Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Crystal structures of $Ca_{4+x}Y_{3-x}Si_7O_{15+x}N_{5-x}$ ($0 \leq x \leq 1$) comprising of an isolated $[Si_7(O,N)_{19}]$ unit

Makoto Kobayashi,[a]*‡ Takuya Yasunaga,[a] Hideki Kato,[a]* Kotaro Fujii,[b] Masatomo Yashima[b] and Masato Kakihana[a]

[a]Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577, Japan, and [b]Department of Chemistry, School of Science, Tokyo Institute of Technology, 2-12-1-W4-17, Ookayama, Meguro-ku, To-kyo 152-8551, Japan. *Correspondence e-mail: mkoba@imass.nagoya-u.ac.jp, hideki.kato.e2@tohoku.ac.jp

Received 8 January 2019
Accepted 23 January 2019

Edited by M. Weil, Vienna University of Technology, Austria

‡ Present address: Institute of Materials and Systems for Sustainability, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464-8601, Japan.

Keywords: oxynitride; silicate; crystal structure.

CCDC references: 1892876; 1892875; 1892874

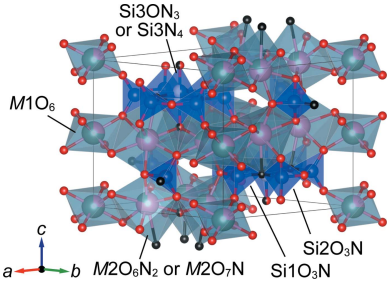
Supporting information: this article has supporting information at journals.iucr.org/e

Single crystals of the solid solution series $Ca_{4+x}Y_{3-x}Si_7O_{15+x}N_{5-x}$ were obtained by a solid-state reaction method using a flux for x = 0, 0.5 and 1, resulting in $Ca_4Y_3Si_7O_{15}N_5$ (tetracalcium triyttrium heptasilicon oxynitride), $Ca_{4.5}Y_{2.5}Si_7O_{15.5}N_{4.5}$ and $Ca_5Y_2Si_7O_{16}N_4$ (pentacalcium diyttrium heptasilicon oxynitride). Single-crystal X-ray analysis revealed that the three compounds are isotypic and belong to space-group type $P6_3/m$. Ca^{2+} and Y^{3+} cations are distributed over two crystallographic sites (site symmetry $\overline{3}$.. and 1) in a disordered manner. The corresponding (Ca,Y)-centred polyhedra are connected by edge-sharing, resulting in the formation of a layer structure extending parallel to (001). Three $[Si(O,N)]_4$ tetrahedra (two with point group symmetry m.., one with 3.. and half-occupancy) are condensed into an isolated $[Si_7(O,N)_{19}]$ unit, in which an $[Si(O,N)]_4$ tetrahedron is located at the center of a 12-membered oxynitride ring with composition $[Si_6O_{15}N_3]$. The present compounds are the first to have such an $[Si_7(O,N)_{19}]$ unit in their structures.

1. Chemical context

Silicon oxynitrides (or oxynitridosilicates) containing an alkaline-earth or a rare-earth metal cation have been extensively studied due to their potential applications as phosphors for white-light-emitting diodes (Takeda *et al.*, 2018). Recently, the exploration range for new silicon oxynitrides has been expanded to compounds with alkaline-earth and rare-earth metal cations. In this regard, $Lu_4Ba_2[Si_9ON_{16}]O$, $Y_4Ba_2[Si_9ON_{16}]O$ (Maak *et al.*, 2017), $La_3BaSi_5N_9O_2$ (Durach *et al.*, 2015), $Ca_{1.4}Ce_{2.6}Si_{12}O_{4.4}N_{16.6}$ (Park *et al.*, 2013), $Ca_{1.46}La_{2.54}Si_{12}O_{4.45}N_{16.55}$ (Park *et al.*, 2012) or $BaYSi_2O_5N$ (Kobayashi *et al.*, 2017) were synthesized and their crystal structures determined. The corresponding oxide or nitride forms are unknown for these materials. At the same time, the introduction of multiple anions contributes to the formation of otherwise unattainable silicate units in single anion compounds. In addition to the compounds mentioned above, for example, $Ce_4[Si_4O_4N_6]O$ has a hyperbolic layer structure, which is composed of an $[SiO_3N]$ unit connected by three cyclic $[Si_3O_3N_6]$ units through corner-sharing (Irran *et al.*, 2000).

While exploring new oxynitrides, we obtained $SrSiO_{2.64}N_{0.24}$ with a single-chain inosilicate structure, which has not been realized for Sr- or Sr-rich metasilicate oxides and nitrides (Kobayashi *et al.*, 2018). In the present work, the synthesis and



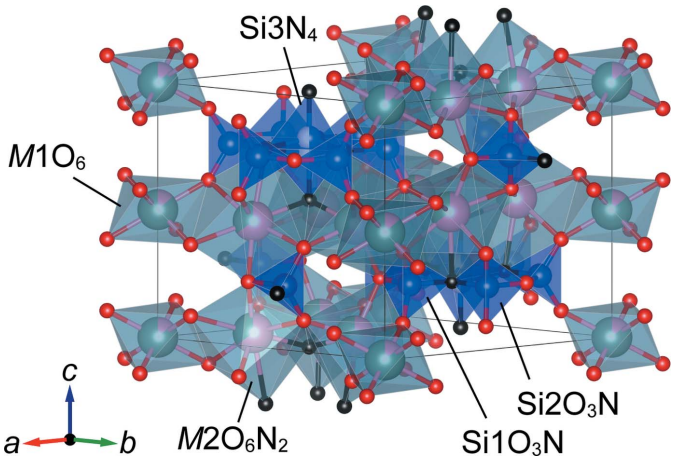


Figure 1
Crystal structure of $Ca_4Y_3Si_7O_{15}N_5$ (**1**) drawn with cation-centered polyhedra. Pink, green, blue, red and black spheres indicate calcium, yttrium, silicon, oxygen, and nitrogen ions, respectively. Mixed colours of the Si3 and associated (N,O) positions indicate the fraction of vacancy/occupancy.

structure determination of three silicon oxynitrides, denoted by the solid solution series $Ca_{4+x}Y_{3-x}Si_7O_{15+x}N_{5-x}$, with compositions of $Ca_4Y_3Si_7O_{15}N_5$ (**1**, $x = 0$), $Ca_{4.5}Y_{2.5}Si_7O_{15.5}N_{4.5}$ (**2**, $x = 0.5$) and $Ca_5Y_2Si_7O_{16}N_4$ (**3**, $x = 1$) are reported.

2. Structural commentary

Compounds **1**–**3** are isotypic and crystallize in space group $P6_3/m$. Figs. 1–4 show the crystal structures and atomic arrangements of **1**–**3**. There are five sites in the structure associated with oxygen and/or nitrogen positions. Two sites at Wyckoff position 12*i*, O1 and O2, and one 6*h* site, O3, are solely occupied by oxygen, and one 6*h* site, N5, is solely occupied by nitrogen, irrespective of the value for *x*. Oxygen and nitrogen atoms are disordered for (O,N)4 situated on a 4*f* site. For **2** and **3**, the O:N ratio at this site amounts to 0.25:0.75 for **2** and 0.5:0.5 for **3**, respectively, whereas for **1** this site is exclusively occupied by nitrogen atoms.

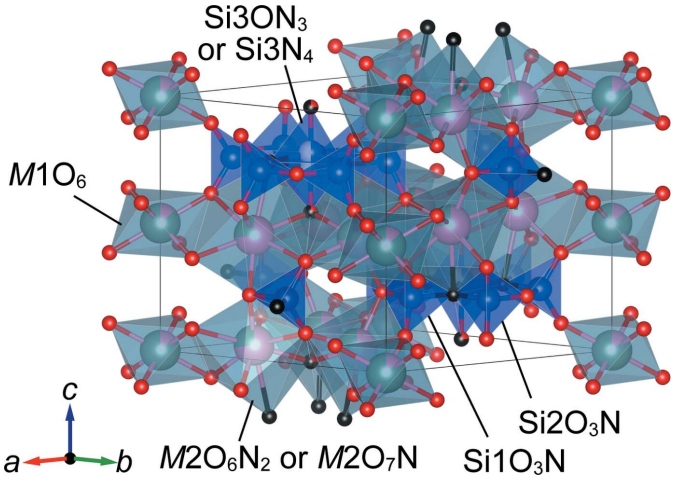


Figure 2
Crystal structure of $Ca_{4.5}Y_{2.5}Si_7O_{15.5}N_{4.5}$ (**2**) drawn with cation-centered polyhedra. Colour code as in Fig. 1.

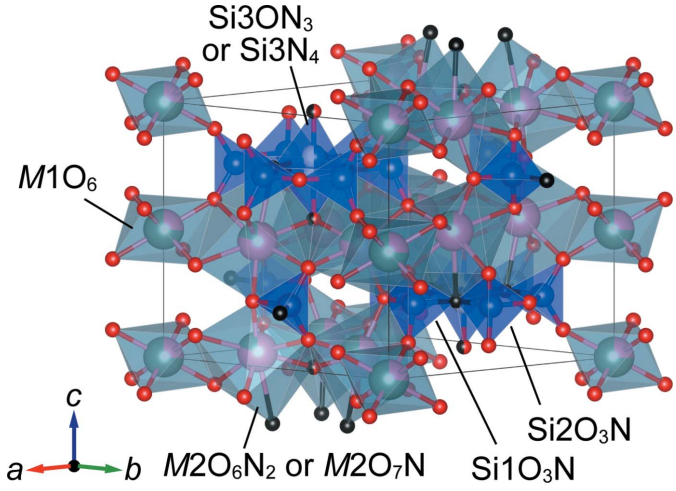


Figure 3
Crystal structure of $Ca_5Y_2Si_7O_{16}N_4$ (**3**) drawn with cation-centered polyhedra. Colour code as in Fig. 1.

Ca^{2+} and Y^{3+} occupy two sites, *viz*. *M*1 with site symmetry $\bar{3}$.. at Wyckoff position 2*b* and *M*2 with site symmetry 1 at Wyckoff position 12*i*. *M*1 is coordinated by six oxygen atoms in the structures of **1**–**3** whereas the coordination environment of *M*2 depends on the value of *x*. In the structure of **1**, six oxygen and two nitrogen atoms define the respective coordination sphere, but there are two possible coordination environments for **2** and **3** because of the disorder of the anionic 4*f* site, *i.e*. two nitrogen and six oxygen atoms, and one nitrogen and seven oxygen atoms, respectively. Site occupancies of Ca^{2+} were refined as 0.1379 (14) (**1**), 0.1338 (14) (**2**)

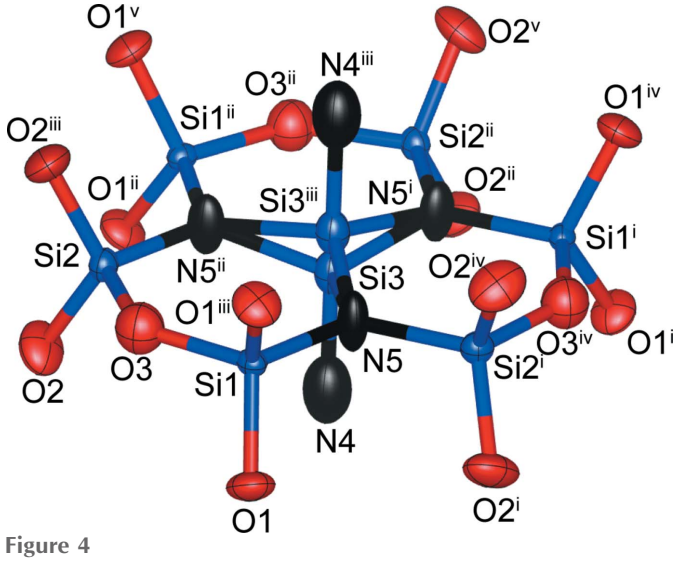


Figure 4
Representative for all structures, the atomic arrangement around Si atoms in the structure of $Ca_4Y_3Si_7O_{15}N_5$ (**1**). Displacement ellipsoids are drawn at the 90% probability level. [Symmetry codes: (i) $1-y, 1+x-y, z$; (ii) $-x+y, 1-x, z$; (iii) $x, y, \frac{1}{2}-z$; (iv) $1-y, 1+x-y, \frac{1}{2}-z$; (v) $-x+y, 1-x, \frac{1}{2}-z$.]

Table 1
Selected bond lengths (Å).

	1	2	3
Si1—O1	1.634 (2) × 2	1.621 (2) × 2	1.623 (2) × 2
Si1—O3	1.686 (3)	1.669 (4)	1.673 (3)
Si1—N5	1.754 (3)	1.788 (4)	1.781 (3)
Si2—O2	1.635 (2) × 2	1.622 (3) × 2	1.624 (2) × 2
Si2—O3	1.684 (3)	1.673 (4)	1.672 (3)
Si2—N5	1.753 (3)	1.798 (4)	1.782 (3)
Si3—(O,N)4	1.804 (6)	1.769 (8)	1.765 (7)
Si3—N5	1.809 (3) × 3	1.730 (5) × 3	1.732 (3) × 3

and 0.2572 (14) (**3**) for *M*1, and 0.6437 (2) (**1**), 0.7277 (2) (**2**) and 0.7905 (2) (**3**) for *M*2. Thus, Ca^{2+} prefers to occupy the larger *M*2 site, in agreement with the larger ionic radius of Ca^{2+} compared to Y^{3+} for six- (1.00 *versus* 0.90 Å) and eight-coordination (1.12 *versus* 1.02 Å; Shannon, 1976). [$M1O_6$] octahedra and [$M2(O,N)_8$] dodecahedra are linked through their edges, resulting in the formation of a layer structure extending parallel to (001). Adjacent layers are connected along [001] through corner-sharing and by silicon atoms in the interstices. There are three Si sites in the crystal structure: Si1, Si2 and Si3 at Wyckhoff positions 6*h* (site symmetry *m*..), 6*h*, and 4*f* (3..), respectively. The latter site is disordered and shows half-occupancy. At both 6*h* sites, [SiO_3N] tetrahedra are present that are condensed into a 12-membered ring, [$Si_6O_{15}N_3$], by corner-sharing. As a result of the disorder and associated splitting of the 4*f* site, tetrahedra above and below the ring are present that share three corners with the ring, resulting in the formation of isolated [$Si_7(O,N)_{19}$] units, as shown in Fig. 4. These units are located at $z = \pm 0.25$ and are situated between the layers formed by layers of [$M1O_6$] octahedra and [$M2(O,N)_8$] dodecahedra.

Bond lengths of the [$Si(O,N)_4$] tetrahedra are collated in Table 1. In agreement with the higher electronegativity of oxygen when compared to nitrogen, the Si—N bonds are systematically longer than Si—O bonds.

3. Synthesis and crystallization

Single crystals of **1**–**3** were obtained from powders synthesized by a solid-state reaction method. $CaCO_3$ (Kanto Chemical, 99.99%), Y_2O_3 (Wako Chemical, 99.99%), SiO_2 (Fuso Chemical, 99.999%), Si_3N_4 (Kojundo Chemical, 99.9%), and CeO_2 (Kanto Chemical, 99.5%) in the molar ratio of $CaCO_3$:Y_2O_3:SiO_2:Si_3N_4 = 5.76:0.62:2.8:1.4 for **2** and of $CaCO_3$:Y_2O_3:CeO_2:SiO_2:Si_3N_4 = 5.76:0.61:0.01:2.8:1.4 (2 mol% Ce to Y) for **1** and **3** were ground in the presence of 20 wt% CaF_2 (Wako Chemical, 99.9%) as a flux. The mixtures were pelletized at 20 MPa, put on an alumina boat with a carbon sheet dish (Toyo Tanso, 0.1 mm of thickness) and calcined at 1733 K for 4 h under 100 ml min^{-1} of flowing nitrogen. The reaction mixtures were slowly cooled under different conditions: to 1373 K at a rate of 30 K h^{-1}, to 1173 K at a rate of 100 K h^{-1} and to RT by turning off the power for **1**, and to 1373 K at a rate of 60 K h^{-1}, to 1173 K at a rate of 100 K h^{-1} and to RT by turning off the power for **2** and **3**. After roughly grinding the recrystallized fused pellets, the powders obtained were washed with 5 *M* HCl(aq.) and distilled water, followed by drying at 353 K. Colourless platelet-like single crystals were selected from the reaction products. Each crystal was cut into two portions. One was affixed to a Mitegen$^{(R)}$ micro-mount device with a drop of Paratone N oil for single-crystal X-ray analysis. The other part was used for elemental analysis by energy dispersive X-ray (EDX) spectrometry using a scanning electron microscope (Hitachi, SU1510) equipped with an EDX detector (Horiba, X-act). EDX analysis indicated a Ca:Y:Si ratio of 0.266 (9):0.237 (4):0.497 (9) for **1**, of 0.325 (9):0.183 (5):0.492 (5) for **2**, and of 0.386 (19):0.146 (10):0.468 (10) for **3**. The ideal ratios according to the formulae of the three title compounds are 0.286:0.214:0.500, 0.321:0.179:0.500, and 0.357:0.143:0.500, respectively.

4. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. In the initial stages of the refinements, all Si3 positions were treated as being located at the the 2*d* site, corresponding to a triangular environment of three N5 atoms. As a result of the strong anisotropy of the displacement ellipsoids along the *c* axis, the Si3 sites were subsequently refined as being split with half occupancy and a mirror symmetry element at $z = \pm 0.25$. When the occupancies of the disordered Ca^{2+} and Y^{3+} sites were refined freely, the ratios of Ca:Y were 7:86:6.14 for **1**, 10.07:3.93 for **2**, and 9:88:4.12 for **3**. Reliability factors for these refinements are summarized in Table 3. All values are almost the same, and the differences between the refined structures are within standard uncertainties. For the final steps of refinements, values obtained by EDX spectrometry were idealized under consideration of charge neutrality. Incorporation of Ce in single crystals of **1** and **3** was confirmed by their photoluminescence (the data are not shown). However, the contamination was ignored because of the small amount (2 mol% relative to Y, that is, $Ca_4Y_{2.93}Ce_{0.06}Si_7O_{15}N_5$ for **1** and $Ca_5Y_{1.96}Ce_{0.04}Si_7O_{15}N_5$ for **3**). Actually, consideration of the presence of Ce had only a marginal effect on refinement parameters and refined structures.

Five sites around the silicon atoms were detected. Although it is difficult to distinguish between oxygen and nitrogen atoms by XRD analysis alone, site occupancies of oxygen and nitrogen sites were determined from coordination environments, bond lengths, and bond-valence sums (Morgan, 1986; Fuertes, 2006; Braun *et al.*, 2010; Maak *et al.*, 2017). Following Pauling's second crystal rule, the site at Wyckoff position 6*h* is coordinated by three Si atoms and thus should be occupied by nitrogen (N5) alone. The relatively long bond length of Si3—(O,N)4, 1.804 (6), 1.769 (8), and 1.765 (7) Å for **1**, **2**, and **3**, respectively, indicate that the (O,N)4 site at the 4*f* position also might be occupied by nitrogen. Under consideration of charge neutrality for the different compositions in **1**–**3**, this site was refined as being occupationally disordered by oxygen and nitrogen for **2** and **3**.

Table 2
Experimental details.

	1	2	3
Crystal data			
Chemical formula	$Ca_4Y_3Si_7O_{15}N_5$	$Ca_{4.5}Y_{2.5}Si_7O_{15.5}N_{4.5}$	$Ca_5Y_2Si_7O_{16}N_4$
M_r	933.73	910.31	886.89
Crystal system, space group	Hexagonal, $P6_3/m$	Hexagonal, $P6_3/m$	Hexagonal, $P6_3/m$
Temperature (K)	293	296	293
a, c (Å)	10.0884 (5), 9.9740 (5)	10.0792 (5), 9.9900 (5)	10.0541 (2), 10.0168 (2)
V (Å^3)	879.11 (10)	878.92 (10)	876.89 (4)
Z	2	2	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	11.56	10.08	8.63
Crystal size (mm)	0.07 × 0.04 × 0.01	0.07 × 0.06 × 0.01	0.05 × 0.03 × 0.02
Data collection			
Diffractometer	Rigaku XtaLAB PRO with a PILATUS 200K	Rigaku R-Axis RAPID II	Rigaku R-Axis RAPID II
Absorption correction	Multi-scan *(CrysAlis PRO*; Rigaku OD, 2015)	Multi-scan (*ABSCOR*; Higashi, 2001)	Multi-scan (*ABSCOR*; Higashi, 2001)
T_{min}, T_{max}	0.684, 1	0.724, 1.000	0.820, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8201, 778, 699	8568, 709, 688	8532, 702, 681
R_{int}	0.039	0.030	0.027
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.685	0.649	0.648
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.025, 0.058, 1.10	0.033, 0.091, 1.19	0.024, 0.062, 1.09
No. of reflections	778	709	702
No. of parameters	62	63	63
No. of restraints	1	1	1
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.25, −0.56	1.83, −0.64	0.50, −0.86

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *RAPID-AUTO* (Rigaku, 2005), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *VESTA* (Momma & Izumi, 2011), *WinGX* (Farrugia, 2012) and *publCIF* (Westrip, 2010).

Table 3
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S depending on the refinement of the site occupation factor of Ca and Y.

	1	2	3
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S at free occupancy	0.025, 0.058, 1.10	0.031, 0.088, 1.14	0.023, 0.062, 1.09
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S at fixed occupancy	0.025, 0.058, 1.10	0.033, 0.091, 1.18	0.024, 0.062, 1.09

Funding information

Funding for this research was provided by: Ministry of Education, Culture, Sports, Science and Technology (grant Nos. JP16H06438, JP16H06439 and JP16H06440); Nippon Sheet Glass Foundation for Materials Science and Engineering; Dynamic Alliance for Open Innovation Bridging Human, Environment and Materials.

References

Braun, C., Seibald, M., Börger, S. L., Oeckler, O., Boyko, T. D., Moewes, A., Miehe, G., Tücks, A. & Schnick, W. (2010). *Chem. Eur. J.* **16**, 9646–9657.
Durach, D., Neudert, L., Schmidt, P. J., Oeckler, O. & Schnick, W. (2015). *Chem. Mater.* **27**, 4832–4838.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Fuertes, A. (2006). *Inorg. Chem.* **45**, 9640–9642.
Higashi, T. (2001). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Irran, E., Köllisch, K., Leoni, S., Nesper, R., Henry, P. F., Weller, M. T. & Schnick, W. (2000). *Chem. Eur. J.* **6**, 2714–2720.
Kobayashi, M., Kim, J., Sato, H., Yasunaga, T., Kato, H., Fujii, K., Shiraiwa, M., Yashima, M. & Kakihana, M. (2018). *Chem. Lett.* **47**, 1327–1329.
Kobayashi, M., Yasunaga, T., Sato, H., Kato, H., Fujii, K., Yashima, M. & Kakihana, M. (2017). *Chem. Lett.* **46**, 795–797.
Maak, C., Niklaus, R., Friedrich, F., Mähringer, A., Schmidt, P. J. & Schnick, W. (2017). *Chem. Mater.* **29**, 8377–8384.
Momma, K. & Izumi, F. (2011). *J. Appl. Cryst.* **44**, 1272–1276.
Morgan, P. E. D. (1986). *J. Mater. Sci.* **21**, 4305–4309.
Park, W. B., Jeong, Y. S., Singh, S. P. & Sohn, K.-S. (2013). *ECS. J. Solid State Sci. Technol.* **2**, R3100–R3106.
Park, W. B., Shin, N., Hong, K.-P., Pyo, M. & Sohn, K.-S. (2012). *Adv. Funct. Mater.* **22**, 2258–2266.
Rigaku (2005). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku O (2015). *CrysAlis PRO*. Rigaku Corporation, Tokyo, Japan.
Shannon, R. D. (1976). *Acta Cryst.* A**32**, 751–767.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Takeda, T., Xie, R.-J., Suehiro, T. & Hirosaki, N. (2018). *Prog. Solid State Chem.* **51**, 41–51.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

Acta Cryst. (2019). E**75**, 260-263 [https://doi.org/10.1107/S2056989019001257]

Crystal structures of $Ca_{4+x}Y_{3-x}Si_7O_{15+x}N_{5-x}$ ($0 \le x \le 1$) comprising of an isolated $[Si_7(O,N)_{19}]$ unit

Makoto Kobayashi, Takuya Yasunaga, Hideki Kato, Kotaro Fujii, Masatomo Yashima and Masato Kakihana

Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2015) for (1); *RAPID-AUTO* (Rigaku, 2005) for (2), (3). Cell refinement: *CrysAlis PRO* (Rigaku OD, 2015) for (1); *RAPID-AUTO* (Rigaku, 2005) for (2), (3). Data reduction: *CrysAlis PRO* (Rigaku OD, 2015) for (1); *RAPID-AUTO* (Rigaku, 2005) for (2), (3). For all structures, program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015b); molecular graphics: *VESTA* (Momma & Izumi, 2011); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *publCIF* (Westrip, 2010).

Tetracalcium triyttrium heptasilicon oxynitride (1)

Crystal data

$Ca_4Y_3Si_7O_{15}N_5$
M_r = 933.73
Hexagonal, $P6_3/m$
Hall symbol: -P 6c
a = 10.0884 (5) Å
c = 9.9740 (5) Å
V = 879.11 (10) Å^3
Z = 2
$F(000)$ = 900
D_x = 3.527 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2781 reflections
θ = 3.0–28.8°
μ = 11.56 mm^{-1}
T = 293 K
Platelet, colorless
0.07 × 0.04 × 0.01 mm

Data collection

Rigaku XtaLAB PRO with a PILATUS 200K diffractometer
Radiation source: fine-focus sealed X-ray tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2015)
T_{min} = 0.684, T_{max} = 1
8201 measured reflections
778 independent reflections
699 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 29.1°, θ_{min} = 2.3°
h = −13→13
k = −13→12
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.058
S = 1.10
778 reflections
62 parameters
1 restraint
0 constraints
Primary atom site location: structure-invariant direct methods

$w = 1/[\sigma^2(F_o^2) + (0.0223P)^2 + 2.2946P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 1.25$ e Å^{-3}
$\Delta\rho_{min} = -0.56$ e Å^{-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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ca1	0	0	0	0.00571 (16)	0.1379 (14)
Y1	0	0	0	0.00571 (16)	0.8620 (14)
Ca2	0.41947 (5)	0.13257 (4)	0.03127 (4)	0.01093 (14)	0.6437 (2)
Y2	0.41947 (5)	0.13257 (4)	0.03127 (4)	0.01093 (14)	0.3563 (2)
Si1	0.10867 (11)	0.31831 (11)	0.25	0.0059 (2)	
Si2	0.56028 (12)	0.01024 (11)	0.25	0.0075 (2)	
Si3	0.3333	0.6667	0.2191 (2)	0.0107 (8)	0.5
O1	0.0791 (2)	0.2237 (2)	0.10980 (19)	0.0136 (4)	
O2	0.4447 (2)	0.3571 (2)	0.1075 (2)	0.0170 (4)	
O3	0.3985 (3)	0.0201 (3)	0.25	0.0180 (6)	
N4	0.3333	0.6667	0.0382 (6)	0.0242 (11)	
N5	0.2961 (4)	0.4743 (4)	0.25	0.0164 (7)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ca1	0.0056 (2)	0.0056 (2)	0.0059 (3)	0.00282 (10)	0	0
Y1	0.0056 (2)	0.0056 (2)	0.0059 (3)	0.00282 (10)	0	0
Ca2	0.0164 (2)	0.0099 (2)	0.0095 (2)	0.00887 (17)	−0.00042 (15)	−0.00065 (14)
Y2	0.0164 (2)	0.0099 (2)	0.0095 (2)	0.00887 (17)	−0.00042 (15)	−0.00065 (14)
Si1	0.0059 (5)	0.0053 (5)	0.0056 (5)	0.0021 (4)	0	0
Si2	0.0061 (5)	0.0069 (5)	0.0087 (5)	0.0026 (4)	0	0
Si3	0.0083 (6)	0.0083 (6)	0.016 (2)	0.0041 (3)	0	0
O1	0.0166 (10)	0.0138 (9)	0.0100 (10)	0.0074 (8)	−0.0004 (8)	−0.0048 (8)
O2	0.0235 (11)	0.0159 (10)	0.0138 (10)	0.0114 (9)	−0.0054 (8)	−0.0069 (8)
O3	0.0171 (15)	0.0169 (15)	0.0204 (16)	0.0089 (12)	0	0
N4	0.0167 (14)	0.0167 (14)	0.039 (3)	0.0083 (7)	0	0
N5	0.0068 (16)	0.0096 (16)	0.032 (2)	0.0038 (13)	0	0

Geometric parameters (Å, º)

Ca1—O1^{i}	2.2646 (19)	Si2—Ca2^{ix}	3.1707 (8)
Ca1—O1^{ii}	2.2646 (19)	Si2—Ca2^{viii}	3.2065 (6)
Ca1—O1^{iii}	2.2646 (19)	Si2—Y2^{viii}	3.2065 (6)
Ca1—O1^{iv}	2.2646 (19)	Si2—Ca2^{xiii}	3.2065 (6)
Ca1—O1^{v}	2.2646 (19)	Si2—Y2^{xiii}	3.2065 (6)

Ca1—O1	2.2646 (19)	Si3—Si3^{ix}	0.617 (5)
Ca1—Y2^{ii}	3.7596 (4)	Si3—N4	1.804 (6)
Ca1—Ca2^{iii}	3.7596 (4)	Si3—N5^{xiv}	1.809 (3)
Ca1—Ca2^{ii}	3.7596 (4)	Si3—N5	1.809 (3)
Ca1—Y2^{iii}	3.7596 (4)	Si3—N5^{xv}	1.809 (4)
Ca1—Ca2^{i}	3.7596 (4)	Si3—Ca2^{xvi}	3.3919 (18)
Ca1—Y2^{i}	3.7596 (4)	Si3—Y2^{xvi}	3.3919 (18)
Ca2—O2	2.280 (2)	Si3—Ca2^{ii}	3.3919 (18)
Ca2—N4^{vi}	2.3979 (17)	Si3—Y2^{ii}	3.3919 (18)
Ca2—O2^{iv}	2.418 (2)	Si3—Ca2^{vi}	3.3919 (18)
Ca2—O3	2.4189 (14)	Si3—Y2^{vi}	3.3919 (18)
Ca2—O1^{iv}	2.477 (2)	O1—Y2^{ii}	2.477 (2)
Ca2—O2^{vii}	2.624 (2)	O1—Ca2^{ii}	2.477 (2)
Ca2—O1^{iii}	2.634 (2)	O1—Ca2^{v}	2.634 (2)
Ca2—N5^{iv}	2.8519 (8)	O1—Y2^{v}	2.634 (2)
Ca2—Si1^{iii}	3.1641 (8)	O2—Si2^{xvii}	1.635 (2)
Ca2—Si2	3.1707 (8)	O2—Y2^{ii}	2.418 (2)
Ca2—Si2^{viii}	3.2065 (6)	O2—Ca2^{ii}	2.418 (2)
Ca2—Si1^{iv}	3.2109 (6)	O2—Ca2^{xvii}	2.624 (2)
Si1—O1	1.6342 (19)	O2—Y2^{xvii}	2.624 (2)
Si1—O1^{ix}	1.6342 (19)	O3—Si1^{iii}	1.686 (3)
Si1—O3^{v}	1.686 (3)	O3—Y2^{ix}	2.4189 (14)
Si1—N5	1.754 (3)	O3—Ca2^{ix}	2.4189 (14)
Si1—Ca2^{v}	3.1641 (8)	N4—Y2^{xvi}	2.3980 (17)
Si1—Y2^{v}	3.1641 (8)	N4—Ca2^{xvi}	2.3980 (17)
Si1—Ca2^{x}	3.1641 (8)	N4—Ca2^{vi}	2.3980 (17)
Si1—Y2^{x}	3.1641 (8)	N4—Y2^{vi}	2.3980 (17)
Si1—Ca2^{xi}	3.2109 (6)	N4—Y2^{ii}	2.3980 (17)
Si1—Y2^{xi}	3.2109 (6)	N4—Ca2^{ii}	2.3980 (17)
Si1—Ca2^{ii}	3.2109 (6)	N5—Si2^{xvii}	1.753 (3)
Si1—Y2^{ii}	3.2109 (6)	N5—Si3^{ix}	1.809 (3)
Si2—O2^{xii}	1.635 (2)	N5—Ca2^{ii}	2.8520 (8)
Si2—O2^{vii}	1.635 (2)	N5—Y2^{ii}	2.8520 (8)
Si2—O3	1.685 (3)	N5—Y2^{xi}	2.8520 (8)
Si2—N5^{vii}	1.753 (3)	N5—Ca2^{xi}	2.8520 (8)
Si2—Y2^{ix}	3.1707 (8)		

O1^{i}—Ca1—O1^{ii}	98.58 (6)	O2^{xii}—Si2—O3	104.46 (9)
O1^{i}—Ca1—O1^{iii}	81.42 (6)	O2^{vii}—Si2—O3	104.46 (9)
O1^{ii}—Ca1—O1^{iii}	180.00 (11)	O2^{xii}—Si2—N5^{vii}	107.17 (9)
O1^{i}—Ca1—O1^{iv}	98.58 (6)	O2^{vii}—Si2—N5^{vii}	107.17 (9)
O1^{ii}—Ca1—O1^{iv}	98.58 (6)	O3—Si2—N5^{vii}	113.01 (16)
O1^{iii}—Ca1—O1^{iv}	81.42 (6)	O2^{xii}—Si2—Y2^{ix}	55.73 (8)
O1^{i}—Ca1—O1^{v}	81.42 (6)	O2^{vii}—Si2—Y2^{ix}	129.27 (9)
O1^{ii}—Ca1—O1^{v}	81.42 (6)	O3—Si2—Y2^{ix}	48.77 (4)
O1^{iii}—Ca1—O1^{v}	98.58 (6)	N5^{vii}—Si2—Y2^{ix}	122.49 (7)
O1^{iv}—Ca1—O1^{v}	180.00 (9)	O2^{xii}—Si2—Ca2^{ix}	55.73 (8)
O1^{i}—Ca1—O1	180	O2^{vii}—Si2—Ca2^{ix}	129.27 (9)

O1^{ii}—Ca1—O1	81.42 (6)	O3—Si2—Ca2^{ix}	48.77 (4)
O1^{iii}—Ca1—O1	98.58 (6)	N5^{vii}—Si2—Ca2^{ix}	122.49 (7)
O1^{iv}—Ca1—O1	81.42 (6)	Y2^{ix}—Si2—Ca2^{ix}	0
O1^{v}—Ca1—O1	98.58 (6)	O2^{xii}—Si2—Ca2	129.27 (9)
O1^{i}—Ca1—Y2^{ii}	140.44 (5)	O2^{vii}—Si2—Ca2	55.73 (8)
O1^{ii}—Ca1—Y2^{ii}	80.35 (5)	O3—Si2—Ca2	48.77 (4)
O1^{iii}—Ca1—Y2^{ii}	99.65 (5)	N5^{vii}—Si2—Ca2	122.49 (7)
O1^{iv}—Ca1—Y2^{ii}	43.64 (5)	Y2^{ix}—Si2—Ca2	87
O1^{v}—Ca1—Y2^{ii}	136.36 (5)	Ca2^{ix}—Si2—Ca2	86.95 (3)
O1—Ca1—Y2^{ii}	39.56 (5)	O2^{xii}—Si2—Ca2^{viii}	147.48 (9)
O1^{i}—Ca1—Ca2^{iii}	39.56 (5)	O2^{vii}—Si2—Ca2^{viii}	47.33 (7)
O1^{ii}—Ca1—Ca2^{iii}	99.65 (5)	O3—Si2—Ca2^{viii}	107.93 (5)
O1^{iii}—Ca1—Ca2^{iii}	80.35 (5)	N5^{vii}—Si2—Ca2^{viii}	62.33 (2)
O1^{iv}—Ca1—Ca2^{iii}	136.36 (5)	Y2^{ix}—Si2—Ca2^{viii}	156.7
O1^{v}—Ca1—Ca2^{iii}	43.64 (5)	Ca2^{ix}—Si2—Ca2^{viii}	156.70 (3)
O1—Ca1—Ca2^{iii}	140.44 (5)	Ca2—Si2—Ca2^{viii}	73.410 (12)
Y2^{ii}—Ca1—Ca2^{iii}	180	O2^{xii}—Si2—Y2^{viii}	147.48 (9)
O1^{i}—Ca1—Ca2^{ii}	140.44 (5)	O2^{vii}—Si2—Y2^{viii}	47.33 (7)
O1^{ii}—Ca1—Ca2^{ii}	80.35 (5)	O3—Si2—Y2^{viii}	107.93 (5)
O1^{iii}—Ca1—Ca2^{ii}	99.65 (5)	N5^{vii}—Si2—Y2^{viii}	62.33 (2)
O1^{iv}—Ca1—Ca2^{ii}	43.64 (5)	Y2^{ix}—Si2—Y2^{viii}	156.70 (3)
O1^{v}—Ca1—Ca2^{ii}	136.36 (5)	Ca2^{ix}—Si2—Y2^{viii}	156.70 (3)
O1—Ca1—Ca2^{ii}	39.56 (5)	Ca2—Si2—Y2^{viii}	73.4
Y2^{ii}—Ca1—Ca2^{ii}	0	Ca2^{viii}—Si2—Y2^{viii}	0.000 (16)
Ca2^{iii}—Ca1—Ca2^{ii}	180.000 (13)	O2^{xii}—Si2—Ca2^{xiii}	47.33 (7)
O1^{i}—Ca1—Y2^{iii}	39.56 (5)	O2^{vii}—Si2—Ca2^{xiii}	147.48 (9)
O1^{ii}—Ca1—Y2^{iii}	99.65 (5)	O3—Si2—Ca2^{xiii}	107.93 (5)
O1^{iii}—Ca1—Y2^{iii}	80.35 (5)	N5^{vii}—Si2—Ca2^{xiii}	62.33 (2)
O1^{iv}—Ca1—Y2^{iii}	136.36 (5)	Y2^{ix}—Si2—Ca2^{xiii}	73.4
O1^{v}—Ca1—Y2^{iii}	43.64 (5)	Ca2^{ix}—Si2—Ca2^{xiii}	73.410 (12)
O1—Ca1—Y2^{iii}	140.44 (5)	Ca2—Si2—Ca2^{xiii}	156.70 (3)
Y2^{ii}—Ca1—Y2^{iii}	180	Ca2^{viii}—Si2—Ca2^{xiii}	122.07 (3)
Ca2^{iii}—Ca1—Y2^{iii}	0.000 (16)	Y2^{viii}—Si2—Ca2^{xiii}	122.1
Ca2^{ii}—Ca1—Y2^{iii}	180	O2^{xii}—Si2—Y2^{xiii}	47.33 (7)
O1^{i}—Ca1—Ca2^{i}	80.35 (5)	O2^{vii}—Si2—Y2^{xiii}	147.48 (9)
O1^{ii}—Ca1—Ca2^{i}	43.64 (5)	O3—Si2—Y2^{xiii}	107.93 (5)
O1^{iii}—Ca1—Ca2^{i}	136.36 (5)	N5^{vii}—Si2—Y2^{xiii}	62.33 (2)
O1^{iv}—Ca1—Ca2^{i}	140.44 (5)	Y2^{ix}—Si2—Y2^{xiii}	73.410 (12)
O1^{v}—Ca1—Ca2^{i}	39.56 (5)	Ca2^{ix}—Si2—Y2^{xiii}	73.410 (12)
O1—Ca1—Ca2^{i}	99.65 (5)	Ca2—Si2—Y2^{xiii}	156.7
Y2^{ii}—Ca1—Ca2^{i}	119.3	Ca2^{viii}—Si2—Y2^{xiii}	122.07 (3)
Ca2^{iii}—Ca1—Ca2^{i}	60.681 (2)	Y2^{viii}—Si2—Y2^{xiii}	122.07 (3)
Ca2^{ii}—Ca1—Ca2^{i}	119.319 (2)	Ca2^{xiii}—Si2—Y2^{xiii}	0.000 (16)
Y2^{iii}—Ca1—Ca2^{i}	60.7	Si3^{ix}—Si3—N4	180
O1^{i}—Ca1—Y2^{i}	80.35 (5)	Si3^{ix}—Si3—N5^{xiv}	80.19 (7)
O1^{ii}—Ca1—Y2^{i}	43.64 (5)	N4—Si3—N5^{xiv}	99.82 (7)
O1^{iii}—Ca1—Y2^{i}	136.36 (5)	Si3^{ix}—Si3—N5	80.18 (7)
O1^{iv}—Ca1—Y2^{i}	140.44 (5)	N4—Si3—N5	99.82 (7)

O1^{v}—Ca1—Y2^{i}	39.56 (5)	N5^{xiv}—Si3—N5	117.15 (4)
O1—Ca1—Y2^{i}	99.65 (5)	Si3^{ix}—Si3—N5^{xv}	80.18 (8)
Y2^{ii}—Ca1—Y2^{i}	119.319 (2)	N4—Si3—N5^{xv}	99.82 (7)
Ca2^{iii}—Ca1—Y2^{i}	60.681 (2)	N5^{xiv}—Si3—N5^{xv}	117.16 (4)
Ca2^{ii}—Ca1—Y2^{i}	119.319 (2)	N5—Si3—N5^{xv}	117.15 (4)
Y2^{iii}—Ca1—Y2^{i}	60.681 (2)	Si3^{ix}—Si3—Ca2^{xvi}	137.41 (3)
Ca2^{i}—Ca1—Y2^{i}	0.000 (13)	N4—Si3—Ca2^{xvi}	42.60 (3)
O2—Ca2—N4^{vi}	72.84 (8)	N5^{xiv}—Si3—Ca2^{xvi}	57.22 (5)
O2—Ca2—O2^{iv}	162.18 (6)	N5—Si3—Ca2^{xvi}	117.10 (9)
N4^{vi}—Ca2—O2^{iv}	107.07 (10)	N5^{xv}—Si3—Ca2^{xvi}	117.54 (9)
O2—Ca2—O3	96.04 (8)	Si3^{ix}—Si3—Y2^{xvi}	137.41 (3)
N4^{vi}—Ca2—O3	117.84 (14)	N4—Si3—Y2^{xvi}	42.60 (3)
O2^{iv}—Ca2—O3	99.44 (8)	N5^{xiv}—Si3—Y2^{xvi}	57.22 (5)
O2—Ca2—O1^{iv}	80.58 (7)	N5—Si3—Y2^{xvi}	117.10 (9)
N4^{vi}—Ca2—O1^{iv}	108.21 (10)	N5^{xv}—Si3—Y2^{xvi}	117.54 (9)
O2^{iv}—Ca2—O1^{iv}	82.66 (7)	Ca2^{xvi}—Si3—Y2^{xvi}	0.00 (2)
O3—Ca2—O1^{iv}	130.56 (8)	Si3^{ix}—Si3—Ca2^{ii}	137.40 (3)
O2—Ca2—O2^{vii}	113.34 (9)	N4—Si3—Ca2^{ii}	42.60 (3)
N4^{vi}—Ca2—O2^{vii}	67.01 (7)	N5^{xiv}—Si3—Ca2^{ii}	117.54 (9)
O2^{iv}—Ca2—O2^{vii}	81.88 (7)	N5—Si3—Ca2^{ii}	57.22 (5)
O3—Ca2—O2^{vii}	62.54 (8)	N5^{xv}—Si3—Ca2^{ii}	117.10 (9)
O1^{iv}—Ca2—O2^{vii}	161.43 (7)	Ca2^{xvi}—Si3—Ca2^{ii}	71.77 (4)
O2—Ca2—O1^{iii}	104.80 (7)	Y2^{xvi}—Si3—Ca2^{ii}	71.8
N4^{vi}—Ca2—O1^{iii}	177.55 (5)	Si3^{ix}—Si3—Y2^{ii}	137.40 (3)
O2^{iv}—Ca2—O1^{iii}	74.97 (6)	N4—Si3—Y2^{ii}	42.60 (3)
O3—Ca2—O1^{iii}	62.73 (8)	N5^{xiv}—Si3—Y2^{ii}	117.54 (9)
O1^{iv}—Ca2—O1^{iii}	70.53 (8)	N5—Si3—Y2^{ii}	57.22 (5)
O2^{vii}—Ca2—O1^{iii}	114.87 (6)	N5^{xv}—Si3—Y2^{ii}	117.10 (9)
O2—Ca2—N5^{iv}	104.57 (9)	Ca2^{xvi}—Si3—Y2^{ii}	71.77 (4)
N4^{vi}—Ca2—N5^{iv}	62.85 (14)	Y2^{xvi}—Si3—Y2^{ii}	71.77 (4)
O2^{iv}—Ca2—N5^{iv}	61.67 (8)	Ca2^{ii}—Si3—Y2^{ii}	0.000 (15)
O3—Ca2—N5^{iv}	158.03 (9)	Si3^{ix}—Si3—Ca2^{vi}	137.40 (3)
O1^{iv}—Ca2—N5^{iv}	61.86 (8)	N4—Si3—Ca2^{vi}	42.60 (3)
O2^{vii}—Ca2—N5^{iv}	101.48 (8)	N5^{xiv}—Si3—Ca2^{vi}	117.10 (9)
O1^{iii}—Ca2—N5^{iv}	117.64 (8)	N5—Si3—Ca2^{vi}	117.54 (9)
O2—Ca2—Si1^{iii}	103.50 (6)	N5^{xv}—Si3—Ca2^{vi}	57.22 (5)
N4^{vi}—Ca2—Si1^{iii}	149.56 (12)	Ca2^{xvi}—Si3—Ca2^{vi}	71.77 (4)
O2^{iv}—Ca2—Si1^{iii}	85.50 (5)	Y2^{xvi}—Si3—Ca2^{vi}	71.8
O3—Ca2—Si1^{iii}	31.72 (7)	Ca2^{ii}—Si3—Ca2^{vi}	71.77 (4)
O1^{iv}—Ca2—Si1^{iii}	100.73 (5)	Y2^{ii}—Si3—Ca2^{vi}	71.8
O2^{vii}—Ca2—Si1^{iii}	88.24 (5)	Si3^{ix}—Si3—Y2^{vi}	137.40 (3)
O1^{iii}—Ca2—Si1^{iii}	31.06 (4)	N4—Si3—Y2^{vi}	42.60 (3)
N5^{iv}—Ca2—Si1^{iii}	143.47 (7)	N5^{xiv}—Si3—Y2^{vi}	117.10 (9)
O2—Ca2—Si2	107.94 (6)	N5—Si3—Y2^{vi}	117.54 (9)
N4^{vi}—Ca2—Si2	92.78 (9)	N5^{xv}—Si3—Y2^{vi}	57.22 (5)
O2^{iv}—Ca2—Si2	89.88 (5)	Ca2^{xvi}—Si3—Y2^{vi}	71.77 (4)
O3—Ca2—Si2	31.59 (7)	Y2^{xvi}—Si3—Y2^{vi}	71.77 (4)
O1^{iv}—Ca2—Si2	158.96 (5)	Ca2^{ii}—Si3—Y2^{vi}	71.77 (4)

O2^{vii}—Ca2—Si2	30.98 (5)	Y2^{ii}—Si3—Y2^{vi}	71.77 (4)
O1^{iii}—Ca2—Si2	88.56 (5)	Ca2^{vi}—Si3—Y2^{vi}	0.000 (18)
N5^{iv}—Ca2—Si2	130.63 (7)	Si1—O1—Ca1	150.03 (12)
Si1^{iii}—Ca2—Si2	58.93 (3)	Si1—O1—Y2^{ii}	100.71 (9)
O2—Ca2—Si2^{viii}	137.54 (6)	Ca1—O1—Y2^{ii}	104.82 (7)
N4^{vi}—Ca2—Si2^{viii}	81.59 (11)	Si1—O1—Ca2^{ii}	100.71 (9)
O2^{iv}—Ca2—Si2^{viii}	29.80 (5)	Ca1—O1—Ca2^{ii}	104.82 (7)
O3—Ca2—Si2^{viii}	126.06 (7)	Y2^{ii}—O1—Ca2^{ii}	0
O1^{iv}—Ca2—Si2^{viii}	75.91 (5)	Si1—O1—Ca2^{v}	92.67 (9)
O2^{vii}—Ca2—Si2^{viii}	85.57 (5)	Ca1—O1—Ca2^{v}	99.97 (7)
O1^{iii}—Ca2—Si2^{viii}	100.00 (5)	Y2^{ii}—O1—Ca2^{v}	95.9
N5^{iv}—Ca2—Si2^{viii}	32.98 (7)	Ca2^{ii}—O1—Ca2^{v}	95.94 (7)
Si1^{iii}—Ca2—Si2^{viii}	115.22 (2)	Si1—O1—Y2^{v}	92.67 (9)
Si2—Ca2—Si2^{viii}	106.589 (12)	Ca1—O1—Y2^{v}	99.97 (7)
O2—Ca2—Si1^{iv}	86.68 (6)	Y2^{ii}—O1—Y2^{v}	95.94 (7)
N4^{vi}—Ca2—Si1^{iv}	82.26 (11)	Ca2^{ii}—O1—Y2^{v}	95.94 (7)
O2^{iv}—Ca2—Si1^{iv}	75.76 (5)	Ca2^{v}—O1—Y2^{v}	0.00 (3)
O3—Ca2—Si1^{iv}	159.66 (7)	Si2^{xvii}—O2—Ca2	139.08 (12)
O1^{iv}—Ca2—Si1^{iv}	30.01 (5)	Si2^{xvii}—O2—Y2^{ii}	102.87 (10)
O2^{vii}—Ca2—Si1^{iv}	134.39 (5)	Ca2—O2—Y2^{ii}	107.8
O1^{iii}—Ca2—Si1^{iv}	97.06 (5)	Si2^{xvii}—O2—Ca2^{ii}	102.87 (10)
N5^{iv}—Ca2—Si1^{iv}	32.96 (7)	Ca2—O2—Ca2^{ii}	107.85 (8)
Si1^{iii}—Ca2—Si1^{iv}	128.11 (3)	Y2^{ii}—O2—Ca2^{ii}	0
Si2—Ca2—Si1^{iv}	162.54 (2)	Si2^{xvii}—O2—Ca2^{xvii}	93.30 (9)
Si2^{viii}—Ca2—Si1^{iv}	56.20 (2)	Ca2—O2—Ca2^{xvii}	108.14 (8)
O1—Si1—O1^{ix}	117.68 (15)	Y2^{ii}—O2—Ca2^{xvii}	98.1
O1—Si1—O3^{v}	105.15 (9)	Ca2^{ii}—O2—Ca2^{xvii}	98.12 (7)
O1^{ix}—Si1—O3^{v}	105.15 (9)	Si2^{xvii}—O2—Y2^{xvii}	93.30 (9)
O1—Si1—N5	108.92 (9)	Ca2—O2—Y2^{xvii}	108.1
O1^{ix}—Si1—N5	108.92 (9)	Y2^{ii}—O2—Y2^{xvii}	98.12 (7)
O3^{v}—Si1—N5	110.87 (16)	Ca2^{ii}—O2—Y2^{xvii}	98.12 (7)
O1—Si1—Ca2^{v}	56.27 (7)	Ca2^{xvii}—O2—Y2^{xvii}	0.00 (3)
O1^{ix}—Si1—Ca2^{v}	128.66 (8)	Si2—O3—Si1^{iii}	135.20 (19)
O3^{v}—Si1—Ca2^{v}	48.97 (4)	Si2—O3—Y2^{ix}	99.64 (8)
N5—Si1—Ca2^{v}	121.33 (7)	Si1^{iii}—O3—Y2^{ix}	99.31 (8)
O1—Si1—Y2^{v}	56.27 (7)	Si2—O3—Ca2^{ix}	99.64 (8)
O1^{ix}—Si1—Y2^{v}	128.66 (8)	Si1^{iii}—O3—Ca2^{ix}	99.31 (8)
O3^{v}—Si1—Y2^{v}	48.97 (4)	Y2^{ix}—O3—Ca2^{ix}	0
N5—Si1—Y2^{v}	121.33 (7)	Si2—O3—Ca2	99.64 (8)
Ca2^{v}—Si1—Y2^{v}	0.000 (16)	Si1^{iii}—O3—Ca2	99.31 (8)
O1—Si1—Ca2^{x}	128.66 (8)	Y2^{ix}—O3—Ca2	128.8
O1^{ix}—Si1—Ca2^{x}	56.27 (7)	Ca2^{ix}—O3—Ca2	128.82 (13)
O3^{v}—Si1—Ca2^{x}	48.97 (4)	Si3—N4—Y2^{xvi}	106.79 (13)
N5—Si1—Ca2^{x}	121.33 (7)	Si3—N4—Ca2^{xvi}	106.79 (13)
Ca2^{v}—Si1—Ca2^{x}	87.18 (3)	Y2^{xvi}—N4—Ca2^{xvi}	0
Y2^{v}—Si1—Ca2^{x}	87.2	Si3—N4—Ca2^{vi}	106.79 (13)
O1—Si1—Y2^{x}	128.66 (8)	Y2^{xvi}—N4—Ca2^{vi}	112
O1^{ix}—Si1—Y2^{x}	56.27 (7)	Ca2^{xvi}—N4—Ca2^{vi}	112.01 (12)

O3^{v}—Si1—Y2^{x}	48.97 (4)	Si3—N4—Y2^{vi}	106.79 (13)
N5—Si1—Y2^{x}	121.33 (7)	Y2^{xvi}—N4—Y2^{vi}	112.01 (12)
Ca2^{v}—Si1—Y2^{x}	87.18 (3)	Ca2^{xvi}—N4—Y2^{vi}	112.01 (12)
Y2^{v}—Si1—Y2^{x}	87.18 (3)	Ca2^{vi}—N4—Y2^{vi}	0.000 (19)
Ca2^{x}—Si1—Y2^{x}	0.000 (11)	Si3—N4—Y2^{ii}	106.79 (13)
O1—Si1—Ca2^{xi}	147.46 (9)	Y2^{xvi}—N4—Y2^{ii}	112.01 (12)
O1^{ix}—Si1—Ca2^{xi}	49.29 (7)	Ca2^{xvi}—N4—Y2^{ii}	112.01 (12)
O3^{v}—Si1—Ca2^{xi}	107.19 (5)	Ca2^{vi}—N4—Y2^{ii}	112.01 (12)
N5—Si1—Ca2^{xi}	62.20 (2)	Y2^{vi}—N4—Y2^{ii}	112.01 (12)
Ca2^{v}—Si1—Ca2^{xi}	156.16 (3)	Si3—N4—Ca2^{ii}	106.79 (13)
Y2^{v}—Si1—Ca2^{xi}	156.2	Y2^{xvi}—N4—Ca2^{ii}	112
Ca2^{x}—Si1—Ca2^{xi}	73.134 (8)	Ca2^{xvi}—N4—Ca2^{ii}	112.01 (12)
Y2^{x}—Si1—Ca2^{xi}	73.1	Ca2^{vi}—N4—Ca2^{ii}	112.01 (12)
O1—Si1—Y2^{xi}	147.46 (9)	Y2^{vi}—N4—Ca2^{ii}	112
O1^{ix}—Si1—Y2^{xi}	49.29 (7)	Y2^{ii}—N4—Ca2^{ii}	0
O3^{v}—Si1—Y2^{xi}	107.19 (5)	Si2^{xvii}—N5—Si1	119.1 (2)
N5—Si1—Y2^{xi}	62.20 (2)	Si2^{xvii}—N5—Si3^{ix}	118.93 (18)
Ca2^{v}—Si1—Y2^{xi}	156.16 (3)	Si1—N5—Si3^{ix}	121.00 (18)
Y2^{v}—Si1—Y2^{xi}	156.16 (3)	Si2^{xvii}—N5—Si3	118.93 (18)
Ca2^{x}—Si1—Y2^{xi}	73.134 (8)	Si1—N5—Si3	121.00 (18)
Y2^{x}—Si1—Y2^{xi}	73.134 (8)	Si3^{ix}—N5—Si3	19.64 (15)
Ca2^{xi}—Si1—Y2^{xi}	0.000 (18)	Si2^{xvii}—N5—Ca2^{ii}	84.69 (7)
O1—Si1—Ca2^{ii}	49.29 (7)	Si1—N5—Ca2^{ii}	84.84 (7)
O1^{ix}—Si1—Ca2^{ii}	147.46 (9)	Si3^{ix}—N5—Ca2^{ii}	110.18 (11)
O3^{v}—Si1—Ca2^{ii}	107.19 (5)	Si3—N5—Ca2^{ii}	90.54 (9)
N5—Si1—Ca2^{ii}	62.20 (2)	Si2^{xvii}—N5—Y2^{ii}	84.69 (7)
Ca2^{v}—Si1—Ca2^{ii}	73.134 (8)	Si1—N5—Y2^{ii}	84.84 (7)
Y2^{v}—Si1—Ca2^{ii}	73.1	Si3^{ix}—N5—Y2^{ii}	110.18 (11)
Ca2^{x}—Si1—Ca2^{ii}	156.16 (3)	Si3—N5—Y2^{ii}	90.54 (9)
Y2^{x}—Si1—Ca2^{ii}	156.2	Ca2^{ii}—N5—Y2^{ii}	0.00 (3)
Ca2^{xi}—Si1—Ca2^{ii}	121.79 (3)	Si2^{xvii}—N5—Y2^{xi}	84.69 (7)
Y2^{xi}—Si1—Ca2^{ii}	121.8	Si1—N5—Y2^{xi}	84.84 (7)
O1—Si1—Y2^{ii}	49.29 (7)	Si3^{ix}—N5—Y2^{xi}	90.54 (9)
O1^{ix}—Si1—Y2^{ii}	147.46 (9)	Si3—N5—Y2^{xi}	110.18 (11)
O3^{v}—Si1—Y2^{ii}	107.19 (5)	Ca2^{ii}—N5—Y2^{xi}	159.27 (14)
N5—Si1—Y2^{ii}	62.20 (2)	Y2^{ii}—N5—Y2^{xi}	159.27 (14)
Ca2^{v}—Si1—Y2^{ii}	73.134 (8)	Si2^{xvii}—N5—Ca2^{xi}	84.69 (7)
Y2^{v}—Si1—Y2^{ii}	73.134 (8)	Si1—N5—Ca2^{xi}	84.84 (7)
Ca2^{x}—Si1—Y2^{ii}	156.16 (3)	Si3^{ix}—N5—Ca2^{xi}	90.54 (9)
Y2^{x}—Si1—Y2^{ii}	156.16 (3)	Si3—N5—Ca2^{xi}	110.18 (11)
Ca2^{xi}—Si1—Y2^{ii}	121.79 (3)	Ca2^{ii}—N5—Ca2^{xi}	159.27 (14)
Y2^{xi}—Si1—Y2^{ii}	121.79 (3)	Y2^{ii}—N5—Ca2^{xi}	159.3
Ca2^{ii}—Si1—Y2^{ii}	0.000 (7)	Y2^{xi}—N5—Ca2^{xi}	0
O2^{xii}—Si2—O2^{vii}	120.73 (16)		

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

Calcium yttrium heptasilicon oxynitride (2)

Crystal data

$Ca_{4.5}Y_{2.5}Si_7O_{15.5}N_{4.5}$
M_r = 910.31
Hexagonal, $P6_3/m$
Hall symbol: -P 6c
a = 10.0792 (5) Å
c = 9.9900 (5) Å
V = 878.92 (10) Å^3
Z = 2
$F(000)$ = 882
D_x = 3.44 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6355 reflections
θ = 3.1–27.5°
μ = 10.08 mm^{-1}
T = 296 K
Platelet, colorless
0.07 × 0.06 × 0.01 mm

Data collection

Rigaku R-Axis RAPID II diffractometer
Radiation source: sealed x-ray tube
Graphite monochromator
Detector resolution: 10 pixels mm^{-1}
phi or ω oscillation scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 2001)
T_{min} = 0.724, T_{max} = 1.000
8568 measured reflections
709 independent reflections
688 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 27.5°, θ_{min} = 3.1°
h = −13→12
k = −12→12
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.091
S = 1.19
709 reflections
63 parameters
1 restraint
0 constraints
Primary atom site location: structure-invariant direct methods
$w = 1/[\sigma^2(F_o^2) + (0.0508P)^2 + 2.6144P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.83 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}
Extinction correction: SHELXL-2014/7 (Sheldrick 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.028 (2)

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.

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Ca1	0	0	0	0.0099 (3)	0.1338 (14)
Y1	0	0	0	0.0099 (3)	0.8662 (14)
Ca2	0.41517 (7)	0.12870 (6)	0.03382 (6)	0.0143 (2)	0.7277 (2)
Y2	0.41517 (7)	0.12870 (6)	0.03382 (6)	0.0143 (2)	0.2723 (2)
Si1	0.11057 (12)	0.31892 (13)	0.25	0.0061 (3)	
Si2	0.55909 (13)	0.01171 (14)	0.25	0.0077 (3)	
Si3	0.3333	0.6667	0.2216 (2)	0.0035 (9)	0.5

O1	0.0838 (3)	0.2250 (3)	0.1115 (2)	0.0143 (5)	
O2	0.4447 (3)	0.3570 (3)	0.1092 (3)	0.0184 (6)	
O3	0.3956 (4)	0.0167 (4)	0.25	0.0186 (8)	
O4	0.3333	0.6667	0.0445 (8)	0.0358 (15)	0.25
N4	0.3333	0.6667	0.0445 (8)	0.0358 (15)	0.75
N5	0.2989 (4)	0.4828 (5)	0.25	0.0251 (11)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ca1	0.0095 (3)	0.0095 (3)	0.0107 (4)	0.00475 (15)	0	0
Y1	0.0095 (3)	0.0095 (3)	0.0107 (4)	0.00475 (15)	0	0
Ca2	0.0209 (3)	0.0137 (3)	0.0117 (4)	0.0111 (2)	−0.0003 (2)	−0.00032 (19)
Y2	0.0209 (3)	0.0137 (3)	0.0117 (4)	0.0111 (2)	−0.0003 (2)	−0.00032 (19)
Si1	0.0049 (5)	0.0078 (6)	0.0045 (6)	0.0024 (4)	0	0
Si2	0.0060 (5)	0.0101 (6)	0.0072 (6)	0.0042 (4)	0	0
Si3	0.0015 (6)	0.0015 (6)	0.008 (3)	0.0007 (3)	0	0
O1	0.0198 (12)	0.0174 (11)	0.0076 (11)	0.0108 (10)	0.0010 (9)	−0.0036 (9)
O2	0.0295 (14)	0.0159 (11)	0.0107 (12)	0.0120 (10)	−0.0052 (10)	−0.0054 (10)
O3	0.0169 (17)	0.0204 (17)	0.0183 (19)	0.0092 (14)	0	0
O4	0.032 (2)	0.032 (2)	0.044 (4)	0.0159 (10)	0	0
N4	0.032 (2)	0.032 (2)	0.044 (4)	0.0159 (10)	0	0
N5	0.0081 (18)	0.020 (2)	0.044 (3)	0.0048 (16)	0	0

Geometric parameters (Å, º)

Ca1—O1	2.276 (2)	Si2—Ca2^{viii}	3.1415 (10)
Ca1—O1^{i}	2.276 (2)	Si2—Y2^{viii}	3.1415 (10)
Ca1—O1^{ii}	2.276 (2)	Si2—Ca2^{xii}	3.2368 (8)
Ca1—O1^{iii}	2.276 (2)	Si2—Y2^{xii}	3.2368 (8)
Ca1—O1^{iv}	2.276 (2)	Si2—Y2^{xiii}	3.2368 (8)
Ca1—O1^{v}	2.276 (2)	Si2—Ca2^{xiii}	3.2368 (8)
Ca1—Ca2	3.7255 (6)	Si3—Si3^{viii}	0.567 (5)
Ca1—Ca2^{iii}	3.7255 (6)	Si3—N5^{xiv}	1.730 (5)
Ca1—Ca2^{ii}	3.7255 (6)	Si3—N5^{xv}	1.730 (5)
Ca1—Y2^{ii}	3.7255 (6)	Si3—N5	1.730 (5)
Ca1—Y2^{iii}	3.7255 (6)	Si3—O4	1.769 (8)
Ca2—O2	2.295 (2)	Si3—N4^{viii}	2.336 (8)
Ca2—O3	2.3990 (17)	Si3—Ca2^{xvi}	3.4587 (19)
Ca2—O2^{iv}	2.422 (3)	Si3—Ca2^{ii}	3.4587 (19)
Ca2—O1^{iv}	2.457 (3)	Si3—Ca2^{vi}	3.4587 (19)
Ca2—N4^{vi}	2.463 (3)	O1—Y2^{ii}	2.457 (3)
Ca2—O4^{vi}	2.463 (3)	O1—Ca2^{ii}	2.457 (3)
Ca2—O1^{iii}	2.627 (2)	O1—Ca2^{v}	2.627 (2)
Ca2—O2^{vii}	2.638 (3)	O1—Y2^{v}	2.627 (2)
Ca2—N5^{iv}	2.9043 (12)	O2—Si2^{xvii}	1.622 (3)
Ca2—Si1^{iii}	3.1302 (10)	O2—Y2^{ii}	2.422 (3)
Ca2—Si2	3.1415 (10)	O2—Ca2^{ii}	2.422 (3)

Ca2—Si1^{iv}	3.2255 (8)	O2—Ca2^{xvii}	2.638 (3)
Si1—O1^{viii}	1.621 (2)	O2—Y2^{xvii}	2.638 (3)
Si1—O1	1.621 (2)	O3—Si1^{iii}	1.669 (4)
Si1—O3^{v}	1.669 (4)	O3—Ca2^{viii}	2.3990 (17)
Si1—N5	1.788 (4)	O3—Y2^{viii}	2.3990 (17)
Si1—Ca2^{v}	3.1302 (10)	O4—Y2^{xvi}	2.463 (3)
Si1—Y2^{v}	3.1302 (10)	O4—Ca2^{xvi}	2.463 (3)
Si1—Ca2^{ix}	3.1302 (10)	O4—Ca2^{vi}	2.463 (3)
Si1—Y2^{ix}	3.1302 (10)	O4—Y2^{vi}	2.463 (3)
Si1—Ca2^{x}	3.2255 (8)	O4—Y2^{ii}	2.463 (3)
Si1—Y2^{x}	3.2255 (8)	O4—Ca2^{ii}	2.463 (3)
Si1—Y2^{ii}	3.2255 (8)	N5—Si3^{viii}	1.730 (5)
Si1—Ca2^{ii}	3.2255 (8)	N5—Si2^{xvii}	1.798 (4)
Si2—O2^{xi}	1.622 (3)	N5—Ca2^{ii}	2.9042 (12)
Si2—O2^{vii}	1.622 (3)	N5—Y2^{ii}	2.9042 (12)
Si2—O3	1.673 (4)	N5—Y2^{x}	2.9042 (12)
Si2—N5^{vii}	1.798 (4)	N5—Ca2^{x}	2.9042 (12)

O1—Ca1—O1^{i}	180	Ca2^{x}—Si1—Ca2^{ii}	123.06 (4)
O1—Ca1—O1^{ii}	81.90 (8)	Y2^{x}—Si1—Ca2^{ii}	123.1
O1^{i}—Ca1—O1^{ii}	98.10 (8)	Y2^{ii}—Si1—Ca2^{ii}	0
O1—Ca1—O1^{iii}	98.10 (8)	O2^{xi}—Si2—O2^{vii}	120.21 (19)
O1^{i}—Ca1—O1^{iii}	81.90 (8)	O2^{xi}—Si2—O3	105.94 (12)
O1^{ii}—Ca1—O1^{iii}	180.00 (14)	O2^{vii}—Si2—O3	105.94 (12)
O1—Ca1—O1^{iv}	81.90 (8)	O2^{xi}—Si2—N5^{vii}	107.38 (12)
O1^{i}—Ca1—O1^{iv}	98.10 (8)	O2^{vii}—Si2—N5^{vii}	107.38 (12)
O1^{ii}—Ca1—O1^{iv}	98.10 (8)	O3—Si2—N5^{vii}	109.7 (2)
O1^{iii}—Ca1—O1^{iv}	81.90 (8)	O2^{xi}—Si2—Ca2	130.42 (11)
O1—Ca1—O1^{v}	98.10 (8)	O2^{vii}—Si2—Ca2	57.07 (10)
O1^{i}—Ca1—O1^{v}	81.90 (8)	O3—Si2—Ca2	48.88 (6)
O1^{ii}—Ca1—O1^{v}	81.90 (8)	N5^{vii}—Si2—Ca2	120.81 (9)
O1^{iii}—Ca1—O1^{v}	98.10 (8)	O2^{xi}—Si2—Ca2^{viii}	57.07 (10)
O1^{iv}—Ca1—O1^{v}	180.0 (2)	O2^{vii}—Si2—Ca2^{viii}	130.42 (11)
O1—Ca1—Ca2	79.39 (6)	O3—Si2—Ca2^{viii}	48.88 (6)
O1^{i}—Ca1—Ca2	100.61 (6)	N5^{vii}—Si2—Ca2^{viii}	120.81 (9)
O1^{ii}—Ca1—Ca2	135.80 (6)	Ca2—Si2—Ca2^{viii}	86.86 (4)
O1^{iii}—Ca1—Ca2	44.20 (6)	O2^{xi}—Si2—Y2^{viii}	57.07 (10)
O1^{iv}—Ca1—Ca2	39.84 (6)	O2^{vii}—Si2—Y2^{viii}	130.42 (11)
O1^{v}—Ca1—Ca2	140.16 (6)	O3—Si2—Y2^{viii}	48.88 (6)
O1—Ca1—Ca2^{iii}	140.16 (6)	N5^{vii}—Si2—Y2^{viii}	120.81 (9)
O1^{i}—Ca1—Ca2^{iii}	39.84 (6)	Ca2—Si2—Y2^{viii}	86.9
O1^{ii}—Ca1—Ca2^{iii}	100.61 (6)	Ca2^{viii}—Si2—Y2^{viii}	0.00 (2)
O1^{iii}—Ca1—Ca2^{iii}	79.39 (6)	O2^{xi}—Si2—Ca2^{xii}	145.99 (11)
O1^{iv}—Ca1—Ca2^{iii}	135.80 (6)	O2^{vii}—Si2—Ca2^{xii}	46.38 (9)
O1^{v}—Ca1—Ca2^{iii}	44.20 (6)	O3—Si2—Ca2^{xii}	107.97 (6)
Ca2—Ca1—Ca2^{iii}	119.187 (3)	N5^{vii}—Si2—Ca2^{xii}	63.05 (3)
O1—Ca1—Ca2^{ii}	39.84 (6)	Ca2—Si2—Ca2^{xii}	73.437 (16)
O1^{i}—Ca1—Ca2^{ii}	140.16 (6)	Ca2^{viii}—Si2—Ca2^{xii}	156.83 (4)

O1^{ii}—Ca1—Ca2^{ii}	79.39 (6)	Y2^{viii}—Si2—Ca2^{xii}	156.8
O1^{iii}—Ca1—Ca2^{ii}	100.61 (6)	O2^{xi}—Si2—Y2^{xii}	145.99 (11)
O1^{iv}—Ca1—Ca2^{ii}	44.20 (6)	O2^{vii}—Si2—Y2^{xii}	46.38 (9)
O1^{v}—Ca1—Ca2^{ii}	135.80 (6)	O3—Si2—Y2^{xii}	107.97 (6)
Ca2—Ca1—Ca2^{ii}	60.813 (3)	N5^{vii}—Si2—Y2^{xii}	63.05 (3)
Ca2^{iii}—Ca1—Ca2^{ii}	180.000 (18)	Ca2—Si2—Y2^{xii}	73.4
O1—Ca1—Y2^{ii}	39.84 (6)	Ca2^{viii}—Si2—Y2^{xii}	156.83 (4)
O1^{i}—Ca1—Y2^{ii}	140.16 (6)	Y2^{viii}—Si2—Y2^{xii}	156.83 (4)
O1^{ii}—Ca1—Y2^{ii}	79.39 (6)	Ca2^{xii}—Si2—Y2^{xii}	0.00 (4)
O1^{iii}—Ca1—Y2^{ii}	100.61 (6)	O2^{xi}—Si2—Y2^{xiii}	46.38 (9)
O1^{iv}—Ca1—Y2^{ii}	44.20 (6)	O2^{vii}—Si2—Y2^{xiii}	145.99 (11)
O1^{v}—Ca1—Y2^{ii}	135.80 (6)	O3—Si2—Y2^{xiii}	107.97 (6)
Ca2—Ca1—Y2^{ii}	60.8	N5^{vii}—Si2—Y2^{xiii}	63.05 (3)
Ca2^{iii}—Ca1—Y2^{ii}	180.000 (18)	Ca2—Si2—Y2^{xiii}	156.8
Ca2^{ii}—Ca1—Y2^{ii}	0.00 (3)	Ca2^{viii}—Si2—Y2^{xiii}	73.437 (16)
O1—Ca1—Y2^{iii}	140.16 (6)	Y2^{viii}—Si2—Y2^{xiii}	73.437 (16)
O1^{i}—Ca1—Y2^{iii}	39.84 (6)	Ca2^{xii}—Si2—Y2^{xiii}	122.32 (4)
O1^{ii}—Ca1—Y2^{iii}	100.61 (6)	Y2^{xii}—Si2—Y2^{xiii}	122.32 (4)
O1^{iii}—Ca1—Y2^{iii}	79.39 (6)	O2^{xi}—Si2—Ca2^{xiii}	46.38 (9)
O1^{iv}—Ca1—Y2^{iii}	135.80 (6)	O2^{vii}—Si2—Ca2^{xiii}	145.99 (11)
O1^{v}—Ca1—Y2^{iii}	44.20 (6)	O3—Si2—Ca2^{xiii}	107.97 (6)
Ca2—Ca1—Y2^{iii}	119.2	N5^{vii}—Si2—Ca2^{xiii}	63.05 (3)
Ca2^{iii}—Ca1—Y2^{iii}	0.00 (2)	Ca2—Si2—Ca2^{xiii}	156.83 (4)
Ca2^{ii}—Ca1—Y2^{iii}	180.000 (14)	Ca2^{viii}—Si2—Ca2^{xiii}	73.437 (16)
Y2^{ii}—Ca1—Y2^{iii}	180.000 (14)	Y2^{viii}—Si2—Ca2^{xiii}	73.4
O2—Ca2—O3	96.63 (11)	Ca2^{xii}—Si2—Ca2^{xiii}	122.32 (4)
O2—Ca2—O2^{iv}	161.52 (8)	Y2^{xii}—Si2—Ca2^{xiii}	122.3
O3—Ca2—O2^{iv}	100.46 (10)	Y2^{xiii}—Si2—Ca2^{xiii}	0
O2—Ca2—O1^{iv}	81.73 (8)	Si3^{viii}—Si3—N5^{xiv}	80.57 (8)
O3—Ca2—O1^{iv}	132.32 (10)	Si3^{viii}—Si3—N5^{xv}	80.56 (9)
O2^{iv}—Ca2—O1^{iv}	81.59 (9)	N5^{xiv}—Si3—N5^{xv}	117.37 (5)
O2—Ca2—N4^{vi}	72.63 (11)	Si3^{viii}—Si3—N5	80.56 (8)
O3—Ca2—N4^{vi}	119.23 (18)	N5^{xiv}—Si3—N5	117.37 (5)
O2^{iv}—Ca2—N4^{vi}	104.53 (14)	N5^{xv}—Si3—N5	117.36 (5)
O1^{iv}—Ca2—N4^{vi}	105.78 (14)	Si3^{viii}—Si3—O4	180
O2—Ca2—O4^{vi}	72.63 (11)	N5^{xiv}—Si3—O4	99.44 (8)
O3—Ca2—O4^{vi}	119.23 (18)	N5^{xv}—Si3—O4	99.44 (8)
O2^{iv}—Ca2—O4^{vi}	104.53 (14)	N5—Si3—O4	99.44 (8)
O1^{iv}—Ca2—O4^{vi}	105.78 (14)	Si3^{viii}—Si3—N4^{viii}	0.0040 (10)
N4^{vi}—Ca2—O4^{vi}	0	N5^{xiv}—Si3—N4^{viii}	80.56 (8)
O2—Ca2—O1^{iii}	106.08 (9)	N5^{xv}—Si3—N4^{viii}	80.56 (8)
O3—Ca2—O1^{iii}	62.93 (10)	N5—Si3—N4^{viii}	80.56 (8)
O2^{iv}—Ca2—O1^{iii}	75.98 (8)	O4—Si3—N4^{viii}	180
O1^{iv}—Ca2—O1^{iii}	71.77 (10)	Si3^{viii}—Si3—Ca2^{xvi}	137.55 (3)
N4^{vi}—Ca2—O1^{iii}	177.46 (11)	N5^{xiv}—Si3—Ca2^{xvi}	56.98 (6)
O4^{vi}—Ca2—O1^{iii}	177.46 (11)	N5^{xv}—Si3—Ca2^{xvi}	117.04 (11)
O2—Ca2—O2^{vii}	112.13 (12)	N5—Si3—Ca2^{xvi}	116.96 (11)
O3—Ca2—O2^{vii}	62.75 (10)	O4—Si3—Ca2^{xvi}	42.46 (3)

O2^{iv}—Ca2—O2^{vii}	82.24 (9)	N4^{viii}—Si3—Ca2^{xvi}	137.54 (3)
O1^{iv}—Ca2—O2^{vii}	159.89 (8)	Si3^{viii}—Si3—Ca2^{ii}	137.54 (3)
N4^{vi}—Ca2—O2^{vii}	67.05 (10)	N5^{xiv}—Si3—Ca2^{ii}	117.04 (11)
O4^{vi}—Ca2—O2^{vii}	67.05 (10)	N5^{xv}—Si3—Ca2^{ii}	116.96 (11)
O1^{iii}—Ca2—O2^{vii}	115.49 (8)	N5—Si3—Ca2^{ii}	56.98 (6)
O2—Ca2—N5^{iv}	103.18 (11)	O4—Si3—Ca2^{ii}	42.46 (3)
O3—Ca2—N5^{iv}	157.70 (11)	N4^{viii}—Si3—Ca2^{ii}	137.54 (3)
O2^{iv}—Ca2—N5^{iv}	61.59 (11)	Ca2^{xvi}—Si3—Ca2^{ii}	71.55 (5)
O1^{iv}—Ca2—N5^{iv}	61.83 (10)	Si3^{viii}—Si3—Ca2^{vi}	137.54 (3)
N4^{vi}—Ca2—N5^{iv}	59.0 (2)	N5^{xiv}—Si3—Ca2^{vi}	116.96 (11)
O4^{vi}—Ca2—N5^{iv}	59.0 (2)	N5^{xv}—Si3—Ca2^{vi}	56.98 (6)
O1^{iii}—Ca2—N5^{iv}	119.67 (11)	N5—Si3—Ca2^{vi}	117.04 (11)
O2^{vii}—Ca2—N5^{iv}	99.76 (10)	O4—Si3—Ca2^{vi}	42.46 (3)
O2—Ca2—Si1^{iii}	104.39 (7)	N4^{viii}—Si3—Ca2^{vi}	137.54 (3)
O3—Ca2—Si1^{iii}	31.79 (9)	Ca2^{xvi}—Si3—Ca2^{vi}	71.55 (5)
O2^{iv}—Ca2—Si1^{iii}	86.87 (6)	Ca2^{ii}—Si3—Ca2^{vi}	71.55 (5)
O1^{iv}—Ca2—Si1^{iii}	102.18 (6)	Si1—O1—Ca1	150.45 (15)
N4^{vi}—Ca2—Si1^{iii}	151.01 (16)	Si1—O1—Y2^{ii}	102.59 (12)
O4^{vi}—Ca2—Si1^{iii}	151.01 (16)	Ca1—O1—Y2^{ii}	103.76 (9)
O1^{iii}—Ca2—Si1^{iii}	31.18 (5)	Si1—O1—Ca2^{ii}	102.59 (12)
O2^{vii}—Ca2—Si1^{iii}	88.78 (6)	Ca1—O1—Ca2^{ii}	103.76 (9)
N5^{iv}—Ca2—Si1^{iii}	145.42 (10)	Y2^{ii}—O1—Ca2^{ii}	0
O2—Ca2—Si2	107.34 (7)	Si1—O1—Ca2^{v}	91.80 (10)
O3—Ca2—Si2	31.69 (8)	Ca1—O1—Ca2^{v}	98.64 (9)
O2^{iv}—Ca2—Si2	90.97 (7)	Y2^{ii}—O1—Ca2^{v}	95.7
O1^{iv}—Ca2—Si2	160.68 (6)	Ca2^{ii}—O1—Ca2^{v}	95.69 (8)
N4^{vi}—Ca2—Si2	93.31 (13)	Si1—O1—Y2^{v}	91.80 (10)
O4^{vi}—Ca2—Si2	93.31 (13)	Ca1—O1—Y2^{v}	98.64 (9)
O1^{iii}—Ca2—Si2	89.16 (6)	Y2^{ii}—O1—Y2^{v}	95.69 (8)
O2^{vii}—Ca2—Si2	31.07 (6)	Ca2^{ii}—O1—Y2^{v}	95.69 (8)
N5^{iv}—Ca2—Si2	129.41 (8)	Ca2^{v}—O1—Y2^{v}	0.00 (4)
Si1^{iii}—Ca2—Si2	59.41 (3)	Si2^{xvii}—O2—Ca2	139.04 (15)
O2—Ca2—Si1^{iv}	86.75 (7)	Si2^{xvii}—O2—Y2^{ii}	104.62 (12)
O3—Ca2—Si1^{iv}	160.80 (9)	Ca2—O2—Y2^{ii}	106.1
O2^{iv}—Ca2—Si1^{iv}	74.80 (7)	Si2^{xvii}—O2—Ca2^{ii}	104.62 (12)
O1^{iv}—Ca2—Si1^{iv}	29.38 (6)	Ca2—O2—Ca2^{ii}	106.14 (10)
N4^{vi}—Ca2—Si1^{iv}	79.85 (16)	Y2^{ii}—O2—Ca2^{ii}	0
O4^{vi}—Ca2—Si1^{iv}	79.85 (16)	Si2^{xvii}—O2—Ca2^{xvii}	91.86 (11)
O1^{iii}—Ca2—Si1^{iv}	97.94 (6)	Ca2—O2—Ca2^{xvii}	109.92 (11)
O2^{vii}—Ca2—Si1^{iv}	133.13 (6)	Y2^{ii}—O2—Ca2^{xvii}	97.8
N5^{iv}—Ca2—Si1^{iv}	33.39 (8)	Ca2^{ii}—O2—Ca2^{xvii}	97.76 (9)
Si1^{iii}—Ca2—Si1^{iv}	129.12 (4)	Si2^{xvii}—O2—Y2^{xvii}	91.86 (11)
Si2—Ca2—Si1^{iv}	161.90 (3)	Ca2—O2—Y2^{xvii}	109.9
O1^{viii}—Si1—O1	117.18 (18)	Y2^{ii}—O2—Y2^{xvii}	97.76 (9)
O1^{viii}—Si1—O3^{v}	106.15 (11)	Ca2^{ii}—O2—Y2^{xvii}	97.76 (9)
O1—Si1—O3^{v}	106.15 (11)	Ca2^{xvii}—O2—Y2^{xvii}	0.00 (2)
O1^{viii}—Si1—N5	109.23 (11)	Si1^{iii}—O3—Si2	136.8 (2)
O1—Si1—N5	109.23 (11)	Si1^{iii}—O3—Ca2	99.02 (10)

O3^{v}—Si1—N5	108.6 (2)	Si2—O3—Ca2	99.42 (10)
O1^{viii}—Si1—Ca2^{v}	129.30 (10)	Si1^{iii}—O3—Ca2^{viii}	99.02 (10)
O1—Si1—Ca2^{v}	57.02 (9)	Si2—O3—Ca2^{viii}	99.42 (10)
O3^{v}—Si1—Ca2^{v}	49.19 (6)	Ca2—O3—Ca2^{viii}	128.37 (16)
N5—Si1—Ca2^{v}	120.21 (10)	Si1^{iii}—O3—Y2^{viii}	99.02 (10)
O1^{viii}—Si1—Y2^{v}	129.30 (10)	Si2—O3—Y2^{viii}	99.42 (10)
O1—Si1—Y2^{v}	57.02 (9)	Ca2—O3—Y2^{viii}	128.4
O3^{v}—Si1—Y2^{v}	49.19 (6)	Ca2^{viii}—O3—Y2^{viii}	0.00 (3)
N5—Si1—Y2^{v}	120.21 (10)	Si3—O4—Y2^{xvi}	108.54 (18)
Ca2^{v}—Si1—Y2^{v}	0.00 (3)	Si3—O4—Ca2^{xvi}	108.54 (18)
O1^{viii}—Si1—Ca2^{ix}	57.02 (9)	Y2^{xvi}—O4—Ca2^{xvi}	0
O1—Si1—Ca2^{ix}	129.30 (10)	Si3—O4—Ca2^{vi}	108.54 (18)
O3^{v}—Si1—Ca2^{ix}	49.19 (6)	Y2^{xvi}—O4—Ca2^{vi}	110.4
N5—Si1—Ca2^{ix}	120.21 (10)	Ca2^{xvi}—O4—Ca2^{vi}	110.39 (17)
Ca2^{v}—Si1—Ca2^{ix}	87.25 (3)	Si3—O4—Y2^{vi}	108.54 (18)
Y2^{v}—Si1—Ca2^{ix}	87.2	Y2^{xvi}—O4—Y2^{vi}	110.39 (17)
O1^{viii}—Si1—Y2^{ix}	57.02 (9)	Ca2^{xvi}—O4—Y2^{vi}	110.39 (17)
O1—Si1—Y2^{ix}	129.30 (10)	Ca2^{vi}—O4—Y2^{vi}	0.00 (3)
O3^{v}—Si1—Y2^{ix}	49.19 (6)	Si3—O4—Y2^{ii}	108.54 (18)
N5—Si1—Y2^{ix}	120.21 (10)	Y2^{xvi}—O4—Y2^{ii}	110.39 (17)
Ca2^{v}—Si1—Y2^{ix}	87.25 (3)	Ca2^{xvi}—O4—Y2^{ii}	110.39 (17)
Y2^{v}—Si1—Y2^{ix}	87.25 (3)	Ca2^{vi}—O4—Y2^{ii}	110.39 (17)
Ca2^{ix}—Si1—Y2^{ix}	0.00 (3)	Y2^{vi}—O4—Y2^{ii}	110.39 (17)
O1^{viii}—Si1—Ca2^{x}	48.03 (9)	Si3—O4—Ca2^{ii}	108.54 (18)
O1—Si1—Ca2^{x}	146.28 (10)	Y2^{xvi}—O4—Ca2^{ii}	110.4
O3^{v}—Si1—Ca2^{x}	107.30 (6)	Ca2^{xvi}—O4—Ca2^{ii}	110.39 (17)
N5—Si1—Ca2^{x}	63.39 (3)	Ca2^{vi}—O4—Ca2^{ii}	110.39 (17)
Ca2^{v}—Si1—Ca2^{x}	156.46 (4)	Y2^{vi}—O4—Ca2^{ii}	110.4
Y2^{v}—Si1—Ca2^{x}	156.5	Y2^{ii}—O4—Ca2^{ii}	0
Ca2^{ix}—Si1—Ca2^{x}	72.773 (9)	Si3^{viii}—N5—Si3	18.88 (17)
Y2^{ix}—Si1—Ca2^{x}	72.8	Si3^{viii}—N5—Si1	122.8 (2)
O1^{viii}—Si1—Y2^{x}	48.03 (9)	Si3—N5—Si1	122.8 (2)
O1—Si1—Y2^{x}	146.28 (10)	Si3^{viii}—N5—Si2^{xvii}	121.1 (2)
O3^{v}—Si1—Y2^{x}	107.30 (6)	Si3—N5—Si2^{xvii}	121.1 (2)
N5—Si1—Y2^{x}	63.39 (3)	Si1—N5—Si2^{xvii}	115.1 (3)
Ca2^{v}—Si1—Y2^{x}	156.46 (4)	Si3^{viii}—N5—Ca2^{ii}	111.94 (15)
Y2^{v}—Si1—Y2^{x}	156.46 (4)	Si3—N5—Ca2^{ii}	93.06 (10)
Ca2^{ix}—Si1—Y2^{x}	72.773 (9)	Si1—N5—Ca2^{ii}	83.21 (9)
Y2^{ix}—Si1—Y2^{x}	72.773 (9)	Si2^{xvii}—N5—Ca2^{ii}	83.45 (9)
Ca2^{x}—Si1—Y2^{x}	0.00 (3)	Si3^{viii}—N5—Y2^{ii}	111.94 (15)
O1^{viii}—Si1—Y2^{ii}	146.28 (10)	Si3—N5—Y2^{ii}	93.06 (10)
O1—Si1—Y2^{ii}	48.03 (9)	Si1—N5—Y2^{ii}	83.21 (9)
O3^{v}—Si1—Y2^{ii}	107.30 (6)	Si2^{xvii}—N5—Y2^{ii}	83.45 (9)
N5—Si1—Y2^{ii}	63.39 (3)	Ca2^{ii}—N5—Y2^{ii}	0.00 (4)
Ca2^{v}—Si1—Y2^{ii}	72.773 (9)	Si3^{viii}—N5—Y2^{x}	93.06 (10)
Y2^{v}—Si1—Y2^{ii}	72.773 (9)	Si3—N5—Y2^{x}	111.94 (15)
Ca2^{ix}—Si1—Y2^{ii}	156.46 (4)	Si1—N5—Y2^{x}	83.21 (9)
Y2^{ix}—Si1—Y2^{ii}	156.46 (4)	Si2^{xvii}—N5—Y2^{x}	83.45 (9)

Ca2^{x}—Si1—Y2^{ii}	123.06 (4)	Ca2^{ii}—N5—Y2^{x}	155.00 (19)
Y2^{x}—Si1—Y2^{ii}	123.06 (4)	Y2^{ii}—N5—Y2^{x}	155.00 (19)
O1^{viii}—Si1—Ca2^{ii}	146.28 (10)	Si3^{viii}—N5—Ca2^{x}	93.06 (10)
O1—Si1—Ca2^{ii}	48.03 (9)	Si3—N5—Ca2^{x}	111.94 (15)
O3^{v}—Si1—Ca2^{ii}	107.30 (6)	Si1—N5—Ca2^{x}	83.21 (9)
N5—Si1—Ca2^{ii}	63.39 (3)	Si2^{xvii}—N5—Ca2^{x}	83.45 (9)
Ca2^{v}—Si1—Ca2^{ii}	72.773 (9)	Ca2^{ii}—N5—Ca2^{x}	155.00 (19)
Y2^{v}—Si1—Ca2^{ii}	72.8	Y2^{ii}—N5—Ca2^{x}	155
Ca2^{ix}—Si1—Ca2^{ii}	156.46 (4)	Y2^{x}—N5—Ca2^{x}	0
Y2^{ix}—Si1—Ca2^{ii}	156.5		

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

Pentacalcium diyttrium heptasilicon oxynitride (3)

Crystal data

$Ca_5Y_2Si_7O_{16}N_4$
M_r = 886.89
Hexagonal, $P6_3/m$
Hall symbol: -P 6c
a = 10.0541 (2) Å
c = 10.0168 (2) Å
V = 876.89 (4) Å^3
Z = 2
F(000) = 864
D_x = 3.359 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 7553 reflections
θ = 3.1–27.4°
μ = 8.63 mm^{-1}
T = 293 K
Platelet, colorless
0.05 × 0.03 × 0.02 mm

Data collection

Rigaku R-Axis RAPID II diffractometer
Radiation source: sealed x-ray tube
Graphite monochromator
Detector resolution: 10 pixels mm^{-1}
phi or *ω* oscillation scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 2001)
T_{min} = 0.820, T_{max} = 1.000
8532 measured reflections
702 independent reflections
681 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 27.4°, θ_{min} = 3.1°
h = −13→13
k = −13→13
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.062
S = 1.09
702 reflections
63 parameters
1 restraint
0 constraints
Primary atom site location: structure-invariant direct methods
$w = 1/[\sigma^2(F_o^2) + (0.0366P)^2 + 1.4061P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.86 e Å^{-3}
Extinction correction: SHELXL-2014/7 (Sheldrick 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0135 (11)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ca1	0	0	0	0.00811 (18)	0.2572 (14)
Y1	0	0	0	0.00811 (18)	0.7428 (14)
Ca2	0.41677 (5)	0.13055 (4)	0.03368 (4)	0.01268 (17)	0.7905 (2)
Y2	0.41677 (5)	0.13055 (4)	0.03368 (4)	0.01268 (17)	0.2095 (2)
Si1	0.11074 (9)	0.31954 (9)	0.25	0.0073 (2)	
Si2	0.55788 (9)	0.00978 (9)	0.25	0.0087 (2)	
Si3	0.3333	0.6667	0.21626 (19)	0.0077 (5)	0.5
O1	0.08563 (19)	0.22613 (19)	0.11149 (17)	0.0150 (4)	
O2	0.4430 (2)	0.35772 (19)	0.10933 (18)	0.0187 (4)	
O3	0.3963 (3)	0.0190 (3)	0.25	0.0197 (5)	
O4	0.3333	0.6667	0.0400 (6)	0.0452 (13)	0.5
N4	0.3333	0.6667	0.0400 (6)	0.0452 (13)	0.5
N5	0.2988 (3)	0.4832 (3)	0.25	0.0208 (7)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ca1	0.0084 (2)	0.0084 (2)	0.0076 (3)	0.00418 (10)	0	0
Y1	0.0084 (2)	0.0084 (2)	0.0076 (3)	0.00418 (10)	0	0
Ca2	0.0191 (2)	0.0123 (2)	0.0098 (2)	0.01028 (16)	−0.00029 (14)	−0.00046 (13)
Y2	0.0191 (2)	0.0123 (2)	0.0098 (2)	0.01028 (16)	−0.00029 (14)	−0.00046 (13)
Si1	0.0074 (4)	0.0071 (4)	0.0064 (4)	0.0029 (3)	0	0
Si2	0.0070 (4)	0.0089 (4)	0.0097 (4)	0.0035 (3)	0	0
Si3	0.0054 (5)	0.0054 (5)	0.0123 (14)	0.0027 (2)	0	0
O1	0.0173 (8)	0.0165 (8)	0.0097 (8)	0.0073 (7)	−0.0001 (6)	−0.0043 (7)
O2	0.0257 (9)	0.0186 (8)	0.0143 (8)	0.0130 (7)	−0.0049 (7)	−0.0055 (7)
O3	0.0185 (12)	0.0207 (12)	0.0206 (13)	0.0103 (10)	0	0
O4	0.0318 (14)	0.0318 (14)	0.072 (4)	0.0159 (7)	0	0
N4	0.0318 (14)	0.0318 (14)	0.072 (4)	0.0159 (7)	0	0
N5	0.0077 (12)	0.0102 (13)	0.043 (2)	0.0033 (10)	0	0

Geometric parameters (Å, º)

Ca1—O1^{i}	2.2804 (16)	Si2—Ca2^{viii}	3.1472 (7)
Ca1—O1^{ii}	2.2804 (16)	Si2—Ca2^{xii}	3.2387 (5)
Ca1—O1	2.2804 (16)	Si2—Y2^{xii}	3.2387 (5)
Ca1—O1^{iii}	2.2804 (16)	Si2—Ca2^{xiii}	3.2387 (5)
Ca1—O1^{iv}	2.2804 (16)	Si2—Y2^{xiii}	3.2387 (5)
Ca1—O1^{v}	2.2804 (16)	Si3—Si3^{viii}	0.676 (4)

Ca1—Ca2	3.7276 (4)	Si3—N5^{xiv}	1.732 (3)
Ca1—Ca2^{ii}	3.7276 (4)	Si3—N5^{xv}	1.732 (3)
Ca1—Ca2^{i}	3.7276 (4)	Si3—N5	1.732 (3)
Ca1—Y2^{i}	3.7276 (4)	Si3—O4	1.765 (7)
Ca1—Y2^{ii}	3.7276 (4)	Si3—Ca2^{xvi}	3.4080 (15)
Ca2—O2	2.2930 (17)	Si3—Y2^{xvi}	3.4080 (15)
Ca2—O3	2.4010 (12)	Si3—Ca2^{i}	3.4080 (15)
Ca2—O2^{iii}	2.4136 (18)	Si3—Y2^{i}	3.4080 (15)
Ca2—N4^{vi}	2.4274 (19)	Si3—Y2^{vi}	3.4080 (15)
Ca2—O4^{vi}	2.4274 (19)	Si3—Ca2^{vi}	3.4080 (15)
Ca2—O1^{iii}	2.4475 (17)	O1—Y2^{i}	2.4475 (17)
Ca2—O2^{vii}	2.6369 (18)	O1—Ca2^{i}	2.4475 (17)
Ca2—O1^{ii}	2.6475 (17)	O1—Ca2^{iv}	2.6475 (17)
Ca2—N5^{iii}	2.9071 (7)	O1—Y2^{iv}	2.6475 (17)
Ca2—Si1^{ii}	3.1432 (7)	O2—Si2^{xvii}	1.6241 (18)
Ca2—Si2	3.1472 (7)	O2—Y2^{i}	2.4136 (18)
Ca2—Si1^{iii}	3.2277 (5)	O2—Ca2^{i}	2.4136 (18)
Si1—O1^{viii}	1.6227 (17)	O2—Ca2^{xvii}	2.6370 (18)
Si1—O1	1.6228 (17)	O2—Y2^{xvii}	2.6370 (18)
Si1—O3^{iv}	1.673 (3)	O3—Si1^{ii}	1.673 (3)
Si1—N5	1.781 (3)	O3—Ca2^{viii}	2.4011 (12)
Si1—Ca2^{iv}	3.1433 (7)	O3—Y2^{viii}	2.4011 (12)
Si1—Y2^{iv}	3.1433 (7)	O4—Y2^{xvi}	2.4273 (19)
Si1—Ca2^{ix}	3.1433 (7)	O4—Ca2^{xvi}	2.4273 (19)
Si1—Y2^{ix}	3.1433 (7)	O4—Ca2^{vi}	2.4273 (19)
Si1—Ca2^{x}	3.2277 (5)	O4—Y2^{vi}	2.4273 (19)
Si1—Y2^{x}	3.2277 (5)	O4—Y2^{i}	2.4273 (19)
Si1—Y2^{i}	3.2277 (5)	O4—Ca2^{i}	2.4273 (19)
Si1—Ca2^{i}	3.2277 (5)	N5—Si3^{viii}	1.732 (3)
Si2—O2^{xi}	1.6241 (18)	N5—Si2^{xvii}	1.782 (3)
Si2—O2^{vii}	1.6241 (18)	N5—Ca2^{i}	2.9071 (7)
Si2—O3	1.672 (3)	N5—Y2^{i}	2.9071 (7)
Si2—N5^{vii}	1.782 (3)	N5—Y2^{x}	2.9071 (7)
Si2—Y2^{viii}	3.1472 (7)	N5—Ca2^{x}	2.9071 (7)

O1^{i}—Ca1—O1^{ii}	180.00 (9)	O2^{xi}—Si2—Y2^{viii}	56.86 (7)
O1^{i}—Ca1—O1	81.94 (6)	O2^{vii}—Si2—Y2^{viii}	130.39 (7)
O1^{ii}—Ca1—O1	98.06 (6)	O3—Si2—Y2^{viii}	48.78 (4)
O1^{i}—Ca1—O1^{iii}	98.06 (6)	N5^{vii}—Si2—Y2^{viii}	121.36 (6)
O1^{ii}—Ca1—O1^{iii}	81.94 (6)	O2^{xi}—Si2—Ca2^{viii}	56.86 (7)
O1—Ca1—O1^{iii}	81.94 (6)	O2^{vii}—Si2—Ca2^{viii}	130.39 (7)
O1^{i}—Ca1—O1^{iv}	81.94 (6)	O3—Si2—Ca2^{viii}	48.78 (4)
O1^{ii}—Ca1—O1^{iv}	98.06 (6)	N5^{vii}—Si2—Ca2^{viii}	121.36 (6)
O1—Ca1—O1^{iv}	98.06 (6)	Y2^{viii}—Si2—Ca2^{viii}	0
O1^{iii}—Ca1—O1^{iv}	180.00 (12)	O2^{xi}—Si2—Ca2	130.39 (7)
O1^{i}—Ca1—O1^{v}	98.06 (6)	O2^{vii}—Si2—Ca2	56.86 (7)
O1^{ii}—Ca1—O1^{v}	81.94 (6)	O3—Si2—Ca2	48.78 (4)
O1—Ca1—O1^{v}	180	N5^{vii}—Si2—Ca2	121.36 (6)

O1^{iii}—Ca1—O1^{v}	98.06 (6)	Y2^{viii}—Si2—Ca2	87
O1^{iv}—Ca1—O1^{v}	81.94 (6)	Ca2^{viii}—Si2—Ca2	87.02 (2)
O1^{i}—Ca1—Ca2	135.31 (4)	O2^{xi}—Si2—Ca2^{xii}	145.93 (8)
O1^{ii}—Ca1—Ca2	44.69 (4)	O2^{vii}—Si2—Ca2^{xii}	46.05 (6)
O1—Ca1—Ca2	78.88 (4)	O3—Si2—Ca2^{xii}	108.32 (4)
O1^{iii}—Ca1—Ca2	39.57 (4)	N5^{vii}—Si2—Ca2^{xii}	63.15 (2)
O1^{iv}—Ca1—Ca2	140.43 (4)	Y2^{viii}—Si2—Ca2^{xii}	157.1
O1^{v}—Ca1—Ca2	101.12 (4)	Ca2^{viii}—Si2—Ca2^{xii}	157.07 (3)
O1^{i}—Ca1—Ca2^{ii}	101.12 (4)	Ca2—Si2—Ca2^{xii}	73.312 (11)
O1^{ii}—Ca1—Ca2^{ii}	78.88 (4)	O2^{xi}—Si2—Y2^{xii}	145.93 (8)
O1—Ca1—Ca2^{ii}	140.43 (4)	O2^{vii}—Si2—Y2^{xii}	46.05 (6)
O1^{iii}—Ca1—Ca2^{ii}	135.31 (4)	O3—Si2—Y2^{xii}	108.32 (4)
O1^{iv}—Ca1—Ca2^{ii}	44.69 (4)	N5^{vii}—Si2—Y2^{xii}	63.15 (2)
O1^{v}—Ca1—Ca2^{ii}	39.57 (4)	Y2^{viii}—Si2—Y2^{xii}	157.07 (3)
Ca2—Ca1—Ca2^{ii}	119.190 (2)	Ca2^{viii}—Si2—Y2^{xii}	157.07 (3)
O1^{i}—Ca1—Ca2^{i}	78.88 (4)	Ca2—Si2—Y2^{xii}	73.3
O1^{ii}—Ca1—Ca2^{i}	101.12 (4)	Ca2^{xii}—Si2—Y2^{xii}	0.000 (15)
O1—Ca1—Ca2^{i}	39.57 (4)	O2^{xi}—Si2—Ca2^{xiii}	46.05 (6)
O1^{iii}—Ca1—Ca2^{i}	44.69 (4)	O2^{vii}—Si2—Ca2^{xiii}	145.93 (8)
O1^{iv}—Ca1—Ca2^{i}	135.31 (4)	O3—Si2—Ca2^{xiii}	108.32 (4)
O1^{v}—Ca1—Ca2^{i}	140.43 (4)	N5^{vii}—Si2—Ca2^{xiii}	63.15 (2)
Ca2—Ca1—Ca2^{i}	60.810 (2)	Y2^{viii}—Si2—Ca2^{xiii}	73.3
Ca2^{ii}—Ca1—Ca2^{i}	180.000 (12)	Ca2^{viii}—Si2—Ca2^{xiii}	73.312 (11)
O1^{i}—Ca1—Y2^{i}	78.88 (4)	Ca2—Si2—Ca2^{xiii}	157.07 (3)
O1^{ii}—Ca1—Y2^{i}	101.12 (4)	Ca2^{xii}—Si2—Ca2^{xiii}	122.65 (3)
O1—Ca1—Y2^{i}	39.57 (4)	Y2^{xii}—Si2—Ca2^{xiii}	122.7
O1^{iii}—Ca1—Y2^{i}	44.69 (4)	O2^{xi}—Si2—Y2^{xiii}	46.05 (6)
O1^{iv}—Ca1—Y2^{i}	135.31 (4)	O2^{vii}—Si2—Y2^{xiii}	145.93 (8)
O1^{v}—Ca1—Y2^{i}	140.43 (4)	O3—Si2—Y2^{xiii}	108.32 (4)
Ca2—Ca1—Y2^{i}	60.8	N5^{vii}—Si2—Y2^{xiii}	63.15 (2)
Ca2^{ii}—Ca1—Y2^{i}	180.000 (12)	Y2^{viii}—Si2—Y2^{xiii}	73.312 (11)
Ca2^{i}—Ca1—Y2^{i}	0.000 (12)	Ca2^{viii}—Si2—Y2^{xiii}	73.312 (11)
O1^{i}—Ca1—Y2^{ii}	101.12 (4)	Ca2—Si2—Y2^{xiii}	157.1
O1^{ii}—Ca1—Y2^{ii}	78.88 (4)	Ca2^{xii}—Si2—Y2^{xiii}	122.65 (3)
O1—Ca1—Y2^{ii}	140.43 (4)	Y2^{xii}—Si2—Y2^{xiii}	122.65 (3)
O1^{iii}—Ca1—Y2^{ii}	135.31 (4)	Ca2^{xiii}—Si2—Y2^{xiii}	0.000 (16)
O1^{iv}—Ca1—Y2^{ii}	44.69 (4)	Si3^{viii}—Si3—N5^{xiv}	78.75 (7)
O1^{v}—Ca1—Y2^{ii}	39.57 (4)	Si3^{viii}—Si3—N5^{xv}	78.74 (7)
Ca2—Ca1—Y2^{ii}	119.2	N5^{xiv}—Si3—N5^{xv}	116.29 (4)
Ca2^{ii}—Ca1—Y2^{ii}	0.000 (16)	Si3^{viii}—Si3—N5	78.74 (6)
Ca2^{i}—Ca1—Y2^{ii}	180	N5^{xiv}—Si3—N5	116.29 (4)
Y2^{i}—Ca1—Y2^{ii}	180	N5^{xv}—Si3—N5	116.29 (4)
O2—Ca2—O3	96.16 (7)	Si3^{viii}—Si3—O4	180
O2—Ca2—O2^{iii}	161.05 (5)	N5^{xiv}—Si3—O4	101.25 (6)
O3—Ca2—O2^{iii}	100.98 (7)	N5^{xv}—Si3—O4	101.25 (6)
O2—Ca2—N4^{vi}	73.06 (8)	N5—Si3—O4	101.25 (6)
O3—Ca2—N4^{vi}	118.54 (14)	Si3^{viii}—Si3—Ca2^{xvi}	137.28 (2)
O2^{iii}—Ca2—N4^{vi}	105.11 (11)	N5^{xiv}—Si3—Ca2^{xvi}	58.53 (4)

O2—Ca2—O4^{vi}	73.06 (8)	N5^{xv}—Si3—Ca2^{xvi}	118.42 (8)
O3—Ca2—O4^{vi}	118.54 (14)	N5—Si3—Ca2^{xvi}	118.45 (8)
O2^{iii}—Ca2—O4^{vi}	105.11 (11)	O4—Si3—Ca2^{xvi}	42.73 (2)
N4^{vi}—Ca2—O4^{vi}	0	Si3^{viii}—Si3—Y2^{xvi}	137.28 (2)
O2—Ca2—O1^{iii}	81.84 (6)	N5^{xiv}—Si3—Y2^{xvi}	58.53 (4)
O3—Ca2—O1^{iii}	132.03 (7)	N5^{xv}—Si3—Y2^{xvi}	118.42 (8)
O2^{iii}—Ca2—O1^{iii}	80.71 (6)	N5—Si3—Y2^{xvi}	118.45 (8)
N4^{vi}—Ca2—O1^{iii}	106.72 (11)	O4—Si3—Y2^{xvi}	42.73 (2)
O4^{vi}—Ca2—O1^{iii}	106.72 (11)	Ca2^{xvi}—Si3—Y2^{xvi}	0.00 (2)
O2—Ca2—O2^{vii}	113.34 (8)	Si3^{viii}—Si3—Ca2^{i}	137.27 (2)
O3—Ca2—O2^{vii}	62.62 (7)	N5^{xiv}—Si3—Ca2^{i}	118.42 (8)
O2^{iii}—Ca2—O2^{vii}	82.05 (6)	N5^{xv}—Si3—Ca2^{i}	118.45 (8)
N4^{vi}—Ca2—O2^{vii}	67.30 (8)	N5—Si3—Ca2^{i}	58.53 (4)
O4^{vi}—Ca2—O2^{vii}	67.30 (8)	O4—Si3—Ca2^{i}	42.73 (2)
O1^{iii}—Ca2—O2^{vii}	159.44 (6)	Ca2^{xvi}—Si3—Ca2^{i}	71.97 (4)
O2—Ca2—O1^{ii}	105.75 (6)	Y2^{xvi}—Si3—Ca2^{i}	72
O3—Ca2—O1^{ii}	62.69 (7)	Si3^{viii}—Si3—Y2^{i}	137.27 (2)
O2^{iii}—Ca2—O1^{ii}	75.59 (5)	N5^{xiv}—Si3—Y2^{i}	118.42 (8)
N4^{vi}—Ca2—O1^{ii}	178.26 (6)	N5^{xv}—Si3—Y2^{i}	118.45 (8)
O4^{vi}—Ca2—O1^{ii}	178.26 (6)	N5—Si3—Y2^{i}	58.53 (4)
O1^{iii}—Ca2—O1^{ii}	71.75 (7)	O4—Si3—Y2^{i}	42.73 (2)
O2^{vii}—Ca2—O1^{ii}	114.42 (5)	Ca2^{xvi}—Si3—Y2^{i}	71.97 (4)
O2—Ca2—N5^{iii}	103.67 (7)	Y2^{xvi}—Si3—Y2^{i}	71.97 (4)
O3—Ca2—N5^{iii}	157.98 (8)	Ca2^{i}—Si3—Y2^{i}	0.00 (2)
O2^{iii}—Ca2—N5^{iii}	61.16 (7)	Si3^{viii}—Si3—Y2^{vi}	137.27 (2)
N4^{vi}—Ca2—N5^{iii}	60.10 (15)	N5^{xiv}—Si3—Y2^{vi}	118.45 (8)
O4^{vi}—Ca2—N5^{iii}	60.10 (15)	N5^{xv}—Si3—Y2^{vi}	58.53 (4)
O1^{iii}—Ca2—N5^{iii}	61.53 (7)	N5—Si3—Y2^{vi}	118.42 (8)
O2^{vii}—Ca2—N5^{iii}	100.12 (7)	O4—Si3—Y2^{vi}	42.73 (2)
O1^{ii}—Ca2—N5^{iii}	119.31 (7)	Ca2^{xvi}—Si3—Y2^{vi}	71.97 (4)
O2—Ca2—Si1^{ii}	103.99 (5)	Y2^{xvi}—Si3—Y2^{vi}	71.97 (4)
O3—Ca2—Si1^{ii}	31.66 (6)	Ca2^{i}—Si3—Y2^{vi}	71.97 (4)
O2^{iii}—Ca2—Si1^{ii}	86.88 (4)	Y2^{i}—Si3—Y2^{vi}	71.97 (4)
N4^{vi}—Ca2—Si1^{ii}	150.19 (13)	Si3^{viii}—Si3—Ca2^{vi}	137.27 (2)
O4^{vi}—Ca2—Si1^{ii}	150.19 (13)	N5^{xiv}—Si3—Ca2^{vi}	118.45 (8)
O1^{iii}—Ca2—Si1^{ii}	102.05 (4)	N5^{xv}—Si3—Ca2^{vi}	58.53 (4)
O2^{vii}—Ca2—Si1^{ii}	88.07 (4)	N5—Si3—Ca2^{vi}	118.42 (8)
O1^{ii}—Ca2—Si1^{ii}	31.07 (4)	O4—Si3—Ca2^{vi}	42.73 (2)
N5^{iii}—Ca2—Si1^{ii}	145.05 (6)	Ca2^{xvi}—Si3—Ca2^{vi}	71.97 (4)
O2—Ca2—Si2	107.89 (5)	Y2^{xvi}—Si3—Ca2^{vi}	72
O3—Ca2—Si2	31.59 (6)	Ca2^{i}—Si3—Ca2^{vi}	71.97 (4)
O2^{iii}—Ca2—Si2	91.00 (5)	Y2^{i}—Si3—Ca2^{vi}	72
N4^{vi}—Ca2—Si2	93.24 (10)	Y2^{vi}—Si3—Ca2^{vi}	0
O4^{vi}—Ca2—Si2	93.24 (10)	Si1—O1—Ca1	150.18 (10)
O1^{iii}—Ca2—Si2	159.75 (4)	Si1—O1—Y2^{i}	103.06 (8)
O2^{vii}—Ca2—Si2	31.04 (4)	Ca1—O1—Y2^{i}	104.02 (6)
O1^{ii}—Ca2—Si2	88.33 (4)	Si1—O1—Ca2^{i}	103.06 (8)
N5^{iii}—Ca2—Si2	129.71 (5)	Ca1—O1—Ca2^{i}	104.02 (6)

Si1^{ii}—Ca2—Si2	58.79 (2)	Y2^{i}—O1—Ca2^{i}	0
O2—Ca2—Si1^{iii}	86.92 (5)	Si1—O1—Ca2^{iv}	91.58 (7)
O3—Ca2—Si1^{iii}	160.52 (6)	Ca1—O1—Ca2^{iv}	98.02 (6)
O2^{iii}—Ca2—Si1^{iii}	74.24 (5)	Y2^{i}—O1—Ca2^{iv}	95.5
N4^{vi}—Ca2—Si1^{iii}	80.79 (13)	Ca2^{i}—O1—Ca2^{iv}	95.48 (6)
O4^{vi}—Ca2—Si1^{iii}	80.79 (13)	Si1—O1—Y2^{iv}	91.58 (7)
O1^{iii}—Ca2—Si1^{iii}	29.32 (4)	Ca1—O1—Y2^{iv}	98.02 (6)
O2^{vii}—Ca2—Si1^{iii}	133.34 (4)	Y2^{i}—O1—Y2^{iv}	95.48 (6)
O1^{ii}—Ca2—Si1^{iii}	97.93 (4)	Ca2^{i}—O1—Y2^{iv}	95.48 (6)
N5^{iii}—Ca2—Si1^{iii}	33.23 (5)	Ca2^{iv}—O1—Y2^{iv}	0.000 (18)
Si1^{ii}—Ca2—Si1^{iii}	129.00 (3)	Si2^{xvii}—O2—Ca2	139.12 (11)
Si2—Ca2—Si1^{iii}	161.82 (2)	Si2^{xvii}—O2—Y2^{i}	104.98 (8)
O1^{viii}—Si1—O1	117.51 (13)	Ca2—O2—Y2^{i}	106.5
O1^{viii}—Si1—O3^{iv}	106.16 (8)	Si2^{xvii}—O2—Ca2^{i}	104.98 (8)
O1—Si1—O3^{iv}	106.16 (8)	Ca2—O2—Ca2^{i}	106.55 (7)
O1^{viii}—Si1—N5	108.71 (8)	Y2^{i}—O2—Ca2^{i}	0
O1—Si1—N5	108.71 (8)	Si2^{xvii}—O2—Ca2^{xvii}	92.10 (8)
O3^{iv}—Si1—N5	109.35 (13)	Ca2—O2—Ca2^{xvii}	108.46 (7)
O1^{viii}—Si1—Ca2^{iv}	129.73 (7)	Y2^{i}—O2—Ca2^{xvii}	98
O1—Si1—Ca2^{iv}	57.35 (6)	Ca2^{i}—O2—Ca2^{xvii}	97.95 (6)
O3^{iv}—Si1—Ca2^{iv}	48.90 (4)	Si2^{xvii}—O2—Y2^{xvii}	92.10 (8)
N5—Si1—Ca2^{iv}	120.32 (6)	Ca2—O2—Y2^{xvii}	108.5
O1^{viii}—Si1—Y2^{iv}	129.73 (7)	Y2^{i}—O2—Y2^{xvii}	97.95 (6)
O1—Si1—Y2^{iv}	57.35 (6)	Ca2^{i}—O2—Y2^{xvii}	97.95 (6)
O3^{iv}—Si1—Y2^{iv}	48.90 (4)	Ca2^{xvii}—O2—Y2^{xvii}	0.00 (2)
N5—Si1—Y2^{iv}	120.32 (6)	Si2—O3—Si1^{ii}	134.77 (16)
Ca2^{iv}—Si1—Y2^{iv}	0.00 (2)	Si2—O3—Ca2	99.63 (7)
O1^{viii}—Si1—Ca2^{ix}	57.35 (6)	Si1^{ii}—O3—Ca2	99.44 (7)
O1—Si1—Ca2^{ix}	129.73 (7)	Si2—O3—Ca2^{viii}	99.63 (7)
O3^{iv}—Si1—Ca2^{ix}	48.90 (4)	Si1^{ii}—O3—Ca2^{viii}	99.44 (7)
N5—Si1—Ca2^{ix}	120.32 (6)	Ca2—O3—Ca2^{viii}	128.97 (11)
Ca2^{iv}—Si1—Ca2^{ix}	87.16 (2)	Si2—O3—Y2^{viii}	99.63 (7)
Y2^{iv}—Si1—Ca2^{ix}	87.2	Si1^{ii}—O3—Y2^{viii}	99.44 (7)
O1^{viii}—Si1—Y2^{ix}	57.35 (6)	Ca2—O3—Y2^{viii}	129
O1—Si1—Y2^{ix}	129.73 (7)	Ca2^{viii}—O3—Y2^{viii}	0.00 (4)
O3^{iv}—Si1—Y2^{ix}	48.90 (4)	Si3—O4—Y2^{xvi}	107.71 (14)
N5—Si1—Y2^{ix}	120.32 (6)	Si3—O4—Ca2^{xvi}	107.71 (14)
Ca2^{iv}—Si1—Y2^{ix}	87.16 (2)	Y2^{xvi}—O4—Ca2^{xvi}	0
Y2^{iv}—Si1—Y2^{ix}	87.16 (2)	Si3—O4—Ca2^{vi}	107.71 (14)
Ca2^{ix}—Si1—Y2^{ix}	0.00 (2)	Y2^{xvi}—O4—Ca2^{vi}	111.2
O1^{viii}—Si1—Ca2^{x}	47.62 (6)	Ca2^{xvi}—O4—Ca2^{vi}	111.18 (13)
O1—Si1—Ca2^{x}	146.23 (7)	Si3—O4—Y2^{vi}	107.71 (14)
O3^{iv}—Si1—Ca2^{x}	107.33 (4)	Y2^{xvi}—O4—Y2^{vi}	111.18 (13)
N5—Si1—Ca2^{x}	63.45 (2)	Ca2^{xvi}—O4—Y2^{vi}	111.18 (13)
Ca2^{iv}—Si1—Ca2^{x}	156.21 (3)	Ca2^{vi}—O4—Y2^{vi}	0.00 (3)
Y2^{iv}—Si1—Ca2^{x}	156.2	Si3—O4—Y2^{i}	107.71 (14)
Ca2^{ix}—Si1—Ca2^{x}	72.618 (6)	Y2^{xvi}—O4—Y2^{i}	111.18 (13)
Y2^{ix}—Si1—Ca2^{x}	72.6	Ca2^{xvi}—O4—Y2^{i}	111.18 (13)

O1^{viii}—Si1—Y2^{x}	47.62 (6)	Ca2^{vi}—O4—Y2^{i}	111.18 (13)
O1—Si1—Y2^{x}	146.23 (7)	Y2^{vi}—O4—Y2^{i}	111.18 (13)
O3^{iv}—Si1—Y2^{x}	107.33 (4)	Si3—O4—Ca2^{i}	107.71 (14)
N5—Si1—Y2^{x}	63.45 (2)	Y2^{xvi}—O4—Ca2^{i}	111.2
Ca2^{iv}—Si1—Y2^{x}	156.21 (3)	Ca2^{xvi}—O4—Ca2^{i}	111.18 (13)
Y2^{iv}—Si1—Y2^{x}	156.21 (3)	Ca2^{vi}—O4—Ca2^{i}	111.18 (13)
Ca2^{ix}—Si1—Y2^{x}	72.618 (6)	Y2^{vi}—O4—Ca2^{i}	111.2
Y2^{ix}—Si1—Y2^{x}	72.618 (6)	Y2^{i}—O4—Ca2^{i}	0
Ca2^{x}—Si1—Y2^{x}	0.00 (3)	Si3^{viii}—N5—Si3	22.51 (13)
O1^{viii}—Si1—Y2^{i}	146.23 (7)	Si3^{viii}—N5—Si1	122.61 (15)
O1—Si1—Y2^{i}	47.62 (6)	Si3—N5—Si1	122.61 (15)
O3^{iv}—Si1—Y2^{i}	107.33 (4)	Si3^{viii}—N5—Si2^{xvii}	120.70 (15)
N5—Si1—Y2^{i}	63.45 (2)	Si3—N5—Si2^{xvii}	120.70 (15)
Ca2^{iv}—Si1—Y2^{i}	72.618 (6)	Si1—N5—Si2^{xvii}	115.29 (16)
Y2^{iv}—Si1—Y2^{i}	72.618 (6)	Si3^{viii}—N5—Ca2^{i}	113.45 (10)
Ca2^{ix}—Si1—Y2^{i}	156.21 (3)	Si3—N5—Ca2^{i}	90.94 (7)
Y2^{ix}—Si1—Y2^{i}	156.21 (3)	Si1—N5—Ca2^{i}	83.32 (6)
Ca2^{x}—Si1—Y2^{i}	123.37 (3)	Si2^{xvii}—N5—Ca2^{i}	83.70 (6)
Y2^{x}—Si1—Y2^{i}	123.37 (3)	Si3^{viii}—N5—Y2^{i}	113.45 (10)
O1^{viii}—Si1—Ca2^{i}	146.23 (7)	Si3—N5—Y2^{i}	90.94 (7)
O1—Si1—Ca2^{i}	47.62 (6)	Si1—N5—Y2^{i}	83.32 (6)
O3^{iv}—Si1—Ca2^{i}	107.33 (4)	Si2^{xvii}—N5—Y2^{i}	83.70 (6)
N5—Si1—Ca2^{i}	63.45 (2)	Ca2^{i}—N5—Y2^{i}	0.00 (3)
Ca2^{iv}—Si1—Ca2^{i}	72.618 (6)	Si3^{viii}—N5—Y2^{x}	90.94 (7)
Y2^{iv}—Si1—Ca2^{i}	72.6	Si3—N5—Y2^{x}	113.45 (10)
Ca2^{ix}—Si1—Ca2^{i}	156.21 (3)	Si1—N5—Y2^{x}	83.32 (6)
Y2^{ix}—Si1—Ca2^{i}	156.2	Si2^{xvii}—N5—Y2^{x}	83.70 (6)
Ca2^{x}—Si1—Ca2^{i}	123.37 (3)	Ca2^{i}—N5—Y2^{x}	155.61 (11)
Y2^{x}—Si1—Ca2^{i}	123.4	Y2^{i}—N5—Y2^{x}	155.61 (11)
Y2^{i}—Si1—Ca2^{i}	0	Si3^{viii}—N5—Ca2^{x}	90.94 (7)
O2^{xi}—Si2—O2^{vii}	120.36 (13)	Si3—N5—Ca2^{x}	113.45 (10)
O2^{xi}—Si2—O3	105.60 (8)	Si1—N5—Ca2^{x}	83.32 (6)
O2^{vii}—Si2—O3	105.60 (8)	Si2^{xvii}—N5—Ca2^{x}	83.70 (6)
O2^{xi}—Si2—N5^{vii}	107.03 (8)	Ca2^{i}—N5—Ca2^{x}	155.61 (11)
O2^{vii}—Si2—N5^{vii}	107.03 (8)	Y2^{i}—N5—Ca2^{x}	155.6
O3—Si2—N5^{vii}	111.18 (13)	Y2^{x}—N5—Ca2^{x}	0

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