Abstract

Table 1

Experimental details

Crystal data	
Chemical formula	$Al_{3.25}Fe$
M_r	143.53
Crystal system, space group	Monoclinic, *C*2/*m*
Temperature (K)	300
a, *b*, *c* (Å)	15.498 (4), 8.0814 (17), 12.488 (3)
β (°)	107.790 (8)
V (Å^3)	1489.2 (6)
Z	24
Radiation type	Mo *K*α
μ (mm^{-1})	6.82
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}	0.552, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	3922, 1423, 756
R_{int}	0.102
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.080, 0.223, 1.06
No. of reflections	1423
No. of parameters	128
No. of restraints	104
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.71, −2.04

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

References

NOT FOUND

full crystallographic data

Computing details

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

(Al13Fe4_a)

Crystal data

$Al_{3.25}Fe$
M_r = 143.53
Monoclinic, *C*2/*m*
a = 15.498 (4) Å
b = 8.0814 (17) Å
c = 12.488 (3) Å
β = 107.790 (8)°
V = 1489.2 (6) Å^3
Z = 24
F(000) = 1638
D_x = 3.841 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 3129 reflections
θ = 3.1–27.5°
μ = 6.82 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} = 0.552, T_{max} = 0.746
3922 measured reflections
1423 independent reflections
756 reflections with $I > 2\sigma(I)$
R_{int} = 0.102
θ_{max} = 27.5°, θ_{min} = 2.8°
h = −18→11
k = −9→9
l = −16→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.080
$wR(F^2)$ = 0.223
S = 1.06
1423 reflections
128 parameters
104 restraints
$w = 1/[\sigma^2(F_o^2) + (0.0834P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.71 e Å^{-3}
$\Delta\rho_{min}$ = −2.04 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 (Al13Fe4_a)

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.0855 (3)	0.000000	0.3823 (3)	0.0043 (9)
Fe2	0.4019 (3)	0.000000	0.6228 (3)	0.0065 (9)
Fe3	0.0908 (3)	0.000000	0.9885 (3)	0.0056 (10)
Fe4	0.4028 (3)	0.000000	0.9863 (3)	0.0046 (9)
Fe5	0.32011 (18)	0.2933 (3)	0.27793 (19)	0.0068 (7)
Al1	0.0670 (6)	0.000000	0.1738 (6)	0.0113 (18)

Al2	0.3213 (6)	0.000000	0.2812 (6)	0.0112 (11)
Al3	0.2381 (6)	0.000000	0.5339 (6)	0.0112 (11)
Al4	0.0734 (6)	0.000000	0.5801 (6)	0.0111 (18)
Al5	0.2415 (6)	0.000000	0.9614 (7)	0.0104 (17)
Al6	0.4786 (6)	0.000000	0.8297 (6)	0.0112 (11)
Al7	0.500000	0.000000	0.500000	0.011 (2)
Al8	0.3060 (6)	0.000000	0.7729 (6)	0.0109 (17)
Al9	0.0862 (6)	0.000000	0.7888 (6)	0.0098 (18)
Al10	0.1859 (4)	0.2172 (7)	0.1112 (4)	0.0096 (14)
Al11	0.3673 (4)	0.2116 (7)	0.1101 (4)	0.0103 (13)
Al12	0.1772 (4)	0.2211 (7)	0.3343 (4)	0.0118 (13)
Al13	0.4920 (4)	0.2328 (6)	0.3296 (4)	0.0082 (13)
Al14	0.3636 (4)	0.2198 (7)	0.4781 (4)	0.0108 (13)
Al15	0.000000	0.2495 (9)	0.000000	0.0086 (19)

Atomic displacement parameters (Å²) for (Al13Fe4_a)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.004 (2)	0.0021 (18)	0.0064 (17)	0.000	0.0011 (16)	0.000
Fe2	0.008 (2)	0.0018 (18)	0.0055 (17)	0.000	−0.0047 (16)	0.000
Fe3	0.006 (2)	0.0039 (18)	0.0052 (17)	0.000	−0.0009 (16)	0.000
Fe4	0.005 (2)	0.0023 (18)	0.0073 (17)	0.000	0.0020 (16)	0.000
Fe5	0.0063 (17)	0.0076 (14)	0.0046 (12)	−0.0001 (12)	−0.0012 (11)	−0.0001 (10)
Al1	0.014 (5)	0.014 (4)	0.004 (3)	0.000	−0.001 (3)	0.000
Al2	0.011 (3)	0.008 (2)	0.0100 (19)	0.000	−0.0040 (18)	0.000
Al3	0.011 (3)	0.008 (2)	0.0100 (19)	0.000	−0.0040 (18)	0.000
Al4	0.009 (4)	0.015 (4)	0.007 (3)	0.000	0.000 (3)	0.000
Al5	0.006 (4)	0.004 (4)	0.017 (4)	0.000	−0.004 (3)	0.000
Al6	0.011 (3)	0.008 (2)	0.0100 (19)	0.000	−0.0040 (18)	0.000
Al7	0.016 (6)	0.011 (5)	0.003 (4)	0.000	−0.002 (4)	0.000
Al8	0.017 (4)	0.005 (4)	0.008 (3)	0.000	0.001 (3)	0.000
Al9	0.011 (5)	0.008 (4)	0.007 (3)	0.000	−0.002 (3)	0.000
Al10	0.008 (3)	0.012 (3)	0.007 (3)	0.002 (2)	−0.001 (2)	−0.002 (2)
Al11	0.007 (3)	0.012 (3)	0.008 (2)	0.001 (3)	−0.003 (2)	−0.003 (2)
Al12	0.014 (3)	0.010 (3)	0.007 (3)	−0.004 (2)	−0.002 (2)	−0.001 (2)
Al13	0.011 (3)	0.009 (3)	0.004 (3)	−0.002 (2)	0.002 (2)	−0.001 (2)
Al14	0.007 (3)	0.014 (3)	0.009 (2)	0.000 (2)	−0.001 (2)	0.002 (2)
Al15	0.010 (4)	0.003 (4)	0.006 (3)	0.000	−0.006 (3)	0.000

Bond lengths (Å) for (Al13Fe4_a)

Fe1—Al12^{i}	2.468 (6)	Al2—Al11^{i}	2.989 (9)
Fe1—Al12	2.468 (6)	Al2—Al11	2.989 (9)
Fe1—Al1	2.530 (8)	Al3—Al14^{vi}	2.736 (8)
Fe1—Al4	2.534 (8)	Al3—Al14^{v}	2.736 (8)
Fe1—Al3	2.538 (9)	Al3—Al4	2.783 (14)
Fe1—Al13^{ii}	2.572 (6)	Al3—Al8	2.845 (10)
Fe1—Al13^{iii}	2.572 (6)	Al3—Al12^{v}	2.862 (7)
Fe1—Al4^{iv}	2.645 (10)	Al3—Al12^{vi}	2.862 (7)
Fe1—Al14^{v}	2.819 (6)	Al3—Al14^{i}	2.872 (9)
Fe1—Al14^{vi}	2.819 (6)	Al3—Al14	2.872 (9)

Fe1—Al9^{iv}	2.859 (8)	Al3—Al12^{i}	2.977 (8)
Fe2—Al3	2.440 (9)	Al3—Al12	2.977 (8)
Fe2—Al13^{vii}	2.449 (6)	Al4—Al4^{iv}	2.530 (15)
Fe2—Al13^{viii}	2.449 (6)	Al4—Al9	2.552 (11)
Fe2—Al7	2.468 (4)	Al4—Al14^{v}	2.654 (7)
Fe2—Al14^{i}	2.473 (6)	Al4—Al14^{vi}	2.654 (7)
Fe2—Al14	2.473 (6)	Al4—Al13^{v}	2.768 (8)
Fe2—Al6	2.492 (8)	Al4—Al13^{vi}	2.768 (8)
Fe2—Al12^{vi}	2.697 (6)	Al5—Al9	2.695 (11)
Fe2—Al12^{v}	2.697 (6)	Al5—Al10^{v}	2.817 (8)
Fe2—Al8	2.725 (10)	Al5—Al10^{vi}	2.817 (8)
Fe3—Al1^{ix}	2.453 (9)	Al5—Al11^{ix}	2.822 (8)
Fe3—Al5	2.459 (10)	Al5—Al11^{x}	2.822 (8)
Fe3—Al9	2.473 (8)	Al5—Al8	2.824 (12)
Fe3—Al15^{iv}	2.488 (6)	Al5—Al11^{vi}	2.855 (7)
Fe3—Al15^{ix}	2.488 (6)	Al5—Al11^{v}	2.855 (7)
Fe3—Al10^{ix}	2.494 (6)	Al5—Al10^{ix}	2.883 (9)
Fe3—Al10^{x}	2.494 (6)	Al5—Al10^{x}	2.883 (9)
Fe3—Al1^{iv}	2.657 (9)	Al6—Al8	2.550 (12)
Fe3—Al11^{vi}	2.803 (6)	Al6—Al11^{vii}	2.845 (9)
Fe3—Al11^{v}	2.803 (6)	Al6—Al11^{viii}	2.845 (9)
Fe3—Fe3^{xi}	2.916 (8)	Al6—Al13^{viii}	2.873 (8)
Fe4—Al5	2.424 (10)	Al6—Al13^{vii}	2.873 (8)
Fe4—Al6^{xii}	2.465 (8)	Al6—Al15^{v}	2.881 (7)
Fe4—Al11^{ix}	2.477 (6)	Al6—Al15^{xiii}	2.881 (7)
Fe4—Al11^{x}	2.477 (6)	Al7—Al14	2.711 (6)
Fe4—Al15^{v}	2.497 (6)	Al7—Al14^{i}	2.711 (6)
Fe4—Al15^{xiii}	2.497 (6)	Al7—Al14^{vii}	2.711 (6)
Fe4—Al6	2.571 (10)	Al7—Al14^{viii}	2.711 (6)
Fe4—Al8	2.628 (8)	Al7—Al13^{vii}	2.814 (5)
Fe4—Al10^{vi}	2.752 (6)	Al7—Al13^{i}	2.814 (5)
Fe4—Al10^{v}	2.752 (6)	Al7—Al13^{viii}	2.814 (5)
Fe4—Fe4^{xii}	2.926 (8)	Al7—Al13	2.814 (5)
Fe5—Al2	2.370 (2)	Al8—Al12^{vi}	2.675 (7)
Fe5—Al14	2.455 (6)	Al8—Al12^{v}	2.675 (7)
Fe5—Al8^{v}	2.501 (7)	Al8—Al10^{v}	2.687 (7)
Fe5—Al11	2.510 (6)	Al8—Al10^{vi}	2.687 (7)
Fe5—Al9^{v}	2.516 (7)	Al9—Al11^{v}	2.644 (6)
Fe5—Al10	2.529 (6)	Al9—Al11^{vi}	2.644 (6)
Fe5—Al12	2.586 (7)	Al9—Al13^{vi}	2.688 (7)
Fe5—Al13	2.589 (6)	Al9—Al13^{v}	2.688 (7)
Fe5—Al4^{v}	2.621 (6)	Al10—Al11^{xv}	2.694 (7)
Al1—Al9^{iv}	2.556 (14)	Al10—Al15	2.802 (6)
Al1—Al10^{i}	2.822 (9)	Al10—Al11	2.817 (9)
Al1—Al10	2.822 (9)	Al10—Al12	2.829 (8)
Al1—Al12^{i}	2.834 (8)	Al11—Al15^{xv}	2.819 (6)
Al1—Al12	2.834 (8)	Al11—Al13	2.836 (7)
Al1—Al15^{xiv}	2.912 (7)	Al12—Al14^{v}	2.650 (8)
Al1—Al15	2.912 (7)	Al12—Al13^{iii}	2.878 (8)
Al2—Al14	2.941 (8)	Al12—Al14	2.897 (8)
Al2—Al14^{i}	2.941 (8)	Al13—Al14^{vii}	2.739 (7)

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