Abstract

Table 1

Experimental details

Crystal data	
Chemical formula	$Al_{78}Fe_{18}$
M_r	3109.74
Crystal system, space group	Trigonal, $R\bar{3}c$:*H*
Temperature (K)	300
a, *c* (Å)	14.5956 (9), 7.6929 (4)
V (Å^3)	1419.27 (19)
Z	1
Radiation type	Mo *K*α
μ (mm^{-1})	5.69
Crystal size (mm)	0.10 × 0.06 × 0.06
Data collection	
Diffractometer	Bruker D8 Venture Photon 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Krause et al., 2015)
T_{min}, T_{max}	0.655, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19200, 367, 341
R_{int}	0.077
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.071, 1.33
No. of reflections	367
No. of parameters	28
	$w = 1/[\sigma^2(F_o^2) + (0.0136P)^2 + 27.4348P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.52, −0.71

Computer programs: *SHELXL2019*/1 (Sheldrick, 2019).

References

NOT FOUND

full crystallographic data

Computing details

Program(s) used to refine structure: *SHELXL2019*/1 (Sheldrick, 2019).

(Al13Fe3)

Crystal data

$Al_{78}Fe_{18}$
$M_r = 3109.74$
Trigonal, $R\bar{3}c$:*H*
$a = 14.5956$ (9) Å
$c = 7.6929$ (4) Å
$V = 1419.27$ (19) Å^3
$Z = 1$
$F(000) = 1482$
$D_x = 3.638$ Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 5370 reflections
θ = 4.8–27.3°
μ = 5.69 mm^{-1}
$T = 300$ K
Lump, gray
0.10 × 0.06 × 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)
$T_{min} = 0.655$, $T_{max} = 0.746$
19200 measured reflections
367 independent reflections
341 reflections with $I > 2\sigma(I)$
$R_{int} = 0.077$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.8°$
$h = -18 \rightarrow 18$
$k = -18 \rightarrow 18$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.071$
$S = 1.33$
367 reflections
28 parameters
0 restraints
$w = 1/[\sigma^2(F_o^2) + (0.0136P)^2 + 27.4348P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.52$ e Å^{-3}
$\Delta\rho_{min} = -0.71$ 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 (Å^2) for (Al13Fe3)

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.333333	0.49355 (6)	0.416667	0.0061 (2)
Al1	0.35988 (13)	0.35988 (13)	0.250000	0.0110 (4)
Al2	0.333333	0.666667	0.416667	0.0180 (8)
Al3	0.48065 (11)	0.63616 (12)	0.24732 (18)	0.0188 (4)
Al4	0.166667	0.333333	0.333333	0.0183 (5)

Atomic displacement parameters (Å^2) for (Al13Fe3)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0066 (4)	0.0062 (3)	0.0056 (4)	0.0033 (2)	0.0014 (3)	0.00069 (14)
Al1	0.0167 (7)	0.0167 (7)	0.0072 (9)	0.0142 (8)	0.0011 (3)	−0.0011 (3)
Al2	0.0085 (10)	0.0085 (10)	0.037 (2)	0.0042 (5)	0.000	0.000
Al3	0.0165 (8)	0.0167 (7)	0.0108 (7)	−0.0009 (6)	0.0058 (5)	0.0001 (5)
Al4	0.0078 (9)	0.0082 (9)	0.0356 (12)	0.0016 (8)	−0.0039 (8)	0.0012 (8)

Geometric parameters (Å, º) for (Al13Fe3)

Fe1—Al4	2.4715 (4)	Al1—Al4^{i}	2.8074 (14)
Fe1—Al4^{i}	2.4715 (4)	Al1—Al4^{v}	2.8074 (14)
Fe1—Al3	2.4855 (14)	Al2—Al3^{viii}	2.7342 (15)
Fe1—Al3^{i}	2.4855 (14)	Al2—Al3^{ix}	2.7342 (15)
Fe1—Al1^{ii}	2.5211 (9)	Al2—Al3^{x}	2.7342 (15)
Fe1—Al1	2.5211 (9)	Al2—Al3^{i}	2.7342 (15)
Fe1—Al2	2.5268 (8)	Al2—Al3	2.7343 (15)
Fe1—Al3^{iii}	2.5774 (14)	Al2—Al3^{xi}	2.7343 (15)
Fe1—Al3^{iv}	2.5774 (14)	Al3—Al3^{iii}	2.705 (2)
Al1—Al1^{v}	2.6507 (9)	Al3—Al3^{xii}	2.705 (2)
Al1—Al1^{ii}	2.6507 (9)	Al3—Al3^{viii}	2.717 (3)
Al1—Al3^{vi}	2.7195 (15)	Al3—Al4^{v}	2.8654 (15)
Al1—Al3^{iii}	2.7195 (15)	Al3—Al4^{ix}	2.8771 (14)
Al1—Al4	2.7242 (12)	Al3—Al4^{i}	2.8929 (16)
Al1—Al4^{vii}	2.7243 (12)		
Al4—Fe1—Al4^{i}	126.00 (3)	Al3^{x}—Al2—Al3^{xi}	112.44 (6)
Al4—Fe1—Al3	133.35 (3)	Al3^{i}—Al2—Al3^{xi}	99.18 (4)
Al4^{i}—Fe1—Al3	71.41 (4)	Al3—Al2—Al3^{xi}	143.67 (6)
Al4—Fe1—Al3^{i}	71.41 (4)	Fe1—Al3—Fe1^{xii}	130.73 (6)
Al4^{i}—Fe1—Al3^{i}	133.35 (3)	Fe1—Al3—Al3^{iii}	59.36 (4)
Al3—Fe1—Al3^{i}	132.23 (8)	Fe1^{xii}—Al3—Al3^{iii}	71.57 (7)
Al4—Fe1—Al1^{ii}	68.42 (3)	Fe1—Al3—Al3^{xii}	134.62 (5)
Al4^{i}—Fe1—Al1^{ii}	66.13 (4)	Fe1^{xii}—Al3—Al3^{xii}	56.07 (6)
Al3—Fe1—Al1^{ii}	135.30 (6)	Al3^{iii}—Al3—Al3^{xii}	100.62 (7)
Al3^{i}—Fe1—Al1^{ii}	88.75 (5)	Fe1—Al3—Al3^{viii}	72.74 (6)
Al4—Fe1—Al1	66.13 (4)	Fe1^{xii}—Al3—Al3^{viii}	154.67 (9)
Al4^{i}—Fe1—Al1	68.42 (3)	Al3^{iii}—Al3—Al3^{viii}	129.43 (7)
Al3—Fe1—Al1	88.75 (5)	Al3^{xii}—Al3—Al3^{viii}	101.77 (7)
Al3^{i}—Fe1—Al1	135.30 (6)	Fe1—Al3—Al1^{xii}	144.37 (8)
Al1^{ii}—Fe1—Al1	63.43 (4)	Fe1^{xii}—Al3—Al1^{xii}	56.77 (3)
Al4—Fe1—Al2	117.002 (17)	Al3^{iii}—Al3—Al1^{xii}	116.41 (8)
Al4^{i}—Fe1—Al2	117.002 (17)	Al3^{xii}—Al3—Al1^{xii}	80.40 (7)
Al3—Fe1—Al2	66.11 (4)	Al3^{viii}—Al3—Al1^{xii}	111.69 (4)
Al3^{i}—Fe1—Al2	66.11 (4)	Fe1—Al3—Al2	57.67 (3)
Al1^{ii}—Fe1—Al2	148.28 (2)	Fe1^{xii}—Al3—Al2	120.06 (6)
Al1—Fe1—Al2	148.29 (2)	Al3^{iii}—Al3—Al2	80.09 (3)
Al4—Fe1—Al3^{iii}	69.12 (4)	Al3^{xii}—Al3—Al2	80.09 (3)
Al4^{i}—Fe1—Al3^{iii}	114.25 (3)	Al3^{viii}—Al3—Al2	60.20 (3)
Al3—Fe1—Al3^{iii}	64.57 (4)	Al1^{xii}—Al3—Al2	156.51 (7)

Al3^{i}—Fe1—Al3^{iii}	112.40 (3)	Fe1—Al3—Al4^{v}	96.38 (5)
Al1^{ii}—Fe1—Al3^{iii}	122.20 (4)	Fe1^{xii}—Al3—Al4^{v}	53.70 (3)
Al1—Fe1—Al3^{iii}	64.46 (4)	Al3^{iii}—Al3—Al4^{v}	62.11 (6)
Al2—Fe1—Al3^{iii}	86.57 (4)	Al3^{xii}—Al3—Al4^{v}	109.56 (8)
Al4—Fe1—Al3^{iv}	114.25 (3)	Al3^{viii}—Al3—Al4^{v}	143.82 (6)
Al4^{i}—Fe1—Al3^{iv}	69.12 (4)	Al1^{xii}—Al3—Al4^{v}	58.32 (4)
Al3—Fe1—Al3^{iv}	112.40 (3)	Al2—Al3—Al4^{v}	141.96 (6)
Al3^{i}—Fe1—Al3^{iv}	64.57 (4)	Fe1—Al3—Al4^{ix}	134.89 (6)
Al1^{ii}—Fe1—Al3^{iv}	64.46 (4)	Fe1^{xii}—Al3—Al4^{ix}	94.06 (4)
Al1—Fe1—Al3^{iv}	122.20 (4)	Al3^{iii}—Al3—Al4^{ix}	161.99 (7)
Al2—Fe1—Al3^{iv}	86.58 (4)	Al3^{xii}—Al3—Al4^{ix}	61.67 (5)
Al3^{iii}—Fe1—Al3^{iv}	173.15 (8)	Al3^{viii}—Al3—Al4^{ix}	62.20 (5)
Fe1—Al1—Fe1^{v}	143.87 (9)	Al1^{xii}—Al3—Al4^{ix}	60.14 (4)
Fe1—Al1—Al1^{v}	131.43 (5)	Al2—Al3—Al4^{ix}	98.81 (5)
Fe1^{v}—Al1—Al1^{v}	58.28 (2)	Al4^{v}—Al3—Al4^{ix}	118.39 (5)
Fe1—Al1—Al1^{ii}	58.28 (2)	Fe1—Al3—Al4^{i}	54.07 (3)
Fe1^{v}—Al1—Al1^{ii}	131.43 (5)	Fe1^{xii}—Al3—Al4^{i}	136.54 (6)
Al1^{v}—Al1—Al1^{ii}	154.67 (12)	Al3^{iii}—Al3—Al4^{i}	98.43 (5)
Fe1—Al1—Al3^{vi}	113.50 (4)	Al3^{xii}—Al3—Al4^{i}	160.30 (7)
Fe1^{v}—Al1—Al3^{vi}	58.77 (3)	Al3^{viii}—Al3—Al4^{i}	61.61 (5)
Al1^{v}—Al1—Al3^{vi}	112.43 (5)	Al1^{xii}—Al3—Al4^{i}	95.55 (6)
Al1^{ii}—Al1—Al3^{vi}	72.72 (5)	Al2—Al3—Al4^{i}	98.43 (4)
Fe1—Al1—Al3^{iii}	58.77 (3)	Al4^{v}—Al3—Al4^{i}	83.82 (4)
Fe1^{v}—Al1—Al3^{iii}	113.50 (4)	Al4^{ix}—Al3—Al4^{i}	99.51 (5)
Al1^{v}—Al1—Al3^{iii}	72.72 (5)	Fe1—Al4—Fe1^{xiii}	180.00 (3)
Al1^{ii}—Al1—Al3^{iii}	112.43 (5)	Fe1—Al4—Al1^{xiii}	122.19 (3)
Al3^{vi}—Al1—Al3^{iii}	157.75 (10)	Fe1^{xiii}—Al4—Al1^{xiii}	57.81 (3)
Fe1—Al1—Al4	56.061 (10)	Fe1—Al4—Al1	57.81 (3)
Fe1^{v}—Al1—Al4	157.43 (6)	Fe1^{xiii}—Al4—Al1	122.19 (3)
Al1^{v}—Al1—Al4	101.33 (3)	Al1^{xiii}—Al4—Al1	180.00 (2)
Al1^{ii}—Al1—Al4	62.96 (6)	Fe1—Al4—Al1^{ii}	56.627 (15)
Al3^{vi}—Al1—Al4	132.30 (5)	Fe1^{xiii}—Al4—Al1^{ii}	123.373 (15)
Al3^{iii}—Al1—Al4	63.52 (3)	Al1^{xiii}—Al4—Al1^{ii}	122.76 (3)
Fe1—Al1—Al4^{vii}	157.43 (6)	Al1—Al4—Al1^{ii}	57.24 (3)
Fe1^{v}—Al1—Al4^{vii}	56.058 (9)	Fe1—Al4—Al1^{iii}	123.372 (15)
Al1^{v}—Al1—Al4^{vii}	62.96 (6)	Fe1^{xiii}—Al4—Al1^{iii}	56.628 (15)
Al1^{ii}—Al1—Al4^{vii}	101.33 (3)	Al1^{xiii}—Al4—Al1^{iii}	57.24 (3)
Al3^{vi}—Al1—Al4^{vii}	63.52 (3)	Al1—Al4—Al1^{iii}	122.76 (3)
Al3^{iii}—Al1—Al4^{vii}	132.30 (5)	Al1^{ii}—Al4—Al1^{iii}	180.0
Al4—Al1—Al4^{vii}	107.87 (7)	Fe1—Al4—Al3^{iii}	57.18 (3)
Fe1—Al1—Al4^{i}	54.95 (2)	Fe1^{xiii}—Al4—Al3^{iii}	122.82 (3)
Fe1^{v}—Al1—Al4^{i}	97.04 (5)	Al1^{xiii}—Al4—Al3^{iii}	121.84 (3)
Al1^{v}—Al1—Al4^{i}	145.33 (8)	Al1—Al4—Al3^{iii}	58.16 (3)
Al1^{ii}—Al1—Al4^{i}	59.80 (4)	Al1^{ii}—Al4—Al3^{iii}	103.78 (3)
Al3^{vi}—Al1—Al4^{i}	62.72 (4)	Al1^{iii}—Al4—Al3^{iii}	76.22 (3)
Al3^{iii}—Al1—Al4^{i}	100.21 (5)	Fe1—Al4—Al3^{ii}	122.82 (3)
Al4—Al1—Al4^{i}	105.525 (8)	Fe1^{xiii}—Al4—Al3^{ii}	57.18 (3)
Al4^{vii}—Al1—Al4^{i}	126.163 (12)	Al1^{xiii}—Al4—Al3^{ii}	58.16 (3)
Fe1—Al1—Al4^{v}	97.04 (5)	Al1—Al4—Al3^{ii}	121.84 (3)
Fe1^{v}—Al1—Al4^{v}	54.95 (2)	Al1^{ii}—Al4—Al3^{ii}	76.22 (3)
Al1^{v}—Al1—Al4^{v}	59.80 (4)	Al1^{iii}—Al4—Al3^{ii}	103.78 (3)

Al1^{ii}—Al1—Al4^{v}	145.33 (8)	Al3^{iii}—Al4—Al3^{ii}	180.0
Al3^{vi}—Al1—Al4^{v}	100.21 (5)	Fe1—Al4—Al3^{x}	70.13 (4)
Al3^{iii}—Al1—Al4^{v}	62.72 (4)	Fe1^{xiii}—Al4—Al3^{x}	109.87 (4)
Al4—Al1—Al4^{v}	126.163 (12)	Al1^{xiii}—Al4—Al3^{x}	69.23 (5)
Al4^{vii}—Al1—Al4^{v}	105.524 (9)	Al1—Al4—Al3^{x}	110.77 (5)
Al4^{i}—Al1—Al4^{v}	86.48 (6)	Al1^{ii}—Al4—Al3^{x}	122.85 (3)
Fe1^{x}—Al2—Fe1^{ix}	120.0	Al1^{iii}—Al4—Al3^{x}	57.14 (3)
Fe1^{x}—Al2—Fe1	120.0	Al3^{iii}—Al4—Al3^{x}	56.21 (5)
Fe1^{ix}—Al2—Fe1	120.0	Al3^{ii}—Al4—Al3^{x}	123.79 (5)
Fe1^{x}—Al2—Al3^{viii}	150.21 (3)	Fe1—Al4—Al3^{xiv}	109.87 (4)
Fe1^{ix}—Al2—Al3^{viii}	56.22 (3)	Fe1^{xiii}—Al4—Al3^{xiv}	70.13 (4)
Fe1—Al2—Al3^{viii}	71.83 (3)	Al1^{xiii}—Al4—Al3^{xiv}	110.77 (5)
Fe1^{x}—Al2—Al3^{ix}	71.83 (3)	Al1—Al4—Al3^{xiv}	69.23 (5)
Fe1^{ix}—Al2—Al3^{ix}	56.22 (3)	Al1^{ii}—Al4—Al3^{xiv}	57.15 (3)
Fe1—Al2—Al3^{ix}	150.21 (3)	Al1^{iii}—Al4—Al3^{xiv}	122.86 (3)
Al3^{viii}—Al2—Al3^{ix}	112.44 (6)	Al3^{iii}—Al4—Al3^{xiv}	123.79 (5)
Fe1^{x}—Al2—Al3^{x}	56.22 (3)	Al3^{ii}—Al4—Al3^{xiv}	56.21 (5)
Fe1^{ix}—Al2—Al3^{x}	150.21 (3)	Al3^{x}—Al4—Al3^{xiv}	180.0
Fe1—Al2—Al3^{x}	71.83 (3)	Fe1—Al4—Al3^{xv}	125.48 (3)
Al3^{viii}—Al2—Al3^{x}	143.67 (6)	Fe1^{xiii}—Al4—Al3^{xv}	54.52 (3)
Al3^{ix}—Al2—Al3^{x}	99.18 (4)	Al1^{xiii}—Al4—Al3^{xv}	111.01 (4)
Fe1^{x}—Al2—Al3^{i}	71.83 (3)	Al1—Al4—Al3^{xv}	68.99 (4)
Fe1^{ix}—Al2—Al3^{i}	150.21 (3)	Al1^{ii}—Al4—Al3^{xv}	104.22 (3)
Fe1—Al2—Al3^{i}	56.22 (3)	Al1^{iii}—Al4—Al3^{xv}	75.78 (3)
Al3^{viii}—Al2—Al3^{i}	99.18 (4)	Al3^{iii}—Al4—Al3^{xv}	86.12 (5)
Al3^{ix}—Al2—Al3^{i}	143.67 (6)	Al3^{ii}—Al4—Al3^{xv}	93.88 (5)
Al3^{x}—Al2—Al3^{i}	59.59 (6)	Al3^{x}—Al4—Al3^{xv}	123.81 (5)
Fe1^{x}—Al2—Al3	150.20 (3)	Al3^{xiv}—Al4—Al3^{xv}	56.19 (5)
Fe1^{ix}—Al2—Al3	71.83 (3)	Fe1—Al4—Al3^{i}	54.52 (3)
Fe1—Al2—Al3	56.22 (3)	Fe1^{xiii}—Al4—Al3^{i}	125.48 (3)
Al3^{viii}—Al2—Al3	59.59 (6)	Al1^{xiii}—Al4—Al3^{i}	68.99 (4)
Al3^{ix}—Al2—Al3	99.18 (4)	Al1—Al4—Al3^{i}	111.01 (4)
Al3^{x}—Al2—Al3	99.18 (4)	Al1^{ii}—Al4—Al3^{i}	75.78 (3)
Al3^{i}—Al2—Al3	112.44 (6)	Al1^{iii}—Al4—Al3^{i}	104.22 (3)
Fe1^{x}—Al2—Al3^{xi}	56.22 (3)	Al3^{iii}—Al4—Al3^{i}	93.88 (5)
Fe1^{ix}—Al2—Al3^{xi}	71.84 (3)	Al3^{ii}—Al4—Al3^{i}	86.12 (5)
Fe1—Al2—Al3^{xi}	150.21 (3)	Al3^{x}—Al4—Al3^{i}	56.19 (5)
Al3^{viii}—Al2—Al3^{xi}	99.18 (4)	Al3^{xiv}—Al4—Al3^{i}	123.81 (5)
Al3^{ix}—Al2—Al3^{xi}	59.59 (6)	Al3^{xv}—Al4—Al3^{i}	180.0

Symmetry codes: (i) −*x*+2/3, −*x*+*y*+1/3, −*z*+5/6; (ii) −*y*+2/3, *x*−*y*+1/3, *z*+1/3; (iii) *y*−1/3, −*x*+*y*+1/3, −*z*+1/3; (iv) −*y*+1, −*x*+1, *z*+1/2; (v) −*x*+*y*+1/3, −*x*+2/3, *z*−1/3; (vi) −*x*+*y*+1/3, *y*−1/3, *z*+1/6; (vii) *y*, *x*, −*z*+1/2; (viii) *x*−*y*+2/3, −*y*+4/3, −*z*+5/6; (ix) −*y*+1, *x*−*y*+1, *z*; (x) −*x*+*y*, −*x*+1, *z*; (xi) *y*−1/3, *x*+1/3, −*z*+5/6; (xii) *x*−*y*+2/3, *x*+1/3, −*z*+1/3; (xiii) −*x*+1/3, −*y*+2/3, −*z*+2/3; (xiv) *x*−*y*+1/3, *x*−1/3, −*z*+2/3; (xv) *x*−1/3, *x*−*y*+1/3, *z*−1/6.