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ISSN 2414-3146

Crystal structure of $Al_{8.77}Fe_{0.80}Ni_{1.20}Si_{0.23}$

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Received 7 January 2026
Accepted 11 March 2026

Edited by S. Bernès, Benemérita Universidad Autónoma de Puebla, México

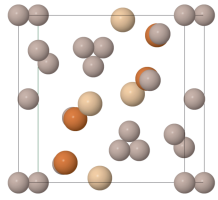
Keywords: crystal structure; high-pressure; intermetallic; quaternary system.

CCDC reference: 2537011

Structural data: full structural data are available from iucrdata.iucr.org

The $Al_{8.77}Fe_{0.80}Ni_{1.20}Si_{0.23}$ (aluminium iron nickel silicate) phase, obtained *via* high-pressure sintering of an Al-rich prealloy (nominal composition $Al_{78.08}Fe_{8.65}Ni_{8.69}Si_{4.58}$), is characterized as a novel phase in the Al—Si—Ni—Fe quaternary system. The obtained phase crystallizes in the space group $P2_1/c$, with lattice parameters a = 6.2093 (9), b = 6.2579 (9), c = 8.5661 (12) Å, and β = 94.877 (5)°. It is isotypic with $Al_9Fe_{0.7}Ni_{1.28}$ [a = 6.2406 (1), b = 6.2993 (1), c = 8.5992 (1) Å, and β = 95.129 (1)°; Chumak *et al.* (2007). *Intermetallics*, **15**, 1416–1424] and Co_2Al_9 [a = 6.2163 (3), b = 6.2883 (3), c = 8.5587 (3) Å, and β = 94.772 (4)°; Boström *et al.* (2005). *Z. Anorg. Allg. Chem.* **631**, 534–541]. It features a co-occupancy of Al and Si atoms with a ratio of the refined site-occupancy factors of 0.88 (10):0.12 (10), as well a co-occupancy Ni/Fe with site-occupancy factors of 0.60 (4):0.40 (4).

3D view



Structure description

It has been reported that the solubility of Si in the Al_9FeNi phase is approximately 4 wt% (Belov *et al.*, 2002), and this conclusion has been further validated by subsequent experimental investigations (Hao *et al.*, 2014). In the current work, the nominal composition of the intermetallic compound $Al_{78.08}Fe_{8.65}Ni_{8.69}Si_{4.58}$ was designed on the basis of the reported Si solubility (4 wt%) in the Al_9FeNi phase. Via high-pressure sintering, laboratory experiments were carried out to investigate the formation behaviour of this phase; consequently, a crystalline intermetallic phase with a composition of $Al_{8.77}Fe_{0.80}Ni_{1.20}Si_{0.23}$ was successfully obtained. This phase shows remarkable structural similarities to $Al_9Fe_{0.7}Ni_{1.3}$ [a = 6.2406 (1), b = 6.2993 (1), c = 8.5992 (1) Å, and β = 95.129 (1)°] reported by Chumak *et al.* (2007), sharing identical space-group symmetry and analogous co-site occupancy characteristics. $Al_{8.77}Fe_{0.80}Ni_{1.20}Si_{0.23}$, along with $Al_9Fe_{0.7}Ni_{1.3}$ and other T_2Al_9-type compounds (T = Co, Rh, Ir), crystallizes in the space

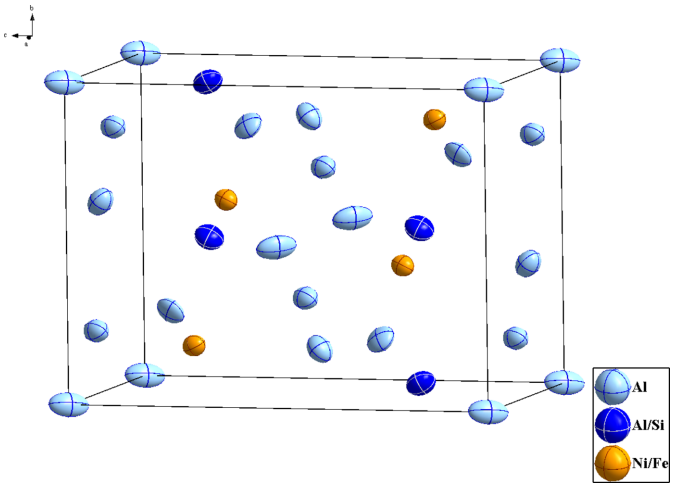


Figure 1
The crystal structure of $Al_{8.77}Fe_{0.80}Ni_{1.20}Si_{0.23}$ (one unit cell), with displacement ellipsoids drawn at the 90% probability level.

group $P2_1/c$ (No. 14). The atomic distribution within the unit cell of $Al_{8.77}Fe_{0.80}Ni_{1.20}Si_{0.23}$ is illustrated in Fig. 1. The environment of atom Al5 is shown in Fig. 2. It is located at special position 2*a* (inversion centre) and is coordinated by 12 atoms, forming the centre of a distorted icosahedron.

In this study, we refined the crystal structure model of $Al_{8.77}Fe_{0.80}Ni_{1.20}Si_{0.23}$ based on single-crystal X-ray diffraction data. Its composition was confirmed by EDX results (see the supporting information).

Synthesis and crystallization

High-purity aluminium (indicated purity 99.9%; 0.6528 g), iron (indicated purity 99.9%; 0.1516 g), nickel (indicated purity 99.9%; 0.1579 g), and silicon (indicated purity 99.9%; 0.0416 g) with a stoichiometric ratio of 78.08:8.65:8.69:4.58 were evenly mixed and fully ground in an agate mortar for 40 min. The homogenized powder was placed in a boron nitride furnace die with a diameter of 5 mm, compacted with a small rod, and subsequently subjected to high-pressure sintering using a six-anvil high-temperature and high-pressure apparatus. Cylindrical blocks without deformation and cracks were obtained. Details of high-pressure sintering experiments using six-anvil high-temperature and high-pressure equipment are described elsewhere (Liu & Fan, 2018). The sample was pressurized to 6 GPa and heated to 1676 K for 30 min., then cooled to 1131 K and held for 60 min., and finally rapidly cooled to room temperature by turning off the furnace power. A single crystal (0.08 × 0.07 × 0.06 mm^3) was selected and mounted on a glass fibre for measurements.

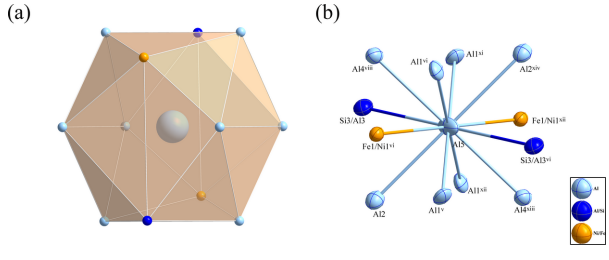


Figure 2
(*a*) The icosahedron formed around the Al5 atom at the 2*a* site and (*b*) the environment of the Al5 atom, with displacement ellipsoids given at the 90% probability level. [Symmetry codes: (v) $-x, -y+1, -z$; (vi) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (viii) $-x+1, -y, -z$; (xi) $x, y-1, z$; (xii) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (xiii) $x-1, y, z$; (xiv) $-x, -y, -z$.]

Table 1
Experimental details.

Crystal data	
Chemical formula	$Al_{8.77}Fe_{0.80}Ni_{1.20}Si_{0.23}$
M_r	358.20
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, *b*, *c* (Å)	6.2093 (9), 6.2579 (9), 8.5661 (12)
β (°)	94.877 (5)
V (Å^3)	331.65 (8)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	6.24
Crystal size (mm)	0.08 × 0.07 × 0.06
Data collection	
Diffractometer	Bruker D8 Venture Photon 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.599, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7812, 769, 606
R_{int}	0.098
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.037, 0.070, 1.08
No. of reflections	769
No. of parameters	54
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.73, −0.68

Computer programs: *APEX5* and *SAINT* (Bruker, 2023), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2017) and *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. To facilitate comparative analysis, the labelling scheme and atomic coordinates for $Al_{8.77}Fe_{0.80}Ni_{1.20}Si_{0.23}$ were taken from the corresponding data for $Al_9Fe_{0.7}Ni_{1.3}$ (Chumak *et al.*, 2007). The occupancy factors for Al3 and Si3 atoms sharing the same site were refined to 0.88 (10) and 0.12 (10); the occupancy factors for Ni1 and Fe1 atoms sharing the same site were refined to 0.60 (4) and 0.40 (4), respectively. The maximum and minimum residual electron densities in the final difference map are located 1.35 Å from Al4 and 0.92 Å from Al3/Si3, respectively.

Funding information

Funding for this research was provided by: The National Natural Science Foundation of China (grant No. 52173231; grant No. U23A20537); The Innovation Ability Promotion Project of Hebei supported by Hebei Key Lab for Optimizing Metal Product Technology and Performance (grant No. 22567609H).

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full crystallographic data

IUCrData (2026). **11**, x260266 [https://doi.org/10.1107/S241431462600266X]

Crystal structure of $Al_{8.77}Fe_{0.80}Ni_{1.20}Si_{0.23}$

Mei Chen, Changzeng Fan, Bin Wen and Lifeng Zhang

Aluminium iron nickel silicate

Crystal data

$Al_{8.77}Fe_{0.80}Ni_{1.20}Si_{0.23}$
M_r = 358.20
Monoclinic, $P2_1/c$
a = 6.2093 (9) Å
b = 6.2579 (9) Å
c = 8.5661 (12) Å
β = 94.877 (5)°
V = 331.65 (8) Å^3
Z = 2
$F(000)$ = 343
D_x = 3.587 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2687 reflections
θ = 3.3–26.8°
μ = 6.24 mm^{-1}
T = 296 K
Lump, grey
0.08 × 0.07 × 0.06 mm

Data collection

Bruker D8 Venture Photon 100 CMOS diffractometer
phi and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.599, T_{max} = 0.746
7812 measured reflections
769 independent reflections
606 reflections with $I > 2\sigma(I)$
R_{int} = 0.098
θ_{max} = 27.5°, θ_{min} = 3.3°
h = −8→8
k = −8→8
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.070
S = 1.08
769 reflections
54 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0247P)^2 + 0.9238P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Al1	0.0887 (2)	0.7113 (2)	0.22978 (17)	0.0100 (4)	
Al2	0.2136 (2)	0.3882 (2)	0.04319 (17)	0.0103 (4)	
Al3	0.4038 (2)	0.0285 (2)	0.26814 (17)	0.0107 (6)	0.88 (10)
Si3	0.4038 (2)	0.0285 (2)	0.26814 (17)	0.0107 (6)	0.12 (10)
Al4	0.6089 (2)	0.1934 (2)	0.00355 (17)	0.0091 (4)	
Ni1	0.26441 (10)	0.37995 (10)	0.33345 (7)	0.0071 (2)	0.60 (4)

Fe1	0.26441 (10)	0.37995 (10)	0.33345 (7)	0.0071 (2)	0.40 (4)
Al5	0.000000	0.000000	0.000000	0.0140 (5)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Al1	0.0075 (8)	0.0099 (8)	0.0121 (8)	0.0032 (6)	−0.0011 (6)	0.0023 (6)
Al2	0.0095 (8)	0.0109 (8)	0.0104 (8)	0.0009 (6)	0.0006 (6)	−0.0026 (6)
Al3	0.0101 (9)	0.0095 (9)	0.0127 (10)	0.0018 (6)	0.0022 (6)	−0.0021 (6)
Si3	0.0101 (9)	0.0095 (9)	0.0127 (10)	0.0018 (6)	0.0022 (6)	−0.0021 (6)
Al4	0.0086 (7)	0.0077 (7)	0.0106 (8)	0.0005 (6)	−0.0010 (6)	−0.0001 (6)
Ni1	0.0060 (4)	0.0068 (4)	0.0085 (4)	−0.0005 (3)	−0.0002 (2)	0.0007 (3)
Fe1	0.0060 (4)	0.0068 (4)	0.0085 (4)	−0.0005 (3)	−0.0002 (2)	0.0007 (3)
Al5	0.0151 (11)	0.0088 (11)	0.0196 (12)	0.0002 (9)	0.0115 (9)	0.0017 (9)

Geometric parameters (Å, º)

Al1—Ni1^{i}	2.4521 (16)	Al3—Ni1	2.4456 (15)
Al1—Fe1	2.4727 (16)	Al3—Ni1^{vii}	2.4842 (15)
Al1—Ni1	2.4727 (16)	Al3—Al4^{viii}	2.706 (2)
Al1—Al5^{ii}	2.6938 (15)	Al3—Al4^{vii}	2.873 (2)
Al1—Al2	2.730 (2)	Al3—Al4^{ix}	2.878 (2)
Al1—Al5^{i}	2.7618 (15)	Al3—Al4	2.884 (2)
Al1—Al3^{ii}	2.787 (2)	Si3—Fe1	2.4456 (15)
Al1—Al4^{iii}	2.833 (2)	Si3—Al4^{viii}	2.706 (2)
Al1—Al4^{iv}	2.918 (2)	Si3—Al4^{vii}	2.873 (2)
Al1—Al2^{v}	2.938 (2)	Si3—Al4^{ix}	2.878 (2)
Al2—Fe1	2.4801 (17)	Si3—Al4	2.884 (2)
Al2—Ni1	2.4801 (17)	Al4—Ni1^{vii}	2.4960 (16)
Al2—Ni1^{vi}	2.4980 (16)	Al4—Ni1^{vi}	2.5260 (16)
Al2—Al3^{vi}	2.773 (2)	Al4—Al5^{x}	2.7158 (15)
Al2—Al5	2.7774 (15)	Al4—Al4^{viii}	2.772 (3)
Al2—Al4	2.787 (2)	Ni1—Al5^{i}	2.3861 (7)
Al2—Al4^{iv}	2.882 (2)	Fe1—Al5^{i}	2.3861 (7)
Al2—Al3^{iii}	2.894 (2)		
Ni1^{i}—Al1—Ni1	143.05 (6)	Ni1^{vii}—Al4—Al1^{vii}	54.85 (4)
Ni1^{i}—Al1—Al5^{ii}	55.01 (3)	Ni1^{vi}—Al4—Al1^{vii}	160.56 (7)
Ni1—Al1—Al5^{ii}	151.81 (6)	Al3^{viii}—Al4—Al1^{vii}	133.06 (7)
Ni1^{i}—Al1—Al2	118.85 (7)	Al5^{x}—Al4—Al1^{vii}	59.65 (4)
Fe1—Al1—Al2	56.67 (5)	Al4^{viii}—Al4—Al1^{vii}	109.93 (8)
Ni1—Al1—Al2	56.67 (5)	Al2—Al4—Al1^{vii}	114.50 (7)
Al5^{ii}—Al1—Al2	96.86 (6)	Ni1^{vii}—Al4—Al3^{iii}	102.61 (6)
Ni1^{i}—Al1—Al5^{i}	98.79 (5)	Ni1^{vi}—Al4—Al3^{iii}	117.03 (6)
Fe1—Al1—Al5^{i}	53.90 (3)	Al3^{viii}—Al4—Al3^{iii}	163.69 (7)
Ni1—Al1—Al5^{i}	53.90 (3)	Al5^{x}—Al4—Al3^{iii}	114.16 (6)
Al5^{ii}—Al1—Al5^{i}	152.94 (6)	Al4^{viii}—Al4—Al3^{iii}	127.65 (8)
Al2—Al1—Al5^{i}	102.88 (6)	Al2—Al4—Al3^{iii}	61.48 (5)

Ni1^{i}—Al1—Al3^{ii}	108.97 (6)	Al1^{vii}—Al4—Al3^{iii}	58.46 (5)
Ni1—Al1—Al3^{ii}	105.73 (6)	Ni1^{vii}—Al4—Al3^{vi}	165.23 (7)
Al5^{ii}—Al1—Al3^{ii}	72.93 (5)	Ni1^{vi}—Al4—Al3^{vi}	53.34 (4)
Al2—Al1—Al3^{ii}	111.41 (6)	Al3^{viii}—Al4—Al3^{vi}	74.27 (4)
Al5^{i}—Al1—Al3^{ii}	115.49 (6)	Al5^{x}—Al4—Al3^{vi}	127.21 (6)
Ni1^{i}—Al1—Al4^{iii}	135.55 (7)	Al4^{viii}—Al4—Al3^{vi}	109.07 (8)
Ni1—Al1—Al4^{iii}	55.63 (4)	Al2—Al4—Al3^{vi}	58.60 (5)
Al5^{ii}—Al1—Al4^{iii}	134.11 (6)	Al1^{vii}—Al4—Al3^{vi}	139.88 (7)
Al2—Al1—Al4^{iii}	103.95 (6)	Al3^{iii}—Al4—Al3^{vi}	89.98 (6)
Al5^{i}—Al1—Al4^{iii}	58.06 (4)	Ni1^{vii}—Al4—Al2^{iv}	133.30 (7)
Al3^{ii}—Al1—Al4^{iii}	61.49 (5)	Ni1^{vi}—Al4—Al2^{iv}	113.59 (6)
Ni1^{i}—Al1—Al4^{iv}	112.10 (6)	Al3^{viii}—Al4—Al2^{iv}	109.29 (6)
Ni1—Al1—Al4^{iv}	97.32 (6)	Al5^{x}—Al4—Al2^{iv}	92.90 (5)
Al5^{ii}—Al1—Al4^{iv}	57.72 (4)	Al4^{viii}—Al4—Al2^{iv}	169.21 (9)
Al2—Al1—Al4^{iv}	61.25 (5)	Al2—Al4—Al2^{iv}	88.33 (6)
Al5^{i}—Al1—Al4^{iv}	149.07 (6)	Al1^{vii}—Al4—Al2^{iv}	80.86 (6)
Al3^{ii}—Al1—Al4^{iv}	56.57 (5)	Al3^{iii}—Al4—Al2^{iv}	57.62 (5)
Al4^{iii}—Al1—Al4^{iv}	98.02 (6)	Al3^{vi}—Al4—Al2^{iv}	60.33 (5)
Ni1^{i}—Al1—Al2^{v}	54.31 (4)	Ni1^{vii}—Al4—Al3	54.43 (4)
Ni1—Al1—Al2^{v}	109.91 (6)	Ni1^{vi}—Al4—Al3	88.81 (5)
Al5^{ii}—Al1—Al2^{v}	58.91 (4)	Al3^{viii}—Al4—Al3	120.65 (6)
Al2—Al1—Al2^{v}	64.61 (6)	Al5^{x}—Al4—Al3	107.72 (6)
Al5^{i}—Al1—Al2^{v}	113.96 (6)	Al4^{viii}—Al4—Al3	57.12 (6)
Al3^{ii}—Al1—Al2^{v}	129.75 (7)	Al2—Al4—Al3	66.94 (5)
Al4^{iii}—Al1—Al2^{v}	165.48 (7)	Al1^{vii}—Al4—Al3	71.77 (6)
Al4^{iv}—Al1—Al2^{v}	84.43 (6)	Al3^{iii}—Al4—Al3	71.74 (4)
Ni1—Al2—Ni1^{vi}	133.95 (6)	Al3^{vi}—Al4—Al3	124.64 (7)
Fe1—Al2—Al1	56.41 (5)	Al2^{iv}—Al4—Al3	129.35 (7)
Ni1—Al2—Al1	56.41 (5)	Al5^{x}—Al4—Si3	107.72 (6)
Ni1^{vi}—Al2—Al1	167.97 (7)	Al4^{viii}—Al4—Si3	57.12 (6)
Ni1—Al2—Al3^{vi}	145.96 (7)	Al2—Al4—Si3	66.94 (5)
Ni1^{vi}—Al2—Al3^{vi}	54.99 (4)	Al1^{vii}—Al4—Si3	71.77 (6)
Al1—Al2—Al3^{vi}	121.39 (7)	Al2^{iv}—Al4—Si3	129.35 (7)
Fe1—Al2—Al5	97.70 (5)	Al5^{i}—Ni1—Al3	134.01 (4)
Ni1—Al2—Al5	97.70 (5)	Al5^{i}—Ni1—Al1^{xii}	67.65 (4)
Ni1^{vi}—Al2—Al5	53.47 (3)	Al3—Ni1—Al1^{xii}	83.66 (5)
Al1—Al2—Al5	124.72 (6)	Al5^{i}—Ni1—Al1	69.25 (4)
Al3^{vi}—Al2—Al5	106.51 (6)	Al3—Ni1—Al1	145.68 (6)
Fe1—Al2—Al4	94.29 (6)	Al1^{xii}—Ni1—Al1	85.56 (3)
Ni1—Al2—Al4	94.29 (6)	Al5^{i}—Ni1—Al2	123.88 (4)
Ni1^{vi}—Al2—Al4	56.78 (4)	Al3—Ni1—Al2	78.86 (5)
Al1—Al2—Al4	133.79 (7)	Al1^{xii}—Ni1—Al2	75.66 (5)
Al3^{vi}—Al2—Al4	62.33 (5)	Al1—Ni1—Al2	66.91 (5)
Al5—Al2—Al4	90.96 (5)	Al5^{i}—Ni1—Al3^{iii}	136.46 (4)
Ni1—Al2—Al4^{iv}	98.08 (6)	Al3—Ni1—Al3^{iii}	86.35 (3)
Ni1^{vi}—Al2—Al4^{iv}	115.93 (6)	Al1^{xii}—Ni1—Al3^{iii}	146.76 (6)
Al1—Al2—Al4^{iv}	62.58 (5)	Al1—Ni1—Al3^{iii}	85.07 (5)
Al3^{vi}—Al2—Al4^{iv}	61.04 (5)	Al2—Ni1—Al3^{iii}	71.32 (5)

Al5—Al2—Al4^{iv}	163.76 (6)	Al5^{i}—Ni1—Al4^{iii}	67.55 (4)
Al4—Al2—Al4^{iv}	91.67 (6)	Al3—Ni1—Al4^{iii}	137.22 (6)
Ni1—Al2—Al3^{iii}	54.41 (4)	Al1^{xii}—Ni1—Al4^{iii}	134.03 (5)
Ni1^{vi}—Al2—Al3^{iii}	117.23 (6)	Al1—Ni1—Al4^{iii}	69.52 (5)
Al1—Al2—Al3^{iii}	73.08 (6)	Al2—Ni1—Al4^{iii}	123.48 (5)
Al3^{vi}—Al2—Al3^{iii}	91.65 (6)	Al3^{iii}—Ni1—Al4^{iii}	70.77 (5)
Al5—Al2—Al3^{iii}	134.41 (6)	Al5^{i}—Ni1—Al2^{ix}	69.27 (4)
Al4—Al2—Al3^{iii}	60.72 (5)	Al3—Ni1—Al2^{ix}	68.24 (5)
Al4^{iv}—Al2—Al3^{iii}	59.76 (5)	Al1^{xii}—Ni1—Al2^{ix}	72.81 (5)
Ni1—Al2—Al1^{v}	144.26 (6)	Al1—Ni1—Al2^{ix}	137.97 (5)
Ni1^{vi}—Al2—Al1^{v}	52.87 (4)	Al2—Ni1—Al2^{ix}	136.22 (4)
Al1—Al2—Al1^{v}	115.39 (6)	Al3^{iii}—Ni1—Al2^{ix}	131.50 (5)
Al3^{vi}—Al2—Al1^{v}	69.70 (5)	Al4^{iii}—Ni1—Al2^{ix}	100.29 (6)
Al5—Al2—Al1^{v}	56.15 (4)	Al5^{i}—Ni1—Al4^{ix}	107.72 (4)
Al4—Al2—Al1^{v}	108.67 (6)	Al3—Ni1—Al4^{ix}	70.71 (5)
Al4^{iv}—Al2—Al1^{v}	107.94 (6)	Al1^{xii}—Ni1—Al4^{ix}	138.31 (6)
Al3^{iii}—Al2—Al1^{v}	161.34 (7)	Al1—Ni1—Al4^{ix}	133.30 (5)
Ni1—Al3—Ni1^{vii}	137.46 (7)	Al2—Ni1—Al4^{ix}	127.69 (5)
Ni1—Al3—Al4^{viii}	132.33 (7)	Al3^{iii}—Ni1—Al4^{ix}	65.36 (5)
Ni1^{vii}—Al3—Al4^{viii}	58.06 (4)	Al4^{iii}—Ni1—Al4^{ix}	66.99 (6)
Ni1—Al3—Al2^{ix}	56.78 (4)	Al2^{ix}—Ni1—Al4^{ix}	67.39 (5)
Ni1^{vii}—Al3—Al2^{ix}	142.53 (7)	Al5^{i}—Fe1—Si3	134.01 (4)
Al4^{viii}—Al3—Al2^{ix}	147.55 (7)	Al5^{i}—Fe1—Al1^{xii}	67.65 (4)
Ni1—Al3—Al1^{xi}	114.14 (6)	Al5^{i}—Fe1—Al1	69.25 (4)
Ni1^{vii}—Al3—Al1^{xi}	106.68 (6)	Si3—Fe1—Al1	145.68 (6)
Al4^{viii}—Al3—Al1^{xi}	64.16 (5)	Al1^{xii}—Fe1—Al1	85.56 (3)
Al2^{ix}—Al3—Al1^{xi}	83.61 (6)	Al5^{i}—Fe1—Al2	123.88 (4)
Ni1—Al3—Al4^{vii}	118.03 (6)	Si3—Fe1—Al2	78.86 (5)
Ni1^{vii}—Al3—Al4^{vii}	92.11 (6)	Al1^{xii}—Fe1—Al2	75.66 (5)
Al4^{viii}—Al3—Al4^{vii}	102.15 (5)	Al1—Fe1—Al2	66.91 (5)
Al2^{ix}—Al3—Al4^{vii}	61.35 (5)	Al5^{i}—Fe1—Al4^{iii}	67.55 (4)
Al1^{xi}—Al3—Al4^{vii}	60.05 (5)	Al1^{xii}—Fe1—Al4^{iii}	134.03 (5)
Ni1—Al3—Al4^{ix}	55.95 (4)	Al1—Fe1—Al4^{iii}	69.52 (5)
Ni1^{vii}—Al3—Al4^{ix}	98.09 (6)	Al2—Fe1—Al4^{iii}	123.48 (5)
Al4^{viii}—Al3—Al4^{ix}	153.13 (6)	Al5^{i}—Fe1—Al2^{ix}	69.27 (4)
Al2^{ix}—Al3—Al4^{ix}	59.07 (5)	Al1^{xii}—Fe1—Al2^{ix}	72.81 (5)
Al1^{xi}—Al3—Al4^{ix}	141.07 (7)	Al1—Fe1—Al2^{ix}	137.97 (5)
Al4^{vii}—Al3—Al4^{ix}	90.02 (6)	Al2—Fe1—Al2^{ix}	136.22 (4)
Ni1—Al3—Al4	92.66 (6)	Al4^{iii}—Fe1—Al2^{ix}	100.29 (6)
Ni1^{vii}—Al3—Al4	54.81 (4)	Al5^{i}—Fe1—Al4^{ix}	107.72 (4)
Al4^{viii}—Al3—Al4	59.35 (6)	Al1^{xii}—Fe1—Al4^{ix}	138.31 (6)
Al2^{ix}—Al3—Al4	148.10 (7)	Al1—Fe1—Al4^{ix}	133.30 (5)
Al1^{xi}—Al3—Al4	120.99 (7)	Al2—Fe1—Al4^{ix}	127.69 (5)
Al4^{vii}—Al3—Al4	146.70 (7)	Al4^{iii}—Fe1—Al4^{ix}	66.99 (6)
Al4^{ix}—Al3—Al4	97.79 (5)	Al2^{ix}—Fe1—Al4^{ix}	67.39 (5)
Ni1—Al3—Al2^{vii}	115.77 (6)	Ni1^{vi}—Al5—Ni1^{xii}	180.00 (4)
Ni1^{vii}—Al3—Al2^{vii}	54.27 (4)	Ni1^{vi}—Al5—Al1^{xi}	122.66 (3)
Al4^{viii}—Al3—Al2^{vii}	106.69 (6)	Ni1^{xii}—Al5—Al1^{xi}	57.34 (3)

Al2^{ix}—Al3—Al2^{vii}	88.35 (6)	Ni1^{vi}—Al5—Al1^{v}	57.34 (3)
Al1^{xi}—Al3—Al2^{vii}	112.61 (6)	Ni1^{xii}—Al5—Al1^{v}	122.66 (3)
Al4^{vii}—Al3—Al2^{vii}	57.80 (5)	Al1^{xi}—Al5—Al1^{v}	180.0
Al4^{ix}—Al3—Al2^{vii}	59.90 (5)	Ni1^{vi}—Al5—Al4^{viii}	58.15 (3)
Al4—Al3—Al2^{vii}	98.68 (6)	Ni1^{xii}—Al5—Al4^{viii}	121.85 (3)
Al4^{viii}—Si3—Al2^{ix}	147.55 (7)	Al1^{xi}—Al5—Al4^{viii}	65.28 (4)
Al4^{viii}—Si3—Al1^{xi}	64.16 (5)	Al1^{v}—Al5—Al4^{viii}	114.72 (4)
Al2^{ix}—Si3—Al1^{xi}	83.61 (6)	Ni1^{vi}—Al5—Al4^{xiii}	121.85 (3)
Al4^{viii}—Si3—Al4^{vii}	102.15 (5)	Ni1^{xii}—Al5—Al4^{xiii}	58.15 (3)
Al2^{ix}—Si3—Al4^{vii}	61.35 (5)	Al1^{xi}—Al5—Al4^{xiii}	114.72 (4)
Al1^{xi}—Si3—Al4^{vii}	60.05 (5)	Al1^{v}—Al5—Al4^{xiii}	65.28 (4)
Al4^{viii}—Si3—Al4^{ix}	153.13 (6)	Al4^{viii}—Al5—Al4^{xiii}	180.00 (3)
Al2^{ix}—Si3—Al4^{ix}	59.07 (5)	Ni1^{vi}—Al5—Al1^{xii}	123.15 (3)
Al1^{xi}—Si3—Al4^{ix}	141.07 (7)	Ni1^{xii}—Al5—Al1^{xii}	56.85 (3)
Al4^{vii}—Si3—Al4^{ix}	90.02 (6)	Al1^{xi}—Al5—Al1^{xii}	75.622 (19)
Fe1—Si3—Al4	92.66 (6)	Al1^{v}—Al5—Al1^{xii}	104.378 (19)
Al4^{viii}—Si3—Al4	59.35 (6)	Al4^{viii}—Al5—Al1^{xii}	117.72 (4)
Al2^{ix}—Si3—Al4	148.10 (7)	Al4^{xiii}—Al5—Al1^{xii}	62.28 (4)
Al1^{xi}—Si3—Al4	120.99 (7)	Ni1^{vi}—Al5—Al1^{vi}	56.85 (3)
Al4^{vii}—Si3—Al4	146.70 (7)	Ni1^{xii}—Al5—Al1^{vi}	123.15 (3)
Al4^{ix}—Si3—Al4	97.79 (5)	Al1^{xi}—Al5—Al1^{vi}	104.378 (19)
Al4^{viii}—Si3—Al2^{vii}	106.69 (6)	Al1^{v}—Al5—Al1^{vi}	75.622 (19)
Al2^{ix}—Si3—Al2^{vii}	88.35 (6)	Al4^{viii}—Al5—Al1^{vi}	62.28 (4)
Al1^{xi}—Si3—Al2^{vii}	112.61 (6)	Al4^{xiii}—Al5—Al1^{vi}	117.72 (4)
Al4^{vii}—Si3—Al2^{vii}	57.80 (5)	Al1^{xii}—Al5—Al1^{vi}	180.00 (3)
Al4^{ix}—Si3—Al2^{vii}	59.90 (5)	Ni1^{vi}—Al5—Al2^{xiv}	122.74 (3)
Al4—Si3—Al2^{vii}	98.68 (6)	Ni1^{xii}—Al5—Al2^{xiv}	57.26 (3)
Ni1^{vii}—Al4—Ni1^{vi}	113.01 (6)	Al1^{xi}—Al5—Al2^{xiv}	64.94 (4)
Ni1^{vii}—Al4—Al3^{viii}	93.58 (6)	Al1^{v}—Al5—Al2^{xiv}	115.06 (4)
Ni1^{vi}—Al4—Al3^{viii}	56.57 (5)	Al4^{viii}—Al5—Al2^{xiv}	91.48 (4)
Ni1^{vii}—Al4—Al5^{x}	54.30 (3)	Al4^{xiii}—Al5—Al2^{xiv}	88.52 (4)
Ni1^{vi}—Al4—Al5^{x}	128.81 (6)	Al1^{xii}—Al5—Al2^{xiv}	113.79 (4)
Al3^{viii}—Al4—Al5^{x}	73.87 (5)	Al1^{vi}—Al5—Al2^{xiv}	66.21 (4)
Ni1^{vii}—Al4—Al4^{viii}	57.02 (5)	Ni1^{vi}—Al5—Al2	57.26 (3)
Ni1^{vi}—Al4—Al4^{viii}	55.99 (5)	Ni1^{xii}—Al5—Al2	122.74 (3)
Al3^{viii}—Al4—Al4^{viii}	63.53 (6)	Al1^{xi}—Al5—Al2	115.06 (4)
Al5^{x}—Al4—Al4^{viii}	92.61 (7)	Al1^{v}—Al5—Al2	64.94 (4)
Ni1^{vii}—Al4—Al2	120.96 (6)	Al4^{viii}—Al5—Al2	88.52 (4)
Ni1^{vi}—Al4—Al2	55.83 (5)	Al4^{xiii}—Al5—Al2	91.48 (4)
Al3^{viii}—Al4—Al2	111.57 (7)	Al1^{xii}—Al5—Al2	66.21 (4)
Al5^{x}—Al4—Al2	173.66 (7)	Al1^{vi}—Al5—Al2	113.79 (4)
Al4^{viii}—Al4—Al2	87.21 (7)	Al2^{xiv}—Al5—Al2	180.0

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