱⁱⁱ —Lu1—O2 ^{iv}	90.1 (3)	O2 ^{xi} —Si2—O2 ^{iv}	108.6 (4)
N2 ⁱⁱⁱ —Lu1—O2 ^{iv}	90.1 (3)	N2 ^{xi} —Si2—O2 ^{iv}	108.6 (4)
O1 ⁱ —Lu1—N2 ^{iv}	179.5 (3)	O2 ^{xi} —Si2—N2 ^{iv}	108.6
N1 ⁱ —Lu1—N2 ^{iv}	179.5 (3)	N2 ^{xi} —Si2—N2 ^{iv}	108.6 (4)
O1 ⁱⁱ —Lu1—N2 ^{iv}	90.2 (2)	O2 ^{iv} —Si2—N2 ^{iv}	0.0
N1 ⁱⁱ —Lu1—N2 ^{iv}	90.2 (2)	O2 ^{xi} —Si2—O2 ^{xii}	108.6 (4)
N1—Lu1—N2 ^{iv}	90.2 (2)	N2 ^{xi} —Si2—O2 ^{xii}	108.6 (4)
O2 ⁱⁱⁱ —Lu1—N2 ^{iv}	90.1	O2 ^{iv} —Si2—O2 ^{xii}	108.6 (4)
N2 ⁱⁱⁱ —Lu1—N2 ^{iv}	90.1 (3)	N2 ^{iv} —Si2—O2 ^{xii}	108.6 (4)
O2 ^{iv} —Lu1—N2 ^{iv}	0.0	O2 ^{xi} —Si2—N2 ^{xii}	108.6
O1 ⁱ —Lu1—O2 ^v	90.2 (2)	N2 ^{xi} —Si2—N2 ^{xii}	108.6 (4)
N1 ⁱ —Lu1—O2 ^v	90.2 (2)	O2 ^{iv} —Si2—N2 ^{xii}	108.6
O1 ⁱⁱ —Lu1—O2 ^v	179.5 (3)	N2 ^{iv} —Si2—N2 ^{xii}	108.6 (4)
N1 ⁱⁱ —Lu1—O2 ^v	179.5 (3)	O2 ^{xii} —Si2—N2 ^{xii}	0.0
N1—Lu1—O2 ^v	90.2 (2)	O2 ^{xi} —Si2—N3	110.3 (3)
O2 ⁱⁱⁱ —Lu1—O2 ^v	90.1 (3)	N2 ^{xi} —Si2—N3	110.3 (3)
N2 ⁱⁱⁱ —Lu1—O2 ^v	90.1 (3)	O2 ^{iv} —Si2—N3	110.3 (3)
O2 ^{iv} —Lu1—O2 ^v	90.1 (3)	N2 ^{iv} —Si2—N3	110.3 (3)
N2 ^{iv} —Lu1—O2 ^v	90.1 (3)	O2 ^{xii} —Si2—N3	110.3 (3)
O1 ⁱ —Lu1—N2 ^v	90.2 (2)	N2 ^{xii} —Si2—N3	110.3 (3)
N1 ⁱ —Lu1—N2 ^v	90.2 (2)	O2 ^{xi} —Si2—Ba2 ^{xiii}	59.07 (3)
O1 ⁱⁱ —Lu1—N2 ^v	179.5 (3)	N2 ^{xi} —Si2—Ba2 ^{xiii}	59.07 (3)
N1 ⁱⁱ —Lu1—N2 ^v	179.5 (3)	O2 ^{iv} —Si2—Ba2 ^{xiii}	151.4 (4)
N1—Lu1—N2 ^v	90.2 (2)	N2 ^{iv} —Si2—Ba2 ^{xiii}	151.4 (4)
O2 ⁱⁱⁱ —Lu1—N2 ^v	90.1	O2 ^{xii} —Si2—Ba2 ^{xiii}	59.07 (3)
N2 ⁱⁱⁱ —Lu1—N2 ^v	90.1 (3)	N2 ^{xii} —Si2—Ba2 ^{xiii}	59.07 (3)
O2 ^{iv} —Lu1—N2 ^v	90.1	N3—Si2—Ba2 ^{xiii}	98.27 (11)
N2 ^{iv} —Lu1—N2 ^v	90.1 (3)	O2 ^{xi} —Si2—Ba2 ^{xiv}	151.4 (4)
O2 ^v —Lu1—N2 ^v	0.0	N2 ^{xi} —Si2—Ba2 ^{xiv}	151.4 (4)
N1—Ba2—O1 ⁱⁱ	65.0	O2 ^{iv} —Si2—Ba2 ^{xiv}	59.07 (3)
N1—Ba2—N1 ⁱⁱ	65.0 (3)	N2 ^{iv} —Si2—Ba2 ^{xiv}	59.07 (3)
O1 ⁱⁱ —Ba2—N1 ⁱⁱ	0.0	O2 ^{xii} —Si2—Ba2 ^{xiv}	59.07 (3)
N1—Ba2—O1 ⁱ	65.0	N2 ^{xii} —Si2—Ba2 ^{xiv}	59.07 (3)
O1 ⁱⁱ —Ba2—O1 ⁱ	65.0 (3)	N3—Si2—Ba2 ^{xiv}	98.27 (11)
N1 ⁱⁱ —Ba2—O1 ⁱ	65.0 (3)	Ba2 ^{xiii} —Si2—Ba2 ^{xiv}	117.97 (6)
N1—Ba2—N1 ⁱ	65.0 (3)	O2 ^{xi} —Si2—Ba2 ^v	59.07 (3)
O1 ⁱⁱ —Ba2—N1 ⁱ	65.0	N2 ^{xi} —Si2—Ba2 ^v	59.07 (3)
N1 ⁱⁱ —Ba2—N1 ⁱ	65.0 (3)	O2 ^{iv} —Si2—Ba2 ^v	59.07 (3)
O1 ⁱ —Ba2—N1 ⁱ	0.0	N2 ^{iv} —Si2—Ba2 ^v	59.07 (3)
N1—Ba2—O2 ^{vi}	57.1 (2)	O2 ^{xii} —Si2—Ba2 ^v	151.4 (4)
O1 ⁱⁱ —Ba2—O2 ^{vi}	87.01 (17)	N2 ^{xii} —Si2—Ba2 ^v	151.4 (4)
N1 ⁱⁱ —Ba2—O2 ^{vi}	87.01 (17)	N3—Si2—Ba2 ^v	98.27 (11)
O1 ⁱ —Ba2—O2 ^{vi}	122.0 (3)	Ba2 ^{xiii} —Si2—Ba2 ^v	117.97 (6)

N1 ⁱ —Ba2—O2 ^{vi}	122.0 (3)	Ba2 ^{xiv} —Si2—Ba2 ^v	117.97 (6)
N1—Ba2—N2 ^{vi}	57.1 (2)	Al1 ^{vii} —N1—Si1 ^{vii}	0.0
O1 ⁱⁱ —Ba2—N2 ^{vi}	87.01 (17)	Al1 ^{vii} —N1—Al1 ^{vi}	113.4 (6)
N1 ⁱⁱ —Ba2—N2 ^{vi}	87.01 (17)	Si1 ^{vii} —N1—Al1 ^{vi}	113.4 (6)
O1 ⁱ —Ba2—N2 ^{vi}	122.0 (3)	Al1 ^{vii} —N1—Si1 ^{vi}	113.4
N1 ⁱ —Ba2—N2 ^{vi}	122.0 (3)	Si1 ^{vii} —N1—Si1 ^{vi}	113.4 (6)
O2 ^{vi} —Ba2—N2 ^{vi}	0.0	Al1 ^{vi} —N1—Si1 ^{vi}	0.0
N1—Ba2—O2 ^{vii}	57.1 (2)	Al1 ^{vii} —N1—Lu1	123.3 (3)
O1 ⁱⁱ —Ba2—O2 ^{vii}	122.0 (3)	Si1 ^{vii} —N1—Lu1	123.3 (3)
N1 ⁱⁱ —Ba2—O2 ^{vii}	122.0 (3)	Al1 ^{vi} —N1—Lu1	123.3 (3)
O1 ⁱ —Ba2—O2 ^{vii}	87.01 (17)	Si1 ^{vi} —N1—Lu1	123.3 (3)
N1 ⁱ —Ba2—O2 ^{vii}	87.01 (17)	Al1 ^{vii} —N1—Ba2	92.8 (4)
O2 ^{vi} —Ba2—O2 ^{vii}	65.6 (3)	Si1 ^{vii} —N1—Ba2	92.8 (4)
N2 ^{vi} —Ba2—O2 ^{vii}	65.6 (3)	Al1 ^{vi} —N1—Ba2	92.8 (4)
N1—Ba2—N2 ^{vii}	57.1 (2)	Si1 ^{vi} —N1—Ba2	92.8 (4)
O1 ⁱⁱ —Ba2—N2 ^{vii}	122.0 (3)	Lu1—N1—Ba2	87.4 (2)
N1 ⁱⁱ —Ba2—N2 ^{vii}	122.0 (3)	Al1 ^{vii} —N1—Ba2 ^{xiv}	90.4 (3)
O1 ⁱ —Ba2—N2 ^{vii}	87.01 (17)	Si1 ^{vii} —N1—Ba2 ^{xiv}	90.4 (3)
N1 ⁱ —Ba2—N2 ^{vii}	87.01 (17)	Al1 ^{vi} —N1—Ba2 ^{xiv}	90.4 (3)
O2 ^{vi} —Ba2—N2 ^{vii}	65.6	Si1 ^{vi} —N1—Ba2 ^{xiv}	90.4 (3)
N2 ^{vi} —Ba2—N2 ^{vii}	65.6 (3)	Lu1—N1—Ba2 ^{xiv}	86.8 (3)
O2 ^{vii} —Ba2—N2 ^{vii}	0.0	Ba2—N1—Ba2 ^{xiv}	174.2 (4)
N1—Ba2—O2 ^{viii}	87.01 (17)	Al2 ^{xv} —N2—Si2 ^{xv}	0.0
O1 ⁱⁱ —Ba2—O2 ^{viii}	57.1 (2)	Al2 ^{xv} —N2—Si1	117.2 (5)
N1 ⁱⁱ —Ba2—O2 ^{viii}	57.1 (2)	Si2 ^{xv} —N2—Si1	117.2 (5)
O1 ⁱ —Ba2—O2 ^{viii}	122.0 (3)	Al2 ^{xv} —N2—Lu1 ^{xv}	124.5 (5)
N1 ⁱ —Ba2—O2 ^{viii}	122.0 (3)	Si2 ^{xv} —N2—Lu1 ^{xv}	124.5 (5)
O2 ^{vi} —Ba2—O2 ^{viii}	54.4 (3)	Si1—N2—Lu1 ^{xv}	118.3 (4)
N2 ^{vi} —Ba2—O2 ^{viii}	54.4 (3)	Al2 ^{xv} —N2—Ba2 ^{ix}	92.07 (17)
O2 ^{vii} —Ba2—O2 ^{viii}	119.924 (18)	Si2 ^{xv} —N2—Ba2 ^{ix}	92.07 (17)
N2 ^{vii} —Ba2—O2 ^{viii}	119.924 (18)	Si1—N2—Ba2 ^{ix}	91.25 (18)
N1—Ba2—N2 ^{viii}	87.01 (17)	Lu1 ^{xv} —N2—Ba2 ^{ix}	86.80 (17)
O1 ⁱⁱ —Ba2—N2 ^{viii}	57.1 (2)	Al2 ^{xv} —N2—Ce2 ^{ix}	92.07 (17)
N1 ⁱⁱ —Ba2—N2 ^{viii}	57.1 (2)	Si2 ^{xv} —N2—Ce2 ^{ix}	92.07 (17)
O1 ⁱ —Ba2—N2 ^{viii}	122.0 (3)	Si1—N2—Ce2 ^{ix}	91.25 (18)
N1 ⁱ —Ba2—N2 ^{viii}	122.0 (3)	Lu1 ^{xv} —N2—Ce2 ^{ix}	86.80 (17)
O2 ^{vi} —Ba2—N2 ^{viii}	54.4	Ba2 ^{ix} —N2—Ce2 ^{ix}	0.0
N2 ^{vi} —Ba2—N2 ^{viii}	54.4 (3)	Al2 ^{xv} —N2—Ce2 ^x	92.07 (17)
O2 ^{vii} —Ba2—N2 ^{viii}	119.9	Si2 ^{xv} —N2—Ce2 ^x	92.07 (17)
N2 ^{vii} —Ba2—N2 ^{viii}	119.924 (18)	Si1—N2—Ce2 ^x	91.25 (18)
O2 ^{viii} —Ba2—N2 ^{viii}	0.0	Lu1 ^{xv} —N2—Ce2 ^x	86.80 (17)
N2—Si1—O1 ^{vi}	111.0 (4)	Ba2 ^{ix} —N2—Ce2 ^x	173.6 (3)
N2—Si1—N1 ^{vi}	111.0 (4)	Ce2 ^{ix} —N2—Ce2 ^x	173.6 (3)
O1 ^{vi} —Si1—N1 ^{vi}	0.0	Al2 ^{xv} —N2—Ba2 ^x	92.07 (17)
N2—Si1—O1 ^{vii}	111.0 (4)	Si2 ^{xv} —N2—Ba2 ^x	92.07 (17)
O1 ^{vi} —Si1—O1 ^{vii}	109.3 (6)	Si1—N2—Ba2 ^x	91.25 (18)
N1 ^{vi} —Si1—O1 ^{vii}	109.3 (6)	Lu1 ^{xv} —N2—Ba2 ^x	86.80 (17)
N2—Si1—N1 ^{vii}	111.0 (4)	Ba2 ^{ix} —N2—Ba2 ^x	173.6 (3)

O1 ^{vi} —Si1—N1 ^{vii}	109.3	Ce2 ^{ix} —N2—Ba2 ^x	173.6
N1 ^{vi} —Si1—N1 ^{vii}	109.3 (6)	Ce2 ^x —N2—Ba2 ^x	0.0
O1 ^{vii} —Si1—N1 ^{vii}	0.0	Si2—N3—Al1 ^{vi}	112.6 (5)
N2—Si1—O3 ^{ix}	105.7 (6)	Si2—N3—Si1 ^{vi}	112.6 (5)
O1 ^{vi} —Si1—O3 ^{ix}	109.9 (4)	Al1 ^{vi} —N3—Si1 ^{vi}	0.0
N1 ^{vi} —Si1—O3 ^{ix}	109.9 (4)	Si2—N3—Al1 ^{xvi}	112.6 (5)
O1 ^{vii} —Si1—O3 ^{ix}	109.9 (4)	Al1 ^{vi} —N3—Al1 ^{xvi}	106.2 (5)
N1 ^{vii} —Si1—O3 ^{ix}	109.9 (4)	Si1 ^{vi} —N3—Al1 ^{xvi}	106.2 (5)
N2—Si1—N3 ^{ix}	105.7 (6)	Si2—N3—Si1 ^{xvi}	112.6 (5)
O1 ^{vi} —Si1—N3 ^{ix}	109.9 (4)	Al1 ^{vi} —N3—Si1 ^{xvi}	106.2
N1 ^{vi} —Si1—N3 ^{ix}	109.9 (4)	Si1 ^{vi} —N3—Si1 ^{xvi}	106.2 (5)
O1 ^{vii} —Si1—N3 ^{ix}	109.9 (4)	Al1 ^{xvi} —N3—Si1 ^{xvi}	0.0
N1 ^{vii} —Si1—N3 ^{ix}	109.9 (4)	Si2—N3—Si1 ^{viii}	112.6 (5)
O3 ^{ix} —Si1—N3 ^{ix}	0.0	Al1 ^{vi} —N3—Si1 ^{viii}	106.2
N2—Si1—Al1 ^{vii}	96.0 (2)	Si1 ^{vi} —N3—Si1 ^{viii}	106.2 (5)
O1 ^{vi} —Si1—Al1 ^{vii}	33.3 (3)	Al1 ^{xvi} —N3—Si1 ^{viii}	106.2
N1 ^{vi} —Si1—Al1 ^{vii}	33.3 (3)	Si1 ^{xvi} —N3—Si1 ^{viii}	106.2 (5)
O1 ^{vii} —Si1—Al1 ^{vii}	88.8 (2)	Si2—N3—Al1 ^{viii}	112.6 (5)
N1 ^{vii} —Si1—Al1 ^{vii}	88.8 (2)	Al1 ^{vi} —N3—Al1 ^{viii}	106.2 (5)
O3 ^{ix} —Si1—Al1 ^{vii}	143.1 (3)	Si1 ^{vi} —N3—Al1 ^{viii}	106.2 (5)
N3 ^{ix} —Si1—Al1 ^{vii}	143.1 (3)	Al1 ^{xvi} —N3—Al1 ^{viii}	106.2 (5)
N2—Si1—Al1 ^{vi}	96.0 (2)	Si1 ^{xvi} —N3—Al1 ^{viii}	106.2 (5)
O1 ^{vi} —Si1—Al1 ^{vi}	88.8 (2)	Si1 ^{viii} —N3—Al1 ^{viii}	0.0 (2)

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