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La₃Si₆N₁₁

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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{Si-N}) = 0.003$ Å; R factor = 0.017; wR factor = 0.030; data-to-parameter ratio = 16.0.

Colorless transparent single crystals of trilanthanum hexasilicon undecanitrogen, La₃Si₆N₁₁, were prepared at 0.85 MPa of N₂ and 2273 K. The title compound is isotypic with Sm₃Si₆N₁₁. Silicon-centered nitrogen tetrahedra form a three-dimensional network structure by sharing their corners. Layers of one type of SiN₄ tetrahedra and slabs composed of the two different La³⁺ cations and the other type of SiN₄ tetrahedra are alternately stacked along the c axis of the tetragonal unit cell. The site symmetries of the two La³⁺ cations are $\dots m$ and $4\dots$, respectively.

Related literature

For the lattice parameters of La₃Si₆N₁₁, see: Woike & Jeitschko (1995). For isotypic Ce₃Si₆N₁₁, Pr₃Si₆N₁₁, Nd₃Si₆N₁₁, Sm₃Si₆N₁₁ and La₃Si₅AlON₁₀, see: Gaudé *et al.* (1983); Woike & Jeitschko (1995); Schlieper & Schnick (1995, 1996); Lauterbach & Schnick (2000). Recently, La₃Si₆N₁₁ has received attention as a host crystal of phosphors by Ce³⁺ doping; for La₃Si₆N₁₁:Ce, (La,Ca)₃Si₆N₁₁:Ce, see: Seto *et al.* (2009); Suehiro *et al.* (2011); George *et al.* (2013). For the ionic radii of La³⁺ and Sm³⁺ cations in nitrides, see: Baur (1987). For the Madelung energies of La₃Si₆N₁₁, LaN and Si₃N₄, see: Hoppe (1966, 1970), Klemm & Winkelmann (1956) and Boulay *et al.* (2004), respectively.

Experimental

Crystal data

La₃Si₆N₁₁
 $M_r = 739.38$
 Tetragonal, $P4bm$
 $a = 10.1988$ (4) Å
 $c = 4.84153$ (19) Å
 $V = 503.60$ (3) Å³

$Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 13.22$ mm⁻¹
 $T = 293$ K
 $0.15 \times 0.14 \times 0.03$ mm

Data collection

Rigaku R-Axis RAPID II
 diffractometer
 Absorption correction: numerical
 (NUMABS; Higashi, 1999)
 $T_{\min} = 0.219$, $T_{\max} = 0.726$

4700 measured reflections
 624 independent reflections
 599 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.039$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.017$
 $wR(F^2) = 0.030$
 $S = 1.20$
 624 reflections
 39 parameters
 1 restraint

$\Delta\rho_{\max} = 0.83$ e Å⁻³
 $\Delta\rho_{\min} = -0.90$ e Å⁻³
 Absolute structure: Flack (1983),
 275 Friedel pairs
 Absolute structure parameter:
 0.05 (3)

Table 1

Selected bond lengths (Å).

La1—N1 ⁱ	2.551 (3)	La2—N1 ^{xii}	2.649 (3)
La1—N1 ⁱⁱ	2.551 (3)	La2—N1 ^{xiii}	2.649 (3)
La1—N4	2.6227 (7)	La2—N1 ^{xiiii}	2.649 (3)
La1—N2 ⁱⁱⁱ	2.674 (3)	La2—N1 ^{xv}	2.649 (3)
La1—N2 ^{iv}	2.674 (3)	Si1—N1 ^x	1.724 (3)
La1—N2 ^v	2.853 (3)	Si1—N2	1.729 (4)
La1—N2 ^{vi}	2.853 (3)	Si1—N1	1.743 (3)
La1—N3 ^{vii}	2.864 (5)	Si1—N3 ^{xv}	1.776 (3)
La2—N2	2.644 (3)	Si2—N4 ^{xvi}	1.6868 (14)
La2—N2 ^{viii}	2.644 (3)	Si2—N2 ^{xvii}	1.725 (4)
La2—N2 ^{ix}	2.644 (3)	Si2—N2 ^{xviii}	1.725 (4)
La2—N2 ^x	2.644 (3)	Si2—N3 ^{xiv}	1.764 (5)

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

Data collection: *PROCESS-AUTO* (Rigaku/MSC, 2005); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-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: RU2057).

References

- Baur, H. (1987). *Crystallogr. Rev.* **1**, 59–83.
 Boulay, D. du, Ishizawa, N., Atake, T., Streltsov, V., Furuya, K. & Munakata, F. (2004). *Acta Cryst.* **B60**, 388–405.
 Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
 Gaudé, J., Lange, J. & Louër, D. (1983). *Rev. Chim. Miner.* **20**, 523–527.
 George, N. C., Birkel, A., Brgoch, J., Hong, B.-C., Mikhailovsky, A. A., Page, K., Llobet, A. & Seshadri, R. (2013). *Inorg. Chem.* **52**, 13730–13741.
 Higashi, T. (1999). *NUMABS*. Rigaku Corporation, Tokyo, Japan.
 Hoppe, R. (1966). *Angew. Chem. Int. Ed.* **5**, 95–106.
 Hoppe, R. (1970). *Angew. Chem. Int. Ed.* **9**, 25–34.
 Klemm, W. & Winkelmann, G. (1956). *Z. Anorg. Allg. Chem.* **288**, 87–90.

- Lauterbach, R. & Schnick, W. (2000). *Z. Anorg. Allg. Chem.* **626**, 56–61.
Momma, K. & Izumi, F. (2008). *J. Appl. Cryst.* **41**, 653–658.
Rigaku/MS (2005). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
Schlieper, T. & Schnick, W. (1995). *Z. Anorg. Allg. Chem.* **621**, 1535–1538.
Schlieper, T. & Schnick, W. (1996). *Z. Kristallogr.* **211**, 254–254.
- Seto, T., Kijima, N. & Hirosaki, N. (2009). *ECS Trans.* **25**, 247–252.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Suehiro, T., Hirosaki, N. & Xie, R.-J. (2011). *ACS Appl. Mater. Inter.* **3**, 811–816.
Woike, M. & Jeitschko, W. (1995). *Inorg. Chem.* **34**, 5105–5108.

supplementary materials

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La₃Si₆N₁₁**Hisanori Yamane, Toshiki Nagura and Tomohiro Miyazaki****1. Comment**

Woike and Jeitschko (1995) measured the tetragonal unit cell parameters of La₃Si₆N₁₁ by X-ray powder diffraction and showed that Ln₃Si₆N₁₁, Ln = Sr, as well as Ce, Pr, Nd, is isostructural with Sm₃Si₆N₁₁ firstly reported by Gaudé *et al.* (1983). The crystal structure of Sm₃Si₆N₁₁ was analyzed by single crystal X-ray diffraction with the noncentrosymmetric space group *P4bm* (Woike & Jeitschko, 1995). The crystal structures of isotopic compounds, Ce₃Si₆N₁₁, Pr₃Si₆N₁₁ and La₃Si₅AlON₁₀ (Schlieper & Schnick, 1995, 1996; Lauterbach & Schinick, 2000), have also been studied, while there is no report on the structure parameters of La₃Si₆N₁₁. Recently, La₃Si₆N₁₁ has received attention as host crystals of phosphors by Ce³⁺ doping (Seto *et al.*, 2009; Suehiro *et al.*, 2011; George *et al.*, 2013).

The cell parameters and volume determined by single crystal X-ray diffraction are close to those ($a = 10.189(1) \text{ \AA}$, $c = 4.837(2) \text{ \AA}$, $V = 502.2(2) \text{ \AA}^3$) reported in the previous study (Woike & Jeitschko, 1995). Fig. 1 shows the coordination environments of the Si1, Si2, La1 and La2 atoms. Si1 atoms are at general positions $8d$ and Si2 at special position $4c$. Si1—N and Si2—N bond lengths are in the ranges of 1.724(3)–1.776(3) Å, and 1.6868(14)–1.764(5) Å, respectively. These ranges are comparable with those (1.709–1.775 Å and 1.675–1.753 Å) reported for Sm₃Si₆N₁₁ (Woike & Jeitschko, 1995).

La1 atoms at $4c$ site with site symmetry ($..m$) and La2 atom at $2a$ site with ($4..$) are surrounded by 8 N atoms. La1—N distances of 2.551(3)–2.864(5) Å and La2—N distances of 2.644(3) Å and 2.649(3) Å are longer than the distances of Sm1—N (2.417–2.866 Å) and Sm2—N (2.557 Å and 2.571 Å) in Sm₃Si₆N₁₁, which is in accordance with the difference between the effective ionic radii of La (1.25 Å) and Sm (1.15 Å) atoms in nitrides (Baur, 1987).

The site potentials calculated with the structure parameters using VESTA program (Momma & Izumi 2008) are -27.3 V (La1³⁺), 28.5 V (La2³⁺), -51.9 V (Si1⁴⁺), -51.6 V (Si2⁴⁺) and 36.6–39.4 V (N³⁻ sites). The value of the Madelung energy for La₃Si₆N₁₁ (MAPLE, MAdelung Part of Lattice Energy, Hoppe 1966, 1970) is -132,000 kJ/mol, which are almost identical to the value of -131,300 kJ/mol (difference $\Delta = 0.5\%$) of the Madelung energies: LaN (-8,240 kJ/mol, Klemm & Winkelmann, 1956) and Si₃N₄ (-53,300 kJ/mol, Boulay *et al.*, 2004) with the formula $3\text{LaN} + 2\text{Si}_3\text{N}_4 \rightarrow \text{La}_3\text{Si}_6\text{N}_{11}$.

2. Experimental

Starting powders of LaN (0.6205 g, Koujundo Chemical Laboratory Co., Ltd.) and Si₃N₄ (0.3795 g, SN—E10, Ube Industries, Ltd.) were weighed and mixed in an aluminum mortar with a pestle in an Ar gas-filled glove box (O₂ and H₂O < 1 ppm). A sintered BN crucible (UHS-FL, inside diameter 18 mm; depth 18 mm, Showa Denko K. K., 99.5%) was loaded with the powder mixture and heated at 0.9 MPa of N₂ (99.9995%) and 1800°C for 2 h with a gas pressure carbon furnace (VESTA, Shimadzu Mectem, Inc.). The obtained product was powdered with the mortar and pestle and heated at 0.85 MPa of N₂ and 2000°C for 4 h. Colorless transparent single crystals (size less than 0.15 mm) were obtained in the product.

3. Refinement

Because the principal mean square atomic displacement for the N2 site was not positive definite, isotropic displacement parameters were refined for all nitrogen sites. The highest peak in the difference electron density map was 1.11 Å from La2 while the deepest hole was 0.79 Å from the same atom.

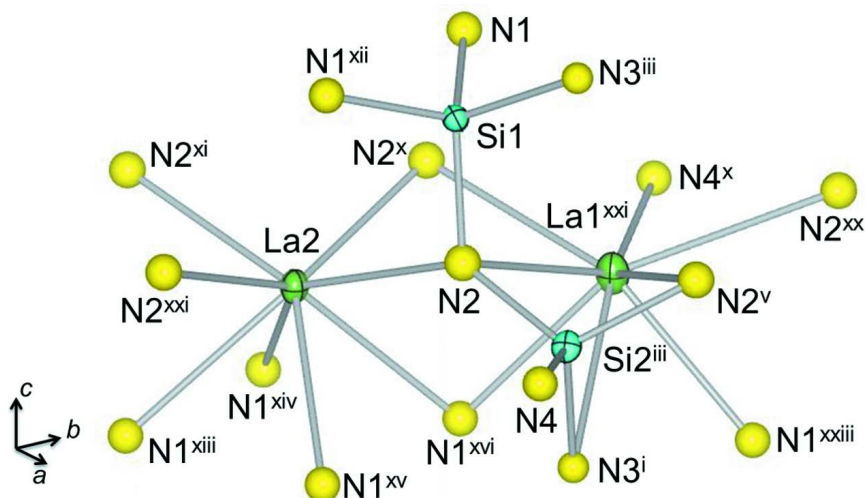


Figure 1

The atomic arrangement around La and Si atoms in the structure of $\text{La}_3\text{Si}_6\text{N}_{11}$. The displacement ellipsoids of La1, La2, Si1 and Si2 are drawn at the 95%. Symmetry codes are listed in *Geometric parameters*.

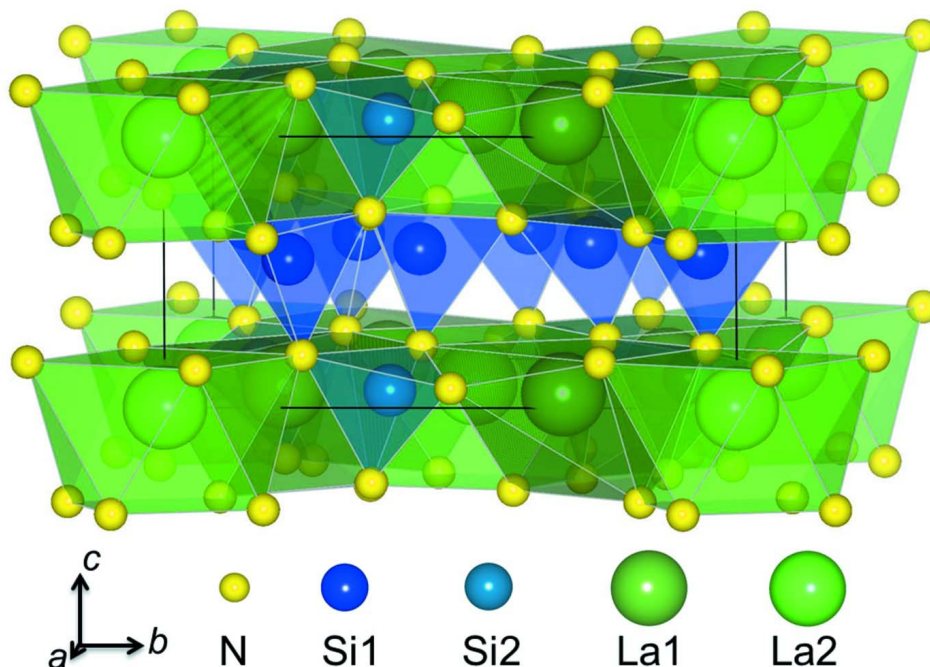


Figure 2

The crystal structure of $\text{La}_3\text{Si}_6\text{N}_{11}$ in a representation using cation-centered nitrogen polyhedra.

Trilanthanum hexasilicon undecanitrogen

Crystal data

La ₃ Si ₆ N ₁₁	$D_x = 4.876 \text{ Mg m}^{-3}$
$M_r = 739.38$	Mo $K\alpha$ radiation, $\lambda = 0.71075 \text{ \AA}$
Tetragonal, $P4bm$	Cell parameters from 4239 reflections
Hall symbol: P 4 -2ab	$\theta = 4.0\text{--}27.5^\circ$
$a = 10.1988 (4) \text{ \AA}$	$\mu = 13.22 \text{ mm}^{-1}$
$c = 4.84153 (19) \text{ \AA}$	$T = 293 \text{ K}$
$V = 503.60 (3) \text{ \AA}^3$	Chunk, colorless
$Z = 2$	$0.15 \times 0.14 \times 0.03 \text{ mm}$
$F(000) = 664$	

Data collection

Rigaku R-AXIS RAPID II diffractometer	4700 measured reflections
Radiation source: fine-focus sealed tube	624 independent reflections
Graphite monochromator	599 reflections with $I > 2\sigma(I)$
Detector resolution: 10.0 pixels mm^{-1}	$R_{\text{int}} = 0.039$
ω scans	$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 4.0^\circ$
Absorption correction: numerical (NUMABS; Higashi, 1999)	$h = -13 \rightarrow 13$
$T_{\text{min}} = 0.219$, $T_{\text{max}} = 0.726$	$k = -13 \rightarrow 12$
	$l = -6 \rightarrow 6$

Refinement

Refinement on F^2	$(\Delta/\sigma)_{\text{max}} = 0.002$
Least-squares matrix: full	$\Delta\rho_{\text{max}} = 0.83 \text{ e \AA}^{-3}$
$R[F^2 > 2\sigma(F^2)] = 0.017$	$\Delta\rho_{\text{min}} = -0.90 \text{ e \AA}^{-3}$
$wR(F^2) = 0.030$	Extinction correction: SHELXL,
$S = 1.20$	$F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
624 reflections	Extinction coefficient: 0.0007 (2)
39 parameters	Absolute structure: Flack (1983), 275 Friedel pairs
1 restraint	Absolute structure parameter: 0.05 (3)
$w = 1/[\sigma^2(F_o^2) + (0.0093P)^2 + 0.0181P]$	
where $P = (F_o^2 + 2F_c^2)/3$	

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ 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	$U_{\text{iso}}^*/U_{\text{eq}}$
La1	0.680962 (17)	0.180962 (17)	0.01861 (13)	0.00578 (9)
La2	0.0000	0.0000	0.00000 (11)	0.00427 (11)
Si1	0.20985 (9)	0.07807 (8)	0.5344 (4)	0.0038 (2)
Si2	0.11658 (9)	0.61658 (9)	0.0439 (5)	0.0039 (3)
N1	0.0803 (3)	0.1779 (3)	0.6388 (7)	0.0056 (7)*

N2	0.2332 (3)	0.0739 (3)	0.1807 (8)	0.0060 (8)*
N3	0.1527 (3)	0.6527 (3)	0.6958 (10)	0.0044 (10)*
N4	0.5000	0.0000	0.0717 (14)	0.0055 (14)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.00443 (11)	0.00443 (11)	0.00849 (17)	-0.00036 (9)	0.0001 (2)	0.0001 (2)
La2	0.00378 (13)	0.00378 (13)	0.0053 (2)	0.000	0.000	0.000
Si1	0.0037 (4)	0.0036 (4)	0.0040 (6)	-0.0006 (3)	0.0005 (7)	-0.0008 (7)
Si2	0.0038 (4)	0.0038 (4)	0.0042 (10)	0.0000 (5)	0.0005 (6)	0.0005 (6)

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

La1—N1 ⁱ	2.551 (3)	Si1—N1	1.743 (3)
La1—N1 ⁱⁱ	2.551 (3)	Si1—N3 ^{ix}	1.776 (3)
La1—N4	2.6227 (7)	Si1—La2 ^{xvii}	3.2089 (16)
La1—N2 ⁱⁱⁱ	2.674 (3)	Si1—La1 ^{xviii}	3.4093 (16)
La1—N2 ^{iv}	2.674 (3)	Si1—La1 ^{xix}	3.5159 (17)
La1—N2 ^v	2.853 (3)	Si2—N4 ^{xx}	1.6868 (14)
La1—N2 ^{vi}	2.853 (3)	Si2—N2 ^{xxi}	1.725 (4)
La1—N3 ^{vii}	2.864 (5)	Si2—N2 ^{xx}	1.725 (4)
La1—Si2 ^{viii}	2.9227 (13)	Si2—N3 ^{xvi}	1.764 (5)
La1—Si2 ^{ix}	3.1072 (7)	Si2—La1 ^{viii}	2.9228 (13)
La1—Si2 ^{iv}	3.1072 (7)	Si2—La1 ^{xx}	3.1072 (7)
La1—Si1 ⁱⁱ	3.4093 (16)	Si2—La1 ^{xix}	3.1072 (7)
La2—N2	2.644 (3)	N1—Si1 ^x	1.724 (3)
La2—N2 ^x	2.644 (3)	N1—La1 ^{xviii}	2.551 (3)
La2—N2 ^{xi}	2.644 (3)	N1—La2 ^{xvii}	2.649 (3)
La2—N2 ^{xii}	2.644 (3)	N2—Si2 ^{ix}	1.725 (4)
La2—N1 ^{xiii}	2.649 (3)	N2—La1 ^{xix}	2.674 (3)
La2—N1 ^{xiv}	2.649 (3)	N2—La1 ^{vi}	2.853 (3)
La2—N1 ^{xv}	2.649 (3)	N3—Si2 ^{xvii}	1.764 (5)
La2—N1 ^{xvi}	2.649 (3)	N3—Si1 ^{xxi}	1.776 (3)
La2—Si1 ^{xiii}	3.2089 (16)	N3—Si1 ^{xx}	1.776 (3)
La2—Si1 ^{xv}	3.2089 (16)	N3—La1 ^{xxii}	2.864 (5)
La2—Si1 ^{xiv}	3.2089 (16)	N4—Si2 ^{iv}	1.6868 (14)
La2—Si1 ^{xvi}	3.2089 (16)	N4—Si2 ^{ix}	1.6868 (14)
Si1—N1 ^{xii}	1.724 (3)	N4—La1 ^{vi}	2.6227 (7)
Si1—N2	1.729 (4)		
N1 ⁱ —La1—N1 ⁱⁱ	86.25 (15)	N2 ^{xii} —La2—Si1 ^{xv}	64.01 (8)
N1 ⁱ —La1—N4	100.64 (13)	N1 ^{xiii} —La2—Si1 ^{xv}	32.47 (7)
N1 ⁱⁱ —La1—N4	100.64 (13)	N1 ^{xiv} —La2—Si1 ^{xv}	84.97 (8)
N1 ⁱ —La1—N2 ⁱⁱⁱ	76.36 (10)	N1 ^{xv} —La2—Si1 ^{xv}	32.88 (7)
N1 ⁱⁱ —La1—N2 ⁱⁱⁱ	118.37 (10)	N1 ^{xvi} —La2—Si1 ^{xv}	85.19 (8)
N4—La1—N2 ⁱⁱⁱ	140.30 (11)	Si1 ^{xiii} —La2—Si1 ^{xv}	60.42 (3)
N1 ⁱ —La1—N2 ^{iv}	118.37 (10)	N2—La2—Si1 ^{xiv}	105.41 (8)
N1 ⁱⁱ —La1—N2 ^{iv}	76.36 (10)	N2 ^x —La2—Si1 ^{xiv}	64.01 (8)
N4—La1—N2 ^{iv}	140.30 (11)	N2 ^{xi} —La2—Si1 ^{xiv}	101.50 (8)

N2 ⁱⁱⁱ —La1—N2 ^{iv}	62.68 (14)	N2 ^{xii} —La2—Si1 ^{xiv}	154.58 (9)
N1 ⁱ —La1—N2 ^v	146.72 (10)	N1 ^{xiii} —La2—Si1 ^{xiv}	85.19 (8)
N1 ⁱⁱ —La1—N2 ^v	70.04 (11)	N1 ^{xiv} —La2—Si1 ^{xiv}	32.88 (7)
N4—La1—N2 ^v	63.11 (8)	N1 ^{xv} —La2—Si1 ^{xiv}	84.97 (8)
N2 ⁱⁱⁱ —La1—N2 ^v	135.23 (11)	N1 ^{xvi} —La2—Si1 ^{xiv}	32.47 (7)
N2 ^{iv} —La1—N2 ^v	79.28 (14)	Si1 ^{xiii} —La2—Si1 ^{xiv}	60.42 (3)
N1 ⁱ —La1—N2 ^{vi}	70.04 (11)	Si1 ^{xv} —La2—Si1 ^{xiv}	90.73 (6)
N1 ⁱⁱ —La1—N2 ^{vi}	146.72 (10)	N2—La2—Si1 ^{xvi}	64.01 (8)
N4—La1—N2 ^{vi}	63.11 (8)	N2 ^x —La2—Si1 ^{xvi}	101.50 (8)
N2 ⁱⁱⁱ —La1—N2 ^{vi}	79.28 (14)	N2 ^{xi} —La2—Si1 ^{xvi}	154.58 (9)
N2 ^{iv} —La1—N2 ^{vi}	135.23 (11)	N2 ^{xii} —La2—Si1 ^{xvi}	105.41 (8)
N2 ^v —La1—N2 ^{vi}	118.90 (14)	N1 ^{xiii} —La2—Si1 ^{xvi}	84.97 (8)
N1 ⁱ —La1—N3 ^{vii}	60.70 (9)	N1 ^{xiv} —La2—Si1 ^{xvi}	85.19 (8)
N1 ⁱⁱ —La1—N3 ^{vii}	60.70 (9)	N1 ^{xv} —La2—Si1 ^{xvi}	32.47 (7)
N4—La1—N3 ^{vii}	152.55 (18)	N1 ^{xvi} —La2—Si1 ^{xvi}	32.88 (7)
N2 ⁱⁱⁱ —La1—N3 ^{vii}	59.21 (11)	Si1 ^{xiii} —La2—Si1 ^{xvi}	90.73 (6)
N2 ^{iv} —La1—N3 ^{vii}	59.21 (11)	Si1 ^{xv} —La2—Si1 ^{xvi}	60.42 (3)
N2 ^v —La1—N3 ^{vii}	120.55 (7)	Si1 ^{xiv} —La2—Si1 ^{xvi}	60.42 (3)
N2 ^{vi} —La1—N3 ^{vii}	120.55 (7)	N1 ^{xii} —Si1—N2	107.06 (17)
N1 ⁱ —La1—Si2 ^{viii}	85.17 (8)	N1 ^{xii} —Si1—N1	108.6 (2)
N1 ⁱⁱ —La1—Si2 ^{viii}	85.17 (8)	N2—Si1—N1	113.98 (17)
N4—La1—Si2 ^{viii}	171.97 (16)	N1 ^{xii} —Si1—N3 ^{ix}	114.9 (2)
N2 ⁱⁱⁱ —La1—Si2 ^{viii}	35.54 (8)	N2—Si1—N3 ^{ix}	109.72 (19)
N2 ^{iv} —La1—Si2 ^{viii}	35.54 (8)	N1—Si1—N3 ^{ix}	102.7 (2)
N2 ^v —La1—Si2 ^{viii}	114.55 (7)	N1 ^{xii} —Si1—La2 ^{xvii}	55.61 (11)
N2 ^{vi} —La1—Si2 ^{viii}	114.55 (7)	N2—Si1—La2 ^{xvii}	141.40 (12)
N3 ^{vii} —La1—Si2 ^{viii}	35.48 (11)	N1—Si1—La2 ^{xvii}	55.63 (11)
N1 ⁱ —La1—Si2 ^{ix}	119.64 (8)	N3 ^{ix} —Si1—La2 ^{xvii}	108.88 (17)
N1 ⁱⁱ —La1—Si2 ^{ix}	75.81 (8)	N1 ^{xii} —Si1—La1 ^{xviii}	117.22 (14)
N4—La1—Si2 ^{ix}	32.88 (2)	N2—Si1—La1 ^{xviii}	135.29 (12)
N2 ⁱⁱⁱ —La1—Si2 ^{ix}	160.67 (9)	N1—Si1—La1 ^{xviii}	46.68 (11)
N2 ^{iv} —La1—Si2 ^{ix}	112.38 (8)	N3 ^{ix} —Si1—La1 ^{xviii}	57.10 (16)
N2 ^v —La1—Si2 ^{ix}	33.29 (7)	La2 ^{xvii} —Si1—La1 ^{xviii}	68.78 (4)
N2 ^{vi} —La1—Si2 ^{ix}	95.52 (7)	N1 ^{xii} —Si1—La2	83.47 (12)
N3 ^{vii} —La1—Si2 ^{ix}	136.50 (7)	N2—Si1—La2	48.51 (12)
Si2 ^{viii} —La1—Si2 ^{ix}	146.89 (2)	N1—Si1—La2	83.23 (12)
N1 ⁱ —La1—Si2 ^{iv}	75.81 (8)	N3 ^{ix} —Si1—La2	156.67 (16)
N1 ⁱⁱ —La1—Si2 ^{iv}	119.64 (8)	La2 ^{xvii} —Si1—La2	93.20 (2)
N4—La1—Si2 ^{iv}	32.88 (2)	La1 ^{xviii} —Si1—La2	128.93 (3)
N2 ⁱⁱⁱ —La1—Si2 ^{iv}	112.38 (8)	N1 ^{xii} —Si1—La1 ^{xix}	147.94 (14)
N2 ^{iv} —La1—Si2 ^{iv}	160.67 (9)	N2—Si1—La1 ^{xix}	47.60 (11)
N2 ^v —La1—Si2 ^{iv}	95.52 (7)	N1—Si1—La1 ^{xix}	74.59 (11)
N2 ^{vi} —La1—Si2 ^{iv}	33.29 (7)	N3 ^{ix} —Si1—La1 ^{xix}	94.54 (14)
N3 ^{vii} —La1—Si2 ^{iv}	136.50 (7)	La2 ^{xvii} —Si1—La1 ^{xix}	128.06 (3)
Si2 ^{viii} —La1—Si2 ^{iv}	146.89 (2)	La1 ^{xviii} —Si1—La1 ^{xix}	88.70 (2)
Si2 ^{ix} —La1—Si2 ^{iv}	65.52 (4)	La2—Si1—La1 ^{xix}	64.97 (3)
N1 ⁱ —La1—Si1 ⁱⁱ	75.26 (8)	N4 ^{xx} —Si2—N2 ^{xxi}	114.67 (16)
N1 ⁱⁱ —La1—Si1 ⁱⁱ	29.80 (7)	N4 ^{xx} —Si2—N2 ^{xx}	114.67 (16)
N4—La1—Si1 ⁱⁱ	129.45 (13)	N2 ^{xxi} —Si2—N2 ^{xx}	107.5 (2)

N2 ⁱⁱⁱ —La1—Si1 ⁱⁱ	88.70 (8)	N4 ^{xx} —Si2—N3 ^{xvi}	111.7 (3)
N2 ^{iv} —La1—Si1 ⁱⁱ	60.70 (8)	N2 ^{xxi} —Si2—N3 ^{xvi}	103.55 (17)
N2 ^v —La1—Si1 ⁱⁱ	92.68 (7)	N2 ^{xx} —Si2—N3 ^{xvi}	103.55 (17)
N2 ^{vi} —La1—Si1 ⁱⁱ	145.04 (8)	N4 ^{xx} —Si2—La1 ^{viii}	177.8 (3)
N3 ^{vii} —La1—Si1 ⁱⁱ	31.39 (5)	N2 ^{xxi} —Si2—La1 ^{viii}	64.35 (12)
Si2 ^{viii} —La1—Si1 ⁱⁱ	57.22 (5)	N2 ^{xx} —Si2—La1 ^{viii}	64.35 (12)
Si2 ^{ix} —La1—Si1 ⁱⁱ	105.30 (4)	N3 ^{xvi} —Si2—La1 ^{viii}	70.43 (16)
Si2 ^{iv} —La1—Si1 ⁱⁱ	138.54 (6)	N4 ^{xx} —Si2—La1 ^{xx}	57.57 (3)
N2—La2—N2 ^x	83.71 (5)	N2 ^{xxi} —Si2—La1 ^{xx}	65.22 (11)
N2—La2—N2 ^{xi}	141.35 (16)	N2 ^{xx} —Si2—La1 ^{xx}	159.37 (17)
N2 ^x —La2—N2 ^{xi}	83.71 (5)	N3 ^{xvi} —Si2—La1 ^{xx}	97.01 (10)
N2—La2—N2 ^{xii}	83.71 (5)	La1 ^{viii} —Si2—La1 ^{xx}	122.62 (2)
N2 ^x —La2—N2 ^{xii}	141.35 (16)	N4 ^{xx} —Si2—La1 ^{xix}	57.57 (3)
N2 ^{xi} —La2—N2 ^{xii}	83.71 (5)	N2 ^{xxi} —Si2—La1 ^{xix}	159.37 (17)
N2—La2—N1 ^{xiii}	133.76 (10)	N2 ^{xx} —Si2—La1 ^{xix}	65.22 (11)
N2 ^x —La2—N1 ^{xiii}	138.27 (10)	N3 ^{xvi} —Si2—La1 ^{xix}	97.01 (10)
N2 ^{xi} —La2—N1 ^{xiii}	75.24 (10)	La1 ^{viii} —Si2—La1 ^{xix}	122.62 (2)
N2 ^{xii} —La2—N1 ^{xiii}	71.98 (11)	La1 ^{xx} —Si2—La1 ^{xix}	114.28 (4)
N2—La2—N1 ^{xiv}	138.27 (10)	Si1 ^x —N1—Si1	137.4 (2)
N2 ^x —La2—N1 ^{xiv}	75.24 (10)	Si1 ^x —N1—La1 ^{xviii}	118.80 (16)
N2 ^{xi} —La2—N1 ^{xiv}	71.98 (11)	Si1—N1—La1 ^{xviii}	103.52 (15)
N2 ^{xii} —La2—N1 ^{xiv}	133.76 (10)	Si1 ^x —N1—La2 ^{xvii}	91.91 (13)
N1 ^{xiii} —La2—N1 ^{xiv}	64.17 (8)	Si1—N1—La2 ^{xvii}	91.49 (13)
N2—La2—N1 ^{xv}	71.98 (11)	La1 ^{xviii} —N1—La2 ^{xvii}	92.01 (11)
N2 ^x —La2—N1 ^{xv}	133.76 (10)	Si2 ^{ix} —N2—Si1	119.8 (2)
N2 ^{xi} —La2—N1 ^{xv}	138.27 (10)	Si2 ^{ix} —N2—La2	138.1 (2)
N2 ^{xii} —La2—N1 ^{xv}	75.24 (10)	Si1—N2—La2	102.16 (15)
N1 ^{xiii} —La2—N1 ^{xv}	64.17 (8)	Si2 ^{ix} —N2—La1 ^{xix}	80.11 (13)
N1 ^{xiv} —La2—N1 ^{xv}	97.40 (14)	Si1—N2—La1 ^{xix}	103.89 (15)
N2—La2—N1 ^{xvi}	75.24 (10)	La2—N2—La1 ^{xix}	89.42 (10)
N2 ^x —La2—N1 ^{xvi}	71.98 (11)	Si2 ^{ix} —N2—La1 ^{vi}	81.48 (12)
N2 ^{xi} —La2—N1 ^{xvi}	133.76 (10)	Si1—N2—La1 ^{vi}	109.71 (15)
N2 ^{xii} —La2—N1 ^{xvi}	138.27 (10)	La2—N2—La1 ^{vi}	85.71 (9)
N1 ^{xiii} —La2—N1 ^{xvi}	97.40 (14)	La1 ^{xix} —N2—La1 ^{vi}	146.33 (15)
N1 ^{xiv} —La2—N1 ^{xvi}	64.17 (8)	Si2 ^{xvii} —N3—Si1 ^{xxi}	119.72 (15)
N1 ^{xv} —La2—N1 ^{xvi}	64.17 (8)	Si2 ^{xvii} —N3—Si1 ^{xx}	119.72 (15)
N2—La2—Si1 ^{xiii}	154.58 (9)	Si1 ^{xxi} —N3—Si1 ^{xx}	118.9 (3)
N2 ^x —La2—Si1 ^{xiii}	105.41 (8)	Si2 ^{xvii} —N3—La1 ^{xxii}	74.09 (17)
N2 ^{xi} —La2—Si1 ^{xiii}	64.01 (8)	Si1 ^{xxi} —N3—La1 ^{xxii}	91.51 (17)
N2 ^{xii} —La2—Si1 ^{xiii}	101.50 (8)	Si1 ^{xx} —N3—La1 ^{xxii}	91.51 (17)
N1 ^{xiii} —La2—Si1 ^{xiii}	32.88 (7)	Si2 ^{iv} —N4—Si2 ^{ix}	170.9 (5)
N1 ^{xiv} —La2—Si1 ^{xiii}	32.47 (7)	Si2 ^{iv} —N4—La1 ^{vi}	89.55 (4)
N1 ^{xv} —La2—Si1 ^{xiii}	85.19 (8)	Si2 ^{ix} —N4—La1 ^{vi}	89.55 (4)
N1 ^{xvi} —La2—Si1 ^{xiii}	84.97 (8)	Si2 ^{iv} —N4—La1	89.55 (4)
N2—La2—Si1 ^{xv}	101.50 (8)	Si2 ^{ix} —N4—La1	89.55 (4)

$N2^x-La2-Si1^{xv}$	154.58 (9)	$La1^{vi}-N4-La1$	168.8 (3)
$N2^{xi}-La2-Si1^{xv}$	105.41 (8)		

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