Crystal structure of the Al$_{20}$Mn$_{5.37}$Ni$_{1.31}$ phase in the Al–Mn–Ni system

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The intermetallic phase with composition Al$_{20}$Mn$_{5.37}$Ni$_{1.31}$ (icosaaluminium pentamanganese nickel) was synthesized by high-temperature sintering of a mixture with initial chemical composition Al$_{60}$Mn$_7$Ni$_3$. Al$_{20}$Mn$_{5.37}$Ni$_{1.31}$ adopts the Co$_2$Al$_5$ structure type in space-group type $P6_3/mmc$, replacing the Co atoms with the transition-metal atoms Mn and Ni. Structure analysis revealed that one of the two transition-metal sites is partially occupied by Ni [refined occupancy 0.342 (2)] and the other is co-occupied by Mn and Ni with a ratio of 0.895 (14):0.105 (14). The present refined chemical composition is supported by complementary energy-dispersive X-ray fluorescence (EDX) analysis and is in agreement with the previously determined Al–Mn–Ni phase diagram [Balanetskyy et al. (2011). J. Alloys Compd, 509, 3795–3805].

Phases in the ternary Al–Mn–Ni alloy system are structurally complex, also including quasicrystals (QC). For example, an aperiodic diffraction pattern was observed for the alloy with composition Al$_{60}$Mn$_{11}$Ni$_4$, exhibiting tenfold rotation symmetry and characterized as a quasi-crystalline phase (Tendeloo et al., 1988). As a result of their applications in industry, relevant stable and metastable phases in the Al–Mn–Ni system have been investigated thoroughly (Balanetskyy et al., 2011). Three thermodynamically stable ternary intermetallics have been reported, among them the $q$ phase adopting the Co$_2$Al$_5$ structure type [$P6_3/mmc$, $Z = 4$, $a = 7.6632$ (16), $c = 7.8296$ (15) Å; Balanetskyy et al., 2011]. However, a detailed crystal-structure analysis of the $q$ phase has not been indicated, although its homogeneity chemical composition regions at 1223, 1123, 1023, 973, 918 and 893 K were determined (see Table S1 of the supporting information). It should be noted that such Co$_2$Al$_5$-type phases have also been found in other systems e.g. in the binary Al–Mn system the phase Al$_{10}$Mn$_3$ with unit-cell parameters $a = 7.543$, $c = 7.898$ Å.
(Taylor, 1959), or the decaaluminium trinickel iron phase Al10Ni3Fe0.83 that was recently obtained in our group by high-pressure sintering (HPS) of a stoichiometric mixture with nominal composition Al71Ni24Fe5 (Wang et al., 2018). In the present study, the crystal-structure refinement of a phase with composition Al20Mn5.37Ni1.31 based on single-crystal X-ray diffraction data is reported, in accordance with the SEM/EDX results (see Tables S2 and S3 along with Fig. S1 compiled in the supporting information). This phase is located within the diagram region of the ϕ phase determined previously (see Table S1 of the supporting information).

With respect to the Co2Al5 structure type (Newkirk et al., 1961), in the crystal structure of the Al20Mn5.37Ni1.31 phase the Co atoms are replaced by the transition metals Mn and Ni (Fig. 1). The asymmetric unit of Al20Mn5.37Ni1.31 comprises five metal sites, three fully occupied by Al atoms at Wyckoff positions 2 a (Al1), 6 h (Al2) and 12 k (Al3), one partially occupied Ni2 site [occupancy 0.342 (2)] at 2 d and one co-occupied (Mn1/Ni1) site [occupancy ratio 0.895 (14): 0.105 (14)] at 6 h. The environment of the co-occupied (Mn1/Ni1) site is shown in Fig. 2, where twelve vertices include ten Al atoms (Al1, Al2, Al3) and two symmetry-related (Mn1/Ni1) sites. In the crystal structure, the distorted icosahedra centered at Al1 and (Mn1/Ni1) and the polyhedron centered at Al2 are fused with each other, as shown in Fig. 3.

**Synthesis and crystallization**

The high-purity elements Al (indicated purity 99.8%; 2.700 g), Mn (indicated purity 99.96%; 0.6417 g) and Ni (indicated purity 99.9%; 0.2935 g) were mixed in the molar ratio 60:7:3 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 sample with a weight of 50.32 mg was selected and subsequently loaded into a Netzsch
STA449C simultaneous thermal analysis apparatus. The sample was heated up to 1373 K for 10 min with a heating rate of 20 K min⁻¹. Finally, the sample was slowly cooled to room temperature by turning off the furnace power. Suitable pieces of single-crystal grains were selected from the products for single-crystal X-ray diffraction experiments.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. For better comparison with the Co₂Al₅ structure type, the labelling scheme and atomic coordinates were adapted from Co₂Al₅ (Newkirk et al., 1961). One of the five metal sites is partially occupied by Ni atoms (Ni2) and one site is co-occupied by Mn and Ni atoms (Mn1/Ni1); all Al atoms show full occupancy. Atoms sharing the same site were constrained to have the same coordinates and anisotropic displacement parameters. The maximum and minimum residual electron densities in the final difference map are located 1.32 Å from the (Mn1/Ni1) site and 0.01 Å from the same site, respectively.

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full crystallographic data

IUCrData (2021). 6, x210981  [https://doi.org/10.1107/S2414314621009810]

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Icosaluminium pentamanganese nickel

Crystal data

Al$_{20}$Mn$_{5.37}$Ni$_{1.31}$  $D_\text{c} = 3.870$ Mg m$^{-3}$

$M_r = 911.74$  Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Hexagonal, $P\overline{6}_3/mmc$

$a = 7.6009$ (3) Å  $\theta = 3.1$–30.5°

c = 7.8187 (5) Å  $\mu = 6.85$ mm$^{-1}$

$V = 391.20$ (4) Å$^3$  $T = 296$ K

$Z = 1$  Fragment, metallic

$F(000) = 431$  0.14 × 0.07 × 0.05 mm

Data collection

Bruker D8 Venture Photon 100 CMOS
diffractometer

$\varphi$ and $\omega$ scans

Absorption correction: multi-scan

(SADABS; Krause et al., 2015)

$T_{\text{min}} = 0.588$, $T_{\text{max}} = 0.746$

14281 measured reflections

260 independent reflections

246 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.048$

$\theta_{\text{max}} = 30.5^\circ$, $\theta_{\text{min}} = 3.1^\circ$

$h = -10\rightarrow10$

$k = -10\rightarrow10$

$l = -11\rightarrow11$

Refinement

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.016$

$wR(F^2) = 0.033$

$S = 1.20$

260 reflections

21 parameters

0 restraints

$\Delta/\sigma$ max: 0.001

$\Delta$$\rho$ max: 0.35 e Å$^{-3}$

$\Delta$$\rho$ min: −0.46 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$^2$)

|       | x     | y     | z     | $U_{eq}$/$U_{eq}$ | Occ. (<1) |
|-------|-------|-------|-------|-------------------|----------|
| Mn1   | 0.12191 (3) | 0.24382 (5) | 0.250000 | 0.00549 (12)       | 0.895 (14)|
| Ni1   | 0.12191 (3) | 0.24382 (5) | 0.250000 | 0.00549 (12)       | 0.105 (14)|
### Atomic displacement parameters (Å²)

|       | $U_{11}$     | $U_{22}$     | $U_{33}$     | $U_{12}$     | $U_{13}$     | $U_{23}$     |
|-------|--------------|--------------|--------------|--------------|--------------|--------------|
| Mn1   | 0.00704 (15) | 0.00404 (17) | 0.00438 (18) | 0.00202 (9)  | 0.000        | 0.000        |
| Ni1   | 0.00704 (15) | 0.00404 (17) | 0.00438 (18) | 0.00202 (9)  | 0.000        | 0.000        |
| Al1   | 0.0067 (3)   | 0.0067 (3)   | 0.0053 (5)   | 0.00333 (17) | 0.000        | 0.000        |
| Al2   | 0.0056 (3)   | 0.0091 (4)   | 0.0095 (3)   | 0.00454 (19) | 0.000        | 0.000        |
| Al3   | 0.0079 (2)   | 0.0095 (3)   | 0.0077 (3)   | 0.00477 (13) | 0.00001 (10) | 0.00003 (19) |
| Ni2   | 0.0050 (5)   | 0.0050 (5)   | 0.0036 (7)   | 0.0025 (3)   | 0.000        | 0.000        |

### Geometric parameters (Å, °)

|       | $d$ (Å)  | $d$ (Å)  |
|-------|----------|----------|
| Mn1—Al2i | 2.4251 (3) | Al1—Al3vi | 2.6698 (5) |
| Mn1—Al2ii | 2.4251 (3) | Al2—Ni2iv | 2.7310 (8) |
| Mn1—Al1   | 2.5292 (2) | Al2—Al3sviii | 2.8132 (6) |
| Mn1—Al1iii | 2.5292 (2) | Al2—Al3sii | 2.8132 (6) |
| Mn1—Al3iv | 2.6438 (6) | Al2—Al3sii | 2.8132 (6) |
| Mn1—Al3v  | 2.6438 (6) | Al2—Al3sii | 2.8132 (6) |
| Mn1—Al3vi | 2.7236 (5) | Al2—Al3sii | 2.8132 (6) |
| Mn1—Al3vii | 2.7236 (5) | Al2—Al3sii | 2.8132 (6) |
| Mn1—Al3viii | 2.7236 (5) | Al2—Al3sii | 2.8132 (6) |
| Mn1—Al3ix | 2.7236 (5) | Al2—Al3sii | 2.8132 (6) |
| Mn1—Mn1x  | 2.7799 (6) | Al2—Al3sii | 2.8132 (6) |
| Mn1—Mn1xi | 2.7799 (6) | Al3—Ni2xiv | 2.9625 (5) |
| Al1—Al3sx | 2.6698 (5) | Al3—Al3sxi | 2.9625 (5) |
| Al1—Al3sii | 2.6698 (5) | Al3—Al3sxi | 2.9625 (5) |
| Al1—Al3v  | 2.6698 (5) | Al3—Al3sxi | 2.9625 (5) |
| Al1—Al3viii | 2.6698 (5) | Al3—Al3sxi | 2.9625 (5) |
| Al1—Mn1—Al2ii | 72.58 (4) | Al3sxi—Al2—Al2i | 107.340 (16) |
| Al1—Mn1—Al1   | 120.763 (8) | Al3sxi—Al2—Al2i | 107.340 (16) |
| Al1—Mn1—Al1iii | 120.763 (8) | Al3sxi—Al2—Al2i | 147.217 (13) |
| Al1—Mn1—Al1ii | 120.763 (9) | Al3sxi—Al2—Al2i | 147.217 (13) |
| Al1—Mn1—Al1iii | 120.763 (8) | Mn1s—Al2—Al2a | 113.710 (19) |
| Al1—Mn1—Al1iv | 101.222 (13) | Mn1s—Al2—Al2a | 147.217 (13) |
| Al1—Al3iv | 71.871 (12) | Mn1s—Al2—Al2a | 147.217 (13) |
| Al1—Al3v  | 71.871 (12) | Ni2s—Al2—Al2a | 147.217 (13) |
| Al1—Mn1—Al3v | 163.319 (18) | Al3s—Al2—Al2a | 147.217 (13) |
| Al1—Mn1—Al3v | 62.097 (12) | Al3s—Al2—Al2a | 107.340 (16) |
| Al1—Mn1—Al3v | 71.871 (12) | Al3s—Al2—Al2a | 107.340 (16) |
| Al1—Mn1—Al3v | 71.871 (12) | Al2—Al2—Al2a | 60.0 |
| Al1—Mn1—Al3v | 62.097 (12) | Mn1s—Al2—Al3sxi | 57.471 (11) |
| Al1—Mn1—Al3v | 163.319 (18) | Mn1s—Al2—Al3sxi | 118.729 (14) |
| Bond | M—M | M—I | I—M |
|------|------|------|------|
| Al3vi—Mn1—Al3vi | 134.58 (3) | Ni2xiv—Al2—Al3xvi | 105.093 (16) |
| Al2—Mn1—Al3vi | 65.942 (17) | Al3xvi—Al2—Al3xvi | 108.722 (19) |
| Al2i—Mn1—Al3vi | 125.493 (18) | Al3xvi—Al2—Al3xvi | 57.684 (15) |
| Al1—Mn1—Al3vi | 60.965 (11) | Al3xvi—Al2—Al3xvi | 151.28 (3) |
| Al1ii—Mn1—Al3vi | 110.438 (11) | Al2iv—Al2—Al3xvi | 91.228 (9) |
| Al3—Mn1—Al3vi | 122.648 (12) | Al2iv—Al2—Al3xvi | 61.207 (14) |
| Al2—Mn1—Al3vi | 65.942 (17) | Mn1iv—Al2—Al3xvi | 91.756 (15) |
| Al2i—Mn1—Al3vi | 125.493 (18) | Mn1iv—Al2—Al3xvi | 57.471 (11) |
| Al1—Mn1—Al3vi | 60.965 (11) | Mn1iv—Al2—Al3xvi | 118.729 (14) |
| Al1iii—Mn1—Al3vi | 62.829 (9) | Ni2xiv—Al2—Al3xvi | 105.093 (16) |
| Al3iv—Mn1—Al3vi | 122.648 (12) | Al3xivi—Al2—Al3xvi | 108.722 (19) |
| Al3v—Mn1—Al3vi | 62.829 (9) | Al3xivi—Al2—Al3xvi | 91.228 (9) |
| Al3vi—Mn1—Al3vi | 65.35 (2) | Al3xv—Al2—Al3xvi | 151.28 (3) |
| Al2—Mn1—Al3vi | 125.493 (18) | Al2v—Al2—Al3xvi | 61.207 (14) |
| Al2i—Mn1—Al3vi | 65.942 (17) | Al2v—Al2—Al3xvi | 91.756 (15) |
| Al1—Mn1—Al3vi | 110.438 (11) | Al3xv—Al2—Al3xvi | 109.848 (19) |
| Al1ii—Mn1—Al3vi | 60.965 (11) | Mn1iv—Al2—Al3xvi | 118.729 (14) |
| Al3—Mn1—Al3vi | 122.648 (12) | Mn1iv—Al2—Al3xvi | 57.471 (10) |
| Al3i—Mn1—Al3vi | 113.20 (2) | Ni2xiv—Al2—Al3xvi | 105.094 (16) |
| Al2—Mn1—Al3ix | 125.493 (18) | Al3xvi—Al2—Al3xvi | 91.227 (9) |
| Al2i—Mn1—Al3ix | 65.942 (17) | Al3xv—Al2—Al3xvi | 151.28 (3) |
| Al1—Mn1—Al3ix | 110.438 (11) | Al3xv—Al2—Al3xvi | 57.684 (15) |
| Al1ii—Mn1—Al3ix | 60.965 (11) | Al3xv—Al2—Al3xvi | 149.81 (3) |
| Al3—Mn1—Al3ix | 122.647 (12) | Al3xv—Al2—Al3xvi | 61.63 (2) |
| Al3i—Mn1—Al3ix | 62.829 (9) | Ni2xiv—Al3—Mn1xvi | 152.54 (3) |
| Al3—Mn1—Al3xvi | 65.35 (2) | Ni2xiv—Al3—Mn1xvi | 150.22 (2) |
| Al2—Mn1—Mn1s | 113.710 (19) | Mn1xxviii—Al3—Mn1xvi | 99.682 (17) |
| Al2i—Mn1—Mn1s | 173.710 (19) | Mn1xxviii—Al3—Mn1xvi | 103.866 (18) |
| Al1—Mn1—Mn1s | 56.663 (5) | Al1xxviii—Al3—Mn1xvi | 55.920 (12) |
| Al1ii—Mn1—Mn1s | 56.663 (5) | Ni2xiv—Al3—Mn1xvi | 99.682 (17) |
| Al3—Mn1—Mn1s | 109.531 (12) | Mn1xxviii—Al3—Mn1xvi | 103.866 (18) |
| Al3i—Mn1—Mn1s | 109.531 (12) | Mn1xxviii—Al3—Mn1xvi | 55.920 (12) |
| Al3—Mn1—Mn1s | 59.314 (9) | Mn1xxviii—Al3—Mn1xvi | 61.373 (18) |
| Al3v—Mn1—Mn1s | 59.314 (9) | Ni2xiv—Al3—Mn1xvi | 125.585 (12) |
| Al3—Mn1—Mn1s | 108.937 (11) | Mn1xxviii—Al3—Mn1xvi | 59.979 (17) |
| Al2—Mn1—Mn1s | 108.937 (11) | Al1xxviii—Al3—Mn1xvi | 58.393 (3) |
| Al2—Mn1—Mn1s | 173.710 (19) | Mn1xxviii—Al3—Mn1xvi | 57.191 (12) |
| Al1—Mn1—Mn1s | 56.663 (5) | Mn1xxviii—Al3—Mn1xvi | 106.707 (14) |
| Al1ii—Mn1—Mn1s | 56.663 (5) | Ni2xiv—Al3—Mn1xvi | 125.584 (12) |
| Al3—Mn1—Mn1s | 109.531 (12) | Mn1xxviii—Al3—Mn1xvi | 59.979 (17) |
| Al3v—Mn1—Mn1s | 109.531 (12) | Al1xxviii—Al3—Mn1xvi | 58.393 (3) |
| Al3—Mn1—Mn1s | 108.937 (11) | Mn1xxviii—Al3—Mn1xvi | 57.191 (12) |
Al$_3^{\text{Vii}}$—Mn$_1$—Mn$_1^{\text{Xii}}$ 108.937 (11)  
Al$_3^{\text{Vii}}$—Mn$_1$—Mn$_1^{\text{X}}$ 59.314 (9)  
Al$_3^{\text{Vii}}$—Mn$_1$—Mn$_1^{\text{Xvii}}$ 59.314 (9)  
Mn$_1$—Mn$_1^{\text{Xii}}$—Mn$_1^{\text{Xvii}}$ 113.326 (11)  
Mn$_1$—Mn$_1^{\text{Xvii}}$—Al$_3$ 113.326 (10)  
Mn$_1$—Al$_1$—Mn$_1^{\text{Xii}}$ 66.764 (10)  
Mn$_1$—Al$_1$—Mn$_1^{\text{Xvii}}$ 113.326 (10)  
Mn$_1$—Al$_1$—Mn$_1^{\text{X}}$ 113.326 (10)  
Mn$_1$—Al$_1$—Mn$_1^{\text{Xii}}$ 113.326 (10)  
Mn$_1$—Al$_1$—Mn$_1^{\text{Xvii}}$ 118.000 (15)  
Mn$_1$—Al$_1$—Al$_3^{\text{Xiv}}$ 63.116 (9)  
Mn$_1^{\text{Vii}}$—Al$_1$—Al$_3^{\text{Xiv}}$ 116.885 (9)  
Mn$_1^{\text{Vii}}$—Al$_1$—Al$_3^{\text{Xv}}$ 116.884 (9)  
Mn$_1^{\text{Vii}}$—Al$_1$—Al$_3^{\text{Xvi}}$ 63.116 (9)  
Al$_3^{\text{Vii}}$—Al$_1$—Al$_3^{\text{Xiv}}$ 118.940 (13)  
Al$_3^{\text{Vii}}$—Al$_1$—Al$_3^{\text{Xv}}$ 61.060 (13)  
Al$_3^{\text{Vii}}$—Al$_1$—Al$_3^{\text{Xvi}}$ 116.884 (9)  
Mn$_1$—Mn$_1^{\text{Vii}}$—Al$_3^{\text{Xiv}}$ 63.115 (9)  
Mn$_1$—Mn$_1^{\text{Vii}}$—Al$_3^{\text{Xv}}$ 116.844 (9)  
Mn$_1$—Mn$_1^{\text{Vii}}$—Al$_3^{\text{Xvi}}$ 63.116 (9)  
Mn$_1$—Mn$_1^{\text{Vii}}$—Al$_3^{\text{Xvii}}$ 118.940 (13)  
Mn$_1^{\text{Vii}}$—Al$_1$—Al$_3^{\text{Xiv}}$ 63.115 (9)  
Mn$_1^{\text{Vii}}$—Al$_1$—Al$_3^{\text{Xv}}$ 116.884 (9)  
Mn$_1^{\text{Vii}}$—Al$_1$—Al$_3^{\text{Xvi}}$ 63.116 (9)  
Mn$_1^{\text{Vii}}$—Al$_1$—Al$_3^{\text{Xvii}}$ 116.884 (9)  
Mn$_1^{\text{Vii}}$—Al$_1$—Al$_3^{\text{Xviii}}$ 63.116 (9)  
Mn$_1^{\text{Xii}}$—Al$_1$—Al$_3^{\text{Xiv}}$ 118.940 (13)  
Mn$_1^{\text{Xii}}$—Al$_1$—Al$_3^{\text{Xv}}$ 61.060 (13)  
Mn$_1^{\text{Xii}}$—Al$_1$—Al$_3^{\text{Xvi}}$ 116.884 (9)  
Mn$_1^{\text{Xii}}$—Al$_1$—Al$_3^{\text{Xvii}}$ 118.940 (13)  
Al$_3^{\text{Xiv}}$—Al$_1$—Al$_3^{\text{Xiv}}$ 180.0  
Al$_3^{\text{Xiv}}$—Al$_1$—Al$_3^{\text{Xv}}$ 61.060 (13)  
Al$_3^{\text{Xiv}}$—Al$_1$—Al$_3^{\text{Xvi}}$ 116.884 (9)  
Al$_3^{\text{Xiv}}$—Al$_1$—Al$_3^{\text{Xvii}}$ 118.940 (13)  
Al$_3^{\text{Xiv}}$—Al$_1$—Al$_3^{\text{Xviii}}$ 63.116 (9)  
Al$_3^{\text{Xiv}}$—Al$_1$—Al$_3^{\text{Xix}}$ 63.214 (7)  
Al$_3^{\text{Xiv}}$—Al$_1$—Al$_3^{\text{Xvi}}$ 116.886 (9)  
Al$_3^{\text{Xiv}}$—Al$_1$—Al$_3^{\text{Xvii}}$ 116.786 (7)  
Al$_3^{\text{Xiv}}$—Al$_1$—Al$_3^{\text{Xviii}}$ 63.214 (7)  
Al$_3^{\text{Xiv}}$—Al$_1$—Al$_3^{\text{Xv}}$ 116.886 (9)  
Al$_3^{\text{Xiv}}$—Al$_1$—Al$_3^{\text{Xvi}}$ 116.786 (7)  
Al$_3^{\text{Xiv}}$—Al$_1$—Al$_3^{\text{Xvii}}$ 63.214 (7)  
Al$_3^{\text{Xiv}}$—Al$_1$—Al$_3^{\text{Xviii}}$ 116.886 (9)  
Al$_3^{\text{Xiv}}$—Al$_1$—Al$_3^{\text{Xv}}$ 116.786 (7)  
Al$_3^{\text{Xiv}}$—Al$_1$—Al$_3^{\text{Xvi}}$ 63.214 (7)  
Al$_3^{\text{Xiv}}$—Al$_1$—Al$_3^{\text{Xvii}}$ 116.886 (9)  
Al$_3^{\text{Xiv}}$—Al$_1$—Al$_3^{\text{Xviii}}$ 116.786 (7)  
Al$_3^{\text{Xiv}}$—Al$_1$—Al$_3^{\text{Xv}}$ 63.214 (7)  
Al$_3^{\text{Xiv}}$—Al$_1$—Al$_3^{\text{Xvi}}$ 116.886 (9)  
Al$_3^{\text{Xiv}}$—Al$_1$—Al$_3^{\text{Xvii}}$ 116.786 (7)  
Al$_3^{\text{Xiv}}$—Al$_1$—Al$_3^{\text{Xviii}}$ 63.214 (7)
| Bond Length (Å) | Symmetry Code | Bond Angle (°) |
|----------------|---------------|---------------|
| Al3—Al1—Al3  | 180.000 (14)  | Ni2—Al3—Ni2  | 83.37 (2)  |
| Mn1—Al1—Al3  | 63.116 (9)    | Al3—Ni2—Al3  | 83.37 (2)  |
| Mn1—Al1—Al3  | 116.884 (9)   | Al3—Ni2—Al3  | 134.842 (9) |
| Ni1—Al1—Al3  | 61.060 (13)   | Al3—Ni2—Al3  | 134.842 (9) |
| Ni1—Al1—Al3  | 118.940 (13)  | Al3—Ni2—Al3  | 83.37 (2)  |
| Mn1—Al1—Al3  | 63.115 (9)    | Al3—Ni2—Al3  | 134.842 (9) |
| Mn1—Al1—Al3  | 116.885 (9)   | Al3—Ni2—Al3  | 79.67 (3)  |
| Al3—Al1—Al3  | 63.214 (7)    | Al3—Ni2—Al3  | 83.37 (2)  |
| Al3—Al1—Al3  | 63.214 (7)    | Al3—Ni2—Al3  | 83.37 (2)  |
| Al3—Al1—Al3  | 116.786 (7)   | Al3—Ni2—Al3  | 83.37 (2)  |
| Mn1—Al2—Mn1i | 167.42 (4)    | Al3—Ni2—Al3  | 79.67 (3)  |
| Mn1—Al2—Mn1i | 96.289 (19)   | Al3—Ni2—Al3  | 134.842 (9) |
| Mn1—Al2—Al3  | 96.290 (19)   | Al3—Ni2—Al3  | 67.421 (5)  |
| Mn1—Al2—Al3  | 62.135 (13)   | Al3—Ni2—Al3  | 67.421 (5)  |
| Ni2—Al2—Al3  | 127.69 (2)    | Al3—Ni2—Al3  | 67.421 (5)  |
| Ni2—Al2—Al3  | 48.892 (16)   | Al3—Ni2—Al3  | 140.167 (13) |
| Mn1—Al2—Al3  | 62.135 (13)   | Al3—Ni2—Al3  | 67.421 (5)  |
| Ni2—Al2—Al3  | 127.69 (2)    | Al3—Ni2—Al3  | 67.421 (5)  |
| Ni2—Al2—Al3  | 48.892 (16)   | Al3—Ni2—Al3  | 140.167 (13) |
| Mn1—Al2—Al3  | 62.135 (13)   | Al3—Ni2—Al3  | 67.421 (5)  |
| Al3—Al2—Al3  | 65.73 (3)     | Al3—Ni2—Al3  | 120.0       |
| Mn1—Al2—Al3  | 97.79 (3)     | Al3—Ni2—Al3  | 140.167 (13) |
| Mn1—Al2—Al3  | 127.69 (2)    | Al3—Ni2—Al3  | 140.167 (13) |
| Mn1—Al2—Al3  | 62.135 (13)   | Al3—Ni2—Al3  | 140.167 (13) |
| Ni2—Al2—Al3  | 48.893 (16)   | Al3—Ni2—Al3  | 140.167 (14) |
| Al3—Al2—Al3  | 65.73 (3)     | Al3—Ni2—Al3  | 67.421 (5)  |
| Al3—Al2—Al3  | 97.79 (3)     | Al3—Ni2—Al3  | 67.421 (5)  |
| Mn1—Al2—Al3  | 127.69 (2)    | Al3—Ni2—Al3  | 120.0       |
| Mn1—Al2—Al3  | 62.135 (13)   | Al3—Ni2—Al3  | 140.167 (13) |
| Ni2—Al2—Al3  | 48.893 (16)   | Al3—Ni2—Al3  | 140.167 (13) |
| Al3—Al2—Al3  | 65.73 (3)     | Al3—Ni2—Al3  | 67.421 (5)  |
| Al3—Al2—Al3  | 97.79 (3)     | Al3—Ni2—Al3  | 67.421 (5)  |
| Mn1—Al2—Al3  | 127.69 (2)    | Al3—Ni2—Al3  | 120.0       |
| Mn1—Al2—Al3  | 62.135 (13)   | Al3—Ni2—Al3  | 120.0       |
| Mn1—Al2—Al3  | 53.710 (19)   | Al3—Ni2—Al3  | 120.0       |
| Mn1—Al2—Al3  | 113.711 (19)  | Al3—Ni2—Al3  | 120.0       |

Symmetry codes: (i) x+y, x−y, z; (ii) −x+y, −x+z, z; (iii) −x, −y, z+1/2; (iv) x, y, −z+3/2; (v) x+y, −z+1/2; (vi) x−y, x, −z+1; (vii) y, −x+y, x, −z+1/2; (viii) y, −x+y, z−1/2; (ix) y, −x+y, −z+1; (x) −y, x−y, z; (xi) −x+y, −x, −z; (xii) −y, x−y, −z; (xiii) x−y, −x+y, −z; (xiv) x−y, y−z, x; (xv) y, −x+y, −z+1/2; (xvi) x+y, y−z, x; (xvii) x+y, x−y, −z; (xviii) x−y, x−y, −z; (xix) −x+y, −x+y, −z; (xx) −x+y, x−y, z−1/2; (xxi) −x+y, x−y, z+1; (xxii) x−y, x−y, z−1; (xxiii) x−y, −x+y, z; (xxiv) x−y, z−1; (xxv) −x+y, −x+y, z; (xxvi) −y, −x+y, z−1; (xxvii) y, −x+y, z; (xxviii) −y, −x+y, z; (xxix) −y, y−z, z; (xxx) x−y, x−y, z; (xxxi) −x+y, −x+y, z; (xxxii) −y, y−z, z; (xxxiii) x−y, x−y, z; (xxxiv) x−y, x−y, z; (xxxv) x−y, x−y, z; (xxxvi) x−y, x−y, z; (xxxvii) x−y, x−y, z; (xxxviii) x−y, x−y, z; (xxxix) x−y, x−y, z; (xxxx) x−y, x−y, z; (xxxxi) x−y, x−y, z; (xxxxii) x−y, x−y, z; (xxxxiii) x−y, x−y, z; (xxxxiv) x−y, x−y, z; (xxxxv) x−y, x−y, z; (xxxxvi) x−y, x−y, z; (xxxxvii) x−y, x−y, z; (xxxxviii) x−y, x−y, z; (xxxxix) x−y, x−y, z; (xxxxx) x−y, x−y, z.