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$Al_{10}Ni_3Fe_{0.83}$, an Fe-depleted phase in the Al–Ni–Fe system

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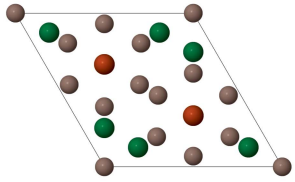
Crystals of the phase $Al_{10}Ni_3Fe_{0.83}$ (decaaluminium trinickel iron) were obtained by high-pressure sintering (HPS) of a stoichiometric mixture with nominal composition $Al_{71}Ni_{24}Fe_5$. $Al_{10}Ni_3Fe_{0.83}$ adopts the Co_2Al_5 structure type in the space group type $P6_3/mmc$ with the unique Fe site on site 2*c* partially occupied (occupancy 0.83).

3D view



Structure description

The second natural quasicrystal named decagonite has the composition $Al_{70.2}Ni_{24.5}Fe_{5.3}$ (Bindi *et al.*, 2015), which is very similar to the synthetic phase $Al_{71}Ni_{24}Fe_5$ (Lemmerz *et al.*, 1994). While simulating the growth mechanism of decagonite under high-pressure and high-temperature conditions (HPHT) by the high-pressure sintering (HPS) process, we obtained another phase in the ternary system Al–Ni–Fe (Raghavan, 2010) with composition $Al_{10}Ni_3Fe_{0.83}$. The occurrence of a phase with composition $Al_{10}Ni_3Fe$ has been reported by Khaidar *et al.* (1982) but it was never observed by other teams afterwards, although the existence of a decagonal phase with composition close to this phase was in argument (Zhang *et al.*, 2008). On the other hand, its Fe-rich counterpart $Al_{10}Fe_3Ni$ was frequently observed, and its crystal structure has also been determined (Chumak *et al.*, 2007).

The new phase $Al_{10}Ni_3Fe_{0.83}$ adopts the Al_5Co_2 structure type (Bradley & Cheng, 1938; Newkirk *et al.*, 1961) in space group type $P6_3/mmc$ with the two Co sites replaced by Ni and Fe, respectively. This structure type can be derived from a distorted closed-packed arrangement of metal atoms (Wells, 1975). The lattice parameters of $Al_{10}Ni_3Fe_{0.83}$ (Table 1) are similar to those of $Al_{10}Fe_3Ni$ (Chumak *et al.*, 2007). The asymmetric unit of $Al_{10}Ni_3Fe_{0.83}$ comprises of five sites, three fully occupied by Al atoms at Wyckoff sites 2*a* (Al3), 6*h* (Al5) and 12*k* (Al4), one fully occupied by Ni atoms (6*h*; Ni1) and one partially occupied (occupancy 0.83) by Fe atoms (2*c*; Fe1). Both the Al3 atom at the 2*a* position

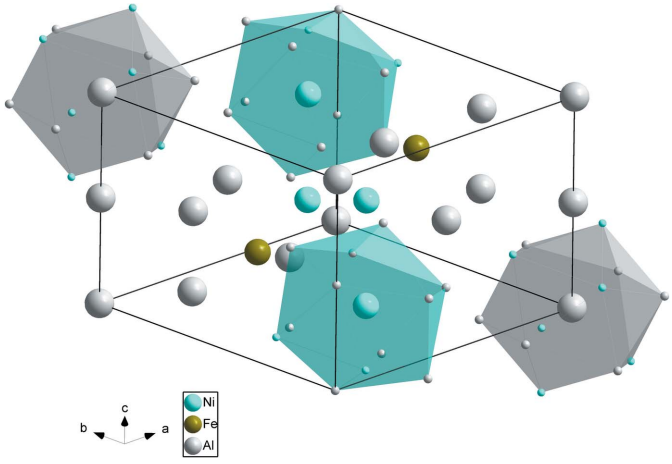


Figure 1
The crystal structure of $Al_{10}Ni_3Fe_{0.83}$ with two Al3 atoms on the 2*a* site and two Ni1 atoms on the 6*h* site displayed with their coordination environments as polyhedra.

and the Ni1 atom at the 6*h* position are surrounded by twelve atoms in the form of a distorted icosahedron (Fig. 1). Al3 is bound to six Ni3 and six Al4 atoms (Fig. 2*a*); Ni1 is bound to two Al3, six Al4, two Al5 and two Ni1 atoms (Fig. 2*b*). The Fe2 atom is surrounded by nine Al atoms (six Al4 and three Al5), forming an irregular polyhedron as shown in Fig. 3.

Synthesis and crystallization

Pure aluminium powder (indicated purity 99.8%), nickel powder (indicated purity 99.95%) and iron powder (indicated purity 99.9%) were mixed according to the atomic ratio 71: 24: 5. The detailed description of the employed HPS process can be found elsewhere (Liu & Fan, 2018). In the current work, the prepared cylindrical block mixture was pressurized up to 5 GPa and heated to 1473 K for 30 min, cooled to 1073 K, held at that temperature for 1 h, and then was rapidly cooled down to room temperature. A fragment was selected and mounted on a glass fiber for single-crystal X-ray diffraction measurements.

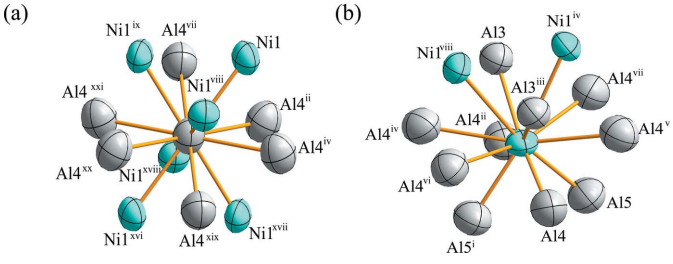


Figure 2
(*a*) The coordination sphere of the Al3 atom at the 2*a* site; (*b*) the coordination sphere of the Ni1 atom at the 6*h* site. Displacement ellipsoids are drawn at the 99.8% probability level. [Symmetry codes: (i) $-y+1, x-y, z$; (ii) $x, y, -z+\frac{1}{2}$; (iii) $-x, -y, z+\frac{1}{2}$; (iv) $y, -x+y, z-\frac{1}{2}$; (v) $x-y, x, -z+1$; (vi) $y, -x+y, -z+1$; (vii) $x-y, x, z-\frac{1}{2}$; (viii) $-x+y, -x, z$; (ix) $-y, x-y, z$; (xvi) $-x, -y, -z$; (xvii) $y, -x+y, -z$; (xviii) $x-y, x, -z$; (xix) $-x+y, -x, -z+\frac{1}{2}$; (xx) $-x, -y, z-\frac{1}{2}$; (xxi) $-y, x-y, -z+\frac{1}{2}$.]

Table 1
Experimental details.

Crystal data	
Chemical formula	$Al_{10}Ni_3Fe_{0.83}$
M_r	492.52
Crystal system, space group	Hexagonal, $P6_3/mmc$
Temperature (K)	293
a, c (Å)	7.6981 (2), 7.6231 (2)
V (Å^3)	391.23 (2)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	30.59
Crystal size (mm)	0.09 × 0.09 × 0.06
Data collection	
Diffractometer	Bruker D8 Venture Photon 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2015)
T_{min}, T_{max}	0.104, 0.170
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5095, 178, 177
R_{int}	0.035
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.624
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.029, 0.090, 1.09
No. of reflections	178
No. of parameters	21
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.53, −0.42

Computer programs: *APEX3* and *SAINT* (Bruker, 2015), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (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. Although iron and nickel atoms have very similar scattering factors and thus cannot be distinguished unambiguously in an X-ray diffraction study, the best model was obtained for the Ni atoms occupying the 6*h* site and the Fe atoms the 2*c* site. Free refinement of the occupation factors revealed the Ni site to be fully occupied and the Fe site to have a partial occupancy of 0.834 (11). The refined composition of $Al_{10}Ni_3Fe_{0.83}$ is in agreement with the results of energy dispersive X-ray spectroscopy (EDS) analysis (see Supporting information).

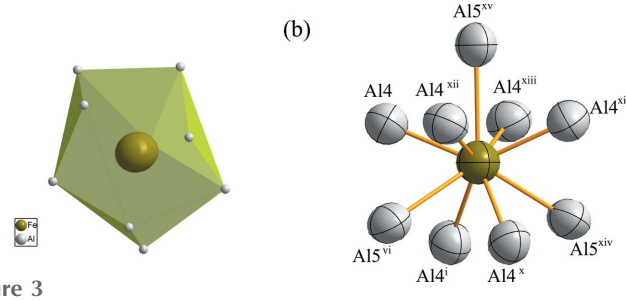


Figure 3
(*a*) The coordination polyhedron of the Fe1 atom at the 2*c* site; (*b*) the coordination sphere of the Fe1 atom showing all atoms as displacement ellipsoids at 99.8% probability level. [Symmetry codes: (i) $-y+1, x-y, z$; (vi) $y, -x+y, -z+1$; (x) $-y+1, x-y, -z+\frac{3}{2}$; (xi) $-x+y+1, -x+1, -z+\frac{3}{2}$; (xii) $x, y, -z+\frac{3}{2}$; (xiii) $-x+y+1, -x+1, z$; (xiv) $x-y+1, x, -z+1$; (xv) $-x+1, -y+1, -z+1$.]

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full crystallographic data

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Decaaluminium trinickel iron

Crystal data

$Al_{10}Ni_3Fe_{0.83}$
M_r = 492.52
Hexagonal, $P6_3/mmc$
a = 7.6981 (2) Å
c = 7.6231 (2) Å
V = 391.23 (2) Å^3
Z = 2
$F(000)$ = 471
D_x = 4.181 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 3731 reflections
θ = 5.8–74.2°
μ = 30.59 mm^{-1}
T = 293 K
Grain, metallic
0.09 × 0.09 × 0.06 mm

Data collection

Bruker APEXII Photon 100 CMOS diffractometer
Phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2015)
T_{min} = 0.104, T_{max} = 0.170
5095 measured reflections
178 independent reflections
177 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 74.2°, θ_{min} = 6.6°
h = −9→9
k = −9→9
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.090
S = 1.09
178 reflections
21 parameters
0 restraints
$w = 1/[\sigma^2(F_o^2) + (0.046P)^2 + 2.8861P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick, 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0025 (7)

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)
Ni1	0.25269 (18)	0.12635 (9)	0.250000	0.0105 (5)	

Fe2	0.666667	0.333333	0.750000	0.0158 (10)	0.834 (11)
Al3	0.000000	0.000000	0.000000	0.0125 (9)	
Al4	0.3919 (3)	0.19597 (13)	0.5598 (2)	0.0155 (6)	
Al5	0.53478 (17)	0.46522 (17)	0.250000	0.0160 (7)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0074 (7)	0.0102 (7)	0.0129 (8)	0.0037 (4)	0.000	0.000
Fe2	0.0147 (12)	0.0147 (12)	0.0181 (15)	0.0073 (6)	0.000	0.000
Al3	0.0114 (11)	0.0114 (11)	0.0148 (18)	0.0057 (6)	0.000	0.000
Al4	0.0155 (9)	0.0140 (7)	0.0177 (9)	0.0077 (4)	−0.0016 (6)	−0.0008 (3)
Al5	0.0129 (9)	0.0129 (9)	0.0205 (13)	0.0052 (9)	0.000	0.000

Geometric parameters (Å, º)

Ni1—Al5	2.4199 (10)	Al3—Al4^{xix}	2.6525 (17)
Ni1—Al5^{i}	2.4199 (10)	Al3—Al4^{vii}	2.6525 (17)
Ni1—Al4	2.5374 (18)	Al3—Al4^{xx}	2.6525 (17)
Ni1—Al4^{ii}	2.5374 (18)	Al3—Al4^{ii}	2.6525 (17)
Ni1—Al3	2.5436 (8)	Al3—Al4^{iv}	2.6525 (17)
Ni1—Al3^{iii}	2.5436 (8)	Al3—Al4^{xxi}	2.6525 (17)
Ni1—Al4^{iv}	2.7141 (15)	Al4—Al3^{iii}	2.6525 (17)
Ni1—Al4^{v}	2.7141 (15)	Al4—Ni1^{vi}	2.7141 (15)
Ni1—Al4^{vi}	2.7141 (15)	Al4—Ni1^{v}	2.7141 (15)
Ni1—Al4^{vii}	2.7141 (15)	Al4—Al4^{vi}	2.767 (2)
Ni1—Ni1^{viii}	2.918 (2)	Al4—Al4^{v}	2.7674 (19)
Ni1—Ni1^{ix}	2.918 (2)	Al4—Al5^{xv}	2.7842 (17)
Fe2—Al4^{x}	2.3360 (17)	Al4—Al5^{vi}	2.7842 (17)
Fe2—Al4^{i}	2.3360 (17)	Al4—Al4^{xii}	2.900 (4)
Fe2—Al4	2.3360 (17)	Al4—Al5^{i}	2.9669 (16)
Fe2—Al4^{xi}	2.3360 (17)	Al4—Al5	2.9669 (16)
Fe2—Al4^{xii}	2.3360 (17)	Al5—Ni1^{xiii}	2.4199 (10)
Fe2—Al4^{xiii}	2.3360 (17)	Al5—Fe2^{xv}	2.686 (2)
Fe2—Al5^{vi}	2.686 (2)	Al5—Al4^{xv}	2.7842 (17)
Fe2—Al5^{xiv}	2.686 (2)	Al5—Al4^{vii}	2.7842 (17)
Fe2—Al5^{xv}	2.686 (2)	Al5—Al4^{xxii}	2.7842 (17)
Al3—Ni1^{xvi}	2.5436 (8)	Al5—Al4^{v}	2.7842 (17)
Al3—Ni1^{xvii}	2.5436 (8)	Al5—Al4^{xiii}	2.9669 (16)
Al3—Ni1^{ix}	2.5436 (8)	Al5—Al4^{ii}	2.9669 (16)
Al3—Ni1^{xviii}	2.5436 (8)	Al5—Al4^{xxiii}	2.9669 (16)
Al3—Ni1^{viii}	2.5436 (8)		
Al5—Ni1—Al5^{i}	78.00 (12)	Al4^{vii}—Al3—Al4^{ii}	62.89 (2)
Al5—Ni1—Al4	73.48 (4)	Al4^{xx}—Al3—Al4^{ii}	180.00 (9)
Al5^{i}—Ni1—Al4	73.48 (4)	Ni1^{xvi}—Al3—Al4^{iv}	117.06 (3)
Al5—Ni1—Al4^{ii}	73.48 (4)	Ni1—Al3—Al4^{iv}	62.94 (3)
Al5^{i}—Ni1—Al4^{ii}	73.48 (4)	Ni1^{xvii}—Al3—Al4^{iv}	58.42 (4)

Al4—Ni1—Al4^{ii}	137.08 (9)	Ni1^{ix}—Al3—Al4^{iv}	121.58 (4)
Al5—Ni1—Al3	120.98 (3)	Ni1^{xviii}—Al3—Al4^{iv}	117.06 (3)
Al5^{i}—Ni1—Al3	120.98 (3)	Ni1^{viii}—Al3—Al4^{iv}	62.94 (3)
Al4—Ni1—Al3	159.99 (6)	Al4^{xix}—Al3—Al4^{iv}	62.89 (2)
Al4^{ii}—Ni1—Al3	62.94 (4)	Al4^{vii}—Al3—Al4^{iv}	117.11 (2)
Al5—Ni1—Al3^{iii}	120.98 (3)	Al4^{xx}—Al3—Al4^{iv}	117.11 (2)
Al5^{i}—Ni1—Al3^{iii}	120.98 (3)	Al4^{ii}—Al3—Al4^{iv}	62.89 (2)
Al4—Ni1—Al3^{iii}	62.94 (4)	Ni1^{xvi}—Al3—Al4^{xxi}	62.94 (3)
Al4^{ii}—Ni1—Al3^{iii}	159.99 (6)	Ni1—Al3—Al4^{xxi}	117.06 (3)
Al3—Ni1—Al3^{iii}	97.05 (4)	Ni1^{xvii}—Al3—Al4^{xxi}	121.58 (4)
Al5—Ni1—Al4^{iv}	129.27 (6)	Ni1^{ix}—Al3—Al4^{xxi}	58.42 (4)
Al5^{i}—Ni1—Al4^{iv}	65.39 (5)	Ni1^{xviii}—Al3—Al4^{xxi}	62.94 (3)
Al4—Ni1—Al4^{iv}	123.24 (4)	Ni1^{viii}—Al3—Al4^{xxi}	117.06 (3)
Al4^{ii}—Ni1—Al4^{iv}	63.50 (3)	Al4^{xix}—Al3—Al4^{xxi}	117.11 (2)
Al3—Ni1—Al4^{iv}	60.49 (4)	Al4^{vii}—Al3—Al4^{xxi}	62.89 (2)
Al3^{iii}—Ni1—Al4^{iv}	107.94 (4)	Al4^{xx}—Al3—Al4^{xxi}	62.89 (2)
Al5—Ni1—Al4^{v}	65.39 (5)	Al4^{ii}—Al3—Al4^{xxi}	117.11 (2)
Al5^{i}—Ni1—Al4^{v}	129.27 (6)	Al4^{iv}—Al3—Al4^{xxi}	180.00 (4)
Al4—Ni1—Al4^{v}	63.50 (3)	Fe2—Al4—Ni1	149.83 (8)
Al4^{ii}—Ni1—Al4^{v}	123.24 (4)	Fe2—Al4—Al3^{iii}	151.52 (8)
Al3—Ni1—Al4^{v}	107.94 (4)	Ni1—Al4—Al3^{iii}	58.65 (5)
Al3^{iii}—Ni1—Al4^{v}	60.49 (4)	Fe2—Al4—Ni1^{vi}	100.36 (6)
Al4^{iv}—Ni1—Al4^{v}	163.98 (7)	Ni1—Al4—Ni1^{vi}	104.98 (6)
Al5—Ni1—Al4^{vi}	129.27 (6)	Al3^{iii}—Al4—Ni1^{vi}	56.57 (4)
Al5^{i}—Ni1—Al4^{vi}	65.39 (5)	Fe2—Al4—Ni1^{v}	100.36 (6)
Al4—Ni1—Al4^{vi}	63.50 (3)	Ni1—Al4—Ni1^{v}	104.98 (6)
Al4^{ii}—Ni1—Al4^{vi}	123.24 (4)	Al3^{iii}—Al4—Ni1^{v}	56.57 (4)
Al3—Ni1—Al4^{vi}	107.94 (4)	Ni1^{vi}—Al4—Ni1^{v}	65.03 (6)
Al3^{iii}—Ni1—Al4^{vi}	60.49 (4)	Fe2—Al4—Al4^{vi}	125.07 (4)
Al4^{iv}—Ni1—Al4^{vi}	64.59 (7)	Ni1—Al4—Al4^{vi}	61.36 (6)
Al4^{v}—Ni1—Al4^{vi}	112.97 (7)	Al3^{iii}—Al4—Al4^{vi}	58.556 (11)
Al5—Ni1—Al4^{vii}	65.39 (5)	Ni1^{vi}—Al4—Al4^{vi}	55.14 (4)
Al5^{i}—Ni1—Al4^{vii}	129.27 (6)	Ni1^{v}—Al4—Al4^{vi}	107.91 (5)
Al4—Ni1—Al4^{vii}	123.24 (4)	Fe2—Al4—Al4^{v}	125.07 (4)
Al4^{ii}—Ni1—Al4^{vii}	63.50 (3)	Ni1—Al4—Al4^{v}	61.36 (6)
Al3—Ni1—Al4^{vii}	60.49 (4)	Al3^{iii}—Al4—Al4^{v}	58.556 (11)
Al3^{iii}—Ni1—Al4^{vii}	107.94 (4)	Ni1^{vi}—Al4—Al4^{v}	107.91 (5)
Al4^{iv}—Ni1—Al4^{vii}	112.97 (7)	Ni1^{v}—Al4—Al4^{v}	55.14 (4)
Al4^{v}—Ni1—Al4^{vii}	64.59 (7)	Al4^{vi}—Al4—Al4^{v}	109.71 (7)
Al4^{vi}—Ni1—Al4^{vii}	163.98 (7)	Fe2—Al4—Al5^{xv}	62.56 (5)
Al5—Ni1—Ni1^{viii}	171.00 (6)	Ni1—Al4—Al5^{xv}	123.29 (4)
Al5^{i}—Ni1—Ni1^{viii}	111.00 (6)	Al3^{iii}—Al4—Al5^{xv}	105.21 (5)
Al4—Ni1—Ni1^{viii}	108.47 (4)	Ni1^{vi}—Al4—Al5^{xv}	106.58 (6)
Al4^{ii}—Ni1—Ni1^{viii}	108.47 (4)	Ni1^{v}—Al4—Al5^{xv}	52.20 (4)
Al3—Ni1—Ni1^{viii}	55.001 (16)	Al4^{vi}—Al4—Al5^{xv}	159.64 (7)
Al3^{iii}—Ni1—Ni1^{viii}	55.001 (16)	Al4^{v}—Al4—Al5^{xv}	64.61 (6)
Al4^{iv}—Ni1—Ni1^{viii}	57.48 (3)	Fe2—Al4—Al5^{vi}	62.56 (5)
Al4^{v}—Ni1—Ni1^{viii}	107.23 (4)	Ni1—Al4—Al5^{vi}	123.29 (4)

Al4^{vi}—Ni1—Ni1^{viii}	57.48 (3)	Al3^{iii}—Al4—Al5^{vi}	105.21 (5)
Al4^{vii}—Ni1—Ni1^{viii}	107.23 (4)	Ni1^{vi}—Al4—Al5^{vi}	52.20 (4)
Al5—Ni1—Ni1^{ix}	111.00 (6)	Ni1^{v}—Al4—Al5^{vi}	106.58 (6)
Al5^{i}—Ni1—Ni1^{ix}	171.00 (6)	Al4^{vi}—Al4—Al5^{vi}	64.61 (6)
Al4—Ni1—Ni1^{ix}	108.47 (4)	Al4^{v}—Al4—Al5^{vi}	159.64 (7)
Al4^{ii}—Ni1—Ni1^{ix}	108.47 (4)	Al5^{xv}—Al4—Al5^{vi}	113.32 (8)
Al3—Ni1—Ni1^{ix}	55.001 (16)	Fe2—Al4—Al4^{xii}	51.63 (4)
Al3^{iii}—Ni1—Ni1^{ix}	55.001 (16)	Ni1—Al4—Al4^{xii}	158.54 (5)
Al4^{iv}—Ni1—Ni1^{ix}	107.23 (4)	Al3^{iii}—Al4—Al4^{xii}	99.89 (4)
Al4^{v}—Ni1—Ni1^{ix}	57.48 (3)	Ni1^{vi}—Al4—Al4^{xii}	57.71 (3)
Al4^{vi}—Ni1—Ni1^{ix}	107.23 (4)	Ni1^{v}—Al4—Al4^{xii}	57.71 (3)
Al4^{vii}—Ni1—Ni1^{ix}	57.48 (3)	Al4^{vi}—Al4—Al4^{xii}	109.23 (7)
Ni1^{viii}—Ni1—Ni1^{ix}	60.0	Al4^{v}—Al4—Al4^{xii}	109.23 (7)
Al4^{x}—Fe2—Al4^{i}	76.74 (9)	Al5^{xv}—Al4—Al4^{xii}	58.61 (4)
Al4^{x}—Fe2—Al4	133.84 (3)	Al5^{vi}—Al4—Al4^{xii}	58.61 (4)
Al4^{i}—Fe2—Al4	85.53 (6)	Fe2—Al4—Al5^{i}	104.03 (5)
Al4^{x}—Fe2—Al4^{xi}	85.53 (6)	Ni1—Al4—Al5^{i}	51.44 (4)
Al4^{i}—Fe2—Al4^{xi}	133.84 (3)	Al3^{iii}—Al4—Al5^{i}	100.34 (5)
Al4—Fe2—Al4^{xi}	133.84 (3)	Ni1^{vi}—Al4—Al5^{i}	111.02 (5)
Al4^{x}—Fe2—Al4^{xii}	85.53 (6)	Ni1^{v}—Al4—Al5^{i}	155.58 (7)
Al4^{i}—Fe2—Al4^{xii}	133.84 (3)	Al4^{vi}—Al4—Al5^{i}	57.97 (7)
Al4—Fe2—Al4^{xii}	76.74 (9)	Al4^{v}—Al4—Al5^{i}	108.01 (9)
Al4^{xi}—Fe2—Al4^{xii}	85.53 (6)	Al5^{xv}—Al4—Al5^{i}	141.91 (7)
Al4^{x}—Fe2—Al4^{xiii}	133.84 (3)	Al5^{vi}—Al4—Al5^{i}	85.95 (3)
Al4^{i}—Fe2—Al4^{xiii}	85.53 (6)	Al4^{xii}—Al4—Al5^{i}	142.74 (3)
Al4—Fe2—Al4^{xiii}	85.53 (6)	Fe2—Al4—Al5	104.03 (5)
Al4^{xi}—Fe2—Al4^{xiii}	76.74 (9)	Ni1—Al4—Al5	51.44 (4)
Al4^{xii}—Fe2—Al4^{xiii}	133.84 (3)	Al3^{iii}—Al4—Al5	100.34 (5)
Al4^{x}—Fe2—Al5^{vi}	66.920 (15)	Ni1^{vi}—Al4—Al5	155.58 (7)
Al4^{i}—Fe2—Al5^{vi}	66.920 (15)	Ni1^{v}—Al4—Al5	111.02 (5)
Al4—Fe2—Al5^{vi}	66.920 (15)	Al4^{vi}—Al4—Al5	108.01 (9)
Al4^{xi}—Fe2—Al5^{vi}	141.63 (4)	Al4^{v}—Al4—Al5	57.97 (7)
Al4^{xii}—Fe2—Al5^{vi}	66.920 (15)	Al5^{xv}—Al4—Al5	85.95 (3)
Al4^{xiii}—Fe2—Al5^{vi}	141.63 (4)	Al5^{vi}—Al4—Al5	141.91 (7)
Al4^{x}—Fe2—Al5^{xiv}	66.920 (15)	Al4^{xii}—Al4—Al5	142.74 (3)
Al4^{i}—Fe2—Al5^{xiv}	66.920 (15)	Al5^{i}—Al4—Al5	61.77 (8)
Al4—Fe2—Al5^{xiv}	141.63 (4)	Ni1^{xiii}—Al5—Ni1	162.00 (12)
Al4^{xi}—Fe2—Al5^{xiv}	66.920 (15)	Ni1^{xiii}—Al5—Fe2^{xv}	99.00 (6)
Al4^{xii}—Fe2—Al5^{xiv}	141.63 (4)	Ni1—Al5—Fe2^{xv}	99.00 (6)
Al4^{xiii}—Fe2—Al5^{xiv}	66.920 (15)	Ni1^{xiii}—Al5—Al4^{xv}	62.41 (4)
Al5^{vi}—Fe2—Al5^{xiv}	120.0	Ni1—Al5—Al4^{xv}	131.46 (7)
Al4^{x}—Fe2—Al5^{xv}	141.63 (4)	Fe2^{xv}—Al5—Al4^{xv}	50.52 (5)
Al4^{i}—Fe2—Al5^{xv}	141.63 (4)	Ni1^{xiii}—Al5—Al4^{vii}	131.46 (7)
Al4—Fe2—Al5^{xv}	66.920 (15)	Ni1—Al5—Al4^{vii}	62.41 (4)
Al4^{xi}—Fe2—Al5^{xv}	66.920 (15)	Fe2^{xv}—Al5—Al4^{vii}	50.52 (5)
Al4^{xii}—Fe2—Al5^{xv}	66.920 (15)	Al4^{xv}—Al5—Al4^{vii}	101.04 (10)
Al4^{xiii}—Fe2—Al5^{xv}	66.920 (15)	Ni1^{xiii}—Al5—Al4^{xxii}	62.41 (4)
Al5^{vi}—Fe2—Al5^{xv}	120.0	Ni1—Al5—Al4^{xxii}	131.46 (7)

Al5^{xiv}—Fe2—Al5^{xv}	120.0	Fe2^{xv}—Al5—Al4^{xxii}	50.52 (5)
Ni1^{xvi}—Al3—Ni1	180.0	Al4^{xv}—Al5—Al4^{xxii}	62.77 (7)
Ni1^{xvi}—Al3—Ni1^{xvii}	70.00 (3)	Al4^{vii}—Al5—Al4^{xxii}	69.46 (8)
Ni1—Al3—Ni1^{xvii}	110.00 (3)	Ni1^{xiii}—Al5—Al4^{v}	131.46 (7)
Ni1^{xvi}—Al3—Ni1^{ix}	110.00 (3)	Ni1—Al5—Al4^{v}	62.41 (4)
Ni1—Al3—Ni1^{ix}	70.00 (3)	Fe2^{xv}—Al5—Al4^{v}	50.52 (5)
Ni1^{xvii}—Al3—Ni1^{ix}	180.00 (3)	Al4^{xv}—Al5—Al4^{v}	69.46 (8)
Ni1^{xvi}—Al3—Ni1^{xviii}	70.00 (3)	Al4^{vii}—Al5—Al4^{v}	62.77 (7)
Ni1—Al3—Ni1^{xviii}	110.00 (3)	Al4^{xxii}—Al5—Al4^{v}	101.04 (10)
Ni1^{xvii}—Al3—Ni1^{xviii}	70.00 (3)	Ni1^{xiii}—Al5—Al4^{xiii}	55.08 (3)
Ni1^{ix}—Al3—Ni1^{xviii}	110.00 (3)	Ni1—Al5—Al4^{xiii}	118.92 (5)
Ni1^{xvi}—Al3—Ni1^{viii}	110.00 (3)	Fe2^{xv}—Al5—Al4^{xiii}	106.50 (5)
Ni1—Al3—Ni1^{viii}	70.00 (3)	Al4^{xv}—Al5—Al4^{xiii}	57.42 (5)
Ni1^{xvii}—Al3—Ni1^{viii}	110.00 (3)	Al4^{vii}—Al5—Al4^{xiii}	154.12 (8)
Ni1^{ix}—Al3—Ni1^{viii}	70.00 (3)	Al4^{xxii}—Al5—Al4^{xiii}	106.89 (6)
Ni1^{xviii}—Al3—Ni1^{viii}	180.00 (5)	Al4^{v}—Al5—Al4^{xiii}	94.05 (3)
Ni1^{xvi}—Al3—Al4^{xix}	62.94 (3)	Ni1^{xiii}—Al5—Al4^{ii}	118.92 (5)
Ni1—Al3—Al4^{xix}	117.06 (3)	Ni1—Al5—Al4^{ii}	55.08 (3)
Ni1^{xvii}—Al3—Al4^{xix}	62.94 (3)	Fe2^{xv}—Al5—Al4^{ii}	106.50 (5)
Ni1^{ix}—Al3—Al4^{xix}	117.06 (3)	Al4^{xv}—Al5—Al4^{ii}	154.12 (8)
Ni1^{xviii}—Al3—Al4^{xix}	121.58 (4)	Al4^{vii}—Al5—Al4^{ii}	57.42 (5)
Ni1^{viii}—Al3—Al4^{xix}	58.42 (4)	Al4^{xxii}—Al5—Al4^{ii}	94.05 (3)
Ni1^{xvi}—Al3—Al4^{vii}	117.06 (3)	Al4^{v}—Al5—Al4^{ii}	106.89 (6)
Ni1—Al3—Al4^{vii}	62.94 (3)	Al4^{xiii}—Al5—Al4^{ii}	146.99 (10)
Ni1^{xvii}—Al3—Al4^{vii}	117.06 (3)	Ni1^{xiii}—Al5—Al4^{xxiii}	55.08 (3)
Ni1^{ix}—Al3—Al4^{vii}	62.94 (3)	Ni1—Al5—Al4^{xxiii}	118.92 (5)
Ni1^{xviii}—Al3—Al4^{vii}	58.42 (4)	Fe2^{xv}—Al5—Al4^{xxiii}	106.50 (5)
Ni1^{viii}—Al3—Al4^{vii}	121.58 (4)	Al4^{xv}—Al5—Al4^{xxiii}	106.89 (6)
Al4^{xix}—Al3—Al4^{vii}	180.00 (7)	Al4^{vii}—Al5—Al4^{xxiii}	94.05 (3)
Ni1^{xvi}—Al3—Al4^{xx}	58.42 (4)	Al4^{xxii}—Al5—Al4^{xxiii}	57.42 (5)
Ni1—Al3—Al4^{xx}	121.58 (4)	Al4^{v}—Al5—Al4^{xxiii}	154.12 (8)
Ni1^{xvii}—Al3—Al4^{xx}	117.06 (3)	Al4^{xiii}—Al5—Al4^{xxiii}	105.49 (6)
Ni1^{ix}—Al3—Al4^{xx}	62.94 (3)	Al4^{ii}—Al5—Al4^{xxiii}	64.63 (6)
Ni1^{xviii}—Al3—Al4^{xx}	117.06 (3)	Ni1^{xiii}—Al5—Al4	118.92 (5)
Ni1^{viii}—Al3—Al4^{xx}	62.94 (3)	Ni1—Al5—Al4	55.08 (3)
Al4^{xix}—Al3—Al4^{xx}	62.89 (2)	Fe2^{xv}—Al5—Al4	106.50 (5)
Al4^{vii}—Al3—Al4^{xx}	117.11 (2)	Al4^{xv}—Al5—Al4	94.05 (3)
Ni1^{xvi}—Al3—Al4^{ii}	121.58 (4)	Al4^{vii}—Al5—Al4	106.89 (6)
Ni1—Al3—Al4^{ii}	58.42 (4)	Al4^{xxii}—Al5—Al4	154.12 (8)
Ni1^{xvii}—Al3—Al4^{ii}	62.94 (3)	Al4^{v}—Al5—Al4	57.42 (5)
Ni1^{ix}—Al3—Al4^{ii}	117.06 (3)	Al4^{xiii}—Al5—Al4	64.63 (6)
Ni1^{xviii}—Al3—Al4^{ii}	62.94 (3)	Al4^{ii}—Al5—Al4	105.49 (6)
Ni1^{viii}—Al3—Al4^{ii}	117.06 (3)	Al4^{xxiii}—Al5—Al4	146.99 (10)
Al4^{xix}—Al3—Al4^{ii}	117.11 (2)		

Symmetry codes: (i) $-y+1, x-y, z$; (ii) $x, y, -z+1/2$; (iii) $-x, -y, z+1/2$; (iv) $y, -x+y, z-1/2$; (v) $x-y, x, -z+1$; (vi) $y, -x+y, -z+1$; (vii) $x-y, x, z-1/2$; (viii) $-x+y, -x, z$; (ix) $-y, x-y, z$; (x) $-y+1, x-y, -z+3/2$; (xi) $-x+y+1, -x+1, -z+3/2$; (xii) $x, y, -z+3/2$; (xiii) $-x+y+1, -x+1, z$; (xiv) $x-y+1, x, -z+1$; (xv) $-x+1, -y+1, -z+1$; (xvi) $-x, -y, -z$; (xvii) $y, -x+y, -z$; (xviii) $x-y, x, -z$; (xix) $-x+y, -x, -z+1/2$; (xx) $-x, -y, z-1/2$; (xxi) $-y, x-y, -z+1/2$; (xxii) $-x+1, -y+1, z-1/2$; (xxiii) $-x+y+1, -x+1, -z+1/2$.