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$Al_{13}Fe_3$

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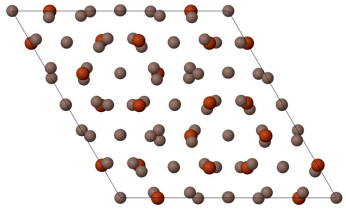
A new trigonal phase with composition $Al_{13}Fe_3$ (tridecaaluminium triiron) was obtained in the binary Fe–Al diagram by high-pressure sintering (HPS) of a stoichiometric Al_3Fe mixture. The refined crystal structure agrees with the descriptions of an unresolved rhombohedral phase reported 30 years ago [Chandrasekaran *et al.* (1988). *Scr. Metall.* **22**, 797–802]. The structure was refined as an inversion twin with a ratio of 0.506 (18):0.494 (18) for the two twin components.

3D view



Structure description

Investigations on the crystal structure of a phase with composition Al_3Fe can be traced back to as early as one century ago (Groth, 1906). Similar efforts continued in the following half century (Osawa, 1933; Bachmetew, 1934; Phragmén, 1950). However, an accurate composition and crystal structure analysis of this phase has been generally accepted to result in a compound with formula λ-$Al_{13}Fe_4$ (Black, 1955*a*,*b*; Armbrüster *et al.*, 2012). A new mineral named hollisterite (Al_3Fe with the λ-$Al_{13}Fe_4$ structure) was discovered very recently during investigation of one fragment of a recovered Khatyrka CV3 carbonaceous chondrite (Ma *et al.*, 2017) while searching for samples to explain the origin of a quasicrystal mineral (Bindi & Steinhardt, 2018). In the present work, a trigonal phase with composition $Al_{13}Fe_3$ was uncovered to be coexistent with the λ-$Al_{13}Fe_4$ phase in the products while simulating the formation of hollisterite under high-pressure and high-temperature conditions (HPHT) by the HPS approach.

There are 96 atoms (78 aluminium plus 18 iron) in the unit cell of the $Al_{13}Fe_3$ structure. The projection of the structure along [001] is shown in Fig. 1, using coordination polyhedra around Al4 atoms for visualization. It is found that there are 18 Al atoms in the unit cell, each of which is coordinated in form of a distorted icosahedron that is formed by two, three, four and three atoms of Fe1, Al2, Al3 and Al6, respectively. All the above

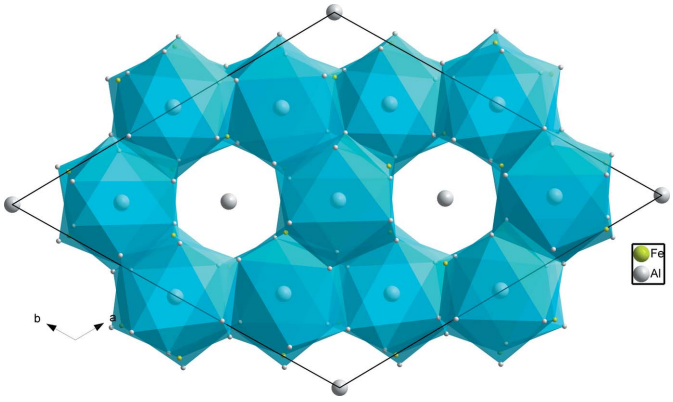


Figure 1
Projection of the new $Al_{13}Fe_3$ phase along the [001] direction showing Al4 atoms with their coordination polyhedra.

mentioned atoms occupy the 18*b* Wyckoff sites while the Al5 atom occupies the 6*a* Wyckoff site.

Fig. 2 shows the environments of the Fe1 and Al5 atoms. Each Fe1 atom is surrounded by ten aluminium atoms including two Al2, two Al3, two Al4, one Al5 and three Al6 atoms, while each Al5 atom is surrounded by three Fe1 atoms, three Al2 and three Al6 atoms.

It should be noted that the present $Al_{13}Fe_3$ phase agrees with the descriptions of an unresolved rhombohedral phase reported 30 years ago (Chandrasekaran *et al.*, 1988).

Synthesis and crystallization

Pure aluminium powder (indicated purity 99.8%) and pure iron powder (indicated purity 99.8%) were mixed according to an atomic ratio of 3:1. The detailed description and the assembled crucible sketch map of the employed HPS process can be found elsewhere (Liu & Fan, 2018). In the current work, the sample was pressurized up to 5 GPa and heated to 1493 K for 30 min, cooled to 1343 K and held at this temperature for one h, and then cooled down rapidly to room temperature. A brick-shaped fragment with dimensions 0.09 × 0.06 × 0.03 mm^3 was selected and mounted on a thin glass fiber for single-crystal X-ray diffraction measurements.

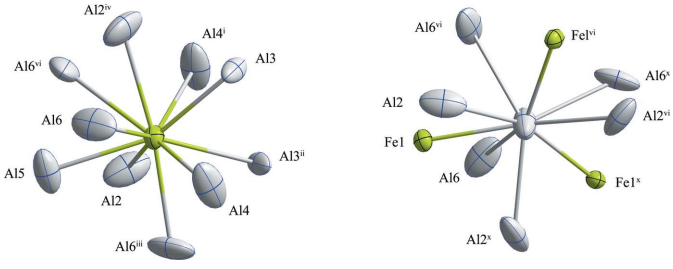


Figure 2
Environments of Fe1 (left) and Al5 (right) atoms. Displacement ellipsoids are given at the 99% probability level. [Symmetry codes: (i) $\frac{1}{3}-x+y,-\frac{1}{3}+y,\frac{1}{6}+z$; (ii) $\frac{1}{3}-x+y,\frac{2}{3}-x,-\frac{1}{3}+z$; (iii) $1-y,1-x,-\frac{1}{2}+z$; (iv) $x,x-y,\frac{1}{2}+z$; (v) $x,x-y,-\frac{1}{2}+z$; (vi) $1-y,x-y,z$; (vii) $\frac{2}{3}-y,\frac{1}{3}+x-y,\frac{1}{3}+z$; (viii) $-\frac{1}{3}+x,\frac{1}{3}+x-y,-\frac{1}{6}+z$; (ix) $1-y,1-x,\frac{1}{2}+z$; (x) $1-x+y,1-x,z$; (xi) $\frac{2}{3}-x+y,\frac{1}{3}+y,-\frac{1}{6}+z$; (xii) $\frac{1}{3}+x,\frac{2}{3}+x-y,\frac{1}{6}+z$.]

Table 1
Experimental details.

Crystal data	
Chemical formula	Al13Fe3
M_r	518.29
Crystal system, space group	Trigonal, *R3c:H*
Temperature (K)	293
a, *c* (Å)	14.5784 (9), 7.7020 (5)
V (Å^3)	1417.6 (2)
Z	6
Radiation type	Mo *Kα*
μ (mm^{-1})	5.69
Crystal size (mm)	0.09 × 0.06 × 0.03
Data collection	
Diffractometer	Bruker D8 Venture Photon 100 COMS
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.590, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	20029, 1017, 954
R_{int}	0.031
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.735
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.020, 0.039, 1.12
No. of reflections	1017
No. of parameters	50
No. of restraints	1
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.45, −0.82
Absolute structure	Refined as an inversion twin.
Absolute structure parameter	0.494 (18)

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. The crystal was refined as an inversion twin with a ratio of 0.506 (18): 0.494 (18) for the two twin components. Although the ADDSYM function in *PLATON* (Spek, 2009) suggested a change from the present space group *R*3*c* to centrosymmetric $R\bar{3}c$, the reliability factors were significantly higher for the centrosymmetric case. Hence the non-centrosymmetric space group was used for the present model.

Acknowledgements

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full crystallographic data

IUCrData (2018). **3**, x180593 [https://doi.org/10.1107/S241431461800593X]

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Tridecaaluminium triiron

Crystal data

Al13Fe3
M_r = 518.29
Trigonal, *R*3*c*:*H*
a = 14.5784 (9) Å
c = 7.7020 (5) Å
V = 1417.6 (2) Å^3
Z = 6
F(000) = 741
D_x = 3.642 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 21502 reflections
θ = 2.8–31.5°
μ = 5.69 mm^{-1}
T = 293 K
Grain, metallic
0.09 × 0.06 × 0.03 mm

Data collection

Bruker D8 Venture Photon 100 COMS diffractometer
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min} = 0.590, T_{max} = 0.746
20029 measured reflections
1017 independent reflections
954 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 31.5°, θ_{min} = 2.8°
h = −21→21
k = −20→21
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.039
S = 1.12
1017 reflections
50 parameters
1 restraint
$w = 1/[\sigma^2(F_o^2) + (0.0208P)^2 + 1.1916P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.81 e Å^{-3}
Absolute structure: Refined as an inversion twin.
Absolute structure parameter: 0.494 (18)

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.
Refinement. Refined as a 2-component inversion twin.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe01	0.49239 (3)	0.33140 (5)	0.49860 (8)	0.00526 (10)

Al02	0.48081 (7)	0.18100 (8)	0.33067 (12)	0.0153 (2)
Al03	0.35885 (7)	0.36146 (7)	0.65909 (13)	0.00896 (16)
Al04	0.50297 (11)	0.49974 (10)	0.4148 (3)	0.01602 (18)
Al05	0.666667	0.333333	0.4775 (3)	0.0134 (3)
Al06	0.63864 (9)	0.47463 (10)	0.66904 (10)	0.0152 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe01	0.00493 (19)	0.00516 (14)	0.00559 (16)	0.00245 (16)	−0.00091 (16)	−0.00119 (11)
Al02	0.0279 (6)	0.0094 (4)	0.0099 (4)	0.0103 (5)	−0.0025 (5)	−0.0030 (4)
Al03	0.0149 (5)	0.0144 (5)	0.0049 (4)	0.0128 (3)	0.0002 (4)	−0.0011 (5)
Al04	0.0114 (3)	0.0066 (3)	0.0311 (5)	0.0053 (3)	0.0047 (3)	0.0037 (3)
Al05	0.0071 (3)	0.0071 (3)	0.0259 (10)	0.00355 (16)	0.000	0.000
Al06	0.0129 (5)	0.0135 (5)	0.0096 (5)	−0.0006 (4)	−0.0016 (4)	−0.0056 (4)

Geometric parameters (Å, º)

Fe01—Al04	2.4667 (16)	Al02—Al04^{ii}	2.832 (2)
Fe01—Al04^{i}	2.4697 (15)	Al02—Al04^{i}	2.8522 (19)
Fe01—Al02	2.4776 (13)	Al03—Al03^{ii}	2.6558 (3)
Fe01—Al06	2.4854 (12)	Al03—Al03^{vii}	2.6558 (4)
Fe01—Al03^{ii}	2.5115 (12)	Al03—Al04^{vii}	2.7230 (19)
Fe01—Al03	2.5226 (12)	Al03—Al04^{i}	2.7254 (18)
Fe01—Al05	2.5319 (4)	Al03—Al06^{viii}	2.7454 (18)
Fe01—Al06^{iii}	2.5797 (11)	Al03—Al04	2.790 (2)
Fe01—Al02^{iv}	2.5893 (13)	Al03—Al04^{ix}	2.821 (2)
Al02—Al06^{iii}	2.6790 (17)	Al04—Al06^{iii}	2.901 (2)
Al02—Al03^{v}	2.7043 (17)	Al04—Al06	2.933 (2)
Al02—Al06^{vi}	2.7269 (11)	Al04—Al06^{viii}	2.9428 (19)
Al02—Al06^{v}	2.7341 (18)	Al05—Al06^{x}	2.7253 (16)
Al02—Al05	2.7450 (13)	Al05—Al06^{vi}	2.7253 (16)
Al02—Al04^{vi}	2.820 (2)	Al05—Al06	2.7254 (16)
Al04—Fe01—Al04^{i}	126.125 (12)	Fe01^{xi}—Al04—Al02^{x}	108.89 (6)
Al04—Fe01—Al02	133.36 (8)	Al03^{ii}—Al04—Al02^{x}	112.86 (6)
Al04^{i}—Fe01—Al02	70.41 (5)	Al03^{xi}—Al04—Al02^{x}	67.36 (4)
Al04—Fe01—Al06	72.65 (5)	Al03—Al04—Al02^{x}	126.10 (6)
Al04^{i}—Fe01—Al06	133.11 (7)	Fe01—Al04—Al03^{iii}	125.60 (8)
Al02—Fe01—Al06	132.02 (4)	Fe01^{xi}—Al04—Al03^{iii}	56.20 (4)
Al04—Fe01—Al03^{ii}	66.31 (4)	Al03^{ii}—Al04—Al03^{iii}	120.99 (10)
Al04^{i}—Fe01—Al03^{ii}	68.99 (6)	Al03^{xi}—Al04—Al03^{iii}	57.19 (3)
Al02—Fe01—Al03^{ii}	86.95 (4)	Al03—Al04—Al03^{iii}	176.46 (8)
Al06—Fe01—Al03^{ii}	137.21 (4)	Al02^{x}—Al04—Al03^{iii}	57.29 (4)
Al04—Fe01—Al03	67.99 (5)	Fe01—Al04—Al02^{vii}	121.54 (9)
Al04^{i}—Fe01—Al03	66.17 (4)	Fe01^{xi}—Al04—Al02^{vii}	57.99 (5)
Al02—Fe01—Al03	133.83 (4)	Al03^{ii}—Al04—Al02^{vii}	122.36 (7)
Al06—Fe01—Al03	90.44 (4)	Al03^{xi}—Al04—Al02^{vii}	58.20 (5)

Al03^{ii}—Fe01—Al03	63.682 (17)	Al03—Al04—Al02^{vii}	75.26 (6)
Al04—Fe01—Al05	114.14 (4)	Al02^{x}—Al04—Al02^{vii}	121.54 (6)
Al04^{i}—Fe01—Al05	119.65 (4)	Al03^{iii}—Al04—Al02^{vii}	103.99 (5)
Al02—Fe01—Al05	66.44 (4)	Fe01—Al04—Al02^{xi}	123.48 (7)
Al06—Fe01—Al05	65.80 (4)	Fe01^{xi}—Al04—Al02^{xi}	54.92 (4)
Al03^{ii}—Fe01—Al05	143.61 (5)	Al03^{ii}—Al04—Al02^{xi}	66.93 (5)
Al03—Fe01—Al05	152.47 (5)	Al03^{xi}—Al04—Al02^{xi}	111.09 (6)
Al04—Fe01—Al06^{iii}	70.15 (6)	Al03—Al04—Al02^{xi}	102.12 (5)
Al04^{i}—Fe01—Al06^{iii}	115.20 (7)	Al02^{x}—Al04—Al02^{xi}	123.32 (8)
Al02—Fe01—Al06^{iii}	63.94 (4)	Al03^{iii}—Al04—Al02^{xi}	74.46 (6)
Al06—Fe01—Al06^{iii}	111.62 (3)	Al02^{vii}—Al04—Al02^{xi}	95.95 (6)
Al03^{ii}—Fe01—Al06^{iii}	65.25 (4)	Fe01—Al04—Al06^{iii}	56.75 (5)
Al03—Fe01—Al06^{iii}	123.20 (4)	Fe01^{xi}—Al04—Al06^{iii}	123.79 (9)
Al05—Fe01—Al06^{iii}	80.44 (6)	Al03^{ii}—Al04—Al06^{iii}	58.33 (5)
Al04—Fe01—Al02^{iv}	113.68 (7)	Al03^{xi}—Al04—Al06^{iii}	121.20 (7)
Al04^{i}—Fe01—Al02^{iv}	68.04 (6)	Al03—Al04—Al06^{iii}	104.09 (5)
Al02—Fe01—Al02^{iv}	112.87 (3)	Al02^{x}—Al04—Al06^{iii}	57.08 (5)
Al06—Fe01—Al02^{iv}	65.16 (4)	Al03^{iii}—Al04—Al06^{iii}	76.79 (6)
Al03^{ii}—Fe01—Al02^{iv}	121.68 (4)	Al02^{vii}—Al04—Al06^{iii}	177.80 (8)
Al03—Fe01—Al02^{iv}	63.86 (4)	Al02^{xi}—Al04—Al06^{iii}	86.24 (6)
Al05—Fe01—Al02^{iv}	92.36 (6)	Fe01—Al04—Al06	53.97 (5)
Al06^{iii}—Fe01—Al02^{iv}	172.79 (4)	Fe01^{xi}—Al04—Al06	127.63 (7)
Fe01—Al02—Fe01^{v}	129.49 (5)	Al03^{ii}—Al04—Al06	110.62 (6)
Fe01—Al02—Al06^{iii}	59.88 (4)	Al03^{xi}—Al04—Al06	71.35 (5)
Fe01^{v}—Al02—Al06^{iii}	69.76 (3)	Al03—Al04—Al06	76.75 (6)
Fe01—Al02—Al03^{v}	148.34 (5)	Al02^{x}—Al04—Al06	56.54 (4)
Fe01^{v}—Al02—Al03^{v}	56.87 (3)	Al03^{iii}—Al04—Al06	106.71 (5)
Al06^{iii}—Al02—Al03^{v}	117.46 (5)	Al02^{vii}—Al04—Al06	86.01 (6)
Fe01—Al02—Al06^{vi}	70.58 (4)	Al02^{xi}—Al04—Al06	177.44 (7)
Fe01^{v}—Al02—Al06^{vi}	154.40 (4)	Al06^{iii}—Al04—Al06	91.80 (6)
Al06^{iii}—Al02—Al06^{vi}	125.55 (5)	Fe01—Al04—Al06^{viii}	110.76 (6)
Al03^{v}—Al02—Al06^{vi}	116.47 (6)	Fe01^{xi}—Al04—Al06^{viii}	67.01 (4)
Fe01—Al02—Al06^{v}	129.03 (5)	Al03^{ii}—Al04—Al06^{viii}	71.23 (5)
Fe01^{v}—Al02—Al06^{v}	55.58 (3)	Al03^{xi}—Al04—Al06^{viii}	108.48 (6)
Al06^{iii}—Al02—Al06^{v}	94.31 (6)	Al03—Al04—Al06^{viii}	57.15 (5)
Al03^{v}—Al02—Al06^{v}	81.63 (4)	Al02^{x}—Al04—Al06^{viii}	175.59 (6)
Al06^{vi}—Al02—Al06^{v}	100.22 (3)	Al03^{iii}—Al04—Al06^{viii}	119.52 (6)
Fe01—Al02—Al05	57.73 (3)	Al02^{vii}—Al04—Al06^{viii}	55.24 (4)
Fe01^{v}—Al02—Al05	113.86 (6)	Al02^{xi}—Al04—Al06^{viii}	56.11 (4)
Al06^{iii}—Al02—Al05	74.96 (5)	Al06^{iii}—Al04—Al06^{viii}	126.25 (7)
Al03^{v}—Al02—Al05	153.71 (5)	Al06—Al04—Al06^{viii}	124.25 (8)
Al06^{vi}—Al02—Al05	59.74 (5)	Fe01^{vi}—Al05—Fe01^{x}	119.592 (12)
Al06^{v}—Al02—Al05	74.09 (5)	Fe01^{vi}—Al05—Fe01	119.591 (12)
Fe01—Al02—Al04^{vi}	134.41 (5)	Fe01^{x}—Al05—Fe01	119.593 (12)
Fe01^{v}—Al02—Al04^{vi}	94.65 (5)	Fe01^{vi}—Al05—Al06^{x}	69.84 (4)
Al06^{iii}—Al02—Al04^{vi}	157.26 (5)	Fe01^{x}—Al05—Al06^{x}	56.28 (3)
Al03^{v}—Al02—Al04^{vi}	61.38 (5)	Fe01—Al05—Al06^{x}	142.70 (10)
Al06^{vi}—Al02—Al04^{vi}	63.83 (5)	Fe01^{vi}—Al05—Al06^{vi}	56.28 (3)

Al06^{v}—Al02—Al04^{vi}	62.96 (5)	Fe01^{x}—Al05—Al06^{vi}	142.70 (10)
Al05—Al02—Al04^{vi}	97.86 (5)	Fe01—Al05—Al06^{vi}	69.84 (4)
Fe01—Al02—Al04^{ii}	98.01 (5)	Al06^{x}—Al05—Al06^{vi}	93.47 (6)
Fe01^{v}—Al02—Al04^{ii}	53.97 (4)	Fe01^{vi}—Al05—Al06	142.70 (10)
Al06^{iii}—Al02—Al04^{ii}	64.48 (4)	Fe01^{x}—Al05—Al06	69.84 (4)
Al03^{v}—Al02—Al04^{ii}	58.92 (4)	Fe01—Al05—Al06	56.28 (3)
Al06^{vi}—Al02—Al04^{ii}	148.11 (6)	Al06^{x}—Al05—Al06	93.47 (6)
Al06^{v}—Al02—Al04^{ii}	109.50 (4)	Al06^{vi}—Al05—Al06	93.47 (6)
Al05—Al02—Al04^{ii}	139.40 (6)	Fe01^{vi}—Al05—Al02	73.73 (3)
Al04^{vi}—Al02—Al04^{ii}	120.25 (6)	Fe01^{x}—Al05—Al02	157.09 (9)
Fe01—Al02—Al04^{i}	54.67 (4)	Fe01—Al05—Al02	55.83 (3)
Fe01^{v}—Al02—Al04^{i}	138.74 (6)	Al06^{x}—Al05—Al02	142.93 (3)
Al06^{iii}—Al02—Al04^{i}	100.82 (5)	Al06^{vi}—Al05—Al02	59.80 (3)
Al03^{v}—Al02—Al04^{i}	99.00 (5)	Al06—Al05—Al02	111.97 (2)
Al06^{vi}—Al02—Al04^{i}	63.62 (5)	Fe01^{vi}—Al05—Al02^{vi}	55.83 (3)
Al06^{v}—Al02—Al04^{i}	162.42 (6)	Fe01^{x}—Al05—Al02^{vi}	73.73 (3)
Al05—Al02—Al04^{i}	101.15 (6)	Fe01—Al05—Al02^{vi}	157.09 (9)
Al04^{vi}—Al02—Al04^{i}	101.74 (6)	Al06^{x}—Al05—Al02^{vi}	59.80 (3)
Al04^{ii}—Al02—Al04^{i}	85.30 (5)	Al06^{vi}—Al05—Al02^{vi}	111.97 (2)
Fe01^{vii}—Al03—Fe01	143.98 (3)	Al06—Al05—Al02^{vi}	142.93 (3)
Fe01^{vii}—Al03—Al03^{ii}	133.94 (6)	Al02—Al05—Al02^{vi}	104.21 (6)
Fe01—Al03—Al03^{ii}	57.96 (4)	Fe01^{vi}—Al05—Al02^{x}	157.09 (9)
Fe01^{vii}—Al03—Al03^{vii}	58.36 (4)	Fe01^{x}—Al05—Al02^{x}	55.83 (3)
Fe01—Al03—Al03^{vii}	129.21 (6)	Fe01—Al05—Al02^{x}	73.73 (3)
Al03^{ii}—Al03—Al03^{vii}	154.39 (4)	Al06^{x}—Al05—Al02^{x}	111.97 (2)
Fe01^{vii}—Al03—Al02^{iv}	111.32 (4)	Al06^{vi}—Al05—Al02^{x}	142.93 (3)
Fe01—Al03—Al02^{iv}	59.27 (4)	Al06—Al05—Al02^{x}	59.80 (3)
Al03^{ii}—Al03—Al02^{iv}	112.41 (7)	Al02—Al05—Al02^{x}	104.21 (6)
Al03^{vii}—Al03—Al02^{iv}	70.04 (4)	Al02^{vi}—Al05—Al02^{x}	104.21 (6)
Fe01^{vii}—Al03—Al04^{vii}	56.05 (5)	Fe01—Al06—Fe01^{ix}	132.10 (5)
Fe01—Al03—Al04^{vii}	158.60 (6)	Fe01—Al06—Al02^{ix}	140.79 (6)
Al03^{ii}—Al03—Al04^{vii}	103.57 (8)	Fe01^{ix}—Al06—Al02^{ix}	56.18 (3)
Al03^{vii}—Al03—Al04^{vii}	62.47 (6)	Fe01—Al06—Al05	57.92 (3)
Al02^{iv}—Al03—Al04^{vii}	129.43 (7)	Fe01^{ix}—Al06—Al05	126.73 (6)
Fe01^{vii}—Al03—Al04^{i}	155.79 (6)	Al02^{ix}—Al06—Al05	86.27 (5)
Fe01—Al03—Al04^{i}	55.99 (5)	Fe01—Al06—Al02^{x}	74.77 (3)
Al03^{ii}—Al03—Al04^{i}	63.22 (7)	Fe01^{ix}—Al06—Al02^{x}	153.01 (4)
Al03^{vii}—Al03—Al04^{i}	99.06 (7)	Al02^{ix}—Al06—Al02^{x}	102.72 (3)
Al02^{iv}—Al03—Al04^{i}	62.88 (6)	Al05—Al06—Al02^{x}	60.46 (5)
Al04^{vii}—Al03—Al04^{i}	107.73 (2)	Fe01—Al06—Al02^{iv}	59.25 (4)
Fe01^{vii}—Al03—Al06^{viii}	58.57 (4)	Fe01^{ix}—Al06—Al02^{iv}	73.19 (3)
Fe01—Al03—Al06^{viii}	115.62 (4)	Al02^{ix}—Al06—Al02^{iv}	106.32 (5)
Al03^{ii}—Al03—Al06^{viii}	75.42 (4)	Al05—Al06—Al02^{iv}	85.20 (6)
Al03^{vii}—Al03—Al06^{viii}	112.38 (7)	Al02^{x}—Al06—Al02^{iv}	132.89 (4)
Al02^{iv}—Al03—Al06^{viii}	157.83 (4)	Fe01—Al06—Al03^{xii}	140.38 (5)
Al04^{vii}—Al03—Al06^{viii}	64.09 (6)	Fe01^{ix}—Al06—Al03^{xii}	56.18 (3)
Al04^{i}—Al03—Al06^{viii}	134.87 (8)	Al02^{ix}—Al06—Al03^{xii}	78.51 (3)
Fe01^{vii}—Al03—Al04	98.30 (5)	Al05—Al06—Al03^{xii}	157.46 (5)

Fe01—Al03—Al04	55.06 (4)	Al02^{x}—Al06—Al03^{xii}	106.64 (6)
Al03^{ii}—Al03—Al04	59.94 (6)	Al02^{iv}—Al06—Al03^{xii}	114.89 (4)
Al03^{vii}—Al03—Al04	145.67 (7)	Fe01—Al06—Al04^{ix}	94.96 (5)
Al02^{iv}—Al03—Al04	100.78 (5)	Fe01^{ix}—Al06—Al04^{ix}	53.10 (4)
Al04^{vii}—Al03—Al04	128.21 (7)	Al02^{ix}—Al06—Al04^{ix}	108.84 (4)
Al04^{i}—Al03—Al04	105.86 (8)	Al05—Al06—Al04^{ix}	144.45 (6)
Al06^{viii}—Al03—Al04	64.23 (5)	Al02^{x}—Al06—Al04^{ix}	139.57 (6)
Fe01^{vii}—Al03—Al04^{ix}	54.81 (4)	Al02^{iv}—Al06—Al04^{ix}	59.96 (4)
Fe01—Al03—Al04^{ix}	96.12 (5)	Al03^{xii}—Al06—Al04^{ix}	57.58 (4)
Al03^{ii}—Al03—Al04^{ix}	145.22 (7)	Fe01—Al06—Al04	53.38 (3)
Al03^{vii}—Al03—Al04^{ix}	59.59 (5)	Fe01^{ix}—Al06—Al04	134.06 (6)
Al02^{iv}—Al03—Al04^{ix}	61.33 (5)	Al02^{ix}—Al06—Al04	157.10 (6)
Al04^{vii}—Al03—Al04^{ix}	105.06 (8)	Al05—Al06—Al04	95.64 (6)
Al04^{i}—Al03—Al04^{ix}	124.15 (7)	Al02^{x}—Al06—Al04	59.63 (5)
Al06^{viii}—Al03—Al04^{ix}	99.98 (5)	Al02^{iv}—Al06—Al04	96.58 (4)
Al04—Al03—Al04^{ix}	86.68 (2)	Al03^{xii}—Al06—Al04	92.20 (6)
Fe01—Al04—Fe01^{xi}	177.68 (6)	Al04^{ix}—Al06—Al04	82.61 (5)
Fe01—Al04—Al03^{ii}	57.63 (4)	Fe01—Al06—Al04^{xii}	134.86 (5)
Fe01^{xi}—Al04—Al03^{ii}	120.42 (7)	Fe01^{ix}—Al06—Al04^{xii}	93.02 (5)
Fe01—Al04—Al03^{xi}	124.13 (7)	Al02^{ix}—Al06—Al04^{xii}	60.28 (4)
Fe01^{xi}—Al04—Al03^{xi}	57.85 (4)	Al05—Al06—Al04^{xii}	99.36 (5)
Al03^{ii}—Al04—Al03^{xi}	177.86 (11)	Al02^{x}—Al06—Al04^{xii}	60.26 (5)
Fe01—Al04—Al03	56.96 (4)	Al02^{iv}—Al06—Al04^{xii}	165.19 (5)
Fe01^{xi}—Al04—Al03	121.17 (7)	Al03^{xii}—Al06—Al04^{xii}	58.62 (5)
Al03^{ii}—Al04—Al03	57.58 (3)	Al04^{ix}—Al06—Al04^{xii}	116.13 (6)
Al03^{xi}—Al04—Al03	124.16 (10)	Al04—Al06—Al04^{xii}	96.98 (5)
Fe01—Al04—Al02^{x}	73.36 (4)		

Symmetry codes: (i) $-x+y+1/3, y-1/3, z+1/6$; (ii) $-x+y+1/3, -x+2/3, z-1/3$; (iii) $-y+1, -x+1, z-1/2$; (iv) $x, x-y, z+1/2$; (v) $x, x-y, z-1/2$; (vi) $-y+1, x-y, z$; (vii) $-y+2/3, x-y+1/3, z+1/3$; (viii) $x-1/3, x-y+1/3, z-1/6$; (ix) $-y+1, -x+1, z+1/2$; (x) $-x+y+1, -x+1, z$; (xi) $-x+y+2/3, y+1/3, z-1/6$; (xii) $x+1/3, x-y+2/3, z+1/6$.