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## Structure Reports

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La<sub>3</sub>Si<sub>6</sub>N<sub>11</sub>

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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, La<sub>3</sub>Si<sub>6</sub>N<sub>11</sub>, were prepared at 0.85 MPa of N<sub>2</sub> and 2273 K. The title compound is isotypic with Sm<sub>3</sub>Si<sub>6</sub>N<sub>11</sub>. Silicon-centered nitrogen tetrahedra form a three-dimensional network structure by sharing their corners. Layers of one type of SiN<sub>4</sub> tetrahedra and slabs composed of the two different La<sup>3+</sup> cations and the other type of SiN<sub>4</sub> tetrahedra are alternately stacked along the  $c$  axis of the tetragonal unit cell. The site symmetries of the two La<sup>3+</sup> cations are  $\dots m$  and  $4\dots$ , respectively.

## Related literature

For the lattice parameters of La<sub>3</sub>Si<sub>6</sub>N<sub>11</sub>, see: Woike & Jeitschko (1995). For isotypic Ce<sub>3</sub>Si<sub>6</sub>N<sub>11</sub>, Pr<sub>3</sub>Si<sub>6</sub>N<sub>11</sub>, Nd<sub>3</sub>Si<sub>6</sub>N<sub>11</sub>, Sm<sub>3</sub>Si<sub>6</sub>N<sub>11</sub> and La<sub>3</sub>Si<sub>5</sub>AlON<sub>10</sub>, see: Gaudé *et al.* (1983); Woike & Jeitschko (1995); Schlieper & Schnick (1995, 1996); Lauterbach & Schnick (2000). Recently, La<sub>3</sub>Si<sub>6</sub>N<sub>11</sub> has received attention as a host crystal of phosphors by Ce<sup>3+</sup> doping; for La<sub>3</sub>Si<sub>6</sub>N<sub>11</sub>:Ce, (La,Ca)<sub>3</sub>Si<sub>6</sub>N<sub>11</sub>:Ce, see: Seto *et al.* (2009); Suehiro *et al.* (2011); George *et al.* (2013). For the ionic radii of La<sup>3+</sup> and Sm<sup>3+</sup> cations in nitrides, see: Baur (1987). For the Madelung energies of La<sub>3</sub>Si<sub>6</sub>N<sub>11</sub>, LaN and Si<sub>3</sub>N<sub>4</sub>, see: Hoppe (1966, 1970), Klemm & Winkelmann (1956) and Boulay *et al.* (2004), respectively.

## Experimental

## Crystal data

La<sub>3</sub>Si<sub>6</sub>N<sub>11</sub>  
 $M_r = 739.38$   
 Tetragonal,  $P4bm$   
 $a = 10.1988$  (4) Å  
 $c = 4.84153$  (19) Å  
 $V = 503.60$  (3) Å<sup>3</sup>

$Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 13.22$  mm<sup>-1</sup>  
 $T = 293$  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<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.90$  e Å<sup>-3</sup>  
 Absolute structure: Flack (1983),  
 275 Friedel pairs  
 Absolute structure parameter:  
 0.05 (3)

Table 1

Selected bond lengths (Å).

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

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## supporting information

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**La<sub>3</sub>Si<sub>6</sub>N<sub>11</sub>****Hisanori Yamane, Toshiki Nagura and Tomohiro Miyazaki****S1. Comment**

Woike and Jeitschko (1995) measured the tetragonal unit cell parameters of La<sub>3</sub>Si<sub>6</sub>N<sub>11</sub> by X-ray powder diffraction and showed that Ln<sub>3</sub>Si<sub>6</sub>N<sub>11</sub>, Ln = Sr, as well as Ce, Pr, Nd, is isostructural with Sm<sub>3</sub>Si<sub>6</sub>N<sub>11</sub> firstly reported by Gaudé *et al.* (1983). The crystal structure of Sm<sub>3</sub>Si<sub>6</sub>N<sub>11</sub> was analyzed by single crystal X-ray diffraction with the noncentrosymmetric space group *P4bm* (Woike & Jeitschko, 1995). The crystal structures of isotopic compounds, Ce<sub>3</sub>Si<sub>6</sub>N<sub>11</sub>, Pr<sub>3</sub>Si<sub>6</sub>N<sub>11</sub> and La<sub>3</sub>Si<sub>5</sub>AlON<sub>10</sub> (Schlieper & Schnick, 1995, 1996; Lauterbach & Schnick, 2000), have also been studied, while there is no report on the structure parameters of La<sub>3</sub>Si<sub>6</sub>N<sub>11</sub>. Recently, La<sub>3</sub>Si<sub>6</sub>N<sub>11</sub> has received attention as host crystals of phosphors by Ce<sup>3+</sup> 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 Sm<sub>3</sub>Si<sub>6</sub>N<sub>11</sub> (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 Sm<sub>3</sub>Si<sub>6</sub>N<sub>11</sub>, 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).

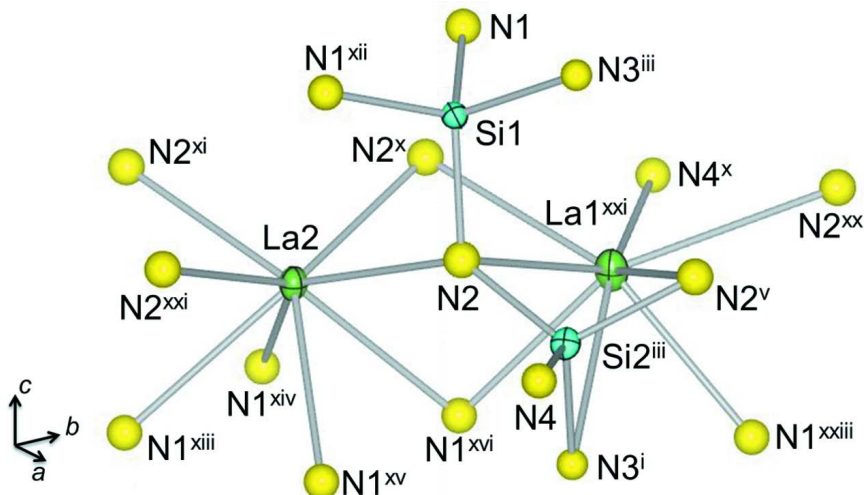
The site potentials calculated with the structure parameters using VESTA program (Momma & Izumi 2008) are -27.3 V (La1<sup>3+</sup>), 28.5 V (La2<sup>3+</sup>), -51.9 V (Si1<sup>4+</sup>), -51.6 V (Si2<sup>4+</sup>) and 36.6–39.4 V (N<sup>3-</sup> sites). The value of the Madelung energy for La<sub>3</sub>Si<sub>6</sub>N<sub>11</sub> (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 Si<sub>3</sub>N<sub>4</sub> (-53,300 kJ/mol, Boulay *et al.*, 2004) with the formula  $3\text{LaN} + 2\text{Si}_3\text{N}_4 \rightarrow \text{La}_3\text{Si}_6\text{N}_{11}$ .

**S2. Experimental**

Starting powders of LaN (0.6205 g, Koujundo Chemical Laboratory Co., Ltd.) and Si<sub>3</sub>N<sub>4</sub> (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 (O<sub>2</sub> and H<sub>2</sub>O < 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 N<sub>2</sub> (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 N<sub>2</sub> and 2000°C for 4 h. Colorless transparent single crystals (size less than 0.15 mm) were obtained in the product.

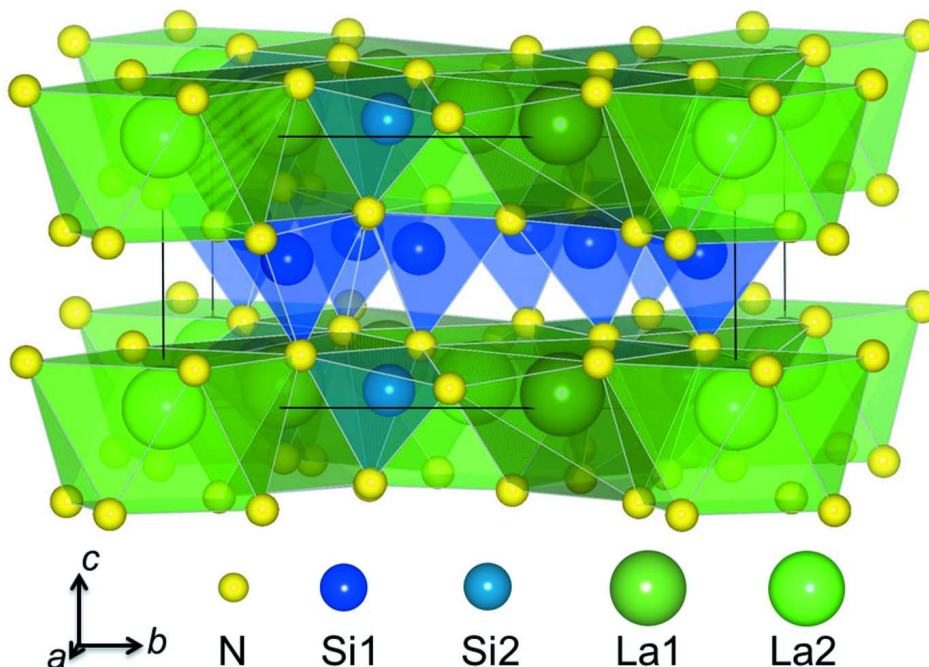
### S3. Refinement

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 <sub>3</sub> Si <sub>6</sub> N <sub>11</sub>	$D_x = 4.876 \text{ Mg m}^{-3}$
$M_r = 739.38$	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: $10.0 \text{ pixels mm}^{-1}$	$R_{\text{int}} = 0.039$
$\omega$ 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,
$S = 1.20$	$\text{Fc}^* = k\text{Fc}[1 + 0.001x\text{Fc}^2\lambda^3/\sin(2\theta)]^{-1/4}$
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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
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 (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
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 (Å, °)*

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

N1 <sup>ii</sup> —La1—N2 <sup>iv</sup>	76.36 (10)	N2 <sup>x</sup> —La2—Si1 <sup>xiv</sup>	64.01 (8)
N4—La1—N2 <sup>iv</sup>	140.30 (11)	N2 <sup>xi</sup> —La2—Si1 <sup>xiv</sup>	101.50 (8)
N2 <sup>iii</sup> —La1—N2 <sup>iv</sup>	62.68 (14)	N2 <sup>xii</sup> —La2—Si1 <sup>xiv</sup>	154.58 (9)
N1 <sup>i</sup> —La1—N2 <sup>v</sup>	146.72 (10)	N1 <sup>xiii</sup> —La2—Si1 <sup>xiv</sup>	85.19 (8)
N1 <sup>ii</sup> —La1—N2 <sup>v</sup>	70.04 (11)	N1 <sup>xiv</sup> —La2—Si1 <sup>xiv</sup>	32.88 (7)
N4—La1—N2 <sup>v</sup>	63.11 (8)	N1 <sup>xv</sup> —La2—Si1 <sup>xiv</sup>	84.97 (8)
N2 <sup>iii</sup> —La1—N2 <sup>v</sup>	135.23 (11)	N1 <sup>xvi</sup> —La2—Si1 <sup>xiv</sup>	32.47 (7)
N2 <sup>iv</sup> —La1—N2 <sup>v</sup>	79.28 (14)	Si1 <sup>xiii</sup> —La2—Si1 <sup>xiv</sup>	60.42 (3)
N1 <sup>i</sup> —La1—N2 <sup>vi</sup>	70.04 (11)	Si1 <sup>xv</sup> —La2—Si1 <sup>xiv</sup>	90.73 (6)
N1 <sup>ii</sup> —La1—N2 <sup>vi</sup>	146.72 (10)	N2—La2—Si1 <sup>xvi</sup>	64.01 (8)
N4—La1—N2 <sup>vi</sup>	63.11 (8)	N2 <sup>x</sup> —La2—Si1 <sup>xvi</sup>	101.50 (8)
N2 <sup>iii</sup> —La1—N2 <sup>vi</sup>	79.28 (14)	N2 <sup>xi</sup> —La2—Si1 <sup>xvi</sup>	154.58 (9)
N2 <sup>iv</sup> —La1—N2 <sup>vi</sup>	135.23 (11)	N2 <sup>xii</sup> —La2—Si1 <sup>xvi</sup>	105.41 (8)
N2 <sup>v</sup> —La1—N2 <sup>vi</sup>	118.90 (14)	N1 <sup>xiii</sup> —La2—Si1 <sup>xvi</sup>	84.97 (8)
N1 <sup>i</sup> —La1—N3 <sup>vii</sup>	60.70 (9)	N1 <sup>xiv</sup> —La2—Si1 <sup>xvi</sup>	85.19 (8)
N1 <sup>ii</sup> —La1—N3 <sup>vii</sup>	60.70 (9)	N1 <sup>xv</sup> —La2—Si1 <sup>xvi</sup>	32.47 (7)
N4—La1—N3 <sup>vii</sup>	152.55 (18)	N1 <sup>xvi</sup> —La2—Si1 <sup>xvi</sup>	32.88 (7)
N2 <sup>iii</sup> —La1—N3 <sup>vii</sup>	59.21 (11)	Si1 <sup>xiii</sup> —La2—Si1 <sup>xvi</sup>	90.73 (6)
N2 <sup>iv</sup> —La1—N3 <sup>vii</sup>	59.21 (11)	Si1 <sup>xv</sup> —La2—Si1 <sup>xvi</sup>	60.42 (3)
N2 <sup>v</sup> —La1—N3 <sup>vii</sup>	120.55 (7)	Si1 <sup>xiv</sup> —La2—Si1 <sup>xvi</sup>	60.42 (3)
N2 <sup>vi</sup> —La1—N3 <sup>vii</sup>	120.55 (7)	N1 <sup>xii</sup> —Si1—N2	107.06 (17)
N1 <sup>i</sup> —La1—Si2 <sup>viii</sup>	85.17 (8)	N1 <sup>xii</sup> —Si1—N1	108.6 (2)
N1 <sup>ii</sup> —La1—Si2 <sup>viii</sup>	85.17 (8)	N2—Si1—N1	113.98 (17)
N4—La1—Si2 <sup>viii</sup>	171.97 (16)	N1 <sup>xii</sup> —Si1—N3 <sup>ix</sup>	114.9 (2)
N2 <sup>iii</sup> —La1—Si2 <sup>viii</sup>	35.54 (8)	N2—Si1—N3 <sup>ix</sup>	109.72 (19)
N2 <sup>iv</sup> —La1—Si2 <sup>viii</sup>	35.54 (8)	N1—Si1—N3 <sup>ix</sup>	102.7 (2)
N2 <sup>v</sup> —La1—Si2 <sup>viii</sup>	114.55 (7)	N1 <sup>xii</sup> —Si1—La2 <sup>xvii</sup>	55.61 (11)
N2 <sup>vi</sup> —La1—Si2 <sup>viii</sup>	114.55 (7)	N2—Si1—La2 <sup>xvii</sup>	141.40 (12)
N3 <sup>vii</sup> —La1—Si2 <sup>viii</sup>	35.48 (11)	N1—Si1—La2 <sup>xvii</sup>	55.63 (11)
N1 <sup>i</sup> —La1—Si2 <sup>ix</sup>	119.64 (8)	N3 <sup>ix</sup> —Si1—La2 <sup>xvii</sup>	108.88 (17)
N1 <sup>ii</sup> —La1—Si2 <sup>ix</sup>	75.81 (8)	N1 <sup>xii</sup> —Si1—La1 <sup>xviii</sup>	117.22 (14)
N4—La1—Si2 <sup>ix</sup>	32.88 (2)	N2—Si1—La1 <sup>xviii</sup>	135.29 (12)
N2 <sup>iii</sup> —La1—Si2 <sup>ix</sup>	160.67 (9)	N1—Si1—La1 <sup>xviii</sup>	46.68 (11)
N2 <sup>iv</sup> —La1—Si2 <sup>ix</sup>	112.38 (8)	N3 <sup>ix</sup> —Si1—La1 <sup>xviii</sup>	57.10 (16)
N2 <sup>v</sup> —La1—Si2 <sup>ix</sup>	33.29 (7)	La2 <sup>xvii</sup> —Si1—La1 <sup>xviii</sup>	68.78 (4)
N2 <sup>vi</sup> —La1—Si2 <sup>ix</sup>	95.52 (7)	N1 <sup>xii</sup> —Si1—La2	83.47 (12)
N3 <sup>vii</sup> —La1—Si2 <sup>ix</sup>	136.50 (7)	N2—Si1—La2	48.51 (12)
Si2 <sup>viii</sup> —La1—Si2 <sup>ix</sup>	146.89 (2)	N1—Si1—La2	83.23 (12)
N1 <sup>i</sup> —La1—Si2 <sup>iv</sup>	75.81 (8)	N3 <sup>ix</sup> —Si1—La2	156.67 (16)
N1 <sup>ii</sup> —La1—Si2 <sup>iv</sup>	119.64 (8)	La2 <sup>xvii</sup> —Si1—La2	93.20 (2)
N4—La1—Si2 <sup>iv</sup>	32.88 (2)	La1 <sup>xviii</sup> —Si1—La2	128.93 (3)
N2 <sup>iii</sup> —La1—Si2 <sup>iv</sup>	112.38 (8)	N1 <sup>xii</sup> —Si1—La1 <sup>xix</sup>	147.94 (14)
N2 <sup>iv</sup> —La1—Si2 <sup>iv</sup>	160.67 (9)	N2—Si1—La1 <sup>xix</sup>	47.60 (11)
N2 <sup>v</sup> —La1—Si2 <sup>iv</sup>	95.52 (7)	N1—Si1—La1 <sup>xix</sup>	74.59 (11)
N2 <sup>vi</sup> —La1—Si2 <sup>iv</sup>	33.29 (7)	N3 <sup>ix</sup> —Si1—La1 <sup>xix</sup>	94.54 (14)
N3 <sup>vii</sup> —La1—Si2 <sup>iv</sup>	136.50 (7)	La2 <sup>xvii</sup> —Si1—La1 <sup>xix</sup>	128.06 (3)
Si2 <sup>viii</sup> —La1—Si2 <sup>iv</sup>	146.89 (2)	La1 <sup>xviii</sup> —Si1—La1 <sup>xix</sup>	88.70 (2)
Si2 <sup>ix</sup> —La1—Si2 <sup>iv</sup>	65.52 (4)	La2—Si1—La1 <sup>xix</sup>	64.97 (3)

N1 <sup>i</sup> —La1—Si1 <sup>ii</sup>	75.26 (8)	N4 <sup>xx</sup> —Si2—N2 <sup>xxi</sup>	114.67 (16)
N1 <sup>ii</sup> —La1—Si1 <sup>ii</sup>	29.80 (7)	N4 <sup>xx</sup> —Si2—N2 <sup>xx</sup>	114.67 (16)
N4—La1—Si1 <sup>ii</sup>	129.45 (13)	N2 <sup>xxi</sup> —Si2—N2 <sup>xx</sup>	107.5 (2)
N2 <sup>iii</sup> —La1—Si1 <sup>ii</sup>	88.70 (8)	N4 <sup>xx</sup> —Si2—N3 <sup>xvi</sup>	111.7 (3)
N2 <sup>iv</sup> —La1—Si1 <sup>ii</sup>	60.70 (8)	N2 <sup>xxi</sup> —Si2—N3 <sup>xvi</sup>	103.55 (17)
N2 <sup>v</sup> —La1—Si1 <sup>ii</sup>	92.68 (7)	N2 <sup>xx</sup> —Si2—N3 <sup>xvi</sup>	103.55 (17)
N2 <sup>vi</sup> —La1—Si1 <sup>ii</sup>	145.04 (8)	N4 <sup>xx</sup> —Si2—La1 <sup>viii</sup>	177.8 (3)
N3 <sup>vii</sup> —La1—Si1 <sup>ii</sup>	31.39 (5)	N2 <sup>xxi</sup> —Si2—La1 <sup>viii</sup>	64.35 (12)
Si2 <sup>viii</sup> —La1—Si1 <sup>ii</sup>	57.22 (5)	N2 <sup>xx</sup> —Si2—La1 <sup>viii</sup>	64.35 (12)
Si2 <sup>ix</sup> —La1—Si1 <sup>ii</sup>	105.30 (4)	N3 <sup>xvi</sup> —Si2—La1 <sup>viii</sup>	70.43 (16)
Si2 <sup>iv</sup> —La1—Si1 <sup>ii</sup>	138.54 (6)	N4 <sup>xx</sup> —Si2—La1 <sup>xx</sup>	57.57 (3)
N2—La2—N2 <sup>x</sup>	83.71 (5)	N2 <sup>xxi</sup> —Si2—La1 <sup>xx</sup>	65.22 (11)
N2—La2—N2 <sup>xi</sup>	141.35 (16)	N2 <sup>xx</sup> —Si2—La1 <sup>xx</sup>	159.37 (17)
N2 <sup>x</sup> —La2—N2 <sup>xi</sup>	83.71 (5)	N3 <sup>xvi</sup> —Si2—La1 <sup>xx</sup>	97.01 (10)
N2—La2—N2 <sup>xii</sup>	83.71 (5)	La1 <sup>viii</sup> —Si2—La1 <sup>xx</sup>	122.62 (2)
N2 <sup>x</sup> —La2—N2 <sup>xii</sup>	141.35 (16)	N4 <sup>xx</sup> —Si2—La1 <sup>xix</sup>	57.57 (3)
N2 <sup>xi</sup> —La2—N2 <sup>xii</sup>	83.71 (5)	N2 <sup>xxi</sup> —Si2—La1 <sup>xix</sup>	159.37 (17)
N2—La2—N1 <sup>xiii</sup>	133.76 (10)	N2 <sup>xx</sup> —Si2—La1 <sup>xix</sup>	65.22 (11)
N2 <sup>x</sup> —La2—N1 <sup>xiii</sup>	138.27 (10)	N3 <sup>xvi</sup> —Si2—La1 <sup>xix</sup>	97.01 (10)
N2 <sup>xi</sup> —La2—N1 <sup>xiii</sup>	75.24 (10)	La1 <sup>viii</sup> —Si2—La1 <sup>xix</sup>	122.62 (2)
N2 <sup>xii</sup> —La2—N1 <sup>xiii</sup>	71.98 (11)	La1 <sup>xx</sup> —Si2—La1 <sup>xix</sup>	114.28 (4)
N2—La2—N1 <sup>xiv</sup>	138.27 (10)	Si1 <sup>x</sup> —N1—Si1	137.4 (2)
N2 <sup>x</sup> —La2—N1 <sup>xiv</sup>	75.24 (10)	Si1 <sup>x</sup> —N1—La1 <sup>xviii</sup>	118.80 (16)
N2 <sup>xi</sup> —La2—N1 <sup>xiv</sup>	71.98 (11)	Si1—N1—La1 <sup>xviii</sup>	103.52 (15)
N2 <sup>xii</sup> —La2—N1 <sup>xiv</sup>	133.76 (10)	Si1 <sup>x</sup> —N1—La2 <sup>xvii</sup>	91.91 (13)
N1 <sup>xiii</sup> —La2—N1 <sup>xiv</sup>	64.17 (8)	Si1—N1—La2 <sup>xvii</sup>	91.49 (13)
N2—La2—N1 <sup>xv</sup>	71.98 (11)	La1 <sup>xviii</sup> —N1—La2 <sup>xvii</sup>	92.01 (11)
N2 <sup>x</sup> —La2—N1 <sup>xv</sup>	133.76 (10)	Si2 <sup>ix</sup> —N2—Si1	119.8 (2)
N2 <sup>xi</sup> —La2—N1 <sup>xv</sup>	138.27 (10)	Si2 <sup>ix</sup> —N2—La2	138.1 (2)
N2 <sup>xii</sup> —La2—N1 <sup>xv</sup>	75.24 (10)	Si1—N2—La2	102.16 (15)
N1 <sup>xiii</sup> —La2—N1 <sup>xv</sup>	64.17 (8)	Si2 <sup>ix</sup> —N2—La1 <sup>xix</sup>	80.11 (13)
N1 <sup>xiv</sup> —La2—N1 <sup>xv</sup>	97.40 (14)	Si1—N2—La1 <sup>xix</sup>	103.89 (15)
N2—La2—N1 <sup>xvi</sup>	75.24 (10)	La2—N2—La1 <sup>xix</sup>	89.42 (10)
N2 <sup>x</sup> —La2—N1 <sup>xvi</sup>	71.98 (11)	Si2 <sup>ix</sup> —N2—La1 <sup>vi</sup>	81.48 (12)
N2 <sup>xi</sup> —La2—N1 <sup>xvi</sup>	133.76 (10)	Si1—N2—La1 <sup>vi</sup>	109.71 (15)
N2 <sup>xii</sup> —La2—N1 <sup>xvi</sup>	138.27 (10)	La2—N2—La1 <sup>vi</sup>	85.71 (9)
N1 <sup>xiii</sup> —La2—N1 <sup>xvi</sup>	97.40 (14)	La1 <sup>xix</sup> —N2—La1 <sup>vi</sup>	146.33 (15)
N1 <sup>xiv</sup> —La2—N1 <sup>xvi</sup>	64.17 (8)	Si2 <sup>xvii</sup> —N3—Si1 <sup>xxi</sup>	119.72 (15)
N1 <sup>xv</sup> —La2—N1 <sup>xvi</sup>	64.17 (8)	Si2 <sup>xvii</sup> —N3—Si1 <sup>xx</sup>	119.72 (15)
N2—La2—Si1 <sup>xiii</sup>	154.58 (9)	Si1 <sup>xxi</sup> —N3—Si1 <sup>xx</sup>	118.9 (3)
N2 <sup>x</sup> —La2—Si1 <sup>xiii</sup>	105.41 (8)	Si2 <sup>xvii</sup> —N3—La1 <sup>xxii</sup>	74.09 (17)
N2 <sup>xi</sup> —La2—Si1 <sup>xiii</sup>	64.01 (8)	Si1 <sup>xxi</sup> —N3—La1 <sup>xxii</sup>	91.51 (17)
N2 <sup>xii</sup> —La2—Si1 <sup>xiii</sup>	101.50 (8)	Si1 <sup>xx</sup> —N3—La1 <sup>xxii</sup>	91.51 (17)
N1 <sup>xiii</sup> —La2—Si1 <sup>xiii</sup>	32.88 (7)	Si2 <sup>iv</sup> —N4—Si2 <sup>ix</sup>	170.9 (5)
N1 <sup>xiv</sup> —La2—Si1 <sup>xiii</sup>	32.47 (7)	Si2 <sup>iv</sup> —N4—La1 <sup>vi</sup>	89.55 (4)
N1 <sup>xv</sup> —La2—Si1 <sup>xiii</sup>	85.19 (8)	Si2 <sup>ix</sup> —N4—La1 <sup>vi</sup>	89.55 (4)
N1 <sup>xvi</sup> —La2—Si1 <sup>xiii</sup>	84.97 (8)	Si2 <sup>iv</sup> —N4—La1	89.55 (4)
N2—La2—Si1 <sup>xv</sup>	101.50 (8)	Si2 <sup>ix</sup> —N4—La1	89.55 (4)



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

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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)  $-x+1, -y+1, z+1$ .