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Crystal structure of the λ-$Al_{13}Fe_4$-type intermetallic $(Al,Cu)_{13}(Fe,Cu)_4$

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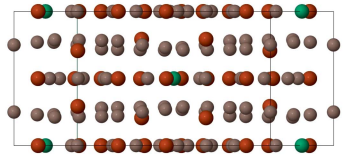
An $(Al,Cu)_{13}(Fe,Cu)_4$ phase of [trideca(aluminium/copper) tetra(iron/copper)] was obtained by the high-pressure sintering (HPS) process of a mixture with composition $Al_{78}Cu_{15}Fe_7$. Structure analysis suggests that Cu atoms can replace both Al and Fe atoms. Such findings support previous anomalous X-ray scattering (AXS) results although deviate from other reports. The new phase adopts the λ-$Al_{13}Fe_4$ structure type where Cu atoms partially occupy the 2*c* and 4*i* sites for Al and Fe atoms, respectively, with occupancies of 0.233 (5) and 0.173 (16).

3D view



Structure description

An unnamed $Al_{78}Cu_{15}Fe_7$ phase was identified in association with icosahedrite (Ma *et al.*, 2016), the first naturally occurring quasicrystal (Bindi *et al.*, 2009). In simulating its growth mechanism by high pressure sintering (HPS), a λ-$Al_{13}Fe_4$-type phase with composition $Al_{4.85}Cu_{0.07}Fe_{1.46}$ [trideca(aluminium/copper) tetra(iron/copper)] was found. The complex intermetallic compound λ-phase possesses more than 100 atoms in the unit cell along with Fe atoms arranged in Fe–Al–Fe groups, which are encapsulated by aluminium atoms (Armbrüster *et al.*, 2012). The synthesized $Al_{4.85}Cu_{0.07}Fe_{1.46}$ phase can also be viewed as a stacking of flat (*F*) and puckered (*P*) layers in a $F_1P_1F_2P_2$ sequence in the [010] direction (Matilainen *et al.*, 2015). The puckered layers are mirrored against the F_2 layer. In total, the unit cell contains 102 atoms, where the flat layer is composed of 16 Al atoms and one commonly occupied Al/Cu atom, 7 Fe atoms and one commonly occupied Fe/Cu atom. The puckered layer has 22 Al and 4 Fe atoms.

Fig. 1 shows the [010] projection of the crystal structure of the new ternary Al–Cu–Fe phase. The environment of the Al/Cu atoms and Fe/Cu atoms are shown in Fig. 2. The Al/Cu atoms share the 2*c* site and are connected by 8 Al atoms and 2 Fe atoms. The Fe/Cu atoms share the 4*i* site and are connected by 11 Al atoms. Therefore, the new phase can

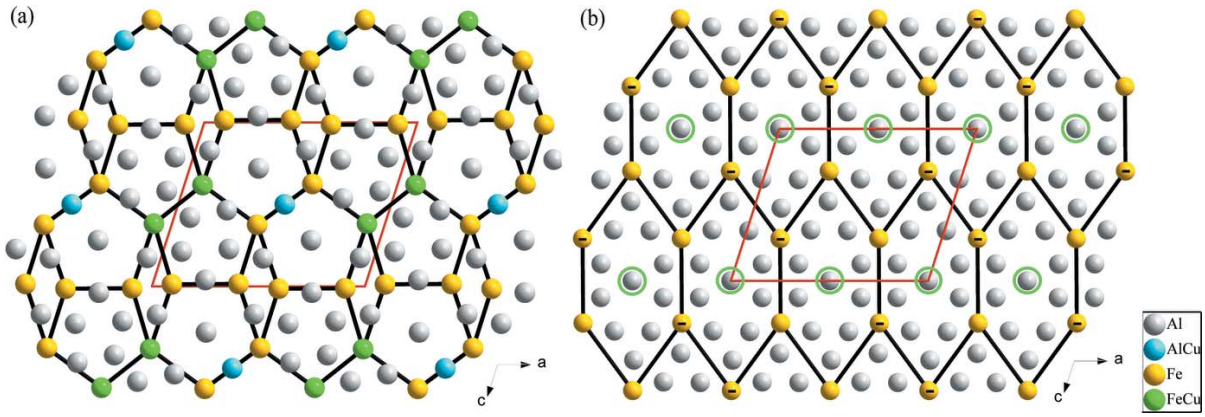


Figure 1
The [010] projection of the crystal structure of the new ternary Al–Cu–Fe phase. The monoclinic unit cell is outlined by a red parallelogram. The tiling formed by (*a*) connecting transition metal atoms for the flat layer with pentagons, rhombi, and (*b*) in the case of the puckered layer with elongated hexagons (edge length around 6.5 Å). The circled Al atoms refer to the glue atoms and the assigned minus Fe atoms mean that they are located below the middle plane position.

be described as $(Al,Cu)_{13}(Fe,Cu)_4$ where Cu atoms replace both Al and Fe atoms, in accordance with the AXS results (Genba *et al.*, 2002) but different from conventional viewpoints (Freiburg & Grushko, 1994).

Synthesis and crystallization

The pure elements Al (indicated purity 99.8%), Cu (indicated purity 99.95%) and Fe (indicated purity 99.8%) were mixed in the stoichiometric ratio 78:15:7 and initially ground in an agate mortar. Blended powders were then placed in a grinding tool of diameter 5 mm and pressed into a tablet at about 4 MPa slowly and continuously for about five minutes. A cylindrical block 5 mm in diameter and 8 mm in height was obtained without cracks or deformations. The cylindrical block was then inserted in a six-anvil high-pressure apparatus for HPS experiments. Inside the anvil, the block was encapsulated into an *h*-BN crucible covered by an *h*-BN gasket and wrapped in a graphite stove. Both ends of the graphite stove were filled with pyrophyllite and dolomite composite medium and sealed by conductive steel. Finally, all of these components were put into pyrophyllite rock that served as pressure transition medium (see Supporting information). The sample was pressurized up to 5 GPa and heated to 1473 K for 30 minutes (similiar conditions as employed by Hollister *et al.*, 2014), cooled to 1073 K and held at this temperature for one hour, and then cooled down rapidly to room temperature. A fragment of dimension 0.08 × 0.05 × 0.03 mm^3 was selected and mounted on a glass fiber for single-crystal X-ray diffraction measurements.

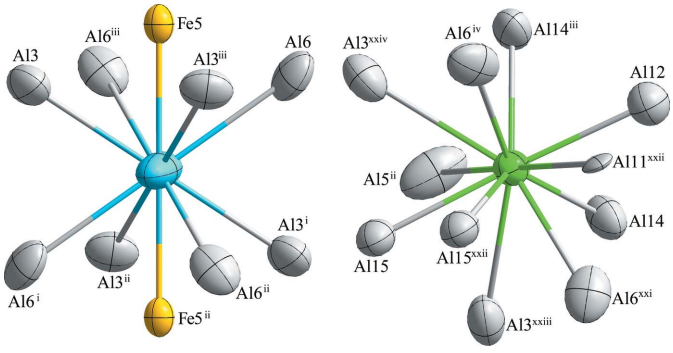


Figure 2
The environment of Al/Cu (left) atoms and Fe/Cu (right) atoms in detail. Displacement ellipsoids are given at the 99.8% probability level. [Symmetry codes: (i) $1-x, 1-y, 1-z$; (ii) $1-x, y, 1-z$; (iii) $x, 1-y, z$; (iv) $\frac{1}{2}+x, \frac{3}{2}-y, z$; (xxi) $-\frac{1}{2}+x, \frac{1}{2}+y, z$; (xxii) $-x, 1-y, 1-z$; (xxiii) $-\frac{1}{2}+x, \frac{3}{2}-y, z$; (xxiv) $-\frac{1}{2}+x, -\frac{1}{2}+y, z$.]

Table 1
Experimental details.

Crystal data	
Chemical formula	$Al_{4.85}Cu_{0.07}Fe_{1.46}$
M_r	216.70
Crystal system, space group	Monoclinic, *C*2/*m*
Temperature (K)	293
a, *b*, *c* (Å)	15.4749 (10), 8.0913 (5), 12.4882 (9)
β (°)	107.768 (2)
V (Å^3)	1489.09 (17)
Z	16
Radiation type	Mo $K\alpha$
μ (mm^{-1})	7.06
Crystal size (mm)	0.08 × 0.05 × 0.03
Data collection	
Diffractometer	Bruker D8 Venture Photon 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.576, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12161, 2319, 1749
R_{int}	0.044
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.715
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.070, 1.07
No. of reflections	2319
No. of parameters	138
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.12, −0.99

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. After considering all atoms in the $Al_{13}Fe_4$ structure, the original Al1 atom (Wyckoff position 2*c*) was modelled as occupied with both Al and Cu atoms with occupancies of 0.767 (5) and 0.233 (5), respectively. In addition, the Fe2 position was modelled by partially occupied Fe atoms [occupancy 0.827 (16)] and Cu atoms [occupancy 0.173 (16)]. Although the refined formula $Al_{4.85}Cu_{0.07}Fe_{1.46}$ shows significant deficiency in Cu compared to that of initial stoichiometry, it is in good agreement with the EDS measurements.

Acknowledgements

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full crystallographic data

IUCrData (2018). **3**, x180363 [https://doi.org/10.1107/S2414314618003632]

Crystal structure of the λ-$Al_{13}Fe_4$-type intermetallic $(Al,Cu)_{13}(Fe,Cu)_4$

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trideca(aluminium/copper) tetra(iron/copper)

Crystal data

$Al_{4.85}Cu_{0.07}Fe_{1.46}$
M_r = 216.70
Monoclinic, *C*2/*m*
a = 15.4749 (10) Å
b = 8.0913 (5) Å
c = 12.4882 (9) Å
β = 107.768 (2)°
V = 1489.09 (17) Å^3
Z = 16
F(000) = 1648
D_x = 3.866 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 1749 reflections
θ = 2.8–30.5°
μ = 7.06 mm^{-1}
T = 293 K
Grain, silver
0.08 × 0.05 × 0.03 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} = 0.576, T_{max} = 0.746
12161 measured reflections
2319 independent reflections
1749 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 30.5°, θ_{min} = 2.8°
h = −21→22
k = −11→10
l = −14→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.070
S = 1.07
2319 reflections
138 parameters
0 restraints
$w = 1/[\sigma^2(F_o^2) + (0.030P)^2 + 1.0855P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.99 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)
Al1	0.500000	0.500000	0.500000	0.0098 (5)	0.767 (5)
Cu1	0.500000	0.500000	0.500000	0.0098 (5)	0.233 (5)

Al2	0.67744 (10)	0.500000	0.71929 (12)	0.0130 (3)	
Al3	0.63633 (7)	0.71530 (13)	0.52217 (8)	0.0092 (2)	
Al4	0.80481 (10)	1.000000	0.77266 (12)	0.0077 (3)	
Al5	0.76330 (10)	0.500000	0.46467 (13)	0.0126 (3)	
Al6	0.49067 (7)	0.27023 (14)	0.33038 (8)	0.0094 (2)	
Al7	0.52074 (9)	0.500000	0.17059 (11)	0.0078 (3)	
Al8	0.500000	0.74935 (18)	0.000000	0.0081 (3)	
Al9	0.36802 (7)	0.71228 (13)	0.11008 (8)	0.0077 (2)	
Al10	0.24072 (10)	0.500000	−0.03857 (13)	0.0118 (3)	
Al11	0.08628 (9)	0.500000	−0.21245 (11)	0.0041 (3)	
Al12	0.06612 (10)	0.500000	0.17389 (11)	0.0079 (3)	
Al13	0.18526 (7)	0.71741 (13)	0.11114 (8)	0.0067 (2)	
Al14	0.17782 (7)	0.72118 (13)	0.33455 (8)	0.0081 (2)	
Al15	0.07414 (9)	0.500000	0.58060 (11)	0.0068 (3)	
Fe1	0.40231 (4)	0.500000	−0.01441 (5)	0.00449 (16)	
Fe2	0.08507 (4)	0.500000	0.38222 (5)	0.0057 (2)	0.827 (16)
Cu2	0.08507 (4)	0.500000	0.38222 (5)	0.0057 (2)	0.173 (16)
Fe3	0.09041 (4)	0.500000	−0.01203 (5)	0.00434 (16)	
Fe4	0.68011 (3)	0.79257 (6)	0.72198 (4)	0.00551 (13)	
Fe5	0.59919 (4)	0.500000	0.37535 (5)	0.00489 (15)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Al1	0.0104 (9)	0.0077 (9)	0.0144 (9)	0.000	0.0082 (7)	0.000
Cu1	0.0104 (9)	0.0077 (9)	0.0144 (9)	0.000	0.0082 (7)	0.000
Al2	0.0183 (9)	0.0072 (8)	0.0132 (8)	0.000	0.0040 (7)	0.000
Al3	0.0100 (5)	0.0113 (6)	0.0066 (5)	−0.0016 (5)	0.0031 (4)	−0.0020 (4)
Al4	0.0066 (7)	0.0062 (8)	0.0090 (7)	0.000	0.0006 (6)	0.000
Al5	0.0066 (7)	0.0088 (8)	0.0189 (8)	0.000	−0.0011 (6)	0.000
Al6	0.0068 (5)	0.0108 (6)	0.0090 (5)	−0.0036 (4)	0.0001 (4)	0.0009 (4)
Al7	0.0062 (7)	0.0101 (8)	0.0059 (7)	0.000	0.0000 (6)	0.000
Al8	0.0070 (7)	0.0064 (8)	0.0113 (7)	0.000	0.0031 (6)	0.000
Al9	0.0076 (5)	0.0093 (6)	0.0060 (5)	0.0016 (4)	0.0016 (4)	−0.0008 (4)
Al10	0.0048 (7)	0.0097 (8)	0.0221 (8)	0.000	0.0061 (6)	0.000
Al11	0.0069 (7)	0.0008 (7)	0.0050 (6)	0.000	0.0025 (5)	0.000
Al12	0.0080 (7)	0.0084 (8)	0.0074 (7)	0.000	0.0023 (6)	0.000
Al13	0.0059 (5)	0.0089 (6)	0.0050 (5)	−0.0015 (4)	0.0011 (4)	−0.0013 (4)
Al14	0.0097 (5)	0.0086 (6)	0.0072 (5)	−0.0023 (4)	0.0044 (4)	−0.0010 (4)
Al15	0.0078 (7)	0.0055 (8)	0.0068 (7)	0.000	0.0018 (6)	0.000
Fe1	0.0036 (3)	0.0049 (4)	0.0050 (3)	0.000	0.0015 (3)	0.000
Fe2	0.0058 (4)	0.0055 (4)	0.0062 (3)	0.000	0.0024 (3)	0.000
Cu2	0.0058 (4)	0.0055 (4)	0.0062 (3)	0.000	0.0024 (3)	0.000
Fe3	0.0037 (3)	0.0049 (4)	0.0044 (3)	0.000	0.0013 (3)	0.000
Fe4	0.0045 (2)	0.0067 (3)	0.0053 (2)	0.0003 (2)	0.00140 (18)	−0.00024 (18)
Fe5	0.0047 (3)	0.0043 (4)	0.0047 (3)	0.000	0.0000 (2)	0.000

Geometric parameters (Å, º)

Al1—Fe5	2.4975 (7)	Al7—Al6	2.8672 (15)
Al1—Fe5^{i}	2.4976 (7)	Al7—Al6^{iii}	2.8672 (15)
Al1—Al6	2.7889 (11)	Al7—Al8^{xiii}	2.8801 (14)
Al1—Al6^{i}	2.7889 (11)	Al7—Al8	2.8801 (14)
Al1—Al6^{ii}	2.7889 (11)	Al8—Fe3^{v}	2.4942 (13)
Al1—Al6^{iii}	2.7889 (11)	Al8—Fe3^{xiv}	2.4942 (13)
Cu1—Fe5	2.4975 (7)	Al8—Fe1^{xiii}	2.4944 (13)
Cu1—Fe5^{i}	2.4976 (7)	Al8—Fe1	2.4945 (13)
Cu1—Al6	2.7889 (11)	Al8—Al13^{iv}	2.7909 (10)
Cu1—Al6^{i}	2.7889 (11)	Al8—Al13^{xiv}	2.7909 (10)
Cu1—Al6^{ii}	2.7889 (11)	Al8—Al9	2.8044 (10)
Cu1—Al6^{iii}	2.7889 (11)	Al8—Al9^{xv}	2.8044 (10)
Al2—Fe4	2.3677 (5)	Al8—Al12^{v}	2.9188 (14)
Al2—Fe4^{iii}	2.3677 (5)	Al8—Al12^{xiv}	2.9188 (14)
Al2—Al3	2.9229 (16)	Al9—Fe1	2.4804 (11)
Al2—Al3^{iii}	2.9229 (16)	Al9—Fe4^{ii}	2.5157 (11)
Al2—Al9^{ii}	2.9834 (16)	Al9—Al11^{xiv}	2.6462 (12)
Al2—Al9^{i}	2.9834 (16)	Al9—Al13^{xiv}	2.6918 (14)
Al3—Fe4	2.4585 (11)	Al9—Fe3^{xiv}	2.7952 (11)
Al3—Fe5	2.4665 (11)	Al9—Al13	2.8327 (14)
Al3—Al14^{iv}	2.6616 (13)	Al9—Al10	2.8364 (16)
Al3—Al15^{v}	2.6821 (12)	Al9—Al10^{xiv}	2.8516 (13)
Al3—Cu1	2.6843 (10)	Al10—Fe1	2.4257 (15)
Al3—Al1	2.6843 (10)	Al10—Fe3	2.4475 (15)
Al3—Al6^{iii}	2.7452 (14)	Al10—Al11	2.694 (2)
Al3—Al5^{vi}	2.7550 (13)	Al10—Al13^{xiv}	2.8277 (13)
Al3—Fe2^{v}	2.8538 (11)	Al10—Al13^{xvi}	2.8277 (13)
Al3—Al5	2.8762 (16)	Al10—Al13^{iii}	2.8820 (15)
Al3—Al14^{ii}	2.8870 (15)	Al10—Al13	2.8820 (15)
Al4—Fe4^{vii}	2.4891 (11)	Al11—Fe3	2.4842 (14)
Al4—Fe4	2.4891 (11)	Al11—Fe4^{xvii}	2.5142 (11)
Al4—Al7^{vi}	2.574 (2)	Al11—Fe4^{xviii}	2.5142 (11)
Al4—Fe1^{viii}	2.6265 (15)	Al11—Al15^{xix}	2.5333 (19)
Al4—Al14^{ii}	2.6785 (13)	Al11—Al12^{xx}	2.547 (2)
Al4—Al14^{ix}	2.6785 (13)	Al11—Fe2^{xx}	2.8452 (15)
Al4—Al13^{ix}	2.6872 (12)	Al12—Fe3	2.4627 (15)
Al4—Al13^{ii}	2.6872 (12)	Al12—Cu2	2.5276 (15)
Al4—Fe5^{vi}	2.7018 (16)	Al12—Fe2	2.5276 (15)
Al4—Al10^{viii}	2.823 (2)	Al12—Fe3^{xx}	2.6391 (16)
Al4—Al5^{vi}	2.827 (2)	Al12—Al13	2.8265 (15)
Al5—Fe5	2.4423 (16)	Al12—Al13^{iii}	2.8265 (15)
Al5—Fe2^{i}	2.5344 (16)	Al12—Al14	2.8460 (15)
Al5—Al15^{i}	2.741 (2)	Al12—Al14^{iii}	2.8460 (15)
Al5—Al14^{x}	2.8580 (14)	Al13—Fe3	2.4974 (11)
Al5—Al14^{iv}	2.8580 (14)	Al13—Fe4^{ii}	2.5305 (11)
Al5—Al14^{ii}	2.9875 (16)	Al13—Fe1^{xiv}	2.7431 (11)

Al5—Al14^{i}	2.9875 (16)	Al13—Al14	2.8274 (14)
Al6—Fe5	2.4528 (11)	Al14—Cu2	2.4776 (11)
Al6—Fe4^{i}	2.5722 (11)	Al14—Fe2	2.4776 (11)
Al6—Fe2^{x}	2.5994 (11)	Al14—Fe4^{ii}	2.5715 (11)
Al6—Al11^{xi}	2.7013 (13)	Al14—Fe5^{xxi}	2.6847 (11)
Al6—Al15^{xii}	2.7755 (13)	Al15—Fe2	2.5342 (15)
Al6—Al9^{iii}	2.8292 (14)	Al15—Cu2	2.5342 (15)
Al6—Al14^{x}	2.9077 (15)	Al15—Al15^{xxii}	2.549 (3)
Al7—Fe1	2.4723 (15)	Al15—Fe4^{xxiii}	2.6185 (12)
Al7—Fe5	2.4734 (15)	Al15—Fe4^{xxiv}	2.6185 (12)
Al7—Fe1^{xiii}	2.5768 (15)	Al15—Fe2^{xxii}	2.6428 (15)
Al7—Al9	2.8313 (15)	Fe1—Fe1^{xiii}	2.9337 (13)
Al7—Al9^{iii}	2.8313 (15)	Fe3—Fe3^{xx}	2.9040 (13)

Fe4^{vii}—Al4—Fe4	84.80 (5)	Al13^{iii}—Al10—Al13	75.23 (5)
Fe4^{vii}—Al4—Al7^{vi}	137.45 (3)	Fe3—Al11—Fe4^{xvii}	119.23 (4)
Fe4—Al4—Al7^{vi}	137.45 (3)	Fe3—Al11—Fe4^{xviii}	119.23 (4)
Fe4^{vii}—Al4—Fe1^{viii}	114.75 (4)	Fe4^{xvii}—Al11—Fe4^{xviii}	83.76 (5)
Fe4—Al4—Fe1^{viii}	114.75 (4)	Fe3—Al11—Al15^{xix}	177.35 (7)
Al7^{vi}—Al4—Fe1^{viii}	59.40 (5)	Fe4^{xvii}—Al11—Al15^{xix}	62.50 (4)
Fe4^{vii}—Al4—Al14^{ii}	128.98 (6)	Fe4^{xviii}—Al11—Al15^{xix}	62.50 (4)
Fe4—Al4—Al14^{ii}	59.55 (3)	Fe3—Al11—Al12^{xx}	63.26 (5)
Al7^{vi}—Al4—Al14^{ii}	83.15 (4)	Fe4^{xvii}—Al11—Al12^{xx}	136.19 (3)
Fe1^{viii}—Al4—Al14^{ii}	113.07 (4)	Fe4^{xviii}—Al11—Al12^{xx}	136.19 (3)
Fe4^{vii}—Al4—Al14^{ix}	59.55 (3)	Al15^{xix}—Al11—Al12^{xx}	114.09 (7)
Fe4—Al4—Al14^{ix}	128.98 (6)	Fe3—Al11—Al9^{xiv}	65.94 (3)
Al7^{vi}—Al4—Al14^{ix}	83.15 (4)	Fe4^{xvii}—Al11—Al9^{xiv}	58.29 (3)
Fe1^{viii}—Al4—Al14^{ix}	113.07 (4)	Fe4^{xviii}—Al11—Al9^{xiv}	130.46 (6)
Al14^{ii}—Al4—Al14^{ix}	114.76 (7)	Al15^{xix}—Al11—Al9^{xiv}	114.74 (4)
Fe4^{vii}—Al4—Al13^{ix}	58.38 (3)	Al12^{xx}—Al11—Al9^{xiv}	92.01 (4)
Fe4—Al4—Al13^{ix}	128.55 (6)	Fe3—Al11—Al9^{xvi}	65.94 (3)
Al7^{vi}—Al4—Al13^{ix}	88.22 (4)	Fe4^{xvii}—Al11—Al9^{xvi}	130.46 (6)
Fe1^{viii}—Al4—Al13^{ix}	62.15 (3)	Fe4^{xviii}—Al11—Al9^{xvi}	58.29 (3)
Al14^{ii}—Al4—Al13^{ix}	171.37 (7)	Al15^{xix}—Al11—Al9^{xvi}	114.74 (4)
Al14^{ix}—Al4—Al13^{ix}	63.60 (3)	Al12^{xx}—Al11—Al9^{xvi}	92.01 (4)
Fe4^{vii}—Al4—Al13^{ii}	128.55 (6)	Al9^{xiv}—Al11—Al9^{xvi}	123.22 (7)
Fe4—Al4—Al13^{ii}	58.38 (3)	Fe3—Al11—Al10	56.23 (4)
Al7^{vi}—Al4—Al13^{ii}	88.22 (4)	Fe4^{xvii}—Al11—Al10	78.70 (4)
Fe1^{viii}—Al4—Al13^{ii}	62.15 (3)	Fe4^{xviii}—Al11—Al10	78.70 (4)
Al14^{ii}—Al4—Al13^{ii}	63.60 (3)	Al15^{xix}—Al11—Al10	126.41 (7)
Al14^{ix}—Al4—Al13^{ii}	171.37 (7)	Al12^{xx}—Al11—Al10	119.50 (7)
Al13^{ix}—Al4—Al13^{ii}	116.62 (7)	Al9^{xiv}—Al11—Al10	64.54 (3)
Fe4^{vii}—Al4—Fe5^{vi}	111.81 (4)	Al9^{xvi}—Al11—Al10	64.54 (3)
Fe4—Al4—Fe5^{vi}	111.81 (4)	Fe3—Al11—Al6^{xi}	114.88 (4)
Al7^{vi}—Al4—Fe5^{vi}	55.86 (4)	Fe4^{xvii}—Al11—Al6^{xi}	124.41 (6)
Fe1^{viii}—Al4—Fe5^{vi}	115.26 (6)	Fe4^{xviii}—Al11—Al6^{xi}	58.97 (3)
Al14^{ii}—Al4—Fe5^{vi}	59.86 (3)	Al15^{xix}—Al11—Al6^{xi}	63.94 (4)
Al14^{ix}—Al4—Fe5^{vi}	59.86 (3)	Al12^{xx}—Al11—Al6^{xi}	79.83 (4)

Al13^{ix}—Al4—Fe5^{vi}	114.62 (4)	Al9^{xiv}—Al11—Al6^{xi}	169.68 (6)
Al13^{ii}—Al4—Fe5^{vi}	114.62 (4)	Al9^{xvi}—Al11—Al6^{xi}	63.87 (3)
Fe4^{vii}—Al4—Al10^{viii}	76.68 (4)	Al10—Al11—Al6^{xi}	125.06 (3)
Fe4—Al4—Al10^{viii}	76.68 (4)	Fe3—Al11—Al6^{xxvi}	114.88 (4)
Al7^{vi}—Al4—Al10^{viii}	112.11 (6)	Fe4^{xvii}—Al11—Al6^{xxvi}	58.97 (3)
Fe1^{viii}—Al4—Al10^{viii}	52.72 (4)	Fe4^{xviii}—Al11—Al6^{xxvi}	124.41 (6)
Al14^{ii}—Al4—Al10^{viii}	122.14 (3)	Al15^{xix}—Al11—Al6^{xxvi}	63.95 (4)
Al14^{ix}—Al4—Al10^{viii}	122.14 (3)	Al12^{xx}—Al11—Al6^{xxvi}	79.83 (4)
Al13^{ix}—Al4—Al10^{viii}	61.70 (3)	Al9^{xiv}—Al11—Al6^{xxvi}	63.87 (3)
Al13^{ii}—Al4—Al10^{viii}	61.70 (3)	Al9^{xvi}—Al11—Al6^{xxvi}	169.68 (6)
Fe5^{vi}—Al4—Al10^{viii}	167.97 (7)	Al10—Al11—Al6^{xxvi}	125.06 (3)
Fe4^{vii}—Al4—Al5^{vi}	73.82 (4)	Al6^{xi}—Al11—Al6^{xxvi}	108.08 (6)
Fe4—Al4—Al5^{vi}	73.82 (4)	Fe3—Al11—Fe2^{xx}	118.84 (5)
Al7^{vi}—Al4—Al5^{vi}	108.23 (6)	Fe4^{xvii}—Al11—Fe2^{xx}	104.89 (4)
Fe1^{viii}—Al4—Al5^{vi}	167.63 (7)	Fe4^{xviii}—Al11—Fe2^{xx}	104.89 (4)
Al14^{ii}—Al4—Al5^{vi}	62.48 (4)	Al15^{xix}—Al11—Fe2^{xx}	58.52 (4)
Al14^{ix}—Al4—Al5^{vi}	62.48 (4)	Al12^{xx}—Al11—Fe2^{xx}	55.57 (4)
Al13^{ix}—Al4—Al5^{vi}	120.52 (3)	Al9^{xiv}—Al11—Fe2^{xx}	114.26 (4)
Al13^{ii}—Al4—Al5^{vi}	120.52 (3)	Al9^{xvi}—Al11—Fe2^{xx}	114.26 (4)
Fe5^{vi}—Al4—Al5^{vi}	52.38 (4)	Al10—Al11—Fe2^{xx}	175.07 (6)
Al10^{viii}—Al4—Al5^{vi}	139.65 (7)	Al6^{xi}—Al11—Fe2^{xx}	55.82 (3)
Fe4—Al2—Fe4^{iii}	177.84 (8)	Al6^{xxvi}—Al11—Fe2^{xx}	55.82 (3)
Fe4—Al2—Al3	54.16 (3)	Fe3—Al12—Cu2	165.30 (7)
Fe4^{iii}—Al2—Al3	127.32 (6)	Fe3—Al12—Fe2	165.30 (7)
Fe4—Al2—Al3^{iii}	127.32 (6)	Fe3—Al12—Al11^{xx}	126.50 (7)
Fe4^{iii}—Al2—Al3^{iii}	54.16 (3)	Fe2—Al12—Al11^{xx}	68.20 (5)
Al3—Al2—Al3^{iii}	73.17 (5)	Fe3—Al12—Fe3^{xx}	69.29 (4)
Fe4—Al2—Al9^{ii}	54.63 (3)	Fe2—Al12—Fe3^{xx}	125.41 (6)
Fe4^{iii}—Al2—Al9^{ii}	124.91 (6)	Al11^{xx}—Al12—Fe3^{xx}	57.21 (5)
Al3—Al2—Al9^{ii}	102.72 (3)	Fe3—Al12—Al13	55.84 (3)
Al3^{iii}—Al2—Al9^{ii}	155.03 (7)	Cu2—Al12—Al13	113.87 (5)
Fe4—Al2—Al9^{i}	124.91 (6)	Fe2—Al12—Al13	113.87 (5)
Fe4^{iii}—Al2—Al9^{i}	54.63 (3)	Al11^{xx}—Al12—Al13	140.57 (3)
Al3—Al2—Al9^{i}	155.02 (7)	Fe3^{xx}—Al12—Al13	108.15 (5)
Al3^{iii}—Al2—Al9^{i}	102.72 (3)	Fe3—Al12—Al13^{iii}	55.84 (3)
Al9^{ii}—Al2—Al9^{i}	70.30 (5)	Fe2—Al12—Al13^{iii}	113.87 (5)
Fe4—Al3—Fe5	149.72 (5)	Al11^{xx}—Al12—Al13^{iii}	140.57 (3)
Fe4—Al3—Al14^{iv}	141.13 (5)	Fe3^{xx}—Al12—Al13^{iii}	108.15 (5)
Fe5—Al3—Al14^{iv}	63.00 (3)	Al13—Al12—Al13^{iii}	76.98 (5)
Fe4—Al3—Al15^{v}	61.06 (4)	Fe3—Al12—Al14	115.47 (5)
Fe5—Al3—Al15^{v}	141.94 (5)	Cu2—Al12—Al14	54.52 (3)
Al14^{iv}—Al3—Al15^{v}	106.06 (5)	Fe2—Al12—Al14	54.52 (3)
Fe4—Al3—Cu1	103.55 (4)	Al11^{xx}—Al12—Al14	105.36 (5)
Fe5—Al3—Cu1	57.82 (3)	Fe3^{xx}—Al12—Al14	139.29 (3)
Al14^{iv}—Al3—Cu1	115.32 (4)	Al13—Al12—Al14	59.79 (4)
Al15^{v}—Al3—Cu1	104.45 (4)	Al13^{iii}—Al12—Al14	106.24 (6)
Fe4—Al3—Al1	103.55 (4)	Fe3—Al12—Al14^{iii}	115.47 (5)
Fe5—Al3—Al1	57.82 (3)	Fe2—Al12—Al14^{iii}	54.52 (3)

Al14^{iv}—Al3—Al1	115.32 (4)	Al11^{xx}—Al12—Al14^{iii}	105.36 (5)
Al15^{v}—Al3—Al1	104.45 (4)	Fe3^{xx}—Al12—Al14^{iii}	139.29 (3)
Fe4—Al3—Al6^{iii}	140.65 (5)	Al13—Al12—Al14^{iii}	106.24 (6)
Fe5—Al3—Al6^{iii}	55.84 (3)	Al13^{iii}—Al12—Al14^{iii}	59.79 (3)
Al14^{iv}—Al3—Al6^{iii}	65.04 (4)	Al14—Al12—Al14^{iii}	77.93 (6)
Al15^{v}—Al3—Al6^{iii}	86.19 (5)	Fe3—Al12—Al8^{xxiv}	54.43 (3)
Al1—Al3—Al6^{iii}	61.80 (3)	Fe2—Al12—Al8^{xxiv}	132.07 (3)
Fe4—Al3—Al5^{vi}	75.59 (4)	Al11^{xx}—Al12—Al8^{xxiv}	90.35 (4)
Fe5—Al3—Al5^{vi}	129.35 (5)	Fe3^{xx}—Al12—Al8^{xxiv}	53.04 (3)
Al14^{iv}—Al3—Al5^{vi}	66.92 (5)	Al13—Al12—Al8^{xxiv}	109.66 (5)
Al15^{v}—Al3—Al5^{vi}	60.54 (4)	Al13^{iii}—Al12—Al8^{xxiv}	58.10 (3)
Al1—Al3—Al5^{vi}	163.70 (5)	Al14—Al12—Al8^{xxiv}	163.95 (6)
Al6^{iii}—Al3—Al5^{vi}	108.31 (5)	Al14^{iii}—Al12—Al8^{xxiv}	95.00 (3)
Fe4—Al3—Fe2^{v}	110.81 (4)	Fe3—Al12—Al8^{xiv}	54.43 (3)
Fe5—Al3—Fe2^{v}	99.01 (4)	Fe2—Al12—Al8^{xiv}	132.07 (3)
Al14^{iv}—Al3—Fe2^{v}	53.25 (3)	Al11^{xx}—Al12—Al8^{xiv}	90.35 (4)
Al15^{v}—Al3—Fe2^{v}	54.38 (4)	Fe3^{xx}—Al12—Al8^{xiv}	53.04 (3)
Al1—Al3—Fe2^{v}	113.45 (4)	Al13—Al12—Al8^{xiv}	58.10 (3)
Al6^{iii}—Al3—Fe2^{v}	55.28 (3)	Al13^{iii}—Al12—Al8^{xiv}	109.66 (5)
Al5^{vi}—Al3—Fe2^{v}	53.69 (4)	Al14—Al12—Al8^{xiv}	95.00 (3)
Fe4—Al3—Al5	114.19 (5)	Al14^{iii}—Al12—Al8^{xiv}	163.95 (6)
Fe5—Al3—Al5	53.74 (4)	Al8^{xxiv}—Al12—Al8^{xiv}	88.03 (6)
Al14^{iv}—Al3—Al5	62.00 (4)	Fe3—Al13—Fe4^{ii}	149.09 (5)
Al15^{v}—Al3—Al5	156.54 (5)	Fe3—Al13—Al4^{ix}	149.09 (5)
Cu1—Al3—Al5	99.00 (4)	Fe4^{ii}—Al13—Al4^{ix}	56.89 (4)
Al1—Al3—Al5	99.00 (4)	Fe3—Al13—Al9^{xiv}	65.06 (3)
Al6^{iii}—Al3—Al5	104.45 (5)	Fe4^{ii}—Al13—Al9^{xiv}	135.38 (5)
Al5^{vi}—Al3—Al5	96.06 (3)	Al4^{ix}—Al13—Al9^{xiv}	108.87 (5)
Fe2^{v}—Al3—Al5	114.79 (4)	Fe3—Al13—Fe1^{xiv}	101.39 (4)
Fe4—Al3—Al14^{ii}	56.83 (3)	Fe4^{ii}—Al13—Fe1^{xiv}	109.53 (4)
Fe5—Al3—Al14^{ii}	115.75 (5)	Al4^{ix}—Al13—Fe1^{xiv}	57.84 (4)
Al14^{iv}—Al3—Al14^{ii}	94.59 (4)	Al9^{xiv}—Al13—Fe1^{xiv}	54.30 (3)
Al15^{v}—Al3—Al14^{ii}	100.92 (5)	Fe3—Al13—Al8^{xiv}	55.95 (4)
Al1—Al3—Al14^{ii}	132.65 (4)	Fe4^{ii}—Al13—Al8^{xiv}	148.11 (5)
Al6^{iii}—Al3—Al14^{ii}	159.63 (5)	Al4^{ix}—Al13—Al8^{xiv}	93.86 (5)
Al5^{vi}—Al3—Al14^{ii}	60.82 (4)	Al9^{xiv}—Al13—Al8^{xiv}	61.50 (3)
Fe2^{v}—Al3—Al14^{ii}	113.85 (4)	Fe1^{xiv}—Al13—Al8^{xiv}	53.57 (4)
Al5—Al3—Al14^{ii}	62.45 (4)	Fe3—Al13—Al12	54.68 (3)
Fe4—Al3—Al2	51.32 (3)	Fe4^{ii}—Al13—Al12	111.35 (5)
Fe5—Al3—Al2	98.43 (4)	Al4^{ix}—Al13—Al12	108.33 (5)
Al14^{iv}—Al3—Al2	143.85 (5)	Al9^{xiv}—Al13—Al12	113.25 (5)
Al15^{v}—Al3—Al2	106.66 (5)	Fe1^{xiv}—Al13—Al12	111.38 (4)
Cu1—Al3—Al2	70.26 (4)	Al8^{xiv}—Al13—Al12	62.61 (4)
Al1—Al3—Al2	70.26 (4)	Fe3—Al13—Al14	114.97 (4)
Al6^{iii}—Al3—Al2	132.07 (5)	Fe4^{ii}—Al13—Al14	57.04 (3)
Al5^{vi}—Al3—Al2	118.31 (5)	Al4^{ix}—Al13—Al14	58.05 (4)
Fe2^{v}—Al3—Al2	160.96 (5)	Al9^{xiv}—Al13—Al14	156.71 (5)
Al5—Al3—Al2	81.93 (5)	Fe1^{xiv}—Al13—Al14	105.20 (4)

Al14^{ii}—Al3—Al2	64.42 (4)	Al8^{xiv}—Al13—Al14	98.32 (4)
Fe5—Al5—Fe2^{i}	159.85 (7)	Al12—Al13—Al14	60.45 (4)
Fe5—Al5—Al15^{i}	142.89 (7)	Fe3—Al13—Al10^{xiv}	126.27 (5)
Fe2^{i}—Al5—Al15^{i}	57.25 (4)	Fe4^{ii}—Al13—Al10^{xiv}	75.96 (4)
Fe5—Al5—Al3^{vi}	121.06 (4)	Al4^{ix}—Al13—Al10^{xiv}	61.51 (4)
Fe2^{i}—Al5—Al3^{vi}	65.15 (4)	Al9^{xiv}—Al13—Al10^{xiv}	61.79 (4)
Al15^{i}—Al5—Al3^{vi}	58.41 (3)	Fe1^{xiv}—Al13—Al10^{xiv}	51.60 (3)
Fe5—Al5—Al3^{xxv}	121.06 (4)	Al8^{xiv}—Al13—Al10^{xiv}	102.58 (5)
Fe2^{i}—Al5—Al3^{xxv}	65.15 (4)	Al12—Al13—Al10^{xiv}	162.64 (5)
Al15^{i}—Al5—Al3^{xxv}	58.41 (3)	Al14—Al13—Al10^{xiv}	116.75 (5)
Al3^{vi}—Al5—Al3^{xxv}	113.47 (7)	Fe3—Al13—Al9	112.75 (4)
Fe5—Al5—Al4^{vi}	61.19 (5)	Fe4^{ii}—Al13—Al9	55.60 (3)
Fe2^{i}—Al5—Al4^{vi}	138.96 (7)	Al4^{ix}—Al13—Al9	97.03 (5)
Al15^{i}—Al5—Al4^{vi}	81.70 (6)	Al9^{xiv}—Al13—Al9	89.53 (4)
Al3^{vi}—Al5—Al4^{vi}	94.91 (5)	Fe1^{xiv}—Al13—Al9	111.71 (4)
Al3^{xxv}—Al5—Al4^{vi}	94.91 (5)	Al8^{xiv}—Al13—Al9	151.00 (4)
Fe5—Al5—Al14^{x}	60.26 (3)	Al12—Al13—Al9	136.79 (5)
Fe2^{i}—Al5—Al14^{x}	126.18 (3)	Al14—Al13—Al9	110.25 (4)
Al15^{i}—Al5—Al14^{x}	100.22 (5)	Al10^{xiv}—Al13—Al9	60.50 (4)
Al3^{vi}—Al5—Al14^{x}	148.06 (7)	Fe3—Al13—Al10	53.55 (3)
Al3^{xxv}—Al5—Al14^{x}	61.87 (3)	Fe4^{ii}—Al13—Al10	110.34 (5)
Al4^{vi}—Al5—Al14^{x}	56.22 (3)	Al4^{ix}—Al13—Al10	152.92 (5)
Fe5—Al5—Al14^{iv}	60.26 (3)	Al9^{xiv}—Al13—Al10	61.43 (4)
Fe2^{i}—Al5—Al14^{iv}	126.18 (3)	Fe1^{xiv}—Al13—Al10	115.34 (4)
Al15^{i}—Al5—Al14^{iv}	100.22 (5)	Al8^{xiv}—Al13—Al10	101.55 (5)
Al3^{vi}—Al5—Al14^{iv}	61.87 (3)	Al12—Al13—Al10	98.54 (4)
Al3^{xxv}—Al5—Al14^{iv}	148.06 (7)	Al14—Al13—Al10	139.16 (5)
Al4^{vi}—Al5—Al14^{iv}	56.22 (3)	Al10^{xiv}—Al13—Al10	93.19 (3)
Al14^{x}—Al5—Al14^{iv}	104.25 (6)	Al9—Al13—Al10	59.51 (4)
Fe5—Al5—Al3^{iii}	54.52 (4)	Fe2—Al14—Fe4^{ii}	146.58 (5)
Fe2^{i}—Al5—Al3^{iii}	110.94 (5)	Fe2—Al14—Al3^{xxiii}	67.35 (4)
Al15^{i}—Al5—Al3^{iii}	142.30 (3)	Fe4^{ii}—Al14—Al3^{xxiii}	130.88 (5)
Al3^{vi}—Al5—Al3^{iii}	155.12 (6)	Fe2—Al14—Al4^{ix}	151.93 (6)
Al3^{xxv}—Al5—Al3^{iii}	83.93 (3)	Fe4^{ii}—Al14—Al4^{ix}	56.56 (4)
Al4^{vi}—Al5—Al3^{iii}	101.38 (5)	Al3^{xxiii}—Al14—Al4^{ix}	111.43 (5)
Al14^{x}—Al5—Al3^{iii}	55.31 (3)	Fe2—Al14—Fe5^{xxi}	103.42 (4)
Al14^{iv}—Al5—Al3^{iii}	112.77 (6)	Fe4^{ii}—Al14—Fe5^{xxi}	109.77 (4)
Fe5—Al5—Al3	54.52 (4)	Al3^{xxiii}—Al14—Fe5^{xxi}	54.95 (3)
Fe2^{i}—Al5—Al3	110.94 (5)	Al4^{ix}—Al14—Fe5^{xxi}	60.50 (4)
Al15^{i}—Al5—Al3	142.30 (3)	Cu2—Al14—Al13	115.49 (4)
Al3^{vi}—Al5—Al3	83.93 (3)	Fe2—Al14—Al13	115.49 (4)
Al3^{xxv}—Al5—Al3	155.12 (6)	Fe4^{ii}—Al14—Al13	55.66 (3)
Al4^{vi}—Al5—Al3	101.38 (5)	Al3^{xxiii}—Al14—Al13	164.61 (5)
Al14^{x}—Al5—Al3	112.77 (6)	Al4^{ix}—Al14—Al13	58.35 (4)
Al14^{iv}—Al5—Al3	55.31 (3)	Fe5^{xxi}—Al14—Al13	110.71 (4)
Al3^{iii}—Al5—Al3	74.56 (6)	Cu2—Al14—Al12	56.18 (4)
Fe5—Al5—Al14^{ii}	113.06 (5)	Fe2—Al14—Al12	56.18 (4)
Fe2^{i}—Al5—Al14^{ii}	52.54 (3)	Fe4^{ii}—Al14—Al12	109.50 (5)

Al15^{i}—Al5—Al14^{ii}	96.26 (5)	Al3^{xxiii}—Al14—Al12	118.96 (5)
Al3^{vi}—Al5—Al14^{ii}	55.04 (3)	Al4^{ix}—Al14—Al12	108.01 (5)
Al3^{xxv}—Al5—Al14^{ii}	115.39 (6)	Fe5^{xxi}—Al14—Al12	116.70 (5)
Al4^{vi}—Al5—Al14^{ii}	143.20 (3)	Al13—Al14—Al12	59.76 (4)
Al14^{x}—Al5—Al14^{ii}	156.89 (6)	Fe2—Al14—Al5^{xxi}	129.43 (5)
Al14^{iv}—Al5—Al14^{ii}	88.51 (3)	Fe4^{ii}—Al14—Al5^{xxi}	72.10 (4)
Al3^{iii}—Al5—Al14^{ii}	102.12 (5)	Al3^{xxiii}—Al14—Al5^{xxi}	62.69 (5)
Al3—Al5—Al14^{ii}	58.95 (4)	Al4^{ix}—Al14—Al5^{xxi}	61.30 (4)
Fe5—Al5—Al14^{i}	113.06 (5)	Fe5^{xxi}—Al14—Al5^{xxi}	52.17 (3)
Fe2^{i}—Al5—Al14^{i}	52.54 (3)	Al13—Al14—Al5^{xxi}	114.73 (5)
Al15^{i}—Al5—Al14^{i}	96.26 (5)	Al12—Al14—Al5^{xxi}	166.75 (5)
Al3^{vi}—Al5—Al14^{i}	115.39 (6)	Fe2—Al14—Al3^{ii}	112.32 (4)
Al3^{xxv}—Al5—Al14^{i}	55.04 (3)	Fe4^{ii}—Al14—Al3^{ii}	53.16 (3)
Al4^{vi}—Al5—Al14^{i}	143.20 (3)	Al3^{xxiii}—Al14—Al3^{ii}	85.41 (4)
Al14^{x}—Al5—Al14^{i}	88.51 (3)	Al4^{ix}—Al14—Al3^{ii}	95.21 (5)
Al14^{iv}—Al5—Al14^{i}	156.89 (6)	Fe5^{xxi}—Al14—Al3^{ii}	108.64 (4)
Al3^{iii}—Al5—Al14^{i}	58.95 (4)	Al13—Al14—Al3^{ii}	106.17 (4)
Al3—Al5—Al14^{i}	102.12 (5)	Al12—Al14—Al3^{ii}	134.62 (5)
Al14^{ii}—Al5—Al14^{i}	73.60 (5)	Al5^{xxi}—Al14—Al3^{ii}	57.31 (4)
Fe5—Al1—Fe5^{i}	180.0	Fe2—Al14—Al6^{xxi}	57.05 (3)
Fe5—Al1—Al3	56.71 (2)	Fe4^{ii}—Al14—Al6^{xxi}	153.47 (5)
Fe5^{i}—Al1—Al3	123.29 (2)	Al3^{xxiii}—Al14—Al6^{xxi}	58.87 (4)
Fe5—Al1—Al3^{i}	123.29 (2)	Al4^{ix}—Al14—Al6^{xxi}	97.32 (5)
Fe5^{i}—Al1—Al3^{i}	56.71 (2)	Fe5^{xxi}—Al14—Al6^{xxi}	51.84 (3)
Al3—Al1—Al3^{i}	180.0	Al13—Al14—Al6^{xxi}	108.91 (4)
Fe5—Al1—Al3^{iii}	56.71 (2)	Al12—Al14—Al6^{xxi}	71.69 (4)
Fe5^{i}—Al1—Al3^{iii}	123.29 (2)	Al5^{xxi}—Al14—Al6^{xxi}	100.84 (5)
Al3—Al1—Al3^{iii}	80.93 (5)	Al3^{ii}—Al14—Al6^{xxi}	144.27 (5)
Al3^{i}—Al1—Al3^{iii}	99.07 (5)	Fe2—Al14—Al5^{i}	54.29 (3)
Fe5—Al1—Al3^{ii}	123.29 (2)	Fe4^{ii}—Al14—Al5^{i}	107.32 (5)
Fe5^{i}—Al1—Al3^{ii}	56.71 (2)	Al3^{xxiii}—Al14—Al5^{i}	58.03 (4)
Al3—Al1—Al3^{ii}	99.07 (5)	Al4^{ix}—Al14—Al5^{i}	150.77 (5)
Al3^{i}—Al1—Al3^{ii}	80.93 (5)	Fe5^{xxi}—Al14—Al5^{i}	112.58 (4)
Al3^{iii}—Al1—Al3^{ii}	180.00 (4)	Al13—Al14—Al5^{i}	136.71 (5)
Fe5—Al1—Al6	54.96 (2)	Al12—Al14—Al5^{i}	100.31 (4)
Fe5^{i}—Al1—Al6	125.04 (2)	Al5^{xxi}—Al14—Al5^{i}	91.49 (3)
Al3—Al1—Al6	111.58 (3)	Al3^{ii}—Al14—Al5^{i}	58.60 (4)
Al3^{i}—Al1—Al6	68.42 (3)	Al6^{xxi}—Al14—Al5^{i}	98.27 (4)
Al3^{iii}—Al1—Al6	60.17 (3)	Al11^{xxvii}—Al15—Fe2	172.31 (7)
Al3^{ii}—Al1—Al6	119.83 (3)	Al11^{xxvii}—Al15—Cu2	172.31 (7)
Fe5—Al1—Al6^{i}	125.04 (2)	Al11^{xxvii}—Al15—Al15^{xxii}	125.05 (9)
Fe5^{i}—Al1—Al6^{i}	54.96 (2)	Fe2—Al15—Al15^{xxii}	62.65 (6)
Al3—Al1—Al6^{i}	68.42 (3)	Al11^{xxvii}—Al15—Fe4^{xxiii}	58.39 (4)
Al3^{i}—Al1—Al6^{i}	111.58 (3)	Fe2—Al15—Fe4^{xxiii}	116.38 (4)
Al3^{iii}—Al1—Al6^{i}	119.83 (3)	Al15^{xxii}—Al15—Fe4^{xxiii}	139.47 (3)
Al3^{ii}—Al1—Al6^{i}	60.17 (3)	Al11^{xxvii}—Al15—Fe4^{xxiv}	58.39 (4)
Al6—Al1—Al6^{i}	180.0	Fe2—Al15—Fe4^{xxiv}	116.38 (4)
Fe5—Al1—Al6^{ii}	125.04 (2)	Al15^{xxii}—Al15—Fe4^{xxiv}	139.47 (3)

Fe5^{i}—Al1—Al6^{ii}	54.96 (2)	Fe4^{xxiii}—Al15—Fe4^{xxiv}	79.73 (4)
Al3—Al1—Al6^{ii}	119.83 (3)	Al11^{xxvii}—Al15—Fe2^{xxii}	66.65 (5)
Al3^{i}—Al1—Al6^{ii}	60.17 (3)	Fe2—Al15—Fe2^{xxii}	121.04 (5)
Al3^{iii}—Al1—Al6^{ii}	68.42 (3)	Al15^{xxii}—Al15—Fe2^{xxii}	58.40 (5)
Al3^{ii}—Al1—Al6^{ii}	111.58 (3)	Fe4^{xxiii}—Al15—Fe2^{xxii}	107.89 (4)
Al6—Al1—Al6^{ii}	96.39 (4)	Fe4^{xxiv}—Al15—Fe2^{xxii}	107.89 (4)
Al6^{i}—Al1—Al6^{ii}	83.62 (4)	Al11^{xxvii}—Al15—Al3^{xxiii}	110.88 (4)
Fe5—Al1—Al6^{iii}	54.96 (2)	Fe2—Al15—Al3^{xxiii}	66.27 (3)
Fe5^{i}—Al1—Al6^{iii}	125.04 (2)	Al15^{xxii}—Al15—Al3^{xxiii}	95.53 (5)
Al3—Al1—Al6^{iii}	60.17 (3)	Fe4^{xxiii}—Al15—Al3^{xxiii}	55.25 (3)
Al3^{i}—Al1—Al6^{iii}	119.83 (3)	Fe4^{xxiv}—Al15—Al3^{xxiii}	122.08 (6)
Al3^{iii}—Al1—Al6^{iii}	111.58 (3)	Fe2^{xxii}—Al15—Al3^{xxiii}	118.62 (3)
Al3^{ii}—Al1—Al6^{iii}	68.42 (3)	Al11^{xxvii}—Al15—Al3^{xxiv}	110.88 (4)
Al6—Al1—Al6^{iii}	83.61 (4)	Fe2—Al15—Al3^{xxiv}	66.26 (3)
Al6^{i}—Al1—Al6^{iii}	96.38 (4)	Al15^{xxii}—Al15—Al3^{xxiv}	95.53 (5)
Al6^{ii}—Al1—Al6^{iii}	180.0	Fe4^{xxiii}—Al15—Al3^{xxiv}	122.08 (6)
Fe5—Cu1—Fe5^{i}	180.0	Fe4^{xxiv}—Al15—Al3^{xxiv}	55.25 (3)
Fe5—Cu1—Al3	56.71 (2)	Fe2^{xxii}—Al15—Al3^{xxiv}	118.62 (3)
Fe5^{i}—Cu1—Al3	123.29 (2)	Al3^{xxiii}—Al15—Al3^{xxiv}	118.38 (7)
Fe5—Cu1—Al3^{i}	123.29 (2)	Al11^{xxvii}—Al15—Al5^{i}	115.05 (7)
Fe5^{i}—Cu1—Al3^{i}	56.71 (2)	Fe2—Al15—Al5^{i}	57.26 (4)
Al3—Cu1—Al3^{i}	180.0	Al15^{xxii}—Al15—Al5^{i}	119.91 (8)
Fe5—Cu1—Al3^{iii}	56.71 (2)	Fe4^{xxiii}—Al15—Al5^{i}	73.37 (4)
Fe5^{i}—Cu1—Al3^{iii}	123.29 (2)	Fe4^{xxiv}—Al15—Al5^{i}	73.37 (4)
Al3—Cu1—Al3^{iii}	80.93 (5)	Fe2^{xxii}—Al15—Al5^{i}	178.30 (7)
Al3^{i}—Cu1—Al3^{iii}	99.07 (5)	Al3^{xxiii}—Al15—Al5^{i}	61.05 (3)
Fe5—Cu1—Al3^{ii}	123.29 (2)	Al3^{xxiv}—Al15—Al5^{i}	61.05 (3)
Fe5^{i}—Cu1—Al3^{ii}	56.71 (2)	Al11^{xxvii}—Al15—Al6^{xxviii}	60.97 (4)
Al3—Cu1—Al3^{ii}	99.07 (5)	Fe2—Al15—Al6^{xxviii}	122.12 (4)
Al3^{i}—Cu1—Al3^{ii}	80.93 (5)	Al15^{xxii}—Al15—Al6^{xxviii}	88.17 (5)
Al3^{iii}—Cu1—Al3^{ii}	180.00 (4)	Fe4^{xxiii}—Al15—Al6^{xxviii}	56.87 (3)
Fe5—Cu1—Al6	54.96 (2)	Fe4^{xxiv}—Al15—Al6^{xxviii}	117.61 (5)
Fe5^{i}—Cu1—Al6	125.04 (2)	Fe2^{xxii}—Al15—Al6^{xxviii}	57.27 (3)
Al3—Cu1—Al6	111.58 (3)	Al3^{xxiii}—Al15—Al6^{xxviii}	68.65 (3)
Al3^{i}—Cu1—Al6	68.42 (3)	Al3^{xxiv}—Al15—Al6^{xxviii}	171.54 (6)
Al3^{iii}—Cu1—Al6	60.17 (3)	Al5^{i}—Al15—Al6^{xxviii}	123.31 (4)
Al3^{ii}—Cu1—Al6	119.83 (3)	Al11^{xxvii}—Al15—Al6^{xii}	60.97 (4)
Fe5—Cu1—Al6^{i}	125.04 (2)	Fe2—Al15—Al6^{xii}	122.12 (4)
Fe5^{i}—Cu1—Al6^{i}	54.96 (2)	Al15^{xxii}—Al15—Al6^{xii}	88.17 (5)
Al3—Cu1—Al6^{i}	68.42 (3)	Fe4^{xxiii}—Al15—Al6^{xii}	117.61 (5)
Al3^{i}—Cu1—Al6^{i}	111.58 (3)	Fe4^{xxiv}—Al15—Al6^{xii}	56.87 (3)
Al3^{iii}—Cu1—Al6^{i}	119.83 (3)	Fe2^{xxii}—Al15—Al6^{xii}	57.27 (3)
Al3^{ii}—Cu1—Al6^{i}	60.17 (3)	Al3^{xxiii}—Al15—Al6^{xii}	171.54 (6)
Al6—Cu1—Al6^{i}	180.0	Al3^{xxiv}—Al15—Al6^{xii}	68.65 (3)
Fe5—Cu1—Al6^{ii}	125.04 (2)	Al5^{i}—Al15—Al6^{xii}	123.31 (4)
Fe5^{i}—Cu1—Al6^{ii}	54.96 (2)	Al6^{xxviii}—Al15—Al6^{xii}	103.96 (6)
Al3—Cu1—Al6^{ii}	119.83 (3)	Al2—Fe4—Al3	74.52 (5)
Al3^{i}—Cu1—Al6^{ii}	60.17 (3)	Al2—Fe4—Al4	133.36 (5)

Al3^{iii}—Cu1—Al6^{ii}	68.42 (3)	Al3—Fe4—Al4	112.44 (4)
Al3^{ii}—Cu1—Al6^{ii}	111.58 (3)	Al2—Fe4—Al11^{viii}	131.51 (5)
Al6—Cu1—Al6^{ii}	96.39 (4)	Al3—Fe4—Al11^{viii}	119.51 (4)
Al6^{i}—Cu1—Al6^{ii}	83.62 (4)	Al4—Fe4—Al11^{viii}	86.96 (4)
Fe5—Cu1—Al6^{iii}	54.96 (2)	Al2—Fe4—Al9^{ii}	75.25 (5)
Fe5^{i}—Cu1—Al6^{iii}	125.04 (2)	Al3—Fe4—Al9^{ii}	136.09 (4)
Al3—Cu1—Al6^{iii}	60.17 (3)	Al4—Fe4—Al9^{ii}	111.46 (4)
Al3^{i}—Cu1—Al6^{iii}	119.83 (3)	Al11^{viii}—Fe4—Al9^{ii}	63.48 (4)
Al3^{iii}—Cu1—Al6^{iii}	111.58 (3)	Al2—Fe4—Al13^{ii}	77.16 (5)
Al3^{ii}—Cu1—Al6^{iii}	68.42 (3)	Al3—Fe4—Al13^{ii}	132.64 (4)
Al6—Cu1—Al6^{iii}	83.61 (4)	Al4—Fe4—Al13^{ii}	64.73 (4)
Al6^{i}—Cu1—Al6^{iii}	96.38 (4)	Al11^{viii}—Fe4—Al13^{ii}	107.72 (4)
Al6^{ii}—Cu1—Al6^{iii}	180.0	Al9^{ii}—Fe4—Al13^{ii}	68.30 (3)
Fe1—Al7—Fe5	162.97 (7)	Al2—Fe4—Al14^{ii}	77.54 (5)
Fe1—Al7—Al4^{vi}	132.34 (7)	Al3—Fe4—Al14^{ii}	70.01 (4)
Fe5—Al7—Al4^{vi}	64.70 (5)	Al4—Fe4—Al14^{ii}	63.89 (4)
Fe1—Al7—Fe1^{xiii}	71.01 (4)	Al11^{viii}—Fe4—Al14^{ii}	150.05 (4)
Fe5—Al7—Fe1^{xiii}	126.02 (6)	Al9^{ii}—Fe4—Al14^{ii}	131.78 (4)
Al4^{vi}—Al7—Fe1^{xiii}	61.32 (5)	Al13^{ii}—Fe4—Al14^{ii}	67.30 (3)
Fe1—Al7—Al9	55.27 (3)	Al2—Fe4—Al6^{i}	77.69 (5)
Fe5—Al7—Al9	112.48 (5)	Al3—Fe4—Al6^{i}	75.42 (4)
Al4^{vi}—Al7—Al9	142.52 (3)	Al4—Fe4—Al6^{i}	148.71 (4)
Fe1^{xiii}—Al7—Al9	109.81 (5)	Al11^{viii}—Fe4—Al6^{i}	64.15 (4)
Fe1—Al7—Al9^{iii}	55.27 (3)	Al9^{ii}—Fe4—Al6^{i}	67.56 (3)
Fe5—Al7—Al9^{iii}	112.48 (5)	Al13^{ii}—Fe4—Al6^{i}	133.29 (4)
Al4^{vi}—Al7—Al9^{iii}	142.52 (3)	Al14^{ii}—Fe4—Al6^{i}	141.63 (4)
Fe1^{xiii}—Al7—Al9^{iii}	109.81 (5)	Al2—Fe4—Al15^{v}	128.80 (5)
Al9—Al7—Al9^{iii}	74.70 (5)	Al3—Fe4—Al15^{v}	63.69 (4)
Fe1—Al7—Al6	114.77 (5)	Al4—Fe4—Al15^{v}	90.95 (4)
Fe5—Al7—Al6	54.07 (3)	Al11^{viii}—Fe4—Al15^{v}	59.11 (4)
Al4^{vi}—Al7—Al6	100.82 (5)	Al9^{ii}—Fe4—Al15^{v}	116.35 (4)
Fe1^{xiii}—Al7—Al6	137.51 (3)	Al13^{ii}—Fe4—Al15^{v}	153.92 (4)
Al9—Al7—Al6	106.24 (5)	Al14^{ii}—Fe4—Al15^{v}	111.77 (4)
Al9^{iii}—Al7—Al6	59.53 (3)	Al6^{i}—Fe4—Al15^{v}	64.64 (4)
Fe1—Al7—Al6^{iii}	114.77 (5)	Al5—Fe5—Al6^{iii}	130.42 (3)
Fe5—Al7—Al6^{iii}	54.07 (3)	Al5—Fe5—Al6	130.42 (3)
Al4^{vi}—Al7—Al6^{iii}	100.82 (5)	Al6^{iii}—Fe5—Al6	98.57 (5)
Fe1^{xiii}—Al7—Al6^{iii}	137.51 (3)	Al5—Fe5—Al3^{iii}	71.73 (4)
Al9—Al7—Al6^{iii}	59.53 (3)	Al6^{iii}—Fe5—Al3^{iii}	133.91 (4)
Al9^{iii}—Al7—Al6^{iii}	106.24 (5)	Al6—Fe5—Al3^{iii}	67.84 (4)
Al6—Al7—Al6^{iii}	80.85 (6)	Al5—Fe5—Al3	71.73 (4)
Fe1—Al7—Al8^{xiii}	54.92 (3)	Al6^{iii}—Fe5—Al3	67.84 (4)
Fe5—Al7—Al8^{xiii}	132.33 (3)	Al6—Fe5—Al3	133.91 (4)
Al4^{vi}—Al7—Al8^{xiii}	94.27 (4)	Al3^{iii}—Fe5—Al3	89.87 (5)
Fe1^{xiii}—Al7—Al8^{xiii}	54.06 (3)	Al5—Fe5—Al7	125.88 (6)
Al9—Al7—Al8^{xiii}	109.39 (5)	Al6^{iii}—Fe5—Al7	71.19 (3)
Al9^{iii}—Al7—Al8^{xiii}	58.81 (3)	Al6—Fe5—Al7	71.18 (3)
Al6—Al7—Al8^{xiii}	93.18 (3)	Al3^{iii}—Fe5—Al7	134.27 (3)

Al6^{iii}—Al7—Al8^{xiii}	164.56 (6)	Al3—Fe5—Al7	134.27 (3)
Fe1—Al7—Al8	54.92 (3)	Al5—Fe5—Al1	117.81 (4)
Fe5—Al7—Al8	132.33 (3)	Al6^{iii}—Fe5—Al1	68.57 (3)
Al4^{vi}—Al7—Al8	94.27 (4)	Al6—Fe5—Al1	68.57 (3)
Fe1^{xiii}—Al7—Al8	54.06 (3)	Al3^{iii}—Fe5—Al1	65.47 (3)
Al9—Al7—Al8	58.81 (3)	Al3—Fe5—Al1	65.47 (3)
Al9^{iii}—Al7—Al8	109.39 (5)	Al7—Fe5—Al1	116.31 (4)
Al6—Al7—Al8	164.56 (6)	Al5—Fe5—Cu1	117.81 (4)
Al6^{iii}—Al7—Al8	93.18 (3)	Al6^{iii}—Fe5—Cu1	68.57 (3)
Al8^{xiii}—Al7—Al8	88.94 (6)	Al6—Fe5—Cu1	68.57 (3)
Fe5—Al6—Fe4^{i}	141.86 (5)	Al3^{iii}—Fe5—Cu1	65.47 (3)
Fe5—Al6—Fe2^{x}	106.68 (4)	Al3—Fe5—Cu1	65.47 (3)
Fe4^{i}—Al6—Fe2^{x}	110.67 (4)	Al7—Fe5—Cu1	116.31 (4)
Fe5—Al6—Al11^{xi}	153.57 (6)	Al5—Fe5—Al14^{iv}	67.57 (3)
Fe4^{i}—Al6—Al11^{xi}	56.88 (4)	Al6^{iii}—Fe5—Al14^{iv}	68.77 (3)
Fe2^{x}—Al6—Al11^{xi}	64.89 (4)	Al6—Fe5—Al14^{iv}	155.74 (4)
Fe5—Al6—Al3^{iii}	56.32 (3)	Al3^{iii}—Fe5—Al14^{iv}	135.91 (4)
Fe4^{i}—Al6—Al3^{iii}	137.44 (5)	Al3—Fe5—Al14^{iv}	62.05 (3)
Fe2^{x}—Al6—Al3^{iii}	64.48 (3)	Al7—Fe5—Al14^{iv}	84.94 (3)
Al11^{xi}—Al6—Al3^{iii}	128.18 (5)	Al1—Fe5—Al14^{iv}	121.24 (2)
Fe5—Al6—Al15^{xii}	144.22 (5)	Al5—Fe5—Al14^{x}	67.57 (3)
Fe4^{i}—Al6—Al15^{xii}	58.49 (4)	Al6^{iii}—Fe5—Al14^{x}	155.74 (4)
Fe2^{x}—Al6—Al15^{xii}	58.80 (4)	Al6—Fe5—Al14^{x}	68.77 (3)
Al11^{xi}—Al6—Al15^{xii}	55.08 (4)	Al3^{iii}—Fe5—Al14^{x}	62.05 (3)
Al3^{iii}—Al6—Al15^{xii}	89.14 (5)	Al3—Fe5—Al14^{x}	135.91 (4)
Fe5—Al6—Cu1	56.47 (3)	Al7—Fe5—Al14^{x}	84.94 (3)
Fe4^{i}—Al6—Cu1	97.80 (4)	Al1—Fe5—Al14^{x}	121.24 (2)
Al11^{xi}—Al6—Cu1	149.96 (5)	Al14^{iv}—Fe5—Al14^{x}	114.34 (5)
Al3^{iii}—Al6—Cu1	58.03 (3)	Al5—Fe5—Al4^{vi}	66.44 (5)
Al15^{xii}—Al6—Cu1	99.33 (4)	Al6^{iii}—Fe5—Al4^{vi}	108.92 (4)
Fe5—Al6—Al1	56.47 (3)	Al6—Fe5—Al4^{vi}	108.92 (4)
Fe4^{i}—Al6—Al1	97.80 (4)	Al3^{iii}—Fe5—Al4^{vi}	117.16 (4)
Fe2^{x}—Al6—Al1	118.47 (4)	Al3—Fe5—Al4^{vi}	117.17 (4)
Al11^{xi}—Al6—Al1	149.96 (5)	Al7—Fe5—Al4^{vi}	59.44 (5)
Al3^{iii}—Al6—Al1	58.03 (3)	Al1—Fe5—Al4^{vi}	175.75 (4)
Al15^{xii}—Al6—Al1	99.33 (4)	Al14^{iv}—Fe5—Al4^{vi}	59.64 (3)
Fe5—Al6—Al9^{iii}	113.21 (5)	Al14^{x}—Fe5—Al4^{vi}	59.64 (3)
Fe4^{i}—Al6—Al9^{iii}	55.27 (3)	Al10—Fe1—Al7	123.94 (6)
Fe2^{x}—Al6—Al9^{iii}	116.33 (5)	Al10—Fe1—Al9^{iii}	70.63 (4)
Al11^{xi}—Al6—Al9^{iii}	57.12 (4)	Al7—Fe1—Al9^{iii}	69.73 (4)
Al3^{iii}—Al6—Al9^{iii}	167.13 (5)	Al10—Fe1—Al9	70.63 (4)
Al15^{xii}—Al6—Al9^{iii}	102.22 (5)	Al7—Fe1—Al9	69.73 (4)
Al1—Al6—Al9^{iii}	124.69 (4)	Al9^{iii}—Fe1—Al9	87.66 (5)
Fe5—Al6—Al7	54.74 (4)	Al10—Fe1—Al8^{xiii}	126.02 (2)
Fe4^{i}—Al6—Al7	108.88 (4)	Al7—Fe1—Al8^{xiii}	70.88 (2)
Fe2^{x}—Al6—Al7	121.37 (5)	Al9^{iii}—Fe1—Al8^{xiii}	68.63 (3)
Al11^{xi}—Al6—Al7	106.48 (5)	Al9—Fe1—Al8^{xiii}	139.09 (4)
Al3^{iii}—Al6—Al7	108.37 (5)	Al10—Fe1—Al8	126.02 (2)

Al15^{xii}—Al6—Al7	160.87 (5)	Al7—Fe1—Al8	70.88 (2)
Cu1—Al6—Al7	96.58 (4)	Al9^{iii}—Fe1—Al8	139.09 (4)
Al1—Al6—Al7	96.58 (4)	Al9—Fe1—Al8	68.62 (3)
Al9^{iii}—Al6—Al7	59.60 (4)	Al8^{xiii}—Fe1—Al8	107.96 (5)
Fe5—Al6—Al14^{x}	59.39 (3)	Al10—Fe1—Al7^{xiii}	127.08 (5)
Fe4^{i}—Al6—Al14^{x}	156.65 (5)	Al7—Fe1—Al7^{xiii}	108.99 (4)
Fe2^{x}—Al6—Al14^{x}	53.11 (3)	Al9^{iii}—Fe1—Al7^{xiii}	135.32 (3)
Al11^{xi}—Al6—Al14^{x}	99.81 (5)	Al9—Fe1—Al7^{xiii}	135.32 (3)
Al3^{iii}—Al6—Al14^{x}	56.09 (3)	Al8^{xiii}—Fe1—Al7^{xiii}	69.19 (2)
Al15^{xii}—Al6—Al14^{x}	111.41 (5)	Al8—Fe1—Al7^{xiii}	69.19 (2)
Al1—Al6—Al14^{x}	104.89 (4)	Al10—Fe1—Al4^{xviii}	67.80 (5)
Al9^{iii}—Al6—Al14^{x}	113.16 (5)	Al7—Fe1—Al4^{xviii}	168.26 (5)
Al7—Al6—Al14^{x}	74.26 (4)	Al9^{iii}—Fe1—Al4^{xviii}	117.90 (4)
Fe3^{v}—Al8—Fe3^{xiv}	71.20 (5)	Al9—Fe1—Al4^{xviii}	117.90 (4)
Fe3^{v}—Al8—Fe1^{xiii}	108.862 (18)	Al8^{xiii}—Fe1—Al4^{xviii}	102.79 (3)
Fe3^{xiv}—Al8—Fe1^{xiii}	172.76 (2)	Al8—Fe1—Al4^{xviii}	102.79 (3)
Fe3^{v}—Al8—Fe1	172.76 (2)	Al7^{xiii}—Fe1—Al4^{xviii}	59.28 (5)
Fe3^{xiv}—Al8—Fe1	108.861 (18)	Al10—Fe1—Al13^{xvi}	66.00 (3)
Fe1^{xiii}—Al8—Fe1	72.04 (5)	Al7—Fe1—Al13^{xvi}	122.50 (2)
Fe3^{v}—Al8—Al13^{iv}	56.06 (3)	Al9^{iii}—Fe1—Al13^{xvi}	61.80 (3)
Fe3^{xiv}—Al8—Al13^{iv}	113.68 (5)	Al9—Fe1—Al13^{xvi}	132.99 (4)
Fe1^{xiii}—Al8—Al13^{iv}	62.23 (3)	Al8^{xiii}—Fe1—Al13^{xvi}	64.19 (3)
Fe1—Al8—Al13^{iv}	128.44 (5)	Al8—Fe1—Al13^{xvi}	155.93 (4)
Fe3^{v}—Al8—Al13^{xiv}	113.68 (5)	Al7^{xiii}—Fe1—Al13^{xvi}	86.96 (3)
Fe3^{xiv}—Al8—Al13^{xiv}	56.06 (3)	Al4^{xviii}—Fe1—Al13^{xvi}	60.01 (3)
Fe1^{xiii}—Al8—Al13^{xiv}	128.44 (5)	Al10—Fe1—Al13^{xiv}	66.00 (3)
Fe1—Al8—Al13^{xiv}	62.23 (3)	Al7—Fe1—Al13^{xiv}	122.50 (2)
Al13^{iv}—Al8—Al13^{xiv}	168.94 (7)	Al9^{iii}—Fe1—Al13^{xiv}	132.99 (4)
Fe3^{v}—Al8—Al9	128.48 (5)	Al9—Fe1—Al13^{xiv}	61.80 (3)
Fe3^{xiv}—Al8—Al9	63.36 (3)	Al8^{xiii}—Fe1—Al13^{xiv}	155.93 (3)
Fe1^{xiii}—Al8—Al9	113.21 (5)	Al8—Fe1—Al13^{xiv}	64.19 (3)
Fe1—Al8—Al9	55.45 (3)	Al7^{xiii}—Fe1—Al13^{xiv}	86.96 (3)
Al13^{iv}—Al8—Al9	123.90 (3)	Al4^{xviii}—Fe1—Al13^{xiv}	60.01 (2)
Al13^{xiv}—Al8—Al9	57.51 (3)	Al13^{xvi}—Fe1—Al13^{xiv}	112.93 (5)
Fe3^{v}—Al8—Al9^{xv}	63.36 (3)	Al10—Fe1—Fe1^{xiii}	179.91 (5)
Fe3^{xiv}—Al8—Al9^{xv}	128.48 (5)	Al7—Fe1—Fe1^{xiii}	56.16 (4)
Fe1^{xiii}—Al8—Al9^{xv}	55.45 (3)	Al9^{iii}—Fe1—Fe1^{xiii}	109.43 (3)
Fe1—Al8—Al9^{xv}	113.21 (5)	Al9—Fe1—Fe1^{xiii}	109.43 (3)
Al13^{iv}—Al8—Al9^{xv}	57.51 (3)	Al8^{xiii}—Fe1—Fe1^{xiii}	53.98 (2)
Al13^{xiv}—Al8—Al9^{xv}	123.90 (3)	Al8—Fe1—Fe1^{xiii}	53.98 (2)
Al9—Al8—Al9^{xv}	167.72 (7)	Al7^{xiii}—Fe1—Fe1^{xiii}	52.83 (4)
Fe3^{v}—Al8—Al7^{xiii}	117.58 (3)	Al4^{xviii}—Fe1—Fe1^{xiii}	112.11 (4)
Fe3^{xiv}—Al8—Al7^{xiii}	132.55 (3)	Al13^{xvi}—Fe1—Fe1^{xiii}	113.96 (3)
Fe1^{xiii}—Al8—Al7^{xiii}	54.20 (4)	Al13^{xiv}—Fe1—Fe1^{xiii}	113.96 (3)
Fe1—Al8—Al7^{xiii}	56.75 (4)	Al10—Fe3—Al12	123.53 (6)
Al13^{iv}—Al8—Al7^{xiii}	107.52 (4)	Al10—Fe3—Al11	66.23 (5)
Al13^{xiv}—Al8—Al7^{xiii}	80.44 (4)	Al12—Fe3—Al11	170.24 (6)
Al9—Al8—Al7^{xiii}	110.75 (5)	Al10—Fe3—Al8^{xxiv}	125.58 (2)

Al9^{xv}—Al8—Al7^{xiii}	59.73 (4)	Al12—Fe3—Al8^{xxiv}	72.15 (2)
Fe3^{v}—Al8—Al7	132.55 (3)	Al11—Fe3—Al8^{xxiv}	102.61 (3)
Fe3^{xiv}—Al8—Al7	117.58 (3)	Al10—Fe3—Al8^{xiv}	125.58 (2)
Fe1^{xiii}—Al8—Al7	56.75 (4)	Al12—Fe3—Al8^{xiv}	72.15 (2)
Fe1—Al8—Al7	54.20 (4)	Al11—Fe3—Al8^{xiv}	102.61 (3)
Al13^{iv}—Al8—Al7	80.44 (4)	Al8^{xxiv}—Fe3—Al8^{xiv}	108.80 (5)
Al13^{xiv}—Al8—Al7	107.52 (4)	Al10—Fe3—Al13^{iii}	71.29 (4)
Al9—Al8—Al7	59.73 (4)	Al12—Fe3—Al13^{iii}	69.48 (4)
Al9^{xv}—Al8—Al7	110.75 (5)	Al11—Fe3—Al13^{iii}	116.75 (4)
Al7^{xiii}—Al8—Al7	91.06 (6)	Al8^{xxiv}—Fe3—Al13^{iii}	67.99 (3)
Fe3^{v}—Al8—Al12^{v}	53.42 (4)	Al8^{xiv}—Fe3—Al13^{iii}	140.41 (4)
Fe3^{xiv}—Al8—Al12^{v}	57.72 (4)	Al10—Fe3—Al13	71.29 (4)
Fe1^{xiii}—Al8—Al12^{v}	116.18 (3)	Al12—Fe3—Al13	69.48 (4)
Fe1—Al8—Al12^{v}	133.06 (3)	Al11—Fe3—Al13	116.75 (4)
Al13^{iv}—Al8—Al12^{v}	59.29 (4)	Al8^{xxiv}—Fe3—Al13	140.41 (4)
Al13^{xiv}—Al8—Al12^{v}	112.13 (5)	Al8^{xiv}—Fe3—Al13	67.99 (3)
Al9—Al8—Al12^{v}	81.49 (4)	Al13^{iii}—Fe3—Al13	89.56 (5)
Al9^{xv}—Al8—Al12^{v}	107.25 (4)	Al10—Fe3—Al12^{xx}	125.76 (5)
Al7^{xiii}—Al8—Al12^{v}	166.33 (4)	Al12—Fe3—Al12^{xx}	110.71 (4)
Al7—Al8—Al12^{v}	90.10 (3)	Al11—Fe3—Al12^{xx}	59.53 (5)
Fe3^{v}—Al8—Al12^{xiv}	57.72 (4)	Al8^{xxiv}—Fe3—Al12^{xx}	69.24 (2)
Fe3^{xiv}—Al8—Al12^{xiv}	53.42 (4)	Al8^{xiv}—Fe3—Al12^{xx}	69.24 (2)
Fe1^{xiii}—Al8—Al12^{xiv}	133.06 (3)	Al13^{iii}—Fe3—Al12^{xx}	134.53 (3)
Fe1—Al8—Al12^{xiv}	116.18 (3)	Al13—Fe3—Al12^{xx}	134.53 (3)
Al13^{iv}—Al8—Al12^{xiv}	112.13 (5)	Al10—Fe3—Al9^{xvi}	65.51 (3)
Al13^{xiv}—Al8—Al12^{xiv}	59.29 (4)	Al12—Fe3—Al9^{xvi}	122.33 (2)
Al9—Al8—Al12^{xiv}	107.25 (4)	Al11—Fe3—Al9^{xvi}	59.82 (2)
Al9^{xv}—Al8—Al12^{xiv}	81.49 (4)	Al8^{xxiv}—Fe3—Al9^{xvi}	63.74 (3)
Al7^{xiii}—Al8—Al12^{xiv}	90.10 (3)	Al8^{xiv}—Fe3—Al9^{xvi}	155.76 (4)
Al7—Al8—Al12^{xiv}	166.33 (4)	Al13^{iii}—Fe3—Al9^{xvi}	60.83 (3)
Al12^{v}—Al8—Al12^{xiv}	91.97 (6)	Al13—Fe3—Al9^{xvi}	133.31 (4)
Fe1—Al9—Fe4^{ii}	151.13 (5)	Al12^{xx}—Fe3—Al9^{xvi}	86.83 (3)
Fe1—Al9—Al11^{xiv}	146.65 (5)	Al10—Fe3—Al9^{xiv}	65.51 (3)
Fe4^{ii}—Al9—Al11^{xiv}	58.23 (4)	Al12—Fe3—Al9^{xiv}	122.33 (2)
Fe1—Al9—Al13^{xiv}	63.91 (3)	Al11—Fe3—Al9^{xiv}	59.82 (2)
Fe4^{ii}—Al9—Al13^{xiv}	136.48 (5)	Al8^{xxiv}—Fe3—Al9^{xiv}	155.76 (4)
Al11^{xiv}—Al9—Al13^{xiv}	105.24 (5)	Al8^{xiv}—Fe3—Al9^{xiv}	63.74 (3)
Fe1—Al9—Fe3^{xiv}	100.39 (4)	Al13^{iii}—Fe3—Al9^{xiv}	133.31 (4)
Fe4^{ii}—Al9—Fe3^{xiv}	108.44 (4)	Al13—Fe3—Al9^{xiv}	60.83 (3)
Al11^{xiv}—Al9—Fe3^{xiv}	54.24 (4)	Al12^{xx}—Fe3—Al9^{xiv}	86.83 (3)
Al13^{xiv}—Al9—Fe3^{xiv}	54.11 (3)	Al9^{xvi}—Fe3—Al9^{xiv}	112.78 (5)
Fe1—Al9—Al8	55.93 (4)	Al10—Fe3—Fe3^{xx}	178.25 (5)
Fe4^{ii}—Al9—Al8	145.71 (5)	Al12—Fe3—Fe3^{xx}	58.22 (4)
Al11^{xiv}—Al9—Al8	90.89 (5)	Al11—Fe3—Fe3^{xx}	112.02 (5)
Al13^{xiv}—Al9—Al8	60.99 (3)	Al8^{xxiv}—Fe3—Fe3^{xx}	54.40 (2)
Fe3^{xiv}—Al9—Al8	52.90 (4)	Al8^{xiv}—Fe3—Fe3^{xx}	54.40 (2)
Fe1—Al9—Al6^{iii}	115.83 (5)	Al13^{iii}—Fe3—Fe3^{xx}	109.88 (3)
Fe4^{ii}—Al9—Al6^{iii}	57.17 (3)	Al13—Fe3—Fe3^{xx}	109.88 (3)

Al11^{xiv}—Al9—Al6^{iii}	59.01 (4)	Al12^{xx}—Fe3—Fe3^{xx}	52.49 (4)
Al13^{xiv}—Al9—Al6^{iii}	153.12 (5)	Al9^{xvi}—Fe3—Fe3^{xx}	113.77 (3)
Fe3^{xiv}—Al9—Al6^{iii}	102.03 (4)	Al9^{xiv}—Fe3—Fe3^{xx}	113.77 (3)
Al8—Al9—Al6^{iii}	95.65 (4)	Al14^{iii}—Fe2—Al14	92.50 (5)
Fe1—Al9—Al7	55.00 (4)	Al14^{iii}—Fe2—Al12	69.30 (3)
Fe4^{ii}—Al9—Al7	111.69 (5)	Al14—Fe2—Al12	69.30 (3)
Al11^{xiv}—Al9—Al7	109.06 (5)	Al14^{iii}—Fe2—Al15	116.82 (3)
Al13^{xiv}—Al9—Al7	111.81 (5)	Al14—Fe2—Al15	116.82 (3)
Fe3^{xiv}—Al9—Al7	109.71 (4)	Al12—Fe2—Al15	170.01 (5)
Al8—Al9—Al7	61.47 (4)	Al14^{iii}—Fe2—Al5^{i}	73.17 (4)
Al6^{iii}—Al9—Al7	60.87 (4)	Al14—Fe2—Al5^{i}	73.17 (4)
Fe1—Al9—Al13	114.71 (4)	Al12—Fe2—Al5^{i}	124.50 (5)
Fe4^{ii}—Al9—Al13	56.10 (3)	Al15—Fe2—Al5^{i}	65.49 (5)
Al11^{xiv}—Al9—Al13	96.02 (5)	Al14^{iii}—Fe2—Al6^{xxix}	69.83 (3)
Al13^{xiv}—Al9—Al13	90.47 (4)	Al14—Fe2—Al6^{xxix}	150.51 (4)
Fe3^{xiv}—Al9—Al13	110.70 (4)	Al12—Fe2—Al6^{xxix}	82.17 (3)
Al8—Al9—Al13	151.44 (4)	Al15—Fe2—Al6^{xxix}	92.49 (3)
Al6^{iii}—Al9—Al13	111.67 (4)	Al5^{i}—Fe2—Al6^{xxix}	120.56 (3)
Al7—Al9—Al13	139.54 (5)	Al14^{iii}—Fe2—Al6^{xxi}	150.52 (4)
Fe1—Al9—Al10	53.78 (4)	Al14—Fe2—Al6^{xxi}	69.83 (3)
Fe4^{ii}—Al9—Al10	112.26 (5)	Al12—Fe2—Al6^{xxi}	82.17 (3)
Al11^{xiv}—Al9—Al10	151.50 (5)	Al15—Fe2—Al6^{xxi}	92.49 (3)
Al13^{xiv}—Al9—Al10	61.46 (4)	Al5^{i}—Fe2—Al6^{xxi}	120.56 (3)
Fe3^{xiv}—Al9—Al10	115.11 (4)	Al6^{xxix}—Fe2—Al6^{xxi}	114.53 (5)
Al8—Al9—Al10	102.02 (5)	Al14^{iii}—Fe2—Al15^{xxii}	132.97 (3)
Al6^{iii}—Al9—Al10	142.43 (5)	Al14—Fe2—Al15^{xxii}	132.97 (3)
Al7—Al9—Al10	99.43 (4)	Al12—Fe2—Al15^{xxii}	111.05 (5)
Al13—Al9—Al10	61.11 (4)	Al15—Fe2—Al15^{xxii}	58.96 (5)
Fe1—Al9—Al10^{xiv}	126.00 (5)	Al5^{i}—Fe2—Al15^{xxii}	124.44 (5)
Fe4^{ii}—Al9—Al10^{xiv}	75.74 (4)	Al6^{xxix}—Fe2—Al15^{xxii}	63.93 (3)
Al11^{xiv}—Al9—Al10^{xiv}	58.55 (4)	Al6^{xxi}—Fe2—Al15^{xxii}	63.93 (3)
Al13^{xiv}—Al9—Al10^{xiv}	62.57 (4)	Al14^{iii}—Fe2—Al11^{xx}	107.31 (3)
Fe3^{xiv}—Al9—Al10^{xiv}	51.36 (3)	Al14—Fe2—Al11^{xx}	107.31 (3)
Al8—Al9—Al10^{xiv}	101.98 (5)	Al12—Fe2—Al11^{xx}	56.22 (4)
Al6^{iii}—Al9—Al10^{xiv}	114.86 (5)	Al15—Fe2—Al11^{xx}	113.79 (5)
Al7—Al9—Al10^{xiv}	160.66 (5)	Al5^{i}—Fe2—Al11^{xx}	179.28 (5)
Al13—Al9—Al10^{xiv}	59.66 (4)	Al6^{xxix}—Fe2—Al11^{xx}	59.29 (3)
Al10—Al9—Al10^{xiv}	93.66 (3)	Al6^{xxi}—Fe2—Al11^{xx}	59.29 (3)
Fe1—Al9—Al2^{i}	101.02 (4)	Al15^{xxii}—Fe2—Al11^{xx}	54.83 (4)
Fe4^{ii}—Al9—Al2^{i}	50.12 (3)	Al14^{iii}—Fe2—Al3^{xxiii}	131.08 (4)
Al11^{xiv}—Al9—Al2^{i}	104.35 (4)	Al14—Fe2—Al3^{xxiii}	59.40 (3)
Al13^{xiv}—Al9—Al2^{i}	142.15 (5)	Al12—Fe2—Al3^{xxiii}	123.62 (3)
Fe3^{xiv}—Al9—Al2^{i}	158.17 (4)	Al15—Fe2—Al3^{xxiii}	59.35 (3)
Al8—Al9—Al2^{i}	141.03 (5)	Al5^{i}—Fe2—Al3^{xxiii}	61.16 (3)
Al6^{iii}—Al9—Al2^{i}	64.45 (4)	Al6^{xxix}—Fe2—Al3^{xxiii}	149.49 (4)
Al7—Al9—Al2^{i}	79.61 (4)	Al6^{xxi}—Fe2—Al3^{xxiii}	60.24 (3)
Al13—Al9—Al2^{i}	63.36 (4)	Al15^{xxii}—Fe2—Al3^{xxiii}	89.55 (3)
Al10—Al9—Al2^{i}	81.42 (5)	Al11^{xx}—Fe2—Al3^{xxiii}	118.56 (3)

Al10^{xiv}—Al9—Al2^{i}	116.65 (5)	Al14^{iii}—Fe2—Al3^{xxiv}	59.40 (3)
Fe1—Al10—Fe3	165.79 (8)	Al14—Fe2—Al3^{xxiv}	131.08 (4)
Fe1—Al10—Al11	136.67 (7)	Al12—Fe2—Al3^{xxiv}	123.62 (3)
Fe3—Al10—Al11	57.54 (4)	Al15—Fe2—Al3^{xxiv}	59.35 (3)
Fe1—Al10—Al4^{xviii}	59.48 (5)	Al5^{i}—Fe2—Al3^{xxiv}	61.16 (3)
Fe3—Al10—Al4^{xviii}	134.73 (7)	Al6^{xxix}—Fe2—Al3^{xxiv}	60.24 (3)
Al11—Al10—Al4^{xviii}	77.19 (6)	Al6^{xxi}—Fe2—Al3^{xxiv}	149.49 (4)
Fe1—Al10—Al13^{xiv}	62.40 (3)	Al15^{xxii}—Fe2—Al3^{xxiv}	89.55 (3)
Fe3—Al10—Al13^{xiv}	122.55 (4)	Al11^{xx}—Fe2—Al3^{xxiv}	118.56 (3)
Al11—Al10—Al13^{xiv}	95.06 (5)	Al3^{xxiii}—Fe2—Al3^{xxiv}	107.65 (5)
Al4^{xviii}—Al10—Al13^{xiv}	56.79 (3)	Al14^{iii}—Cu2—Al14	92.50 (5)
Fe1—Al10—Al13^{xvi}	62.40 (3)	Al14^{iii}—Cu2—Al12	69.30 (3)
Fe3—Al10—Al13^{xvi}	122.55 (4)	Al14—Cu2—Al12	69.30 (3)
Al11—Al10—Al13^{xvi}	95.06 (5)	Al14^{iii}—Cu2—Al15	116.82 (3)
Al4^{xviii}—Al10—Al13^{xvi}	56.79 (3)	Al14—Cu2—Al15	116.82 (3)
Al13^{xiv}—Al10—Al13^{xvi}	107.92 (6)	Al12—Cu2—Al15	170.01 (5)
Fe1—Al10—Al9^{iii}	55.59 (4)	Al14^{iii}—Cu2—Al5^{i}	73.17 (4)
Fe3—Al10—Al9^{iii}	114.23 (5)	Al14—Cu2—Al5^{i}	73.17 (4)
Al11—Al10—Al9^{iii}	142.71 (3)	Al12—Cu2—Al5^{i}	124.50 (5)
Al4^{xviii}—Al10—Al9^{iii}	101.28 (5)	Al15—Cu2—Al5^{i}	65.49 (5)
Al13^{xiv}—Al10—Al9^{iii}	115.53 (6)	Al14^{iii}—Cu2—Al6^{xxix}	69.83 (3)
Al13^{xvi}—Al10—Al9^{iii}	56.75 (3)	Al14—Cu2—Al6^{xxix}	150.51 (4)
Fe1—Al10—Al9	55.59 (4)	Al12—Cu2—Al6^{xxix}	82.17 (3)
Fe3—Al10—Al9	114.23 (5)	Al15—Cu2—Al6^{xxix}	92.49 (3)
Al11—Al10—Al9	142.71 (3)	Al5^{i}—Cu2—Al6^{xxix}	120.56 (3)
Al4^{xviii}—Al10—Al9	101.28 (5)	Al14^{iii}—Cu2—Al6^{xxi}	150.52 (4)
Al13^{xiv}—Al10—Al9	56.75 (3)	Al14—Cu2—Al6^{xxi}	69.83 (3)
Al13^{xvi}—Al10—Al9	115.53 (6)	Al12—Cu2—Al6^{xxi}	82.17 (3)
Al9^{iii}—Al10—Al9	74.54 (6)	Al15—Cu2—Al6^{xxi}	92.49 (3)
Fe1—Al10—Al9^{xvi}	121.76 (4)	Al5^{i}—Cu2—Al6^{xxi}	120.56 (3)
Fe3—Al10—Al9^{xvi}	63.13 (3)	Al6^{xxix}—Cu2—Al6^{xxi}	114.53 (5)
Al11—Al10—Al9^{xvi}	56.91 (3)	Al14^{iii}—Cu2—Al15^{xxii}	132.97 (3)
Al4^{xviii}—Al10—Al9^{xvi}	93.59 (4)	Al14—Cu2—Al15^{xxii}	132.97 (3)
Al13^{xiv}—Al10—Al9^{xvi}	144.87 (7)	Al12—Cu2—Al15^{xxii}	111.05 (5)
Al13^{xvi}—Al10—Al9^{xvi}	59.84 (3)	Al15—Cu2—Al15^{xxii}	58.96 (5)
Al9^{iii}—Al10—Al9^{xvi}	86.34 (3)	Al5^{i}—Cu2—Al15^{xxii}	124.44 (5)
Al9—Al10—Al9^{xvi}	157.66 (6)	Al6^{xxix}—Cu2—Al15^{xxii}	63.93 (3)
Fe1—Al10—Al9^{xiv}	121.76 (4)	Al6^{xxi}—Cu2—Al15^{xxii}	63.93 (3)
Fe3—Al10—Al9^{xiv}	63.13 (3)	Al14^{iii}—Cu2—Al11^{xx}	107.31 (3)
Al11—Al10—Al9^{xiv}	56.91 (3)	Al14—Cu2—Al11^{xx}	107.31 (3)
Al4^{xviii}—Al10—Al9^{xiv}	93.59 (4)	Al12—Cu2—Al11^{xx}	56.22 (4)
Al13^{xiv}—Al10—Al9^{xiv}	59.84 (3)	Al15—Cu2—Al11^{xx}	113.79 (5)
Al13^{xvi}—Al10—Al9^{xiv}	144.87 (7)	Al5^{i}—Cu2—Al11^{xx}	179.28 (5)
Al9^{iii}—Al10—Al9^{xiv}	157.66 (6)	Al6^{xxix}—Cu2—Al11^{xx}	59.29 (3)
Al9—Al10—Al9^{xiv}	86.34 (3)	Al6^{xxi}—Cu2—Al11^{xx}	59.29 (3)
Al9^{xvi}—Al10—Al9^{xiv}	109.45 (6)	Al15^{xxii}—Cu2—Al11^{xx}	54.83 (4)
Fe1—Al10—Al13^{iii}	114.78 (5)	Al14^{iii}—Cu2—Al3^{xxiii}	131.08 (4)
Fe3—Al10—Al13^{iii}	55.16 (3)	Al14—Cu2—Al3^{xxiii}	59.40 (3)

Al11—Al10—Al13^{iii}	99.00 (5)	Al12—Cu2—Al3^{xxiii}	123.62 (3)
Al4^{xviii}—Al10—Al13^{iii}	142.36 (3)	Al15—Cu2—Al3^{xxiii}	59.35 (3)
Al13^{xiv}—Al10—Al13^{iii}	158.67 (6)	Al5^{i}—Cu2—Al3^{xxiii}	61.16 (3)
Al13^{xvi}—Al10—Al13^{iii}	86.81 (3)	Al6^{xxix}—Cu2—Al3^{xxiii}	149.49 (4)
Al9^{iii}—Al10—Al13^{iii}	59.38 (4)	Al6^{xxi}—Cu2—Al3^{xxiii}	60.24 (3)
Al9—Al10—Al13^{iii}	103.29 (6)	Al15^{xxii}—Cu2—Al3^{xxiii}	89.55 (3)
Al9^{xvi}—Al10—Al13^{iii}	56.00 (3)	Al11^{xx}—Cu2—Al3^{xxiii}	118.56 (3)
Al9^{xiv}—Al10—Al13^{iii}	115.94 (6)	Al14^{iii}—Cu2—Al3^{xxiv}	59.40 (3)
Fe1—Al10—Al13	114.78 (5)	Al14—Cu2—Al3^{xxiv}	131.08 (4)
Fe3—Al10—Al13	55.16 (3)	Al12—Cu2—Al3^{xxiv}	123.62 (3)
Al11—Al10—Al13	99.00 (5)	Al15—Cu2—Al3^{xxiv}	59.35 (3)
Al4^{xviii}—Al10—Al13	142.36 (3)	Al5^{i}—Cu2—Al3^{xxiv}	61.16 (3)
Al13^{xiv}—Al10—Al13	86.81 (3)	Al6^{xxix}—Cu2—Al3^{xxiv}	60.24 (3)
Al13^{xvi}—Al10—Al13	158.67 (6)	Al6^{xxi}—Cu2—Al3^{xxiv}	149.49 (4)
Al9^{iii}—Al10—Al13	103.29 (6)	Al15^{xxii}—Cu2—Al3^{xxiv}	89.55 (3)
Al9—Al10—Al13	59.38 (4)	Al11^{xx}—Cu2—Al3^{xxiv}	118.56 (3)
Al9^{xvi}—Al10—Al13	115.94 (6)	Al3^{xxiii}—Cu2—Al3^{xxiv}	107.65 (5)
Al9^{xiv}—Al10—Al13	56.00 (3)		

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