Redetermination of the crystal structure of R_5Si_4 (R = Pr, Nd) from single-crystal X-ray diffraction data

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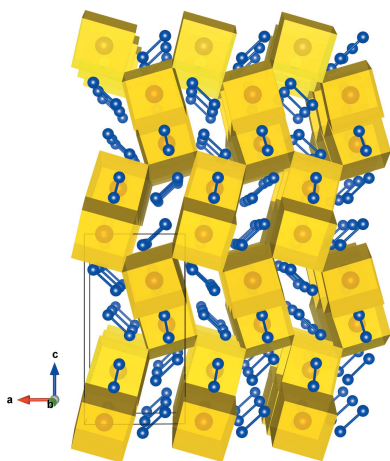[a]Department of Physics, Yokohama National University, 79-5 Tokiwadai, Hodogaya-ku, Yokohama 240-8501, Japan, [b]Department of Chemistry, Yokohama National University, 79-5 Tokiwadai, Hodogaya-ku, Yokohama 240-8501, Japan, and [c]The Institute for Solid State Physics, The University of Tokyo, 5-1-5, Kashiwanoha, Kashiwa, Chiba 277-8581, Japan. *Correspondence e-mail: watanuki-ryuta-sm@ynu.ac.jp

The crystal structures of praseodymium silicide (5/4), Pr_5Si_4, and neodymium silicide (5/4), Nd_5Si_4, were redetermined using high-quality single-crystal X-ray diffraction data. The previous structure reports of Pr_5Si_4 were only based on powder X-ray diffraction data [Smith *et al.* (1967). *Acta Cryst.* 22 940–943; Yang *et al.* (2002b). *J. Alloys Compd.* 339, 189–194; Yang *et al.*, (2003). *J. Alloys Compd.* 263, 146–153]. On the other hand, the structure of Nd_5Si_4 has been determined from powder data [neutron; Cadogan *et al.*, (2002). *J. Phys. Condens. Matter*, 14, 7191–7200] and X-ray [Smith *et al.* (1967). *Acta Cryst.* 22 940–943; Yang *et al.* (2002b). *J. Alloys Compd.* 339, 189–194; Yang *et al.*, (2003). *J. Alloys Compd.* 263, 146–153] and single-crystal data with isotropic atomic displacement parameters [Roger *et al.*, (2006). *J. Alloys Compd.* 415, 73–84]. In addition, the anisotropic atomic displacement parameters for all atomic sites have been determined for the first time. These compounds are confirmed to have the tetragonal Zr_5Si_4-type structure (space group: $P4_12_12$), as reported previously (Smith *et al.*, 1967). The structure is built up by distorted body-centered cubes consisting of Pr(Nd) atoms, which are linked to each other by edge-sharing to form a three-dimensional framework. This framework delimits zigzag channels in which the silicon dimers are situated.

1. Chemical context

In natural science, there are some essential concepts concerned with symmetry, among which chiral symmetry is one of the fundamentals in all fields of physics, especially magnetism in solid-state materials. A chiral magnet in solids is of great interest in both science and technology. These magnets have been studied for novel phenomena such as chiral magnetic soliton lattices and use in future spintronic devices such as magnetic memories and logic gates. The critical point is that the crystal-structure chirality affects the arrangement of magnetic moments in these materials. The symmetry of crystals plays an important role in the spatial arrangement of the magnetic moments. For example, the intermetallic compound $YbNi_3Al_9$ has a trigonal $ErNi_3Al_9$-type structure in space group $R32$, a member of the Sohncke group (Gladyshevskii *et al.*, 1993). This compound exhibits a characteristic helical magnetic structure, reflecting the symmetry of the crystal (Aoki *et al.*, 2018). To study magnetism for chiral symmetry, we focused on the intermetallic compound R_5Si_4 (R = Pr and Nd), which has a

Table 1
Selected bond lengths (Å) for Pr_5Si_4.

Pr1—Pr2[i]	3.4914 (4)	Pr1—Si1[ix]	3.1756 (13)
Pr1—Pr2[ii]	3.5319 (4)	Pr1—Si2[ii]	3.1780 (13)
Pr1—Pr2[iii]	3.5319 (4)	Pr1—Si2[iii]	3.1780 (13)
Pr1—Pr2[iv]	3.4914 (4)	Pr2—Pr2[i]	3.9561 (6)
Pr1—Pr3[v]	3.6423 (3)	Pr2—Pr3[vii]	3.9414 (4)
Pr1—Pr3[vi]	3.6423 (3)	Pr2—Pr3[x]	3.9717 (3)
Pr1—Si1[vii]	3.1756 (13)	Pr2—Pr3[xi]	3.9156 (3)
Pr1—Si1[viii]	3.0985 (13)	Pr3—Pr3[ii]	4.0074 (2)
Pr1—Si1	3.0985 (13)	Si1—Si2	2.4738 (16)

Symmetry codes: (i) $-y+1, -x+1, -z+\frac{1}{2}$; (ii) $-y+\frac{3}{2}, x+\frac{1}{2}, z+\frac{1}{4}$; (iii) $x+\frac{1}{2}, -y+\frac{3}{2}, -z+\frac{3}{4}$; (iv) $-x+1, -y+1, z+\frac{1}{2}$; (v) $-y+2, -x+1, -z+\frac{1}{2}$; (vi) $-x+1, -y+2, z+\frac{1}{2}$; (vii) $-y+\frac{3}{2}, x-\frac{1}{2}, z+\frac{1}{4}$; (viii) $y, x, -z+1$; (ix) $x-\frac{1}{2}, -y+\frac{3}{2}, -z+\frac{3}{4}$.

Table 2
Selected bond lengths (Å) for Nd_5Si_4.

Nd1—Nd2[i]	3.4725 (5)	Nd1—Si1[ix]	3.1528 (16)
Nd1—Nd2[ii]	3.5021 (5)	Nd1—Si2[ii]	3.1661 (16)
Nd1—Nd2[iii]	3.5021 (5)	Nd1—Si2[iii]	3.1661 (16)
Nd1—Nd2[iv]	3.4725 (5)	Nd2—Nd2[i]	3.9202 (7)
Nd1—Nd3[v]	3.6265 (3)	Nd2—Nd3[x]	3.9094 (4)
Nd1—Nd3[vi]	3.6265 (3)	Nd2—Nd3[xi]	3.9378 (4)
Nd1—Si1[vii]	3.1528 (16)	Nd2—Nd3[vii]	3.9061 (4)
Nd1—Si1[viii]	3.0744 (15)	Nd3—Nd3[xii]	3.9752 (2)
Nd1—Si1	3.0744 (15)	Si1—Si2	2.482 (2)

Symmetry codes: (i) $-y+1, -x+1, -z+\frac{1}{2}$; (ii) $-y+\frac{3}{2}, x+\frac{1}{2}, z+\frac{1}{4}$; (iii) $x+\frac{1}{2}, -y+\frac{3}{2}, -z+\frac{3}{4}$; (iv) $-x+1, -y+1, z+\frac{1}{2}$; (v) $-y+2, -x+1, -z+\frac{1}{2}$; (vi) $-x+1, -y+2, z+\frac{1}{2}$; (vii) $-y+\frac{3}{2}, x-\frac{1}{2}, z+\frac{1}{4}$; (viii) $y, x, -z+1$; (ix) $x-\frac{1}{2}, -y+\frac{3}{2}, -z+\frac{3}{4}$.

tetragonal Zr_5Si_4-type crystal structure in the chiral space group $P4_12_12$ (Smith et al., 1967).

Roger et al. (2006) isolated a small single crystal of Nd_5Si_4 by crushing the solidified sample and collected single-crystal X-ray data. Very recently, Sato et al. (2018) reported the single-crystal growth and magnetic properties of Ce_5Si_4, which has the same crystal structure as Pr_5Si_4 and Nd_5Si_4. At present, there has only been a report of large-size single-crystal growth for R = Ce, and there are no reports of a large single crystal having been grown successfully for R = Pr or Nd. In particular,
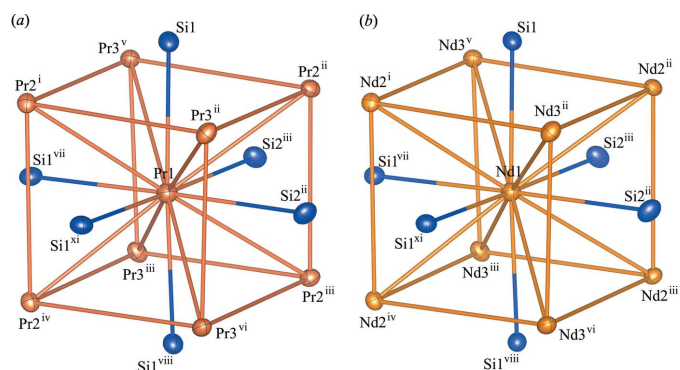
for Pr_5Si_4, the crystal-structure analysis is based only on powder XRD data (Yang et al., 2002a,b,c, 2003; Cadogan et al., 2002; Smith et al., 1967). It is still unknown, however, whether there is a relationship between chiral symmetry and electronic properties, including magnetic ones. In this paper, we report the details of crystallographic studies of single-crystal X-ray analysis of high-quality single-crystalline Pr_5Si_4 and Nd_5Si_4, which are expected to be candidate materials for chiral magnets.

2. Structural commentary

The crystal structures of Pr_5Si_4 and Nd_5Si_4 refined in this study are essentially the same as those determined previously, belonging to chiral space group $P4_12_12$ (No. 92) for R = La, Ce, and Nd (Yang et al., 2002a; Sato et al., 2018). The asymmetric unit of these compounds consists of three Pr (Nd) and two Si atoms. The Pr1(Nd1) atom occupies the Wyckoff 4a site, and the Pr2 (Nd2), Pr3 (Nd3), Si1 and Si2 are located on the general position 8b sites. The principal units in the crystal structures of Pr_5Si_4 and Nd_5Si_4 are illustrated in Fig. 1, and selected bond lengths are given in Tables 1 and 2. The Pr1(Nd1) coordination environment in these compounds can be described as a distorted cube with four Pr2 (Nd2) and four Pr3 (Nd3) [Pr1—Pr2 and Pr1—Pr3 bond lengths ranging from 3.4914 (4) to 3.6423 (3) Å, Pr2—Pr3 bond lengths in the range 3.9156 (3) to 4.0074 (2) Å, Nd1—Nd2 and Nd1—Nd3 bond

Figure 1
Principal units in the structure of (a) Pr_5Si_4 and (b) Nd_5Si_4, illustrated using VESTA (Momma & Izumi, 2011). Displacement ellipsoids are drawn at the 90% probability level. Symmetry codes: (i) $-y+1, -x+1, -z+\frac{1}{2}$; (ii) $-y+\frac{3}{2}, x+\frac{1}{2}, z+\frac{1}{4}$; (iii) $x+\frac{1}{2}, -y+\frac{3}{2}, -z+\frac{3}{4}$; (iv) $-x+1, -y+1, z+\frac{1}{2}$; (v) $-y+2, -x+1, -z+\frac{1}{2}$; (vi) $-x+1, -y+2, z+\frac{1}{2}$; (vii) $-y+\frac{3}{2}, x-\frac{1}{2}, z+\frac{1}{4}$; (viii) $y, x, -z+1$; (ix) $x-\frac{1}{2}, -y+\frac{3}{2}, -z+\frac{3}{4}$.
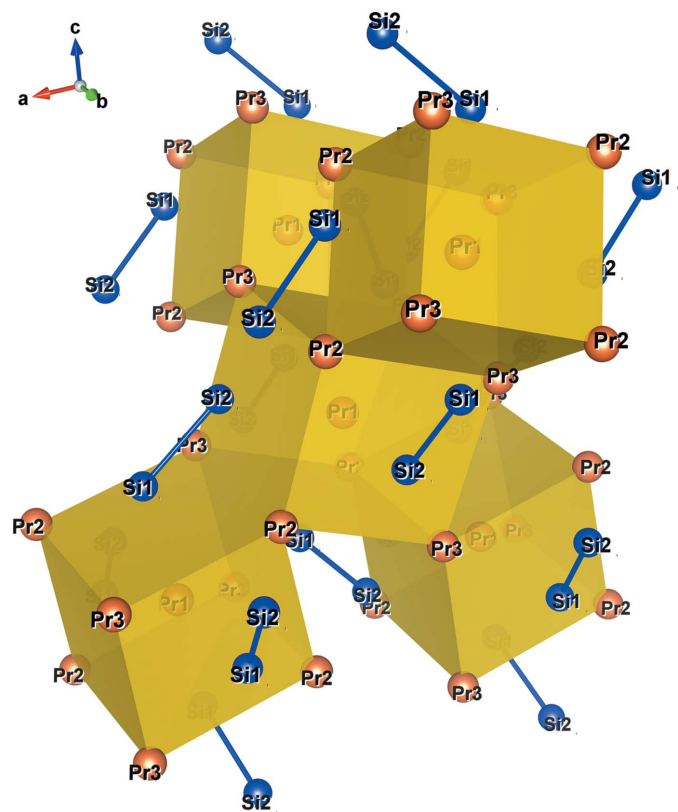

Figure 2
Parts of the crystal structure showing five distorted body-centered cubes sharing Pr2—Pr3 edges (polyhedral drawing). Si1 and Si2 atoms form dimers with atoms Si2 and Si1, respectively, of the adjacent unit.

lengths of 3.4725 (5)–3.6265 (3) Å and Nd2—Nd3 bond lengths of 3.9094 (4)–3.9752 (2) Å]. In addition, the Pr1(Nd1)—Si bonds protruding through the distorted rectangular faces formed by two Pr2 (Nd2) and two Pr3 (Nd3) atoms have Pr1—Si bond lengths ranging from 3.0985 (13) to 3.1780 (13) Å and Nd1—Si bond lengths from 3.0744 (15) to 3.1661 (16) Å. The distorted cubes are connected through common two Pr2—Pr3 (Nd2—Nd3) edges, and Si1 (Si2) atoms form dimers with Si2 (Si1) atoms in the adjacent unit (Fig. 2). The Si1—Si2 bond length in Pr_5Si_4 is 2.4738 (16) Å, and that of Nd_5Si_4 is 2.482 (2) Å. The extended structure is shown in polyhedral representation in Fig. 3. The structure is built up by distorted body-centered cubes consisting of Pr (Nd) atoms, which are linked to each other by edge-sharing to form a three-dimensional framework. This framework delimits zigzag channels oriented along the [100] and [010] directions, in which the Si–Si dimers are situated.

3. Synthesis and crystallization

We have succeeded in growing single-crystalline samples of Pr_5Si_4 for the first time. For Nd_5Si_4, Roger *et al.* (2006) obtained a very small single crystal, but we have succeeded in growing a large single crystal. These compounds are incongruently melting compounds (Shukla *et al.*, 2009), so we synthesized source materials with the non-stoichiometric
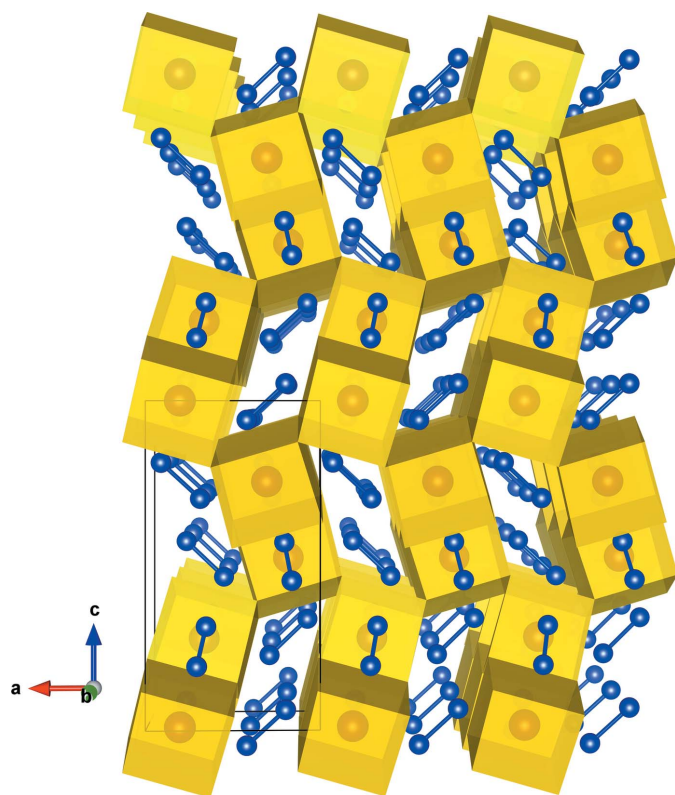

Figure 3
Polyhedral representation of the crystal structure of Pr_5Si_4 showing the Si–Si dimers situated in zigzag channels running along the [100] and [010] directions.

molar ratio of Pr (Nd):Si of 58:42 in a mono-arc furnace. Each melted button of source materials was turned over and remelted three times to ensure homogeneity. Single crystals of Pr_5Si_4 and Nd_5Si_4 were grown by the Czochralski pulling method in a tetra arc furnace in an argon atmosphere on a water-cooled copper hearth. A tungsten rod was used as a pulling axis with no seed crystal, and after optimizing the initial conditions of the growth, the crystal was pulled at a constant rate of 12 mm hour^{-1}. The sizes of the grown ingots were about 30 mm in length and 5 mm in diameter. The grown single-crystal samples were characterized by powder X-ray diffraction using a Rigaku MiniFlexII diffractometer with Cu $K\alpha$ radiation. The powder X-ray diffraction peaks can be well indexed based on the tetragonal Zr_5Si_4-type structure. In addition, it has been confirmed that the whole grown crystal is a single grain crystal by means of the back-reflection Laue method.

4. Database survey

A survey of the Inorganic Crystal Structure Database (ICSD; Belsky *et al.*, 2002) for Pr_5Si_4 yielded three hits. In all three, it is reported that Pr_5Si_4 has a Zr_5Si_4-type structure (Smith *et al.*, 1967; ICSD 649362; Yang *et al.*, 2002*b*; ICSD 95099; Yang *et al.*, 2003; ICSD 98352). On the other hand, for Nd_5Si_4, previous reports have shown that Nd_5Si_4 has two types of crystal structure, a Sm_5Ge_4 type (Raman, 1968; ICSD 645983; Roger *et al.*, 2006; ICSD 154658 and 154659) and a Zr_5Si_4-type structure (Smith *et al.*, 1967; ICSD 645939; Mokra *et al.*, 1978; ICSD 645946; Eremenko *et al.*, 1984; ICSD 600990; Yang *et al.*, 2002*a*; ICSD 94987; Yang *et al.*, 2002*c*; ICSD 190404; Cadogan *et al.*, 2002; ICSD 190404). Roger *et al.* (2006) reported that Sm_5Ge_4-type Nd_5Si_4 could be obtained only with the addition of a tiny amount of boron of less than three at.% in the initial mixture, and that when synthesized with Nd and Si alone, Zr_5Si_4-type Nd_5Si_4 was obtained.

5. Refinement

Crystal data, data collection, and structure refinement details are summarized in Table 3. The highest and deepest remaining difference electron density features are located at 0.90 Å from Pr2 and 1.08 Å from Pr3 for Pr_5Si_4, and 0.74 Å from Nd1 and 1.38 Å from Nd2 for Nd_5Si_4. The absolute structures of the samples were well-defined in space group $P4_12_12$ (No. 92), although the bulk samples possibly also contain the other enantiomer; space group $P4_32_12$ (No. 96).

Table 3
Experimental details.

	Pr$_5$Si$_4$	Nd$_5$Si$_4$
Crystal data		
M_r	816.91	833.56
Crystal system, space group	Tetragonal, $P4_12_12$	Tetragonal, $P4_12_12$
Temperature (K)	223	223
a, c (Å)	7.9001 (2), 14.9568 (6)	7.8644 (2), 14.8085 (5)
V (Å^3)	933.48 (6)	915.89 (6)
Z	4	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	26.03	28.27
Crystal size (mm)	0.13 × 0.08 × 0.03	0.12 × 0.09 × 0.07
Data collection		
Diffractometer	XtaLAB AFC12 (RINC): Kappa dual offset/far	XtaLAB AFC12 (RINC): Kappa dual offset/far
Absorption correction	Analytical [*CrysAlis PRO* (Rigaku OD, 2019) based on Clark & Reid (1995)]	Analytical [*CrysAlis PRO* (Rigaku OD, 2019) based on Clark & Reid (1995)]
T_{min}, T_{max}	0.588, 0.830	0.561, 0.702
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5553, 1260, 1225	6054, 1238, 1203
R_{int}	0.025	0.032
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.710	0.708
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.013, 0.026, 1.10	0.015, 0.028, 1.09
No. of reflections	1260	1238
No. of parameters	43	43
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.69, −0.85	1.10, −0.71
Absolute structure	Flack x determined using 431 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)	Flack x determined using 422 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.04 (2)	−0.01 (3)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2019), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

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Yang, H. F., Rao, G. H., Liu, G. Y., Ouyang, Z. W., Liu, W. F., Feng, X. M., Chu, W. G. & Liang, J. K. (2003). *J. Alloys Compd.* **263**, 146–153.

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Computing details

For both structures, data collection: *CrysAlis PRO* (Rigaku OD, 2019); cell refinement: *CrysAlis PRO* (Rigaku OD, 2019); data reduction: *CrysAlis PRO* (Rigaku OD, 2019); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Pentapraseodymium tetrasiliside (A)

Crystal data

Pr_5Si_4	D_x = 5.813 Mg m^{-3}
M_r = 816.91	Mo $K\alpha$ radiation, λ = 0.71073 Å
Tetragonal, $P4_12_12$	Cell parameters from 4009 reflections
Hall symbol: P 4abw 2nw	θ = 3.8–30.3°
a = 7.9001 (2) Å	μ = 26.03 mm^{-1}
c = 14.9568 (6) Å	T = 223 K
V = 933.48 (6) Å^3	Plate, metallic gray
Z = 4	0.13 × 0.08 × 0.03 mm
$F(000)$ = 1404	

Data collection

XtaLAB AFC12 (RINC): Kappa dual offset/far diffractometer	T_{min} = 0.588, T_{max} = 0.830
Radiation source: micro-focus sealed X-ray tube	5553 measured reflections
Mirror monochromator	1260 independent reflections
Detector resolution: 5.8140 pixels mm^{-1}	1225 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.025
Absorption correction: analytical [CrysAlisPro (Rigaku OD, 2019) based on Clark & Reid (1995)]	θ_{max} = 30.3°, θ_{min} = 3.7°
	h = −11→11
	k = −10→10
	l = −19→17

Refinement

Refinement on F^2	Primary atom site location: dual
Least-squares matrix: full	w = 1/[$\sigma^2(F_o^2)$ + $(0.0078P)^2$ + $0.0556P$]
$R[F^2 > 2\sigma(F^2)]$ = 0.013	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.026	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.10	$\Delta\rho_{max}$ = 0.69 e Å^{-3}
1260 reflections	$\Delta\rho_{min}$ = −0.85 e Å^{-3}
43 parameters	Extinction correction: SHELXL (Sheldrick, 2015b), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
0 restraints	

Extinction coefficient: 0.00247 (9)

Absolute structure: Flack x determined using 431 quotients $[(I^+)\text{-}(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)

Absolute structure parameter: −0.04 (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}
Pr1	0.81086 (3)	0.81086 (3)	0.500000	0.00721 (8)
Pr2	0.51578 (3)	0.37028 (3)	0.12478 (2)	0.00578 (7)
Pr3	0.51088 (3)	0.87144 (3)	0.04758 (2)	0.00676 (7)
Si1	0.92537 (16)	0.71000 (16)	0.30916 (8)	0.0069 (2)
Si2	0.69967 (16)	0.66478 (16)	0.19702 (8)	0.0078 (2)

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pr1	0.00720 (10)	0.00720 (10)	0.00723 (16)	−0.00017 (11)	0.00069 (9)	−0.00069 (9)
Pr2	0.00587 (11)	0.00618 (12)	0.00529 (12)	−0.00033 (9)	0.00050 (9)	−0.00083 (8)
Pr3	0.00630 (12)	0.00650 (12)	0.00748 (12)	−0.00045 (7)	−0.00114 (9)	0.00172 (9)
Si1	0.0074 (5)	0.0078 (6)	0.0056 (6)	−0.0011 (4)	−0.0004 (4)	0.0001 (5)
Si2	0.0066 (5)	0.0074 (6)	0.0094 (6)	−0.0018 (4)	−0.0012 (5)	0.0007 (5)

Geometric parameters (Å, º)

Pr1—Pr2[i]	3.4914 (4)	Pr2—Pr3[xi]	3.9156 (3)
Pr1—Pr2[ii]	3.5319 (4)	Pr2—Si1[xi]	3.0641 (13)
Pr1—Pr2[iii]	3.5319 (4)	Pr2—Si1[i]	3.1005 (14)
Pr1—Pr2[iv]	3.4914 (4)	Pr2—Si1[xii]	3.0668 (14)
Pr1—Pr3[v]	3.6423 (3)	Pr2—Si2	2.9480 (13)
Pr1—Pr3[vi]	3.6423 (3)	Pr2—Si2[xi]	2.9737 (13)
Pr1—Si1[vii]	3.1756 (13)	Pr2—Si2[i]	3.0730 (13)
Pr1—Si1[viii]	3.0985 (13)	Pr3—Pr3[ii]	4.0074 (2)
Pr1—Si1	3.0985 (13)	Pr3—Si1[xiii]	3.1554 (13)
Pr1—Si1[ix]	3.1756 (13)	Pr3—Si1[xii]	3.3434 (12)
Pr1—Si2[ii]	3.1780 (13)	Pr3—Si1[xiv]	3.1957 (12)
Pr1—Si2[iii]	3.1780 (13)	Pr3—Si2[xiii]	3.2566 (12)
Pr2—Pr2[i]	3.9561 (6)	Pr3—Si2[xii]	3.1708 (12)
Pr2—Pr3[vii]	3.9414 (4)	Pr3—Si2	3.1442 (12)
Pr2—Pr3[x]	3.9717 (3)	Si1—Si2	2.4738 (16)
Pr2[i]—Pr1—Pr2[iv]	71.331 (11)	Si2[xi]—Pr2—Si2[i]	124.47 (4)
Pr2[iii]—Pr1—Pr2[ii]	68.120 (11)	Pr1[xvi]—Pr3—Pr1[xii]	97.461 (6)

Pr2^{iv}—Pr1—Pr2^{ii}	176.841 (6)	Pr1^{xvi}—Pr3—Pr2^{x}	99.525 (8)
Pr2^{i}—Pr1—Pr2^{iii}	176.841 (6)	Pr1^{xii}—Pr3—Pr2^{xvii}	158.527 (9)
Pr2^{i}—Pr1—Pr2^{ii}	110.343 (4)	Pr1^{xvi}—Pr3—Pr2^{xiii}	136.554 (9)
Pr2^{iv}—Pr1—Pr2^{iii}	110.343 (4)	Pr1^{xii}—Pr3—Pr2^{x}	97.821 (7)
Pr2^{iv}—Pr1—Pr3^{v}	109.131 (9)	Pr1^{xii}—Pr3—Pr2^{xiii}	99.441 (7)
Pr2^{iii}—Pr1—Pr3^{vi}	74.025 (6)	Pr1^{xvi}—Pr3—Pr2^{xvii}	102.639 (8)
Pr2^{i}—Pr1—Pr3^{v}	70.258 (6)	Pr1^{xvi}—Pr3—Pr3^{ii}	98.905 (6)
Pr2^{ii}—Pr1—Pr3^{v}	74.025 (6)	Pr1^{xii}—Pr3—Pr3^{ii}	56.190 (4)
Pr2^{ii}—Pr1—Pr3^{vi}	106.588 (8)	Pr2^{xiii}—Pr3—Pr2^{xvii}	60.464 (9)
Pr2^{i}—Pr1—Pr3^{vi}	109.131 (9)	Pr2^{xvii}—Pr3—Pr2^{x}	86.316 (6)
Pr2^{iv}—Pr1—Pr3^{vi}	70.258 (6)	Pr2^{xiii}—Pr3—Pr2^{x}	117.252 (7)
Pr2^{iii}—Pr1—Pr3^{v}	106.588 (8)	Pr2^{x}—Pr3—Pr3^{ii}	149.882 (8)
Pr3^{vi}—Pr1—Pr3^{v}	179.290 (14)	Pr2^{xvii}—Pr3—Pr3^{ii}	112.494 (8)
Si1—Pr1—Pr2^{iii}	122.55 (3)	Pr2^{xiii}—Pr3—Pr3^{ii}	60.158 (7)
Si1^{viii}—Pr1—Pr2^{i}	127.07 (3)	Si1^{xii}—Pr3—Pr1^{xvi}	89.84 (2)
Si1—Pr1—Pr2^{ii}	54.63 (3)	Si1^{xiv}—Pr3—Pr1^{xii}	54.18 (2)
Si1^{ix}—Pr1—Pr2^{iii}	128.63 (2)	Si1^{xiii}—Pr3—Pr1^{xvi}	55.14 (2)
Si1^{ix}—Pr1—Pr2^{iv}	54.47 (2)	Si1^{xii}—Pr3—Pr1^{xii}	51.84 (2)
Si1—Pr1—Pr2^{i}	55.75 (3)	Si1^{xiii}—Pr3—Pr1^{xii}	144.17 (3)
Si1^{vii}—Pr1—Pr2^{iv}	54.52 (2)	Si1^{xiv}—Pr3—Pr1^{xvi}	53.40 (2)
Si1^{viii}—Pr1—Pr2^{iii}	54.63 (3)	Si1^{xiii}—Pr3—Pr2^{xiii}	89.98 (2)
Si1^{ix}—Pr1—Pr2^{i}	54.52 (2)	Si1^{xiv}—Pr3—Pr2^{xiii}	108.89 (3)
Si1^{vii}—Pr1—Pr2^{iii}	124.06 (2)	Si1^{xii}—Pr3—Pr2^{xvii}	134.80 (2)
Si1^{vii}—Pr1—Pr2^{i}	54.47 (2)	Si1^{xiv}—Pr3—Pr2^{x}	129.63 (3)
Si1—Pr1—Pr2^{iv}	127.07 (3)	Si1^{xii}—Pr3—Pr2^{xiii}	131.45 (2)
Si1^{viii}—Pr1—Pr2^{ii}	122.55 (3)	Si1^{xiii}—Pr3—Pr2^{xvii}	50.33 (3)
Si1^{viii}—Pr1—Pr2^{iv}	55.75 (3)	Si1^{xii}—Pr3—Pr2^{x}	48.60 (2)
Si1^{ix}—Pr1—Pr2^{ii}	124.06 (2)	Si1^{xiii}—Pr3—Pr2^{x}	108.41 (2)
Si1^{vii}—Pr1—Pr2^{ii}	128.63 (2)	Si1^{xiv}—Pr3—Pr2^{xvii}	136.01 (3)
Si1—Pr1—Pr3^{vi}	124.12 (2)	Si1^{xiii}—Pr3—Pr3^{ii}	101.66 (2)
Si1^{viii}—Pr1—Pr3^{v}	124.12 (2)	Si1^{xii}—Pr3—Pr3^{ii}	108.02 (2)
Si1^{vii}—Pr1—Pr3^{v}	54.62 (2)	Si1^{xiv}—Pr3—Pr3^{ii}	50.43 (2)
Si1^{viii}—Pr1—Pr3^{vi}	55.90 (2)	Si1^{xiv}—Pr3—Si1^{xii}	85.949 (17)
Si1^{ix}—Pr1—Pr3^{v}	124.76 (3)	Si1^{xiii}—Pr3—Si1^{xii}	137.237 (18)
Si1^{ix}—Pr1—Pr3^{vi}	54.62 (2)	Si1^{xiii}—Pr3—Si1^{xiv}	90.036 (12)
Si1^{vii}—Pr1—Pr3^{vi}	124.76 (3)	Si1^{xiv}—Pr3—Si2^{xiii}	90.54 (3)
Si1—Pr1—Pr3^{v}	55.90 (2)	Si1^{xiii}—Pr3—Si2^{xiii}	45.35 (3)
Si1—Pr1—Si1^{vii}	91.45 (4)	Si1^{xiii}—Pr3—Si2^{xii}	92.74 (3)
Si1^{viii}—Pr1—Si1^{ix}	91.45 (4)	Si2^{xii}—Pr3—Pr1^{xii}	87.19 (2)
Si1—Pr1—Si1^{ix}	90.57 (2)	Si2—Pr3—Pr1^{xii}	54.53 (2)
Si1^{viii}—Pr1—Si1^{vii}	90.57 (2)	Si2—Pr3—Pr1^{xvi}	145.87 (2)
Si1—Pr1—Si1^{viii}	177.18 (5)	Si2^{xiii}—Pr3—Pr1^{xii}	123.76 (2)
Si1^{ix}—Pr1—Si1^{vii}	88.74 (5)	Si2^{xiii}—Pr3—Pr1^{xvi}	90.26 (2)
Si1^{vii}—Pr1—Si2^{ii}	178.20 (3)	Si2^{xii}—Pr3—Pr1^{xvi}	55.08 (2)
Si1^{ix}—Pr1—Si2^{ii}	92.22 (3)	Si2^{xiii}—Pr3—Pr2^{xvii}	49.43 (2)
Si1^{vii}—Pr1—Si2^{iii}	92.22 (3)	Si2^{xiii}—Pr3—Pr2^{xiii}	47.45 (2)
Si1—Pr1—Si2^{ii}	90.07 (3)	Si2^{xiii}—Pr3—Pr2^{x}	135.71 (2)
Si1^{ix}—Pr1—Si2^{iii}	178.20 (3)	Si2^{xii}—Pr3—Pr2^{xiii}	164.53 (2)

Si1—Pr1—Si2ⁱⁱⁱ	87.88 (3)	Si2—Pr3—Pr2^{xiii}	48.31 (2)
Si1^{viii}—Pr1—Si2ⁱⁱⁱ	90.07 (3)	Si2—Pr3—Pr2^{xvii}	103.99 (2)
Si1^{viii}—Pr1—Si2ⁱⁱ	87.88 (3)	Si2^{xii}—Pr3—Pr2^{xvii}	110.50 (2)
Si2ⁱⁱⁱ—Pr1—Pr2ⁱⁱ	54.20 (2)	Si2—Pr3—Pr2^x	103.11 (2)
Si2ⁱⁱⁱ—Pr1—Pr2^{iv}	127.29 (2)	Si2^{xii}—Pr3—Pr2^x	47.59 (2)
Si2ⁱⁱ—Pr1—Pr2ⁱⁱ	51.80 (2)	Si2^{xiii}—Pr3—Pr3ⁱⁱ	67.57 (2)
Si2ⁱⁱⁱ—Pr1—Pr2ⁱ	125.04 (2)	Si2—Pr3—Pr3ⁱⁱ	50.90 (2)
Si2ⁱⁱ—Pr1—Pr2^{iv}	125.04 (2)	Si2^{xii}—Pr3—Pr3ⁱⁱ	133.74 (2)
Si2ⁱⁱ—Pr1—Pr2ⁱⁱⁱ	54.20 (2)	Si2^{xii}—Pr3—Si1^{xiv}	86.34 (3)
Si2ⁱⁱⁱ—Pr1—Pr2ⁱⁱⁱ	51.80 (2)	Si2—Pr3—Si1^{xii}	86.35 (3)
Si2ⁱⁱ—Pr1—Pr2ⁱ	127.29 (2)	Si2^{xiii}—Pr3—Si1^{xii}	175.55 (3)
Si2ⁱⁱⁱ—Pr1—Pr3^{vi}	125.73 (2)	Si2^{xii}—Pr3—Si1^{xii}	44.54 (3)
Si2ⁱⁱ—Pr1—Pr3^{vi}	54.90 (2)	Si2—Pr3—Si1^{xiv}	92.48 (3)
Si2ⁱⁱ—Pr1—Pr3^v	125.73 (2)	Si2—Pr3—Si1^{xiii}	136.40 (3)
Si2ⁱⁱⁱ—Pr1—Pr3^v	54.90 (2)	Si2—Pr3—Si2^{xiii}	91.079 (17)
Si2ⁱⁱⁱ—Pr1—Si2ⁱⁱ	86.85 (5)	Si2^{xii}—Pr3—Si2^{xiii}	138.014 (18)
Pr1^{xv}—Pr2—Pr1^{xii}	103.710 (6)	Si2—Pr3—Si2^{xii}	130.86 (2)
Pr1^{xii}—Pr2—Pr2ⁱ	55.940 (5)	Pr1—Si1—Pr1^{xvii}	123.37 (4)
Pr1^{xv}—Pr2—Pr2ⁱ	140.135 (10)	Pr1—Si1—Pr2ⁱ	68.56 (3)
Pr1^{xv}—Pr2—Pr3^{vii}	102.847 (8)	Pr1—Si1—Pr3ⁱⁱ	70.13 (2)
Pr1^{xv}—Pr2—Pr3^x	106.888 (8)	Pr1^{xvii}—Si1—Pr3ⁱⁱ	134.03 (4)
Pr1^{xii}—Pr2—Pr3^{xi}	106.191 (8)	Pr1^{xvii}—Si1—Pr3^v	71.14 (3)
Pr1^{xii}—Pr2—Pr3^{vii}	105.646 (8)	Pr1—Si1—Pr3^v	70.70 (3)
Pr1^{xii}—Pr2—Pr3^x	117.969 (7)	Pr1—Si1—Pr3^{xi}	136.94 (4)
Pr1^{xv}—Pr2—Pr3^{xi}	149.920 (8)	Pr2^{xiii}—Si1—Pr1^{xvii}	68.02 (3)
Pr2ⁱ—Pr2—Pr3^x	112.953 (9)	Pr2ⁱⁱ—Si1—Pr1	69.90 (3)
Pr3^{vii}—Pr2—Pr2ⁱ	59.445 (6)	Pr2^{xiii}—Si1—Pr1	139.92 (4)
Pr3^{xi}—Pr2—Pr2ⁱ	60.092 (6)	Pr2ⁱⁱ—Si1—Pr1^{xvii}	67.99 (3)
Pr3^{xi}—Pr2—Pr3^x	61.068 (5)	Pr2ⁱ—Si1—Pr1^{xvii}	141.38 (4)
Pr3^{xi}—Pr2—Pr3^{vii}	65.880 (8)	Pr2^{xiii}—Si1—Pr2ⁱ	129.66 (4)
Pr3^{vii}—Pr2—Pr3^x	117.851 (7)	Pr2ⁱⁱ—Si1—Pr2ⁱ	138.39 (4)
Si1^{xi}—Pr2—Pr1^{xv}	57.51 (2)	Pr2^{xiii}—Si1—Pr2ⁱⁱ	83.22 (3)
Si1ⁱ—Pr2—Pr1^{xii}	96.00 (2)	Pr2^{xiii}—Si1—Pr3^{xi}	82.63 (3)
Si1^{xii}—Pr2—Pr1^{xii}	55.47 (2)	Pr2^{xiii}—Si1—Pr3ⁱⁱ	76.47 (3)
Si1^{xii}—Pr2—Pr1^{xv}	57.49 (2)	Pr2ⁱⁱ—Si1—Pr3^{xi}	138.21 (4)
Si1ⁱ—Pr2—Pr1^{xv}	55.69 (2)	Pr2ⁱⁱ—Si1—Pr3^v	87.20 (3)
Si1^{xi}—Pr2—Pr1^{xii}	147.18 (3)	Pr2ⁱⁱ—Si1—Pr3ⁱⁱ	79.97 (3)
Si1^{xii}—Pr2—Pr2ⁱ	111.25 (2)	Pr2ⁱ—Si1—Pr3^{xi}	78.10 (3)
Si1^{xi}—Pr2—Pr2ⁱ	155.46 (3)	Pr2ⁱ—Si1—Pr3ⁱⁱ	84.10 (3)
Si1ⁱ—Pr2—Pr2ⁱ	90.03 (3)	Pr2ⁱ—Si1—Pr3^v	81.41 (3)
Si1^{xi}—Pr2—Pr3^{vii}	104.88 (3)	Pr2^{xiii}—Si1—Pr3^v	138.72 (4)
Si1^{xi}—Pr2—Pr3^x	54.93 (2)	Pr3^{xi}—Si1—Pr1^{xvii}	70.24 (3)
Si1ⁱ—Pr2—Pr3^x	145.54 (2)	Pr3^{xi}—Si1—Pr3^v	78.24 (3)
Si1ⁱ—Pr2—Pr3^{vii}	51.57 (2)	Pr3^{xi}—Si1—Pr3ⁱⁱ	133.50 (4)
Si1^{xi}—Pr2—Pr3^{xi}	97.03 (3)	Pr3^v—Si1—Pr3ⁱⁱ	140.82 (4)
Si1^{xii}—Pr2—Pr3^x	101.67 (2)	Si2—Si1—Pr1	116.82 (5)
Si1^{xii}—Pr2—Pr3^{xi}	147.77 (2)	Si2—Si1—Pr1^{xvii}	119.66 (5)
Si1ⁱ—Pr2—Pr3^{xi}	117.17 (2)	Si2—Si1—Pr2^{xiii}	63.92 (4)

Si1ˣⁱⁱ—Pr2—Pr3�vⁱⁱ	140.10 (2)	Si2—Si1—Pr2ⁱⁱ	135.25 (5)
Si1ˣⁱⁱ—Pr2—Si1ⁱ	92.601 (18)	Si2—Si1—Pr2ⁱ	65.79 (4)
Si1ˣⁱ—Pr2—Si1ⁱ	93.56 (3)	Si2—Si1—Pr3ᵛ	137.54 (6)
Si1ˣⁱ—Pr2—Si1ˣⁱⁱ	92.85 (4)	Si2—Si1—Pr3ⁱⁱ	64.03 (4)
Si1ˣⁱ—Pr2—Si2ⁱ	140.79 (3)	Si2—Si1—Pr3ˣⁱ	69.49 (4)
Si1ˣⁱⁱ—Pr2—Si2ⁱ	90.38 (3)	Pr1ˣⁱⁱ—Si2—Pr3ˣⁱ	135.69 (4)
Si2ⁱ—Pr2—Pr1ˣᵛ	92.68 (2)	Pr2—Si2—Pr1ˣⁱⁱ	70.30 (3)
Si2—Pr2—Pr1ˣⁱⁱ	57.90 (2)	Pr2ˣⁱⁱⁱ—Si2—Pr1ˣⁱⁱ	141.97 (4)
Si2ˣⁱ—Pr2—Pr1ˣⁱⁱ	158.04 (2)	Pr2ⁱ—Si2—Pr1ˣⁱⁱ	68.78 (3)
Si2ⁱ—Pr2—Pr1ˣⁱⁱ	57.02 (2)	Pr2—Si2—Pr2ˣⁱⁱⁱ	132.15 (4)
Si2—Pr2—Pr1ˣᵛ	152.08 (2)	Pr2—Si2—Pr2ⁱ	82.12 (3)
Si2ˣⁱ—Pr2—Pr1ˣᵛ	98.16 (2)	Pr2ˣⁱⁱⁱ—Si2—Pr2ⁱ	134.64 (4)
Si2ˣⁱ—Pr2—Pr2ⁱ	107.11 (2)	Pr2ˣⁱⁱⁱ—Si2—Pr3ⁱⁱ	80.47 (3)
Si2—Pr2—Pr2ⁱ	50.30 (2)	Pr2ˣⁱⁱⁱ—Si2—Pr3ˣⁱ	82.34 (3)
Si2ⁱ—Pr2—Pr2ⁱ	47.57 (2)	Pr2—Si2—Pr3ⁱⁱ	140.09 (4)
Si2ⁱ—Pr2—Pr3ᵛⁱⁱ	53.61 (2)	Pr2ⁱ—Si2—Pr3ⁱⁱ	87.54 (3)
Si2ˣⁱ—Pr2—Pr3ˣ	51.94 (2)	Pr2—Si2—Pr3ˣⁱ	78.08 (3)
Si2ˣⁱ—Pr2—Pr3ˣⁱ	52.15 (2)	Pr2ⁱ—Si2—Pr3ˣⁱ	76.97 (3)
Si2ˣⁱ—Pr2—Pr3ᵛⁱⁱ	70.89 (2)	Pr2ˣⁱⁱⁱ—Si2—Pr3	79.53 (3)
Si2ⁱ—Pr2—Pr3ˣⁱ	100.75 (2)	Pr2—Si2—Pr3	85.15 (3)
Si2—Pr2—Pr3ˣⁱ	54.47 (2)	Pr2ⁱ—Si2—Pr3	140.56 (4)
Si2ⁱ—Pr2—Pr3ˣ	160.33 (3)	Pr3—Si2—Pr1ˣⁱⁱ	71.78 (3)
Si2—Pr2—Pr3ˣ	70.64 (3)	Pr3ⁱⁱ—Si2—Pr1ˣⁱⁱ	70.02 (3)
Si2—Pr2—Pr3ᵛⁱⁱ	102.52 (2)	Pr3—Si2—Pr3ˣⁱ	136.07 (4)
Si2—Pr2—Si1ˣⁱⁱ	95.16 (3)	Pr3—Si2—Pr3ⁱⁱ	78.78 (3)
Si2—Pr2—Si1ⁱ	139.57 (4)	Pr3ⁱⁱ—Si2—Pr3ˣⁱ	136.58 (4)
Si2ⁱ—Pr2—Si1ⁱ	47.24 (3)	Si1—Si2—Pr1ˣⁱⁱ	121.26 (5)
Si2ˣⁱ—Pr2—Si1ˣⁱⁱ	140.11 (3)	Si1—Si2—Pr2ⁱ	66.96 (4)
Si2ˣⁱ—Pr2—Si1ⁱ	97.97 (3)	Si1—Si2—Pr2ˣⁱⁱⁱ	67.74 (4)
Si2ˣⁱ—Pr2—Si1ˣⁱ	48.35 (3)	Si1—Si2—Pr2	135.86 (5)
Si2—Pr2—Si1ˣⁱ	125.48 (3)	Si1—Si2—Pr3ⁱⁱ	71.43 (4)
Si2ˣⁱ—Pr2—Si2ˣⁱ	100.995 (18)	Si1—Si2—Pr3	138.49 (5)
Si2—Pr2—Si2ⁱ	93.03 (4)	Si1—Si2—Pr3ˣⁱ	65.16 (4)

Symmetry codes: (i) −*y*+1, −*x*+1, −*z*+1/2; (ii) −*y*+3/2, *x*+1/2, *z*+1/4; (iii) *x*+1/2, −*y*+3/2, −*z*+3/4; (iv) −*x*+1, −*y*+1, *z*+1/2; (v) −*y*+2, −*x*+1, −*z*+1/2; (vi) −*x*+1, −*y*+2, *z*+1/2; (vii) −*y*+3/2, *x*−1/2, *z*+1/4; (viii) *y*, *x*, −*z*+1; (ix) *x*−1/2, −*y*+3/2, −*z*+3/4; (x) *y*, *x*, −*z*; (xi) −*x*+3/2, *y*−1/2, −*z*+1/4; (xii) *y*−1/2, −*x*+3/2, *z*−1/4; (xiii) −*x*+3/2, *y*+1/2, −*z*+1/4; (xiv) −*y*+1, −*x*+2, −*z*+1/2; (xv) −*x*+1, −*y*+1, *z*−1/2; (xvi) −*x*+1, −*y*+2, *z*−1/2; (xvii) *y*+1/2, −*x*+3/2, *z*−1/4.

Pentaneodymium tetrasiliside (B)

Crystal data

Nd₅Si₄	D_x = 6.045 Mg m⁻³
M_r = 833.56	Mo *Kα* radiation, λ = 0.71073 Å
Tetragonal, *P*4₁2₁2	Cell parameters from 3985 reflections
Hall symbol: P 4abw 2nw	θ = 3.8–30.4°
a = 7.8644 (2) Å	µ = 28.27 mm⁻¹
c = 14.8085 (5) Å	*T* = 223 K
V = 915.89 (6) Å³	Plate, metallic gray
Z = 4	0.12 × 0.09 × 0.07 mm
F(000) = 1424	

Data collection

XtaLAB AFC12 (RINC): Kappa dual offset/far diffractometer	$T_{min} = 0.561$, $T_{max} = 0.702$
Radiation source: micro-focus sealed X-ray tube	6054 measured reflections
Mirror monochromator	1238 independent reflections
Detector resolution: 5.8140 pixels mm^{-1}	1203 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.032$
Absorption correction: analytical [CrysAlisPro (Rigaku OD, 2019) based on Clark & Reid (1995)]	$\theta_{max} = 30.2°$, $\theta_{min} = 3.7°$
	$h = -11 \rightarrow 10$
	$k = -10 \rightarrow 10$
	$l = -20 \rightarrow 19$

Refinement

Refinement on F^2	$(\Delta/\sigma)_{max} = 0.001$
Least-squares matrix: full	$\Delta\rho_{max} = 1.10$ e Å^{-3}
$R[F^2 > 2\sigma(F^2)] = 0.015$	$\Delta\rho_{min} = -0.71$ e Å^{-3}
$wR(F^2) = 0.028$	Extinction correction: SHELXL (Sheldrick, 2015b), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
$S = 1.09$	
1238 reflections	Extinction coefficient: 0.00090 (6)
43 parameters	Absolute structure: Flack x determined using 422 quotients [(I^+)-(I^-)]/[(I^+)+(I^-)] (Parsons *et al.*, 2013)
0 restraints	
Primary atom site location: dual	
$w = 1/[\sigma^2(F_o^2) + 0.4858P]$ where $P = (F_o^2 + 2F_c^2)/3$	Absolute structure parameter: −0.01 (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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Nd1	0.81184 (4)	0.81184 (4)	0.500000	0.00637 (9)
Nd2	0.51490 (3)	0.36933 (4)	0.12498 (2)	0.00518 (7)
Nd3	0.51034 (4)	0.87021 (4)	0.04676 (2)	0.00649 (7)
Si1	0.9274 (2)	0.7098 (2)	0.30921 (10)	0.0060 (3)
Si2	0.7003 (2)	0.6636 (2)	0.19543 (10)	0.0078 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Nd1	0.00630 (11)	0.00630 (11)	0.00652 (17)	−0.00026 (13)	0.00064 (11)	−0.00064 (11)
Nd2	0.00538 (14)	0.00534 (14)	0.00483 (12)	0.00002 (12)	0.00035 (11)	−0.00097 (10)
Nd3	0.00617 (15)	0.00631 (14)	0.00700 (13)	−0.00027 (9)	−0.00098 (11)	0.00152 (11)
Si1	0.0060 (7)	0.0066 (7)	0.0054 (6)	−0.0007 (5)	0.0001 (5)	0.0001 (6)
Si2	0.0069 (7)	0.0073 (7)	0.0093 (6)	−0.0016 (5)	−0.0015 (6)	0.0017 (6)

Geometric parameters (Å, º)

Nd1—Nd2^i	3.4725 (5)	Nd2—Nd3^{vii}	3.9061 (4)
Nd1—Nd2^{ii}	3.5021 (5)	Nd2—Si1^x	3.0366 (16)

Nd1—Nd2ⁱⁱⁱ	3.5021 (5)	Nd2—Si1ⁱ	3.0848 (17)
Nd1—Nd2^{iv}	3.4725 (5)	Nd2—Si1^{xii}	3.0436 (17)
Nd1—Nd3^v	3.6265 (3)	Nd2—Si2	2.9272 (17)
Nd1—Nd3^{vi}	3.6265 (3)	Nd2—Si2^x	2.9533 (17)
Nd1—Si1^{vii}	3.1528 (16)	Nd2—Si2ⁱ	3.0565 (15)
Nd1—Si1^{viii}	3.0744 (15)	Nd3—Nd3^{xii}	3.9752 (2)
Nd1—Si1	3.0744 (15)	Nd3—Si1^{xiii}	3.1359 (15)
Nd1—Si1^{ix}	3.1528 (16)	Nd3—Si1^{xii}	3.3315 (14)
Nd1—Si2ⁱⁱ	3.1661 (16)	Nd3—Si1^{xiv}	3.1748 (15)
Nd1—Si2ⁱⁱⁱ	3.1661 (16)	Nd3—Si2^{xiii}	3.2425 (15)
Nd2—Nd2ⁱ	3.9202 (7)	Nd3—Si2^{xii}	3.1619 (16)
Nd2—Nd3^x	3.9094 (4)	Nd3—Si2	3.1177 (14)
Nd2—Nd3^{xi}	3.9378 (4)	Si1—Si2	2.482 (2)
Nd2ⁱ—Nd1—Nd2^{iv}	71.144 (14)	Si2^x—Nd2—Si2ⁱ	123.86 (5)
Nd2ⁱⁱⁱ—Nd1—Nd2ⁱⁱ	68.070 (13)	Nd1^{xvi}—Nd3—Nd1^{xii}	97.355 (7)
Nd2^{iv}—Nd1—Nd2ⁱⁱ	177.032 (7)	Nd1^{xvi}—Nd3—Nd2^{xi}	99.740 (9)
Nd2ⁱ—Nd1—Nd2ⁱⁱⁱ	177.032 (7)	Nd1^{xii}—Nd3—Nd2^{xiii}	99.322 (9)
Nd2ⁱ—Nd1—Nd2ⁱⁱ	110.453 (5)	Nd1^{xvi}—Nd3—Nd2^{xvii}	102.777 (9)
Nd2^{iv}—Nd1—Nd2ⁱⁱⁱ	110.453 (5)	Nd1^{xii}—Nd3—Nd2^{xi}	97.621 (8)
Nd2^{iv}—Nd1—Nd3^v	70.374 (8)	Nd1^{xii}—Nd3—Nd2^{xvii}	158.298 (11)
Nd2ⁱⁱⁱ—Nd1—Nd3^{vi}	106.665 (10)	Nd1^{xvi}—Nd3—Nd2^{xiii}	136.478 (12)
Nd2ⁱ—Nd1—Nd3^v	108.985 (11)	Nd1^{xvi}—Nd3—Nd3^{xii}	57.694 (6)
Nd2ⁱⁱ—Nd1—Nd3^v	106.665 (10)	Nd1^{xii}—Nd3—Nd3^{xii}	137.385 (10)
Nd2ⁱⁱ—Nd1—Nd3^{vi}	73.978 (8)	Nd2^{xvii}—Nd3—Nd2^{xiii}	60.212 (10)
Nd2ⁱ—Nd1—Nd3^{vi}	70.374 (8)	Nd2^{xiii}—Nd3—Nd2^{xi}	117.333 (8)
Nd2^{iv}—Nd1—Nd3^{vi}	108.985 (11)	Nd2^{xvii}—Nd3—Nd2^{xi}	86.968 (8)
Nd2ⁱⁱⁱ—Nd1—Nd3^v	73.978 (8)	Nd2^{xi}—Nd3—Nd3^{xii}	59.212 (7)
Nd3^{vi}—Nd1—Nd3^v	179.256 (17)	Nd2^{xiii}—Nd3—Nd3^{xii}	122.770 (9)
Si1—Nd1—Nd2ⁱⁱⁱ	122.55 (4)	Nd2^{xvii}—Nd3—Nd3^{xii}	62.562 (7)
Si1^{viii}—Nd1—Nd2ⁱ	126.97 (4)	Si1^{xii}—Nd3—Nd1^{xvi}	89.95 (3)
Si1—Nd1—Nd2ⁱⁱ	54.67 (3)	Si1^{xiv}—Nd3—Nd1^{xii}	54.16 (3)
Si1^{ix}—Nd1—Nd2ⁱⁱⁱ	128.53 (3)	Si1^{xiii}—Nd3—Nd1^{xvi}	55.00 (3)
Si1^{ix}—Nd1—Nd2^{iv}	54.30 (3)	Si1^{xii}—Nd3—Nd1^{xii}	51.72 (3)
Si1—Nd1—Nd2ⁱ	55.82 (3)	Si1^{xiii}—Nd3—Nd1^{xii}	143.78 (3)
Si1^{vii}—Nd1—Nd2^{iv}	54.44 (3)	Si1^{xiv}—Nd3—Nd1^{xvi}	53.25 (3)
Si1^{viii}—Nd1—Nd2ⁱⁱⁱ	54.67 (3)	Si1^{xiii}—Nd3—Nd2^{xvii}	50.52 (3)
Si1^{ix}—Nd1—Nd2ⁱ	54.44 (3)	Si1^{xiv}—Nd3—Nd2^{xvii}	135.69 (3)
Si1^{vii}—Nd1—Nd2ⁱⁱⁱ	124.35 (3)	Si1^{xii}—Nd3—Nd2^{xiii}	131.30 (3)
Si1^{vii}—Nd1—Nd2ⁱ	54.30 (3)	Si1^{xiv}—Nd3—Nd2^{xi}	129.50 (3)
Si1—Nd1—Nd2^{iv}	126.97 (4)	Si1^{xii}—Nd3—Nd2^{xvii}	135.35 (3)
Si1^{viii}—Nd1—Nd2ⁱⁱ	122.55 (4)	Si1^{xiii}—Nd3—Nd2^{xiii}	90.04 (3)
Si1^{viii}—Nd1—Nd2^{iv}	55.82 (3)	Si1^{xii}—Nd3—Nd2^{xi}	48.50 (3)
Si1^{ix}—Nd1—Nd2ⁱⁱ	124.35 (3)	Si1^{xiii}—Nd3—Nd2^{xi}	108.97 (3)
Si1^{vii}—Nd1—Nd2ⁱⁱ	128.53 (3)	Si1^{xiv}—Nd3—Nd2^{xiii}	108.81 (3)
Si1—Nd1—Nd3^{vi}	55.83 (3)	Si1^{xiii}—Nd3—Nd3^{xii}	51.39 (3)
Si1^{viii}—Nd1—Nd3^v	55.83 (3)	Si1^{xii}—Nd3—Nd3^{xii}	91.19 (3)
Si1^{vii}—Nd1—Nd3^v	124.78 (3)	Si1^{xiv}—Nd3—Nd3^{xii}	110.85 (3)

Si1^{viii}—Nd1—Nd3^{vi}	124.19 (3)	Si1^{xiv}—Nd3—Si1^{xii}	85.88 (2)
Si1^{ix}—Nd1—Nd3^{v}	54.57 (3)	Si1^{xiii}—Nd3—Si1^{xii}	137.46 (2)
Si1^{ix}—Nd1—Nd3^{vi}	124.78 (3)	Si1^{xiii}—Nd3—Si1^{xiv}	89.678 (15)
Si1^{vii}—Nd1—Nd3^{vi}	54.57 (3)	Si1^{xiv}—Nd3—Si2^{xiii}	90.11 (4)
Si1—Nd1—Nd3^{v}	124.19 (3)	Si1^{xiii}—Nd3—Si2^{xiii}	45.76 (4)
Si1—Nd1—Si1^{vii}	91.21 (4)	Si1^{xiii}—Nd3—Si2^{xii}	92.67 (4)
Si1^{viii}—Nd1—Si1^{ix}	91.21 (4)	Si2^{xii}—Nd3—Nd1^{xii}	87.36 (3)
Si1—Nd1—Si1^{ix}	90.79 (3)	Si2—Nd3—Nd1^{xii}	54.76 (3)
Si1^{viii}—Nd1—Si1^{vii}	90.79 (3)	Si2—Nd3—Nd1^{xvi}	146.00 (3)
Si1—Nd1—Si1^{viii}	177.21 (7)	Si2^{xiii}—Nd3—Nd1^{xii}	123.04 (3)
Si1^{ix}—Nd1—Si1^{vii}	88.51 (6)	Si2^{xiii}—Nd3—Nd1^{xvi}	90.38 (3)
Si1^{vii}—Nd1—Si2^{ii}	178.58 (4)	Si2^{xii}—Nd3—Nd1^{xvi}	55.09 (3)
Si1^{ix}—Nd1—Si2^{ii}	92.27 (4)	Si2^{xiii}—Nd3—Nd2^{xiii}	47.19 (3)
Si1^{vii}—Nd1—Si2^{iii}	92.27 (4)	Si2^{xiii}—Nd3—Nd2^{xvii}	49.57 (3)
Si1—Nd1—Si2^{ii}	89.96 (4)	Si2^{xiii}—Nd3—Nd2^{xi}	136.52 (3)
Si1^{ix}—Nd1—Si2^{iii}	178.58 (4)	Si2^{xii}—Nd3—Nd2^{xvii}	110.79 (3)
Si1—Nd1—Si2^{iii}	88.01 (4)	Si2—Nd3—Nd2^{xvii}	103.54 (3)
Si1^{viii}—Nd1—Si2^{iii}	89.96 (4)	Si2—Nd3—Nd2^{xiii}	48.09 (3)
Si1^{viii}—Nd1—Si2^{ii}	88.01 (4)	Si2^{xii}—Nd3—Nd2^{xiii}	164.61 (3)
Si2^{iii}—Nd1—Nd2^{ii}	54.28 (3)	Si2—Nd3—Nd2^{xi}	102.77 (3)
Si2^{iii}—Nd1—Nd2^{iv}	127.09 (3)	Si2^{xii}—Nd3—Nd2^{xi}	47.63 (3)
Si2^{ii}—Nd1—Nd2^{ii}	51.78 (3)	Si2^{xiii}—Nd3—Nd3^{xii}	93.42 (3)
Si2^{iii}—Nd1—Nd2^{i}	125.25 (3)	Si2—Nd3—Nd3^{xii}	156.02 (3)
Si2^{ii}—Nd1—Nd2^{iv}	125.25 (3)	Si2^{xii}—Nd3—Nd3^{xii}	50.23 (3)
Si2^{ii}—Nd1—Nd2^{iii}	54.28 (3)	Si2^{xii}—Nd3—Si1^{xiv}	86.36 (4)
Si2^{iii}—Nd1—Nd2^{iii}	51.78 (3)	Si2—Nd3—Si1^{xii}	86.26 (4)
Si2^{ii}—Nd1—Nd2^{i}	127.09 (3)	Si2^{xiii}—Nd3—Si1^{xii}	174.74 (4)
Si2^{iii}—Nd1—Nd3^{vi}	54.98 (3)	Si2^{xii}—Nd3—Si1^{xii}	44.85 (4)
Si2^{ii}—Nd1—Nd3^{vi}	125.68 (3)	Si2—Nd3—Si1^{xiv}	92.77 (4)
Si2^{ii}—Nd1—Nd3^{v}	54.98 (3)	Si2—Nd3—Si1^{xiii}	136.26 (4)
Si2^{iii}—Nd1—Nd3^{v}	125.68 (3)	Si2—Nd3—Si2^{xiii}	90.54 (2)
Si2^{iii}—Nd1—Si2^{ii}	86.97 (6)	Si2^{xii}—Nd3—Si2^{xiii}	138.34 (2)
Nd1^{xv}—Nd2—Nd1^{xii}	103.774 (8)	Si2—Nd3—Si2^{xii}	131.07 (3)
Nd1^{xii}—Nd2—Nd2^{i}	55.965 (6)	Nd1—Si1—Nd1^{xvii}	123.58 (5)
Nd1^{xv}—Nd2—Nd2^{i}	140.405 (13)	Nd1—Si1—Nd2^{i}	68.64 (3)
Nd1^{xv}—Nd2—Nd3^{x}	149.935 (9)	Nd1—Si1—Nd3^{ii}	70.00 (3)
Nd1^{xv}—Nd2—Nd3^{xi}	107.244 (10)	Nd1^{xvii}—Si1—Nd3^{ii}	134.15 (5)
Nd1^{xii}—Nd2—Nd3^{vii}	106.182 (10)	Nd1^{xvii}—Si1—Nd3^{vi}	71.13 (3)
Nd1^{xii}—Nd2—Nd3^{x}	106.111 (9)	Nd1—Si1—Nd3^{vi}	70.93 (3)
Nd1^{xii}—Nd2—Nd3^{xi}	117.604 (9)	Nd1—Si1—Nd3^{x}	136.75 (6)
Nd1^{xv}—Nd2—Nd3^{vii}	102.810 (9)	Nd2^{xiii}—Si1—Nd1^{xvii}	68.23 (3)
Nd2^{i}—Nd2—Nd3^{xi}	112.321 (11)	Nd2^{ii}—Si1—Nd1	69.84 (3)
Nd3^{x}—Nd2—Nd2^{i}	59.853 (7)	Nd2^{xiii}—Si1—Nd1	139.62 (5)
Nd3^{vii}—Nd2—Nd2^{i}	59.937 (8)	Nd2^{ii}—Si1—Nd1^{xvii}	68.14 (4)
Nd3^{vii}—Nd2—Nd3^{xi}	117.388 (8)	Nd2^{i}—Si1—Nd1^{xvii}	141.48 (5)
Nd3^{vii}—Nd2—Nd3^{x}	65.627 (10)	Nd2^{xiii}—Si1—Nd2^{i}	129.31 (5)
Nd3^{x}—Nd2—Nd3^{xi}	60.872 (7)	Nd2^{ii}—Si1—Nd2^{i}	138.41 (5)
Si1^{x}—Nd2—Nd1^{xv}	57.47 (3)	Nd2^{xiii}—Si1—Nd2^{ii}	83.28 (4)

Si1[i]—Nd2—Nd1[xii]	96.51 (3)	Nd2[xiii]—Si1—Nd3[x]	83.05 (4)
Si1[xii]—Nd2—Nd1[xii]	55.49 (3)	Nd2[xiii]—Si1—Nd3[ii]	76.24 (3)
Si1[xii]—Nd2—Nd1[xv]	57.42 (3)	Nd2[ii]—Si1—Nd3[x]	138.55 (5)
Si1[i]—Nd2—Nd1[xv]	55.54 (3)	Nd2[ii]—Si1—Nd3[vi]	87.22 (4)
Si1[x]—Nd2—Nd1[xii]	147.02 (3)	Nd2[ii]—Si1—Nd3[ii]	80.06 (4)
Si1[xii]—Nd2—Nd2[i]	111.31 (3)	Nd2[i]—Si1—Nd3[x]	77.79 (4)
Si1[x]—Nd2—Nd2[i]	155.46 (3)	Nd2[i]—Si1—Nd3[ii]	83.83 (4)
Si1[i]—Nd2—Nd2[i]	90.59 (3)	Nd2[i]—Si1—Nd3[vi]	81.65 (4)
Si1[x]—Nd2—Nd3[x]	97.14 (3)	Nd2[xiii]—Si1—Nd3[vi]	138.92 (5)
Si1[x]—Nd2—Nd3[xi]	55.26 (3)	Nd3[x]—Si1—Nd1[xvii]	70.43 (3)
Si1[i]—Nd2—Nd3[xi]	145.44 (3)	Nd3[x]—Si1—Nd3[vi]	78.09 (3)
Si1[i]—Nd2—Nd3[x]	117.05 (3)	Nd3[x]—Si1—Nd3[ii]	133.33 (5)
Si1[x]—Nd2—Nd3[vii]	104.58 (3)	Nd3[vi]—Si1—Nd3[ii]	140.92 (5)
Si1[xii]—Nd2—Nd3[xi]	101.82 (3)	Si2—Si1—Nd1	116.71 (6)
Si1[xii]—Nd2—Nd3[vii]	140.39 (3)	Si2—Si1—Nd1[xvii]	119.56 (6)
Si1[i]—Nd2—Nd3[vii]	51.69 (3)	Si2—Si1—Nd2[xiii]	63.78 (5)
Si1[xii]—Nd2—Nd3[x]	147.88 (3)	Si2—Si1—Nd2[ii]	135.29 (6)
Si1[xii]—Nd2—Si1[i]	92.69 (2)	Si2—Si1—Nd2[i]	65.57 (5)
Si1[x]—Nd2—Si1[i]	93.26 (4)	Si2—Si1—Nd3[vi]	137.48 (7)
Si1[x]—Nd2—Si1[xii]	92.72 (5)	Si2—Si1—Nd3[ii]	63.95 (4)
Si1[x]—Nd2—Si2[i]	140.91 (4)	Si2—Si1—Nd3[x]	69.39 (5)
Si1[xii]—Nd2—Si2[i]	90.60 (4)	Nd1[xii]—Si2—Nd3[x]	135.36 (6)
Si2[i]—Nd2—Nd1[xv]	92.89 (3)	Nd2—Si2—Nd1[xii]	70.04 (4)
Si2—Nd2—Nd1[xii]	58.18 (3)	Nd2[xiii]—Si2—Nd1[xii]	142.04 (5)
Si2[x]—Nd2—Nd1[xii]	157.63 (3)	Nd2[i]—Si2—Nd1[xii]	68.47 (3)
Si2[i]—Nd2—Nd1[xii]	57.24 (3)	Nd2—Si2—Nd2[xiii]	133.24 (5)
Si2—Nd2—Nd1[xv]	151.99 (3)	Nd2—Si2—Nd2[i]	81.83 (4)
Si2[x]—Nd2—Nd1[xv]	98.52 (3)	Nd2[xiii]—Si2—Nd2[i]	134.00 (5)
Si2[x]—Nd2—Nd2[i]	106.53 (3)	Nd2[xiii]—Si2—Nd3[ii]	80.09 (4)
Si2—Nd2—Nd2[i]	50.51 (3)	Nd2[xiii]—Si2—Nd3[x]	82.54 (4)
Si2[i]—Nd2—Nd2[i]	47.66 (3)	Nd2—Si2—Nd3[ii]	139.78 (6)
Si2[i]—Nd2—Nd3[x]	100.42 (3)	Nd2[i]—Si2—Nd3[ii]	87.23 (4)
Si2[x]—Nd2—Nd3[xi]	52.28 (3)	Nd2—Si2—Nd3[x]	78.46 (4)
Si2[x]—Nd2—Nd3[vii]	70.03 (3)	Nd2[i]—Si2—Nd3[x]	76.59 (3)
Si2[x]—Nd2—Nd3[x]	51.78 (3)	Nd2[xiii]—Si2—Nd3	80.12 (4)
Si2[i]—Nd2—Nd3[vii]	53.85 (3)	Nd2—Si2—Nd3	85.51 (4)
Si2—Nd2—Nd3[vii]	102.94 (3)	Nd2[i]—Si2—Nd3	140.17 (6)
Si2[i]—Nd2—Nd3[xi]	159.76 (3)	Nd3—Si2—Nd1[xii]	71.70 (3)
Si2—Nd2—Nd3[xi]	69.76 (3)	Nd3[ii]—Si2—Nd1[xii]	69.93 (3)
Si2—Nd2—Nd3[x]	54.35 (3)	Nd3—Si2—Nd3[x]	137.09 (5)
Si2—Nd2—Si1[xii]	95.25 (4)	Nd3—Si2—Nd3[ii]	78.55 (4)
Si2—Nd2—Si1[i]	140.41 (4)	Nd3[ii]—Si2—Nd3[x]	136.04 (5)
Si2[i]—Nd2—Si1[i]	47.67 (4)	Si1—Si2—Nd1[xii]	120.80 (6)
Si2[x]—Nd2—Si1[xii]	140.61 (4)	Si1—Si2—Nd2[i]	66.76 (5)
Si2[x]—Nd2—Si1[i]	97.55 (4)	Si1—Si2—Nd2[xiii]	67.28 (5)
Si2[x]—Nd2—Si1[x]	48.93 (4)	Si1—Si2—Nd2	135.73 (6)
Si2—Nd2—Si1[x]	124.91 (4)	Si1—Si2—Nd3[ii]	71.20 (5)

Si2—Nd2—Si2^x	100.44 (2)	Si1—Si2—Nd3	138.40 (7)
Si2—Nd2—Si2^i	93.45 (5)	Si1—Si2—Nd3^x	64.85 (5)

Symmetry codes: (i) −y+1, −x+1, −z+1/2; (ii) −y+3/2, x+1/2, z+1/4; (iii) x+1/2, −y+3/2, −z+3/4; (iv) −x+1, −y+1, z+1/2; (v) −x+1, −y+2, z+1/2; (vi) −y+2, −x+1, −z+1/2; (vii) −y+3/2, x−1/2, z+1/4; (viii) y, x, −z+1; (ix) x−1/2, −y+3/2, −z+3/4; (x) −x+3/2, y−1/2, −z+1/4; (xi) y, x, −z; (xii) y−1/2, −x+3/2, z−1/4; (xiii) −x+3/2, y+1/2, −z+1/4; (xiv) −y+1, −x+2, −z+1/2; (xv) −x+1, −y+1, z−1/2; (xvi) −x+1, −y+2, z−1/2; (xvii) y+1/2, −x+3/2, z−1/4.