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ISSN 2414-3146

The structure of the aluminium-abundant γ-brass-type $Al_{8.6}Mn_{4.4}$

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Received 30 July 2021
Accepted 22 September 2021

Edited by S. Bernès, Benemérita Universidad Autónoma de Puebla, México

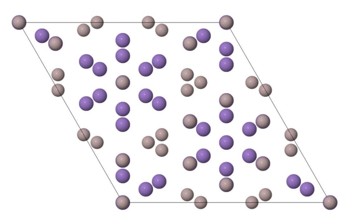
Keywords: crystal structure; Al–Mn; intermetallic; γ-brass phase.

CCDC reference: 2111321

Structural data: full structural data are available from iucrdata.iucr.org

An aluminium-abundant Al_8Mn_5/γ-brass-type intermetallic with formula $Al_{8.6}Mn_{4.4}$, which is isotypic with γ-Al_8Cr_5 and γ-Al_8V_5, was discovered by high-temperature sintering of an Al/Mn mixture with initial composition Al_2Mn. Structure analysis revealed that one special position (Wyckoff site 18*h* in space group $R\overline{3}m$) is shared by Al and Mn, with refined site occupancy factors of 0.7 and 0.3, respectively. The present low-temperature Al_8Mn_5-type phase crystallizes in the centrosymmetric space group $R\overline{3}m$ (No. 166), rather than $R3m$ (No. 160) as previously reported for the same intermetallic characterized by TEM measurements [Zeng *et al.* (2018). *Acta Mater.* **153**, 364–376].

3D view



Structure description

The γ-brasses are common phases with rhombohedral symmetry, and have been observed in many systems, including the Al–Cr, Al–Mn, Al–Cu, Ga–Cr, Ga–Mn and Ga–Fe mixtures (Bradley & Lu, 1937; Meissner *et al.*, 1965; Westman, 1965). However, it has long been known that the structure model of the γ-Al_8Mn_5 phase has some conflicts. For example, the Al_8Mn_5 phase was first reported with a hexagonal unit cell (a = 12.713 Å, c = 15.839 Å) and was believed to be associated with Al_8Cr_5 (Schubert *et al.*, 1960). Subsequently, this structure was checked with the unit-cell parameters a = 12.630 Å and c = 7.933 Å by powder diffraction patterns (Schonover & Mohanty, 1969). In another study, the low-temperature phase Al_8Mn_5 was analysed and considered as a hexagonal structure with unit-cell parameters a = 7.20 Å and c = 22.95 Å. In the meantime, a high-temperature Al_8Mn_5 phase was reported (Koch *et al.*, 1960). Further studies were reported on the transformation from the high-temperature Al–Mn phase to the low-temperature Al_8Mn_5 phase, and on the measured metal concentrations, ranging from $Mn_{48}Al_{52}$ to $Mn_{37}Al_{63}$, with unit-cell parameters in the range a = 12.598–12.671 Å, and c = 7.911–7.942 Å, by powder diffraction patterns (Ellner, 1990). They reached the conclu-

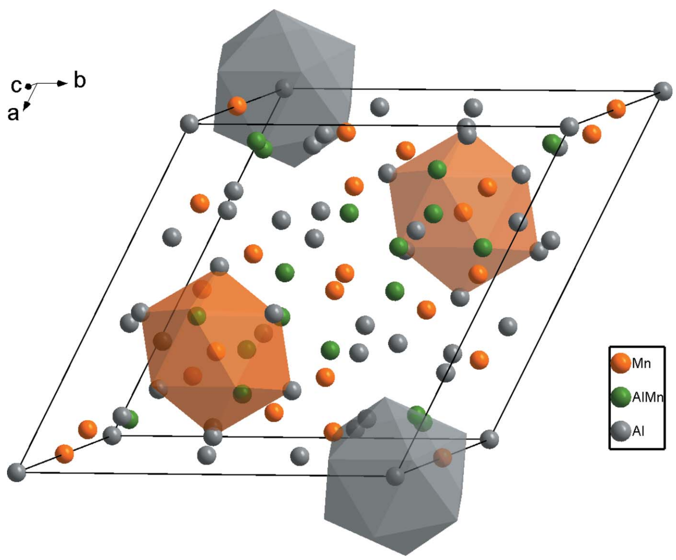


Figure 1
The crystal structure of $Al_{8.6}Mn_{4.4}$ with two Mn02 atoms and two Al04 atoms displayed with their coordination environments as polyhedra.

sion that the axial ratio c/a decreases while the molar fraction of aluminium increases. Very recently, the $D8_{10}$–Al_8Mn_5 phase has been found to nucleate on B2–Al(Mn, Fe) particles in

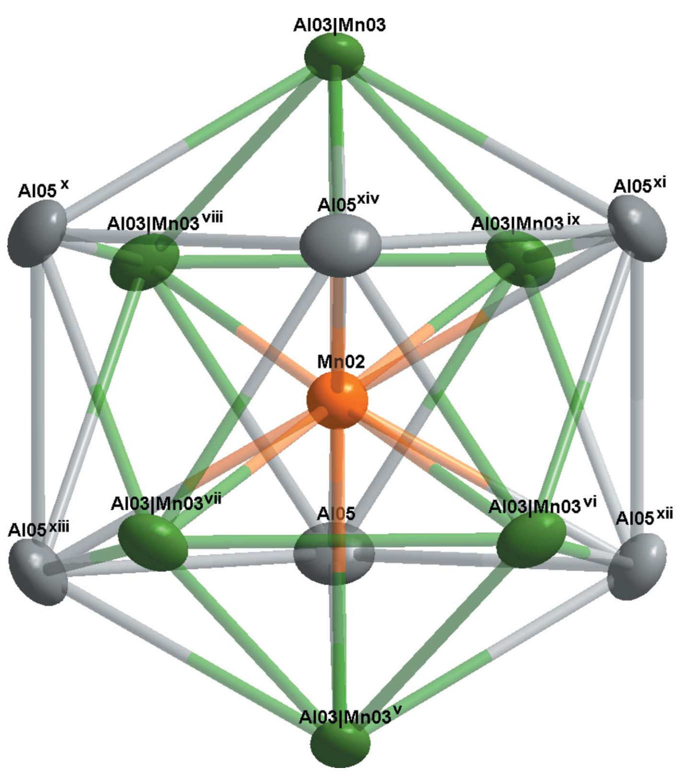


Figure 2
The environment of the Mn02 atom. Displacement ellipsoids are given at the 90% probability level. Symmetry codes: (v) $-x + 4/3, -y + \frac{2}{3}, -z + \frac{5}{3}$; (vi) $y + \frac{1}{3}, -x + y + \frac{2}{3}, -z + \frac{5}{3}$; (vii) $x - y + \frac{1}{3}, x - \frac{1}{3}, -z + \frac{5}{3}$; (viii) $-y + 1, x - y, z$; (ix) $-x + y + 1, -x + 1, z$; (x) $-x + y + \frac{1}{3}, -x + \frac{2}{3}, z + \frac{2}{3}$; (xi) $-y + \frac{4}{3}, x - y + \frac{2}{3}, z + \frac{2}{3}$; (xii) $x - y + 1, x, -z + 1$; (xiii) $y, -x + y, -z + 1$; (xiv) $-x + 1, -y + 1, -z + 1$.

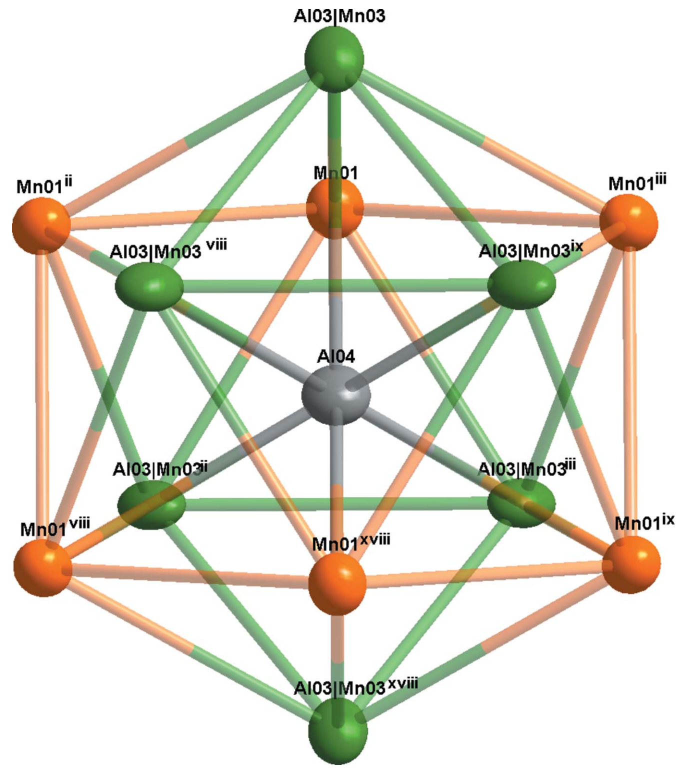


Figure 3
The environment of the Al04 atom. Displacement ellipsoids are given at the 90% probability level. Symmetry codes: (ii) $x - y + \frac{1}{3}, x - \frac{1}{3}, -z + \frac{2}{3}$; (iii) $y + \frac{1}{3}, -x + y + \frac{2}{3}, -z + \frac{2}{3}$; (viii) $-y + 1, x - y, z$; (ix) $-x + y + 1, -x + 1, z$; (xviii) $-x + \frac{4}{3}, -y + \frac{2}{3}, -z + \frac{2}{3}$.

AZ91 magnesium alloys (Zeng *et al.*, 2018). The $D8_{10}$–Al_8Mn_5 structure model closely resembles that described in the present work; however, its composition includes not only Al and Mn, but also other elements such as Fe and Mg.

Although the Al_8Mn_5 intermetallic phase has been reported many times over many years, the atomic coordinates have not so far been determined accurately by single-crystal X-ray diffraction. In the present work, the crystal structure of the low-temperature γ-Al_8Mn_5-type phase with the refined chemical composition $Al_{8.6}Mn_{4.4}$ was determined by single-crystal X-ray diffraction measurements for the first time. Intermetallic $Al_{8.6}Mn_{4.4}$ is a aluminium-rich phase compared to $Mn_{37}Al_{63}$, and its axial ratio, c/a = 0.624 is then slightly reduced ($Mn_{37}Al_{63}$: c/a = 0.626), in agreement with the results reported by Ellner (1990).

Fig. 1 shows the overall atomic distribution of $Al_{8.6}Mn_{4.4}$ in the unit cell. For simplicity, four distorted icosahedra are illustrated here, and the environment of the Mn02 atoms is shown in Fig. 2. The twelve vertices include six Al atoms (Al05) and six co-occupied Al/Mn sites (Al03/Mn03), where the refined site occupancies converged to 0.7 for Al03 and 0.3 for Mn03. In addition, the icosahedron centred at Al04 is shown in Fig. 3; it is constituted of six Mn atoms (Mn01) and six co-occupied Al/Mn sites (Al03/Mn03). In summary, these two icosahedra are packed together and form the main building blocks of $Al_{8.6}Mn_{4.4}$.

Table 1
Experimental details.

Crystal data	
Chemical formula	$Al_{8.6}Mn_{4.4}$
M_r	473.76
Crystal system, space group	Trigonal, $R\overline{3}m:H$
Temperature (K)	296
a, c (Å)	12.6751 (13), 7.9137 (9)
V (Å^3)	1101.1 (3)
Z	6
Radiation type	Mo $K\alpha$
μ (mm^{-1})	8.32
Crystal size (mm)	0.09 × 0.06 × 0.04
Data collection	
Diffractometer	Bruker D8 Venture Photon 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2015)
T_{min}, T_{max}	0.494, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7162, 323, 298
R_{int}	0.078
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.125, 1.19
No. of reflections	323
No. of parameters	29
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.98, −1.23

Computer programs: *APEX3* and *SAINT* (Bruker, 2015), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2016/6* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2017) and *publCIF* (Westrip, 2010).

Synthesis and crystallization

The high-purity elements Al (indicated purity 99.8%; 1.080 g) and Mn (indicated purity 99.96%; 1.100 g) were mixed in the stoichiometric ratio 2:1 and ground in an agate mortar. The blended powders were placed into a cemented carbide grinding mound of 9.6 mm diameter and pressed at 4 MPa for about 5 min. The obtained cylindrical block was crushed and a specimen weighing 50.55 mg was selected and subsequently loaded into the crucible of a Netzsch STA 449 C simultaneous thermal analysis instrument. The sample was heated up to 1250°C for 10 min with a heating rate of 20°C min^{-1}, and then slowly cooled to 700°C with a cooling rate of 10°C min^{-1}. Finally, the sample was cooled down to room temperature by switching off the furnace. Suitable pieces of single-crystal grains were selected from the educts for single-crystal X-ray diffraction experiments. Details of the EDS analysis are given in the supporting information.

Refinement

Table 1 shows the details of data collection and structural refinement. Only one site is co-occupied by Al and Mn atoms (Al03/Mn03). Site occupancies were refined to 0.7 for Al03 and 0.3 for Mn03, and then fixed in the following least-squares cycles. Atoms sharing the same site were constrained to have the same coordinates and displacement parameters. The maximum and minimum residual electron densities in the last difference map are located 0.97 Å from atom Mn01 and 0.85 Å from atom Al05, respectively.

Acknowledgements

We acknowledge the referee for insightful remarks.

Funding information

Funding for this research was provided by: Research Foundation of Education Bureau of Hebei Province (grant No. ZD2018069); The National Natural Science Foundation of China (grant No. 51771165).

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full crystallographic data

IUCrData (2021). **6**, x210988 [https://doi.org/10.1107/S2414314621009883]

The structure of the aluminium-abundant γ-brass-type $Al_{8.6}Mn_{4.4}$

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Octaluminium pentamanganese

Crystal data

$Al_{8.6}Mn_{4.4}$
M_r = 473.76
Trigonal, $R\overline{3}m$:H
a = 12.6751 (13) Å
c = 7.9137 (9) Å
V = 1101.1 (3) Å^3
Z = 6
F(000) = 1331
D_x = 4.287 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3882 reflections
θ = 3.2–30.4°
μ = 8.32 mm^{-1}
T = 296 K
Graininess, silver
0.09 × 0.06 × 0.04 mm

Data collection

Bruker D8 Venture Photon 100 CMOS diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2015)
T_{min} = 0.494, T_{max} = 0.746
7162 measured reflections
323 independent reflections
298 reflections with $I > 2\sigma(I)$
R_{int} = 0.078
θ_{max} = 27.5°, θ_{min} = 3.2°
h = −16→16
k = −15→16
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.125
S = 1.19
323 reflections
29 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0472P)^2 + 72.2358P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.98 e Å^{-3}
$\Delta\rho_{min}$ = −1.23 e Å^{-3}
Extinction correction: SHELXL-2016/6 (Sheldrick, 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0015 (3)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Mn01	0.54960 (7)	0.45040 (7)	0.26408 (19)	0.0082 (5)	
Mn02	0.666667	0.333333	0.833333	0.0082 (8)	
Al03	0.59276 (11)	0.40724 (11)	0.5828 (3)	0.0082 (6)	0.7
Mn03	0.59276 (11)	0.40724 (11)	0.5828 (3)	0.0082 (6)	0.3
Al04	0.666667	0.333333	0.333333	0.0090 (15)	

Al05	0.45078 (13)	0.54922 (13)	0.0926 (4)	0.0101 (7)
Al06	0.333333	0.2900 (3)	0.166667	0.0151 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn01	0.0079 (6)	0.0079 (6)	0.0085 (8)	0.0038 (6)	−0.0004 (3)	0.0004 (3)
Mn02	0.0086 (11)	0.0086 (11)	0.0072 (17)	0.0043 (6)	0.000	0.000
Al03	0.0090 (9)	0.0090 (9)	0.0046 (10)	0.0031 (9)	−0.0011 (4)	0.0011 (4)
Mn03	0.0090 (9)	0.0090 (9)	0.0046 (10)	0.0031 (9)	−0.0011 (4)	0.0011 (4)
Al04	0.011 (2)	0.011 (2)	0.006 (3)	0.0053 (11)	0.000	0.000
Al05	0.0127 (12)	0.0127 (12)	0.0096 (14)	0.0098 (13)	0.0005 (5)	−0.0005 (5)
Al06	0.0121 (15)	0.0156 (12)	0.0163 (16)	0.0060 (8)	−0.0051 (12)	−0.0026 (6)

Geometric parameters (Å, º)

Mn01—Al05	2.559 (3)	Mn02—Al05^{xii}	2.644 (3)
Mn01—Al06	2.5824 (10)	Mn02—Al05^{xiii}	2.644 (3)
Mn01—Al06^{i}	2.5825 (10)	Mn02—Al05^{xiv}	2.644 (3)
Mn01—Al04	2.6278 (15)	Al03—Al04	2.556 (2)
Mn01—Al03^{ii}	2.6650 (17)	Al03—Al06^{iii}	2.650 (3)
Mn01—Al03^{iii}	2.6650 (17)	Al03—Al06^{iv}	2.650 (3)
Mn01—Al06^{iii}	2.667 (2)	Al03—Al05^{xi}	2.655 (3)
Mn01—Al06^{iv}	2.667 (2)	Al03—Al05^{x}	2.655 (3)
Mn01—Al03	2.695 (3)	Al03—Al05^{xiv}	2.741 (4)
Mn01—Mn01^{iii}	2.7941 (18)	Al03—Al03^{ix}	2.810 (4)
Mn01—Mn01^{ii}	2.7941 (18)	Al03—Al03^{viii}	2.810 (4)
Mn02—Al03^{v}	2.562 (2)	Al05—Al05^{xv}	2.611 (6)
Mn02—Al03^{vi}	2.562 (2)	Al05—Al05^{i}	2.832 (4)
Mn02—Al03^{vii}	2.562 (2)	Al05—Al05^{xvi}	2.832 (4)
Mn02—Al03^{viii}	2.562 (2)	Al05—Al06^{i}	2.909 (3)
Mn02—Al03^{ix}	2.562 (2)	Al05—Al06	2.909 (3)
Mn02—Al03	2.562 (2)	Al06—Al06^{iv}	2.804 (2)
Mn02—Al05^{x}	2.644 (3)	Al06—Al06^{xvii}	2.804 (2)
Mn02—Al05^{xi}	2.644 (3)		
Al05—Mn01—Al06	68.92 (8)	Mn02—Al03—Al03^{viii}	56.73 (4)
Al05—Mn01—Al06^{i}	68.92 (8)	Al06^{iii}—Al03—Al03^{viii}	163.86 (5)
Al06—Mn01—Al06^{i}	135.16 (12)	Al06^{iv}—Al03—Al03^{viii}	111.76 (7)
Al05—Mn01—Al04	160.01 (9)	Al05^{xi}—Al03—Al03^{viii}	108.17 (7)
Al06—Mn01—Al04	107.13 (8)	Al05^{x}—Al03—Al03^{viii}	58.04 (6)
Al06^{i}—Mn01—Al04	107.13 (8)	Mn01^{ii}—Al03—Al03^{viii}	58.18 (5)
Al05—Mn01—Al03^{ii}	106.00 (8)	Mn01^{iii}—Al03—Al03^{viii}	107.93 (5)
Al06—Mn01—Al03^{ii}	60.63 (8)	Mn01—Al03—Al03^{viii}	107.73 (5)
Al06^{i}—Mn01—Al03^{ii}	118.97 (8)	Al05^{xiv}—Al03—Al03^{viii}	107.58 (7)
Al04—Mn01—Al03^{ii}	57.74 (5)	Al03^{ix}—Al03—Al03^{viii}	60.0
Al05—Mn01—Al03^{iii}	106.00 (8)	Al03^{xviii}—Al04—Al03^{ii}	66.71 (8)
Al06—Mn01—Al03^{iii}	118.97 (8)	Al03^{xviii}—Al04—Al03^{ix}	113.29 (8)

Al06^{i}—Mn01—Al03^{iii}	60.63 (8)	Al03^{ii}—Al04—Al03^{ix}	180.0
Al04—Mn01—Al03^{iii}	57.74 (5)	Al03^{xviii}—Al04—Al03^{iii}	66.71 (8)
Al03^{ii}—Mn01—Al03^{iii}	63.64 (11)	Al03^{ii}—Al04—Al03^{iii}	66.71 (8)
Al05—Mn01—Al06^{iii}	91.44 (7)	Al03^{ix}—Al04—Al03^{iii}	113.29 (8)
Al06—Mn01—Al06^{iii}	130.82 (5)	Al03^{xviii}—Al04—Al03^{viii}	113.29 (8)
Al06^{i}—Mn01—Al06^{iii}	64.55 (7)	Al03^{ii}—Al04—Al03^{viii}	113.29 (8)
Al04—Mn01—Al06^{iii}	104.67 (5)	Al03^{ix}—Al04—Al03^{viii}	66.71 (8)
Al03^{ii}—Mn01—Al06^{iii}	162.37 (7)	Al03^{iii}—Al04—Al03^{viii}	180.00 (10)
Al03^{iii}—Mn01—Al06^{iii}	109.58 (7)	Al03^{xviii}—Al04—Al03	180.0
Al05—Mn01—Al06^{iv}	91.43 (7)	Al03^{ii}—Al04—Al03	113.29 (8)
Al06—Mn01—Al06^{iv}	64.55 (7)	Al03^{ix}—Al04—Al03	66.71 (8)
Al06^{i}—Mn01—Al06^{iv}	130.82 (5)	Al03^{iii}—Al04—Al03	113.29 (8)
Al04—Mn01—Al06^{iv}	104.67 (5)	Al03^{viii}—Al04—Al03	66.71 (8)
Al03^{ii}—Mn01—Al06^{iv}	109.58 (7)	Al03^{xviii}—Al04—Mn01^{iii}	118.14 (3)
Al03^{iii}—Mn01—Al06^{iv}	162.37 (7)	Al03^{ii}—Al04—Mn01^{iii}	118.14 (3)
Al06^{iii}—Mn01—Al06^{iv}	71.75 (12)	Al03^{ix}—Al04—Mn01^{iii}	61.86 (3)
Al05—Mn01—Al03	142.61 (10)	Al03^{iii}—Al04—Mn01^{iii}	62.63 (6)
Al06—Mn01—Al03	111.28 (5)	Al03^{viii}—Al04—Mn01^{iii}	117.37 (6)
Al06^{i}—Mn01—Al03	111.28 (5)	Al03—Al04—Mn01^{iii}	61.86 (3)
Al04—Mn01—Al03	57.37 (6)	Al03^{xviii}—Al04—Mn01^{ii}	118.14 (3)
Al03^{ii}—Mn01—Al03	105.61 (8)	Al03^{ii}—Al04—Mn01^{ii}	62.63 (6)
Al03^{iii}—Mn01—Al03	105.61 (8)	Al03^{ix}—Al04—Mn01^{ii}	117.37 (6)
Al06^{iii}—Mn01—Al03	59.22 (5)	Al03^{iii}—Al04—Mn01^{ii}	118.14 (3)
Al06^{iv}—Mn01—Al03	59.23 (5)	Al03^{viii}—Al04—Mn01^{ii}	61.86 (3)
Al05—Mn01—Mn01^{iii}	126.73 (2)	Al03—Al04—Mn01^{ii}	61.86 (3)
Al06—Mn01—Mn01^{iii}	164.30 (8)	Mn01^{iii}—Al04—Mn01^{ii}	115.77 (2)
Al06^{i}—Mn01—Mn01^{iii}	59.33 (7)	Al03^{xviii}—Al04—Mn01^{viii}	61.86 (3)
Al04—Mn01—Mn01^{iii}	57.883 (11)	Al03^{ii}—Al04—Mn01^{viii}	61.86 (3)
Al03^{ii}—Mn01—Mn01^{iii}	109.05 (6)	Al03^{ix}—Al04—Mn01^{viii}	118.14 (3)
Al03^{iii}—Mn01—Mn01^{iii}	59.10 (5)	Al03^{iii}—Al04—Mn01^{viii}	117.37 (6)
Al06^{iii}—Mn01—Mn01^{iii}	56.38 (6)	Al03^{viii}—Al04—Mn01^{viii}	62.63 (6)
Al06^{iv}—Mn01—Mn01^{iii}	112.33 (9)	Al03—Al04—Mn01^{viii}	118.14 (3)
Al03—Mn01—Mn01^{iii}	58.06 (5)	Mn01^{iii}—Al04—Mn01^{viii}	180.0
Al05—Mn01—Mn01^{ii}	126.73 (2)	Mn01^{ii}—Al04—Mn01^{viii}	64.23 (2)
Al06—Mn01—Mn01^{ii}	59.33 (7)	Al03^{xviii}—Al04—Mn01^{ix}	61.86 (3)
Al06^{i}—Mn01—Mn01^{ii}	164.30 (8)	Al03^{ii}—Al04—Mn01^{ix}	117.37 (6)
Al04—Mn01—Mn01^{ii}	57.883 (11)	Al03^{ix}—Al04—Mn01^{ix}	62.63 (6)
Al03^{ii}—Mn01—Mn01^{ii}	59.10 (5)	Al03^{iii}—Al04—Mn01^{ix}	61.86 (3)
Al03^{iii}—Mn01—Mn01^{ii}	109.05 (6)	Al03^{viii}—Al04—Mn01^{ix}	118.14 (3)
Al06^{iii}—Mn01—Mn01^{ii}	112.33 (9)	Al03—Al04—Mn01^{ix}	118.14 (3)
Al06^{iv}—Mn01—Mn01^{ii}	56.38 (6)	Mn01^{iii}—Al04—Mn01^{ix}	64.23 (2)
Al03—Mn01—Mn01^{ii}	58.06 (5)	Mn01^{ii}—Al04—Mn01^{ix}	180.0
Mn01^{iii}—Mn01—Mn01^{ii}	105.61 (6)	Mn01^{viii}—Al04—Mn01^{ix}	115.77 (2)
Al03^{v}—Mn02—Al03^{vi}	66.53 (8)	Al03^{xviii}—Al04—Mn01	117.37 (6)
Al03^{v}—Mn02—Al03^{vii}	66.53 (8)	Al03^{ii}—Al04—Mn01	61.86 (3)
Al03^{vi}—Mn02—Al03^{vii}	66.53 (8)	Al03^{ix}—Al04—Mn01	118.14 (3)
Al03^{v}—Mn02—Al03^{viii}	113.47 (8)	Al03^{iii}—Al04—Mn01	61.86 (3)
Al03^{vi}—Mn02—Al03^{viii}	180.0	Al03^{viii}—Al04—Mn01	118.14 (3)

Al03^{vii}—Mn02—Al03^{viii}	113.47 (9)	Al03—Al04—Mn01	62.63 (6)
Al03^{v}—Mn02—Al03^{ix}	113.47 (8)	Mn01^{iii}—Al04—Mn01	64.23 (2)
Al03^{vi}—Mn02—Al03^{ix}	113.47 (9)	Mn01^{ii}—Al04—Mn01	64.23 (2)
Al03^{vii}—Mn02—Al03^{ix}	180.0	Mn01^{viii}—Al04—Mn01	115.77 (2)
Al03^{viii}—Mn02—Al03^{ix}	66.53 (8)	Mn01^{ix}—Al04—Mn01	115.77 (2)
Al03^{v}—Mn02—Al03	180.0	Mn01—Al05—Al05^{xv}	66.17 (13)
Al03^{vi}—Mn02—Al03	113.47 (8)	Mn01—Al05—Mn02^{xix}	135.17 (13)
Al03^{vii}—Mn02—Al03	113.47 (8)	Al05^{xv}—Al05—Mn02^{xix}	158.7 (2)
Al03^{viii}—Mn02—Al03	66.53 (8)	Mn01—Al05—Al03^{xx}	147.49 (7)
Al03^{ix}—Mn02—Al03	66.53 (8)	Al05^{xv}—Al05—Al03^{xx}	104.81 (15)
Al03^{v}—Mn02—Al05^{x}	118.71 (5)	Mn02^{xix}—Al05—Al03^{xx}	57.82 (7)
Al03^{vi}—Mn02—Al05^{x}	118.71 (5)	Mn01—Al05—Al03^{xxi}	147.49 (7)
Al03^{vii}—Mn02—Al05^{x}	63.51 (9)	Al05^{xv}—Al05—Al03^{xxi}	104.81 (15)
Al03^{viii}—Mn02—Al05^{x}	61.29 (5)	Mn02^{xix}—Al05—Al03^{xxi}	57.82 (7)
Al03^{ix}—Mn02—Al05^{x}	116.49 (9)	Al03^{xx}—Al05—Al03^{xxi}	63.92 (12)
Al03—Mn02—Al05^{x}	61.29 (5)	Mn01—Al05—Al03^{xiv}	78.39 (10)
Al03^{v}—Mn02—Al05^{xi}	118.71 (5)	Al05^{xv}—Al05—Al03^{xiv}	144.6 (2)
Al03^{vi}—Mn02—Al05^{xi}	63.51 (9)	Mn02^{xix}—Al05—Al03^{xiv}	56.78 (8)
Al03^{vii}—Mn02—Al05^{xi}	118.71 (5)	Al03^{xx}—Al05—Al03^{xiv}	105.11 (11)
Al03^{viii}—Mn02—Al05^{xi}	116.49 (9)	Al03^{xxi}—Al05—Al03^{xiv}	105.11 (11)
Al03^{ix}—Mn02—Al05^{xi}	61.29 (5)	Mn01—Al05—Mn01^{xv}	122.19 (11)
Al03—Mn02—Al05^{xi}	61.29 (5)	Al05^{xv}—Al05—Mn01^{xv}	56.02 (12)
Al05^{x}—Mn02—Al05^{xi}	115.24 (5)	Mn02^{xix}—Al05—Mn01^{xv}	102.64 (10)
Al03^{v}—Mn02—Al05^{xii}	61.29 (5)	Al03^{xx}—Al05—Mn01^{xv}	58.13 (7)
Al03^{vi}—Mn02—Al05^{xii}	61.29 (5)	Al03^{xxi}—Al05—Mn01^{xv}	58.13 (7)
Al03^{vii}—Mn02—Al05^{xii}	116.49 (9)	Al03^{xiv}—Al05—Mn01^{xv}	159.42 (13)
Al03^{viii}—Mn02—Al05^{xii}	118.71 (5)	Mn01—Al05—Al05^{i}	99.58 (11)
Al03^{ix}—Mn02—Al05^{xii}	63.51 (9)	Al05^{xv}—Al05—Al05^{i}	127.52 (4)
Al03—Mn02—Al05^{xii}	118.71 (5)	Mn02^{xix}—Al05—Al05^{i}	57.62 (2)
Al05^{x}—Mn02—Al05^{xii}	180.0	Al03^{xx}—Al05—Al05^{i}	109.39 (8)
Al05^{xi}—Mn02—Al05^{xii}	64.76 (5)	Al03^{xxi}—Al05—Al05^{i}	59.82 (8)
Al03^{v}—Mn02—Al05^{xiii}	61.29 (5)	Al03^{xiv}—Al05—Al05^{i}	56.87 (10)
Al03^{vi}—Mn02—Al05^{xiii}	116.49 (9)	Mn01^{xv}—Al05—Al05^{i}	114.36 (13)
Al03^{vii}—Mn02—Al05^{xiii}	61.29 (5)	Mn01—Al05—Al05^{xvi}	99.58 (11)
Al03^{viii}—Mn02—Al05^{xiii}	63.50 (9)	Al05^{xv}—Al05—Al05^{xvi}	127.52 (4)
Al03^{ix}—Mn02—Al05^{xiii}	118.71 (5)	Mn02^{xix}—Al05—Al05^{xvi}	57.62 (2)
Al03—Mn02—Al05^{xiii}	118.71 (5)	Al03^{xx}—Al05—Al05^{xvi}	59.82 (8)
Al05^{x}—Mn02—Al05^{xiii}	64.76 (5)	Al03^{xxi}—Al05—Al05^{xvi}	109.39 (8)
Al05^{xi}—Mn02—Al05^{xiii}	180.0	Al03^{xiv}—Al05—Al05^{xvi}	56.87 (10)
Al05^{xii}—Mn02—Al05^{xiii}	115.23 (5)	Mn01^{xv}—Al05—Al05^{xvi}	114.36 (13)
Al03^{v}—Mn02—Al05^{xiv}	116.49 (9)	Al05^{i}—Al05—Al05^{xvi}	104.07 (14)
Al03^{vi}—Mn02—Al05^{xiv}	61.29 (5)	Mn01—Al05—Al06^{i}	55.92 (5)
Al03^{vii}—Mn02—Al05^{xiv}	61.29 (5)	Al05^{xv}—Al05—Al06^{i}	70.76 (8)
Al03^{viii}—Mn02—Al05^{xiv}	118.71 (5)	Mn02^{xix}—Al05—Al06^{i}	118.49 (7)
Al03^{ix}—Mn02—Al05^{xiv}	118.71 (5)	Al03^{xx}—Al05—Al06^{i}	153.69 (11)
Al03—Mn02—Al05^{xiv}	63.51 (9)	Al03^{xxi}—Al05—Al06^{i}	91.59 (6)
Al05^{x}—Mn02—Al05^{xiv}	64.77 (5)	Al03^{xiv}—Al05—Al06^{i}	89.87 (8)
Al05^{xi}—Mn02—Al05^{xiv}	64.77 (5)	Mn01^{xv}—Al05—Al06^{i}	101.71 (7)

$Al05^{xii}$—Mn02—$Al05^{xiv}$	115.23 (5)
$Al05^{xiii}$—Mn02—$Al05^{xiv}$	115.23 (5)
Al04—Al03—Mn02	101.29 (8)
Al04—Al03—$Al06^{iii}$	107.27 (7)
Mn02—Al03—$Al06^{iii}$	132.71 (7)
Al04—Al03—$Al06^{iv}$	107.27 (7)
Mn02—Al03—$Al06^{iv}$	132.71 (7)
$Al06^{iii}$—Al03—$Al06^{iv}$	72.31 (13)
Al04—Al03—$Al05^{xi}$	109.07 (7)
Mn02—Al03—$Al05^{xi}$	60.89 (7)
$Al06^{iii}$—Al03—$Al05^{xi}$	74.36 (8)
$Al06^{iv}$—Al03—$Al05^{xi}$	136.29 (11)
Al04—Al03—$Al05^{x}$	109.07 (7)
Mn02—Al03—$Al05^{x}$	60.89 (7)
$Al06^{iii}$—Al03—$Al05^{x}$	136.30 (11)
$Al06^{iv}$—Al03—$Al05^{x}$	74.36 (8)
$Al05^{xi}$—Al03—$Al05^{x}$	114.53 (15)
Al04—Al03—$Mn01^{ii}$	60.40 (5)
Mn02—Al03—$Mn01^{ii}$	109.51 (6)
$Al06^{iii}$—Al03—$Mn01^{ii}$	117.24 (9)
$Al06^{iv}$—Al03—$Mn01^{ii}$	58.15 (5)
$Al05^{xi}$—Al03—$Mn01^{ii}$	165.50 (11)
$Al05^{x}$—Al03—$Mn01^{ii}$	64.09 (7)
Al04—Al03—$Mn01^{iii}$	60.40 (5)
Mn02—Al03—$Mn01^{iii}$	109.51 (6)
$Al06^{iii}$—Al03—$Mn01^{iii}$	58.14 (5)
$Al06^{iv}$—Al03—$Mn01^{iii}$	117.23 (9)
$Al05^{xi}$—Al03—$Mn01^{iii}$	64.09 (7)
$Al05^{x}$—Al03—$Mn01^{iii}$	165.50 (11)
$Mn01^{ii}$—Al03—$Mn01^{iii}$	113.26 (10)
Al04—Al03—Mn01	60.00 (6)
Mn02—Al03—Mn01	161.29 (11)
$Al06^{iii}$—Al03—Mn01	59.88 (6)
$Al06^{iv}$—Al03—Mn01	59.88 (6)
$Al05^{xi}$—Al03—Mn01	122.45 (7)
$Al05^{x}$—Al03—Mn01	122.45 (7)
$Mn01^{ii}$—Al03—Mn01	62.84 (5)
$Mn01^{iii}$—Al03—Mn01	62.84 (5)
Al04—Al03—$Al05^{xiv}$	161.01 (12)
Mn02—Al03—$Al05^{xiv}$	59.72 (8)
$Al06^{iii}$—Al03—$Al05^{xiv}$	87.92 (8)
$Al06^{iv}$—Al03—$Al05^{xiv}$	87.92 (8)
$Al05^{xi}$—Al03—$Al05^{xiv}$	63.31 (7)
$Al05^{x}$—Al03—$Al05^{xiv}$	63.31 (7)
$Mn01^{ii}$—Al03—$Al05^{xiv}$	123.08 (5)
$Mn01^{iii}$—Al03—$Al05^{xiv}$	123.08 (5)
Mn01—Al03—$Al05^{xiv}$	139.00 (12)
Al04—Al03—$Al03^{ix}$	56.65 (4)

$Al05^{i}$—Al05—$Al06^{i}$	60.87 (6)
$Al05^{xvi}$—Al05—$Al06^{i}$	143.81 (17)
Mn01—Al05—Al06	55.92 (5)
$Al05^{xv}$—Al05—Al06	70.75 (8)
$Mn02^{xix}$—Al05—Al06	118.49 (7)
$Al03^{xx}$—Al05—Al06	91.59 (6)
$Al03^{xxi}$—Al05—Al06	153.69 (11)
$Al03^{xiv}$—Al05—Al06	89.87 (8)
$Mn01^{xv}$—Al05—Al06	101.71 (7)
$Al05^{i}$—Al05—Al06	143.81 (17)
$Al05^{xvi}$—Al05—Al06	60.87 (6)
$Al06^{i}$—Al05—Al06	110.28 (11)
$Mn01^{xvi}$—Al06—Mn01	150.27 (16)
$Mn01^{xvi}$—Al06—$Al03^{xvii}$	61.23 (5)
Mn01—Al06—$Al03^{xvii}$	141.63 (9)
$Mn01^{xvi}$—Al06—$Al03^{ii}$	141.63 (9)
Mn01—Al06—$Al03^{ii}$	61.23 (5)
$Al03^{xvii}$—Al06—$Al03^{ii}$	107.69 (13)
$Mn01^{xvi}$—Al06—$Mn01^{xvii}$	64.29 (6)
Mn01—Al06—$Mn01^{xvii}$	137.27 (7)
$Al03^{xvii}$—Al06—$Mn01^{xvii}$	60.90 (8)
$Al03^{ii}$—Al06—$Mn01^{xvii}$	78.16 (9)
$Mn01^{xvi}$—Al06—$Mn01^{ii}$	137.27 (7)
Mn01—Al06—$Mn01^{ii}$	64.29 (6)
$Al03^{xvii}$—Al06—$Mn01^{ii}$	78.16 (9)
$Al03^{ii}$—Al06—$Mn01^{ii}$	60.90 (8)
$Mn01^{xvii}$—Al06—$Mn01^{ii}$	108.25 (12)
$Mn01^{xvi}$—Al06—$Al06^{iv}$	111.18 (4)
Mn01—Al06—$Al06^{iv}$	59.19 (9)
$Al03^{xvii}$—Al06—$Al06^{iv}$	94.07 (10)
$Al03^{ii}$—Al06—$Al06^{iv}$	106.01 (5)
$Mn01^{xvii}$—Al06—$Al06^{iv}$	154.14 (16)
$Mn01^{ii}$—Al06—$Al06^{iv}$	56.26 (3)
$Mn01^{xvi}$—Al06—$Al06^{xvii}$	59.19 (9)
Mn01—Al06—$Al06^{xvii}$	111.18 (4)
$Al03^{xvii}$—Al06—$Al06^{xvii}$	106.00 (5)
$Al03^{ii}$—Al06—$Al06^{xvii}$	94.07 (10)
$Mn01^{xvii}$—Al06—$Al06^{xvii}$	56.25 (3)
$Mn01^{ii}$—Al06—$Al06^{xvii}$	154.14 (16)
$Al06^{iv}$—Al06—$Al06^{xvii}$	145.82 (19)
$Mn01^{xvi}$—Al06—Al05	97.07 (11)
Mn01—Al06—Al05	55.16 (8)
$Al03^{xvii}$—Al06—Al05	154.93 (11)
$Al03^{ii}$—Al06—Al05	97.17 (6)
$Mn01^{xvii}$—Al06—Al05	123.49 (8)
$Mn01^{ii}$—Al06—Al05	118.16 (7)
$Al06^{iv}$—Al06—Al05	81.81 (14)
$Al06^{xvii}$—Al06—Al05	68.22 (8)

Mn02—Al03—Al03^{ix}	56.73 (4)	Mn01^{xvi}—Al06—Al05^{xvi}	55.15 (8)
Al06^{iii}—Al03—Al03^{ix}	111.75 (7)	Mn01—Al06—Al05^{xvi}	97.07 (11)
Al06^{iv}—Al03—Al03^{ix}	163.86 (5)	Al03^{xvii}—Al06—Al05^{xvi}	97.18 (6)
Al05^{xi}—Al03—Al03^{ix}	58.04 (6)	Al03^{ii}—Al06—Al05^{xvi}	154.93 (11)
Al05^{x}—Al03—Al03^{ix}	108.17 (7)	Mn01^{xvii}—Al06—Al05^{xvi}	118.16 (7)
Mn01^{ii}—Al03—Al03^{ix}	107.93 (5)	Mn01^{ii}—Al06—Al05^{xvi}	123.49 (8)
Mn01^{iii}—Al03—Al03^{ix}	58.18 (5)	Al06^{iv}—Al06—Al05^{xvi}	68.22 (8)
Mn01—Al03—Al03^{ix}	107.73 (5)	Al06^{xvii}—Al06—Al05^{xvi}	81.82 (14)
Al05^{xiv}—Al03—Al03^{ix}	107.58 (7)	Al05—Al06—Al05^{xvi}	58.26 (12)
Al04—Al03—Al03^{viii}	56.65 (4)		

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