The $\text{Al}_{61.49}\text{Mn}_{11.35}\text{Ni}_4$ phase in the Al–Mn–Ni system

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An intermetallic phase in the Al–Mn–Ni system crystallizing in space group $\text{Cmcm}$ (No. 63) and refined formula $\text{Al}_{61.49}\text{Mn}_{11.35}\text{Ni}_4$ (called the $R^0$ phase) has been synthesized by high-temperature sintering of a mixture with initial chemical composition $\text{Al}_{60}\text{Mn}_7\text{Ni}_3$. In comparison with the structure model of the previously reported $R$ phase with composition $\text{Al}_{60}\text{Mn}_{11}\text{Ni}_4$ [Robinson (1954). Acta Cryst. 7, 494–497], there are two mutually exchanged Mn and Ni sites together with one positionally disordered Al site [occupancy ratio 0.811 (8):0.121 (7)] and one partially occupied Mn site [s.o.f. 0.677 (5)] in the current structure model of the $R^0$ phase.

Structure description

The ternary Al–Mn–Ni alloy system contains a variety of phases with complex or even quasicrystalline structures, most of which are not completely determined. Phase equilibria in the Al-rich region of the Al–Mn–Ni alloy system have been investigated previously. In this regard, a ternary phase with composition close to $\text{Al}_{60}\text{Mn}_{11}\text{Ni}_4$ was reported as thermodynamically stable, crystallizing in space group $\text{Bbmm}$ (non-conventional setting of space group $\text{Cmcm}$) with unit-cell parameters of $a = 23.8$, $b = 12.5$, $c = 7.55$ Å (Raynor, 1944). Its chemical composition was determined to be $\text{Al}_{60.0}\text{Mn}_{14.3}\text{Ni}_{5.3}$ for the same sample. This phase was later denominated the $R$ phase (Robinson, 1954). The derived crystal-structure model for the $R$ phase had some ambiguities because at that time it was not possible to accurately model the deficiencies or the type of element for some of the atomic sites (Robinson, 1954). The $R$ phase with similar composition/crystal structure has also been discovered in other systems, such as the $T_3$ phase in the Al–Mn–Zn system or the $\text{Al}_{30}\text{Mn}_3\text{Cu}_2$ phase (Damjanovic, 1961). It is interesting to note that the orthorhombic phase in the Al–Mn system is isostructural with...
Al61.49Mn11.35Ni4, in accordance with complementary Cmcm phase has similar unit-cell parameters to the previously reported phase. This phase has two reversed sites compared to the original model, and vice versa. In addition, the R' phase shows positional disorder of one Al site (Al7), and one Mn site (Mn2) with partial occupancy. Fig. 1 shows the distribution of all atoms in the unit cell of Al61.49Mn11.35Ni4 with four distorted icosahedra illustrated for simplicity. The environments of the Mn3 and Mn4 sites are shown in Fig. 2a and 2b, respectively. The icosahedron centered at Mn3 is surrounded solely by Al atoms (Al1, Al4, Al5, Al6, Al10, Al11, Al12 and Al13) while that centered at Mn4 atom is composed of eleven Al atoms (Al1, Al2, Al4, Al5, Al9, Al11 and Al12) and one Mn atom (Mn4); all of the corresponding atomic sites are fully occupied. The polyhedron centered at Al3 is composed of a pentagonal prism capped by two atoms at the base faces, as shown in Fig. 3a. The environments of Al3 are displayed in Fig. 3b, where ten Al atoms (Al6, Al12 and Al13) and two Mn atoms (Mn3) surround the central atom.

Synthesis and crystallization

The high-purity elements Al (indicated purity 99.8%; 2.4285 g), Mn (indicated purity 99.96%; 0.5768 g) and Ni (indicated purity 99.9%; 0.2641 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 put into a silica glass tube and vacuum-sealed by a home-made sealing machine. The resulting ampoule then was placed in a furnace (SG-XQL1200) and heated up to 473 K for 10 min with a heating rate of 10 K min$^{-1}$ and then heated up to 1373 K for 30 min with the same heating rate. Finally, the sample was slowly cooled to room temperature by turning off the furnace power. Suitable pieces of single-crystal grains were broken and selected from the product for single-crystal X-ray diffraction.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. Manganese site Mn2 is partially

![Diagram](image-url)
Table 1
Experimental details.

| Crystal data |
|--------------|
| Chemical formula | Al_{61.49}Mn_{11.35}Ni_{4} |
| $M_r$ | 2517.49 |
| Crystal system, space group | Orthorhombic, Cmcm |
| Temperature (K) | 296 |
| $a$, $b$, $c$ (Å) | 7.6135 (3), 23.9582 (11), 12.4828 (6) |
| $V$ (Å³) | 2276.93 (18) |
| $Z$ | 2 |
| Radiation type | Mo Ka |
| $\mu$ (mm⁻¹) | 5.85 |
| Crystal size (mm) | 0.10 × 0.10 × 0.05 |

| Data collection |
|----------------|
| Diffractometer | Bruker D8 Venture Photon 100 CMOS |
| Absorption correction | Multi-scan (SADABS; Krause et al., 2015) |
| $T_{\text{min}}$, $T_{\text{max}}$ | 0.648, 0.746 |
| No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections | 40442, 1584, 1269 |
| $R_{\text{int}}$ | 0.090 |
| $(\sin \theta/\lambda)_{\text{max}}$ (Å⁻¹) | 0.666 |

| Refinement |
|-------------|
| $R(F^2 > 2\sigma(F^2))$, $wR(F^2)$, $S$ | 0.039, 0.095, 1.06 |
| No. of reflections | 1584 |
| No. of parameters | 114 |
| $\Delta p_{\text{max}}$, $\Delta p_{\text{min}}$ (e Å⁻³) | 1.85, -1.03 |

Computer programs: APEX3 and SAINT (Bruker, 2015), SHELXT (Sheldrick, 2015a), SHELXL (Sheldrick, 2015b), DIAMOND (Brandenburg & Putz, 2017) and publCIF (Westrip, 2010).

occupied, and its site occupation factor (s.o.f.) was refined to 0.677 (5). The aluminium site Al17 was found to be disordered over two positions with refined s.o.f.s of 0.811 (8) and 0.121 (7) for Al7A and Al7B, respectively. The same anisotropic displacement parameters were used for these two split Al sites. All Ni sites in the present model show full occupancy. The maximum and minimum residual electron densities in the final difference map are located 1.42 Å from site Al11 and 0.57 Å from site Al7A, respectively.

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(I)

Crystal data
Al$_{61.49}$Mn$_{11.35}$Ni$_4$
$D_x$ = 3.672 Mg m$^{-3}$
$M_r$ = 2517.49
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Orthorhombic, $Cmcm$
$\theta$ = 2.4–30.6°
$a$ = 7.6135 (3) Å
$\mu$ = 5.85 mm$^{-1}$
$b$ = 23.9582 (11) Å
$T$ = 296 K
c = 12.4828 (6) Å
$F(000)$ = 2390
$V$ = 2276.93 (18) Å$^3$
Fragment, metallic
$Z$ = 2
$\theta_{\text{min}}$ = 0.648, $\theta_{\text{max}}$ = 0.746
$\phi$ and $\omega$ scans
$\theta_{\text{max}}$ = 28.3°, $\theta_{\text{min}}$ = 2.4°
40442 measured reflections
$\phi = -10$→10
$R_{\text{int}}$ = 0.090
$h$ = −10→10
$T_{\text{min}}$ = 0.648, $T_{\text{max}}$ = 0.746
$k$ = −31→31
$R_{\text{int}}$ = 0.090
$l$ = −16→16

Reefinement
Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2) = 0.095$
$S$ = 1.06
0 restraints
1584 reflections
114 parameters
$\Delta\rho_{\text{max}}$ = 1.85 e Å$^{-3}$
$\Delta\rho_{\text{min}}$ = −1.03 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$^2$)

|        | $x$      | $y$      | $z$      | $U_{eq}$ | Occ. (<1) |
|--------|----------|----------|----------|----------|-----------|
| Ni1    | 0.000000 | 0.91273 (3) | 0.06707 (7) | 0.0123 (2) |           |
| Mn1    | 0.000000 | 0.54113 (5) | 0.750000 | 0.0070 (3) |           |
|   | U<sup>11</sup>  | U<sup>22</sup>  | U<sup>33</sup>  | U<sup>12</sup>  | U<sup>13</sup>  | U<sup>23</sup>  |
|---|----------------|----------------|----------------|----------------|----------------|----------------|
| Mn2 | 0.000000 | 0.92062 (7) | 0.750000 | 0.0071 (6) | 0.677 (5) |
| Mn3 | 0.000000 | 0.63847 (3) | 0.05426 (6) | 0.00525 (19) |
| Mn4 | 0.18574 (11) | 0.71395 (3) | 0.750000 | 0.00517 (19) |
| Al1 | 0.000000 | 0.81074 (10) | 0.750000 | 0.0081 (5) |
| Al2 | 0.000000 | 0.79366 (10) | 0.250000 | 0.0083 (5) |
| Al3 | 0.000000 | 0.63386 (10) | 0.250000 | 0.0111 (5) |
| Al4 | 0.000000 | 0.63837 (6) | 0.84947 (13) | 0.0066 (3) |
| Al5 | 0.000000 | 0.73945 (7) | 0.93387 (13) | 0.0076 (3) |
| Al6 | 0.000000 | 0.53869 (7) | 0.11718 (14) | 0.0129 (4) |
| Al7A | 0.000000 | 0.98517 (9) | 0.9064 (2) | 0.0170 (8) | 0.811 (8) |
| Al7B | 0.000000 | 0.000000 | 0.000000 | 0.0170 (8) | 0.121 (7) |
| Al8 | 0.2272 (3) | 0.01406 (8) | 0.250000 | 0.0250 (5) |
| Al9 | 0.1846 (2) | 0.89615 (7) | 0.250000 | 0.0094 (4) |
| Al10 | 0.18981 (16) | 0.55406 (5) | 0.93399 (9) | 0.0075 (3) |
| Al11 | 0.19159 (16) | 0.82804 (5) | 0.06539 (9) | 0.0074 (3) |
| Al12 | 0.18747 (16) | 0.71601 (5) | 0.12610 (9) | 0.0080 (3) |
| Al13 | 0.18943 (17) | 0.89124 (5) | 0.88587 (11) | 0.0135 (3) |

### Atomic displacement parameters (Å<sup>2</sup>)

|   | U<sup>11</sup>  | U<sup>22</sup>  | U<sup>33</sup>  | U<sup>12</sup>  | U<sup>13</sup>  | U<sup>23</sup>  |
|---|----------------|----------------|----------------|----------------|----------------|----------------|
| Ni1 | 0.0055 (4) | 0.0074 (4) | 0.0241 (5) | 0.000 | 0.000 | −0.0016 (3) |
| Mn1 | 0.0134 (6) | 0.0033 (5) | 0.0044 (5) | 0.000 | 0.000 | 0.000 |
| Mn2 | 0.0057 (10) | 0.0112 (10) | 0.0043 (9) | 0.000 | 0.000 | 0.000 |
| Mn3 | 0.0080 (4) | 0.0039 (4) | 0.0039 (4) | 0.000 | 0.000 | 0.0003 (3) |
| Mn4 | 0.0049 (4) | 0.0059 (4) | 0.0046 (4) | 0.0000 (3) | 0.000 | 0.000 |
| Al1 | 0.0099 (12) | 0.0074 (11) | 0.0071 (11) | 0.000 | 0.000 | 0.000 |
| Al2 | 0.0051 (12) | 0.0117 (12) | 0.0080 (11) | 0.000 | 0.000 | 0.000 |
| Al3 | 0.0182 (14) | 0.0106 (12) | 0.0045 (11) | 0.000 | 0.000 | 0.000 |
| Al4 | 0.0074 (8) | 0.0060 (8) | 0.0065 (8) | 0.000 | 0.000 | 0.0008 (6) |
| Al5 | 0.0077 (8) | 0.0072 (8) | 0.0079 (8) | 0.000 | 0.000 | 0.0011 (6) |
| Al6 | 0.0241 (11) | 0.0051 (8) | 0.0094 (8) | 0.000 | 0.000 | 0.0021 (6) |
| Al7A | 0.0102 (12) | 0.0087 (12) | 0.0320 (15) | 0.000 | 0.000 | −0.0034 (10) |
| Al7B | 0.0102 (12) | 0.0087 (12) | 0.0320 (15) | 0.000 | 0.000 | −0.0034 (10) |
| Al8 | 0.0427 (14) | 0.0160 (10) | 0.0162 (10) | 0.0111 (9) | 0.000 | 0.000 |
| Al9 | 0.0088 (9) | 0.0125 (8) | 0.0068 (8) | −0.0031 (7) | 0.000 | 0.000 |
| Al10 | 0.0073 (6) | 0.0069 (5) | 0.0082 (6) | −0.0003 (4) | −0.0009 (5) | −0.0003 (4) |
| Al11 | 0.0073 (6) | 0.0074 (5) | 0.0074 (6) | 0.0009 (4) | 0.0006 (5) | 0.0013 (4) |
| Al12 | 0.0077 (6) | 0.0067 (5) | 0.0098 (6) | −0.0012 (5) | 0.0003 (5) | −0.0028 (4) |
| Al13 | 0.0130 (7) | 0.0101 (6) | 0.0174 (7) | −0.0008 (5) | −0.0003 (5) | 0.0021 (5) |

### Geometric parameters (Å, °)

|   | Ni1—Al7B<sup>i</sup> | 2.2523 (7) | Al2—Al9<sup>v</sup> | 2.829 (3) |
|---|-------------------|------------|---------------------|----------|
| Ni1—Al7A<sup>ii</sup> | 2.468 (2) | Al2—Al9 | 2.829 (3) |
| Ni1—Al10<sup>iv</sup> | 2.4921 (12) | Al2—Al11<sup>xx</sup> | 2.8490 (13) |
| Ni1—Al10<sup>v</sup> | 2.4921 (12) | Al2—Al11<sup>v</sup> | 2.8490 (13) |
| Ni1—Al11 | 2.4989 (13) | Al2—Al11<sup>vii</sup> | 2.8490 (13) |
Ni1—Al11 2.4989 (13) Al2—Al11 2.8490 (13)
Ni1—Al17A 2.652 (3) Al3—Al6 2.819 (3)
Ni1—Al9 2.7106 (12) Al3—Al12 2.819 (3)
Ni1—Al9vii 2.7107 (12) Al3—Al12 2.881 (2)
Ni1—Al13 2.7315 (15) Al3—Al12vii 2.881 (2)
Ni1—Al13vi 2.7315 (15) Al3—Al12v 2.881 (2)
Mn1—Al8v 2.462 (2) Al3—Al12v 2.9714 (14)
Mn1—Al8vii 2.462 (2) Al3—Al12iv 2.9714 (14)
Mn1—Al6v 2.5310 (19) Al3—Al12v 2.9714 (14)
Mn1—Al6vi 2.5310 (19) Al3—Al12iv 2.9714 (14)
Mn1—Al14 2.6399 (19) Al3—Al12iv 2.9714 (14)
Mn1—Al14vii 2.6400 (19) Al4—Al14vii 2.483 (3)
Mn1—Al10v 2.7312 (12) Al4—Al5 2.641 (2)
Mn1—Al10v 2.7312 (12) Al4—Al10 2.6985 (18)
Mn1—Al10xiv 2.7312 (12) Al4—Al10 2.6985 (18)
Mn1—Al10xii 2.7312 (12) Al4—Al10 2.7001 (15)
Mn1—Al9 2.8328 (18) Al4—Al10 2.7001 (14)
Mn1—Al9xi 2.8328 (18) Al4—Al10 2.8270 (18)
Mn2—Al8xvi 2.333 (2) Al4—Al9iii 2.8270 (18)
Mn2—Al8xii 2.333 (2) Al5—Al12ii 2.7131 (15)
Mn2—Al13xiv 2.3349 (14) Al5—Al12iv 2.7131 (15)
Mn2—Al13xiii 2.3349 (14) Al5—Al12xxiii 2.8480 (18)
Mn2—Al13vi 2.3349 (14) Al5—Al12xxiv 2.8480 (18)
Mn2—Al13 2.3349 (14) Al5—Al12xxv 2.8480 (18)
Mn2—Al13 2.3349 (14) Al6—Al10ii 2.8510 (15)
Mn2—Al17A 2.491 (3) Al6—Al10ii 2.8510 (15)
Mn2—Al17A 2.491 (3) Al6—Al10vi 2.722 (2)
Mn2—Al17 2.633 (3) Al6—Al10vi 2.722 (2)
Mn3—Al13 2.4459 (8) Al6—Al10xxiv 2.722 (2)
Mn3—Al12 2.5085 (13) Al6—Al10xxv 2.7266 (19)
Mn3—Al12 2.5085 (13) Al6—Al10xxvii 2.7266 (19)
Mn3—Al6 2.5162 (19) Al6—Al10xxviii 2.7300 (19)
Mn3—Al6 2.5162 (19) Al6—Al10xxix 2.7300 (19)
Mn3—Al14vi 2.5563 (18) Al6—Al13 2.9000 (16)
Mn3—Al13iv 2.5563 (18) Al6—Al13iv 2.9000 (16)
Mn3—Al13iv 2.5563 (18) Al7A—Al7Axxvii 2.442 (5)
Mn3—Al13ii 2.5800 (14) Al7A—Al7Axxviii 2.608 (3)
Mn3—Al5vii 2.8481 (18) Al7A—Al7Axxix 2.608 (3)
Mn3—Al11vii 2.8962 (13) Al7A—Al7Axv 2.685 (2)
Mn3—Al11viii 2.8962 (13) Al7A—Al13 2.685 (2)
Mn3—Al10viii 2.9039 (13) Al7A—Al13 2.685 (2)
Mn3—Al10v 2.9039 (13) Al7A—Al10xxix 2.9016 (17)
Mn4—Al12iii 2.3996 (9) Al7A—Al10xxvii 2.9016 (17)
Mn4—Al12iii 2.4779 (13) Al7A—Al10xxvii 2.9016 (17)
Mn4—Al12ix 2.4779 (13) Al7B—Al10xxvii 2.8166 (12)
Mn4—Al4 2.6116 (15) Al7B—Al10xxvii 2.8166 (12)
Mn4—Al4ii 2.6116 (15) Al7B—Al10xxvii 2.8166 (12)
Mn4—Al11ix 2.6823 (12) Al8—Al9xxiii 2.843 (3)
Mn4—Al11iii 2.6823 (12) Al8—Al9xxiii 2.843 (3)
Mn4—Al11 2.716 (2) Al8—Al13xxvii 2.847 (2)
Mn4—Al5 2.7642 (15) Al8—Al10v 2.8874 (16)
| Bond                  | Distance | Eps   | Bond                  | Distance | Eps   |
|-----------------------|----------|-------|-----------------------|----------|-------|
| Mn4—Al5               | 2.7642   | 15    | Al8—Al10             | 2.8874   | 16    |
| Mn4—Al9               | 2.8163   | 19    | Al9—Al10             | 2.7591   | 15    |
| Mn4—Mn4              | 2.8282   | 17    | Al9—Al10             | 2.7591   | 15    |
| Al1—Al5              | 2.861    | 2     | Al9—Al11             | 2.811    | 4     |
| Al1—Al5xiii         | 2.861    | 2     | Al9—Al11             | 2.8242   | 15    |
| Al1—Al12xvi         | 2.9093   | 14    | Al9—Al11             | 2.8242   | 15    |
| Al1—Al12i            | 2.9093   | 14    | Al10—Al13xxxvi       | 2.7603   | 17    |
| Al1—Al12ii           | 2.9093   | 14    | Al10—Al10            | 2.890    | 2     |
| Al1—Al12xix          | 2.9093   | 14    | Al11—Al13v           | 2.7046   | 17    |
| Al1—Al13             | 2.946    | 2     | Al11—Al12xxvii       | 2.7705   | 16    |
| Al1—Al13x            | 2.946    | 2     | Al11—Al12xxvii       | 2.7891   | 16    |
| Al1—Al13xxi         | 2.946    | 2     | Al11—Al11v           | 2.917    | 2     |
| Al2—Al12             | 2.809    | 2     | Al12—Al13xxii        | 2.7393   | 17    |
| Al2—Al12x            | 2.809    | 2     | Al12—Al12x           | 2.855    | 3     |
| Al2—Al12ii           | 2.809    | 2     | Al13—Al13v           | 2.884    | 3     |
| Al2—Al12xxx          | 2.809    | 2     |                       |          |       |
| Al7Aiv—Ni1—Al10xxxii | 71.59    | 3     | Al11v—Al4—Al9xxxiii | 177.12   | 7     |
| Al7Aiv—Ni1—Al10xiv  | 71.59    | 3     | Al9v—Al4—Al9xxxiii  | 116.30   | 7     |
| Al7Aiv—Ni1—Al10xvi  | 142.75   | 6     | Al4—Al5—Al12i       | 104.51   | 5     |
| Al7Aiv—Ni1—Al11v    | 138.65   | 3     | Al4—Al5—Al12v       | 104.51   | 5     |
| Al7Aiv—Ni1—Al11v    | 143.68   | 3     | Al12iii—Al5—Al12iv  | 122.57   | 8     |
| Al10iv—Ni1—Al11     | 72.91    | 4     | Al4—Al5—Mn4         | 57.73    | 5     |
| Al10iv—Ni1—Al11v    | 144.33   | 5     | Al12iii—Al5—Mn4     | 53.78    | 4     |
| Al7Aiv—Ni1—Al11     | 56.83    | 10    | Al12iv—Al5—Mn4xxxv   | 61.54    | 5     |
| Al10iv—Ni1—Al11v    | 77.70    | 3     | Al12iv—Al5—Mn4xxxv   | 98.93    | 6     |
| Al11—Ni1—Al11v      | 121.67   | 5     | Al12iv—Al5—Mn4xxxv   | 118.66   | 4     |
| Al7B—Ni1—Al9        | 116.69   | 4     | Mn4—Al5—Mn4xxxv      | 55.36    | 5     |
| Al7B—Ni1—Al10        | 91.85    | 7     | Al4—Al5—Mn3xxxv     | 104.50   | 5     |
| Al10v—Ni1—Al11v     | 63.89    | 4     | Al4—Al5—Mn3xxxv     | 113.56   | 4     |
| Al10v—Ni1—Al11     | 122.86   | 5     | Al12iv—Al5—Mn3xxxv  | 62.46    | 7     |
| Al9—Ni1—Al10v       | 65.51    | 4     | Al4—Al5—Al12xxxv    | 113.56   | 4     |
| Al11v—Ni1—Al10v     | 101.00   | 5     | Mn4—Al5—Al12xxxv    | 155.84   | 7     |
| Al7Aiv—Ni1—Al10     | 137.13   | 5     | Al4—Al5—Al12xxxv    | 155.84   | 7     |
| Al7Aiv—Ni1—Al10v    | 91.85    | 7     | Al4—Al5—Mn3xxxv     | 155.84   | 7     |
| Al10iv—Ni1—Al10v    | 122.86   | 5     | Al12iv—Al5—Mn3xxxv  | 155.84   | 7     |
| Al10iv—Ni1—Al10     | 63.89    | 4     | Al12iv—Al5—Mn3xxxv  | 155.84   | 7     |
| Al11—Ni1—Al10v      | 100.99   | 5     | Mn4—Al5—Mn3xxxv     | 113.56   | 4     |
| Al11—Ni1—Al10v      | 65.51    | 4     | Al4—Al5—Mn3xxxv     | 113.56   | 4     |
| Al7Aiv—Ni1—Al10v    | 137.13   | 5     | Al4—Al5—Mn3xxxv     | 113.56   | 4     |
| Al9—Ni1—Al10v       | 62.46    | 7     | Al4—Al5—Al11v       | 58.75    | 4     |
| Al7Aiv—Ni1—Al13     | 107.32   | 6     | Al4—Al5—Al11v       | 58.75    | 4     |
| Bond | Angle (°) | Error (°) |
|------|----------|-----------|
| Al10<sup>iii</sup>—Ni1—Al13<sup>vi</sup> | 123.79 | (5) |
| Al10<sup>vi</sup>—Ni1—Al13<sup>xiii</sup> | 63.61 | (4) |
| A11—Ni1—Al13<sup>vi</sup> | 98.53 | (4) |
| A11<sup>+</sup>—Ni1—Al13<sup>iii</sup> | 62.09 | (4) |
| A17A<sup>xii</sup>—Ni1—Al13<sup>vi</sup> | 59.81 | (5) |
| A9—Ni1—Al13<sup>vi</sup> | 160.69 | (5) |
| Al9<sup>xii</sup>—Ni1—Al13<sup>iii</sup> | 113.34 | (4) |
| A17A<sup>iii</sup>—Ni1—Al1<sup>iii</sup> | 107.32 | (6) |
| A10<sup>iii</sup>—Ni1—Al1<sup>iii</sup> | 63.61 | (4) |
| A10<sup>xiv</sup>—Ni1—Al1<sup>iii</sup> | 123.79 | (5) |
| A11—Ni1—Al1<sup>iii</sup> | 62.09 | (4) |
| A11<sup>+</sup>—Ni1—Al1<sup>iii</sup> | 98.53 | (4) |
| A17A<sup>xiii</sup>—Ni1—Al1<sup>iii</sup> | 59.81 | (5) |
| A9—Ni1—Al13<sup>vi</sup> | 113.34 | (4) |
| A9<sup>xii</sup>—Ni1—Al13<sup>iii</sup> | 160.69 | (5) |
| A13<sup>xiii</sup>—Ni1—Al13<sup>xvi</sup> | 63.74 | (6) |
| A18<sup>xii</sup>—Mn1—A18<sup>xii</sup> | 66.07 | (5) |
| A18<sup>xii</sup>—Mn1—Al6<sup>xii</sup> | 66.07 | (5) |
| A18<sup>xii</sup>—Mn1—Al6<sup>xvi</sup> | 66.07 | (5) |
| A18<sup>xii</sup>—Mn1—Al6<sup>xii</sup> | 66.07 | (5) |
| Al6<sup>xii</sup>—Mn1—Al6<sup>xii</sup> | 81.85 | (9) |
| A18<sup>xii</sup>—Mn1—A4 | 118.28 | (5) |
| A18<sup>xii</sup>—Mn1—A4 | 118.28 | (5) |
| A16<sup>+</sup>—Mn1—A4 | 167.13 | (6) |
| A16<sup>+</sup>—Mn1—A4 | 111.02 | (5) |
| A18<sup>xii</sup>—Mn1—A14<sup>xii</sup> | 118.28 | (5) |
| A18<sup>xii</sup>—Mn1—A14<sup>xii</sup> | 118.28 | (5) |
| A16<sup>xii</sup>—Mn1—A14<sup>xii</sup> | 111.02 | (5) |
| A14—Mn1—A4 | 167.13 | (6) |
| A14—Mn1—A4 | 111.02 | (5) |
| A18<sup>xii</sup>—Mn1—A10<sup>xiv</sup> | 67.33 | (3) |
| A18<sup>xii</sup>—Mn1—A10<sup>xiv</sup> | 67.33 | (3) |
| A16<sup>xii</sup>—Mn1—A10<sup>xiv</sup> | 62.28 | (4) |
| A16<sup>xii</sup>—Mn1—A10<sup>xiv</sup> | 129.53 | (5) |
| A14—Mn1—A10<sup>xiv</sup> | 107.18 | (5) |
| A14<sup>xii</sup>—Mn1—A10<sup>xiv</sup> | 60.29 | (4) |
| A18<sup>xii</sup>—Mn1—A10<sup>xiv</sup> | 67.33 | (3) |
| A18<sup>xii</sup>—Mn1—A10<sup>xiv</sup> | 67.33 | (3) |
| A16<sup>xii</sup>—Mn1—A10<sup>xiv</sup> | 129.53 | (5) |
| A16<sup>xii</sup>—Mn1—A10<sup>xiv</sup> | 62.28 | (4) |
| A14—Mn1—A10<sup>xiv</sup> | 60.29 | (4) |
| A14<sup>xii</sup>—Mn1—A10<sup>xiv</sup> | 60.29 | (4) |
| A14<sup>xii</sup>—Mn1—A10<sup>xiv</sup> | 107.18 | (5) |
| A110<sup>xvi</sup>—Mn1—A10<sup>xiv</sup> | 114.48 | (5) |
| A18<sup>xii</sup>—Mn1—A10<sup>xiv</sup> | 129.48 | (3) |
| A18<sup>xii</sup>—Mn1—A10<sup>xiv</sup> | 67.33 | (3) |
| A16<sup>xii</sup>—Mn1—A10<sup>xiv</sup> | 62.28 | (4) |
| A16<sup>xii</sup>—Mn1—A10<sup>xiv</sup> | 129.53 | (5) |
| A14—Mn1—A10<sup>xiv</sup> | 60.29 | (4) |
| A14<sup>xii</sup>—Mn1—A10<sup>xiv</sup> | 107.18 | (5) |
| A110<sup>xvi</sup>—Mn1—A10<sup>xiv</sup> | 114.48 | (5) |
| A18<sup>xii</sup>—Mn1—A10<sup>xiv</sup> | 129.48 | (3) |
| A18<sup>xii</sup>—Mn1—A10<sup>xiv</sup> | 67.33 | (3) |
| A16<sup>xii</sup>—Mn1—A10<sup>xiv</sup> | 62.28 | (4) |
| A16<sup>xii</sup>—Mn1—A10<sup>xiv</sup> | 129.53 | (5) |
| Bond | Al4—Mn1—Al10 | 107.18 (5) | Mn1—Al6—Al10 | 130.58 (6) |
|------|---------------|------------|---------------|------------|
|      | Al4—Mn1—Al10i | 60.29 (4)  | Al8—Al6—Al10i | 97.78 (4)  |
|      | Al10—Mn1—Al10i | 63.89 (5)  | Al10—Al6—Al10i | 160.60 (7) |
|      | Al10—Mn1—Al10i | 166.98 (7) | Al10—Al6—Al10i | 101.20 (7) |
|      | Al10—Mn1—Al10i | 120.48 (3) | Al10—Al6—Al10i | 68.47 (6)  |
|      | Al6—Mn1—Al10i | 67.33 (3)  | Al10—Al6—Al10i | 63.92 (6)  |
|      | Al6—Mn1—Al10i | 129.54 (5) | Mn3—Al6—Al13  | 54.21 (5)  |
|      | Al4—Mn1—Al10i | 62.28 (4)  | Mn1—Al6—Al13  | 103.05 (7) |
|      | Al4—Mn1—Al10i | 60.29 (4)  | Al8—Al6—Al13  | 79.47 (6)  |
|      | Al4—Mn1—Al10i | 107.18 (5) | Al10—Al6—Al13  | 79.47 (6)  |
|      | Al10—Mn1—Al10i | 166.98 (7) | Al10—Al6—Al13  | 142.84 (5) |
|      | Al10—Mn1—Al10i | 63.89 (5)  | Al10—Al6—Al13  | 142.84 (5) |
|      | Al10—Mn1—Al10i | 114.48 (5) | Al10—Al6—Al13  | 112.56 (6) |
|      | Al8—Mn1—Al9  | 179.56 (8) | Al10—Al6—Al13  | 112.56 (6) |
|      | Al8—Mn1—Al9  | 64.51 (6)  | Mn3—Al6—Al13  | 56.36 (4)  |
|      | Al6—Mn1—Al9  | 113.63 (3) | Mn1—Al6—Al13  | 116.48 (5) |
|      | Al6—Mn1—Al9  | 113.63 (3) | Al8—Al6—Al13  | 60.75 (5)  |
|      | Al4—Mn1—Al9  | 62.08 (4)  | Al8—Al6—Al13  | 139.08 (8) |
|      | Al4—Mn1—Al9  | 60.29 (4)  | Al10—Al6—Al13  | 154.26 (6) |
|      | Al10—Mn1—Al9  | 112.85 (4) | Al10—Al6—Al13  | 92.09 (4)  |
|      | Al10—Mn1—Al9  | 112.85 (4) | Al10—Al6—Al13  | 110.04 (7) |
|      | Al10—Mn1—Al9  | 59.42 (3)  | Al10—Al6—Al13  | 58.63 (4)  |
|      | Al10—Mn1—Al9  | 59.42 (3)  | A3—Al6—Al13  | 62.59 (4)  |
|      | A18—Mn1—Al9  | 64.51 (6)  | Mn3—Al6—Al13  | 56.36 (4)  |
|      | A18—Mn1—Al9  | 179.56 (8) | Mn1—Al6—Al13  | 116.48 (5) |
|      | A18—Mn1—Al9  | 113.63 (3) | Al8—Al6—Al13  | 60.75 (5)  |
|      | A18—Mn1—Al9  | 113.63 (3) | Al8—Al6—Al13  | 139.08 (8) |
|      | Al4—Mn1—Al9  | 62.09 (4)  | Al10—Al6—Al13  | 154.26 (6) |
|      | Al4—Mn1—Al9  | 60.29 (4)  | Al10—Al6—Al13  | 58.63 (4)  |
|      | Al4—Mn1—Al9  | 59.42 (3)  | Al10—Al6—Al13  | 110.04 (7) |
|      | Al4—Mn1—Al9  | 59.42 (3)  | A3—Al6—Al13  | 62.59 (4)  |
|      | Al4—Mn1—Al9  | 112.85 (4) | Al13—Al6—Al13  | 109.24 (7) |
|      | A19—Mn1—Al9  | 115.92 (8) | A17A—Al17A—Ni1  | 65.38 (9)  |
|      | A19—Mn1—Al9  | 95.71 (13) | A17A—Al17A—Mn2  | 158.53 (16) |
|      | A18—Mn2—Al8i | 131.32 (5) | Ni1—Al17A—Mn2  | 136.09 (12) |
|      | A18—Mn2—Al8i | 75.18 (5)  | A17A—Al17A—Ni1  | 135.57 (7) |
|      | A18—Mn2—Al8i | 75.18 (5)  | Ni1—Al17A—Al8  | 95.36 (8)  |
|      | A18—Mn2—Al8i | 131.32 (5) | Mn2—Al17A—Al8  | 54.39 (7)  |
|      | A18—Mn2—Al8i | 75.18 (5)  | Al8—Al17A—Al8  | 83.07 (11) |
|      | A18—Mn2—Al8i | 93.17 (7)  | Al7A—Al17A—Ni1  | 57.79 (10) |
|      | A18—Mn2—Al8i | 144.92 (10) | Ni1—Al17A—Al8  | 123.17 (10) |
|      | A18—Mn2—Al8i | 75.18 (5)  | Mn2—Al17A—Ni1  | 100.74 (8) |
|      | A18—Mn2—Al8i | 131.32 (5) | Al8—Al17A—Ni1  | 124.80 (8) |
|      | A18—Mn2—Al8i | 75.18 (5)  | Al8—Al17A—Ni1  | 124.80 (8) |
| Bond                  | Angle (°)       |
|----------------------|----------------|
| Al$_{13}v$—Mn$_2$—Al$_{13}$ | 76.30 (7)       |
| Al$_{18}vi$—Mn$_2$—Al$_{17}A_{xxiii}$ | 65.38 (5)       |
| Al$_{18}vii$—Mn$_2$—Al$_{17}A_{xxiii}$ | 65.38 (5)       |
| Al$_{13}vi$—Mn$_2$—Al$_{17}A_{xxiii}$ | 67.53 (5)       |
| Al$_{13}v$—Mn$_2$—Al$_{17}A_{xxiii}$ | 139.16 (5)      |
| Al$_{13}$—Mn$_2$—Al$_{17}A$      | 67.53 (5)       |
| Al$_{18}vii$—Mn$_2$—Al$_{17}A$    | 65.38 (5)       |
| Al$_{13}vi$—Mn$_2$—Al$_{17}A$     | 139.16 (5)      |
| Al$_{13}$—Mn$_2$—Al$_{17}A$       | 67.53 (5)       |
| Al$_{17}A_{xxiii}$—Mn$_2$—Al$_{17}A$ | 103.23 (13)     |
| Al$_{18}vi$—Mn$_2$—Al$_{11}$      | 132.14 (7)      |
| Al$_{18}vii$—Mn$_2$—Al$_{11}$     | 132.14 (7)      |
| Al$_{13}vi$—Mn$_2$—Al$_{11}$      | 72.46 (5)       |
| Al$_{13}$—Mn$_2$—Al$_{11}$        | 72.46 (5)       |
| Al$_{17}A_{xxiii}$—Mn$_2$—Al$_{11}$ | 128.38 (6)     |
| Al$_{17}A_{xx}$—Mn$_2$—Al$_{11}$  | 128.38 (6)      |
| Al$_3$—Mn$_3$—Al$_{12}v$         | 71.11 (6)       |
| Al$_3$—Mn$_3$—Al$_{12}$           | 71.11 (6)       |
| Al$_{12}$—Mn$_3$—Al$_{12}$        | 69.36 (6)       |
| Al$_3$—Mn$_3$—Al$_{16}$           | 69.22 (7)       |
| Al$_{12}$—Mn$_3$—Al$_{16}$        | 126.30 (5)      |
| Al$_{12}$—Mn$_3$—Al$_{16}$        | 126.30 (5)      |
| Al$_3$—Mn$_3$—Al$_{14}vi$        | 177.36 (8)      |
| Al$_{12}$—Mn$_3$—Al$_{14}vi$     | 110.99 (5)      |
| Al$_{12}$—Mn$_3$—Al$_{14}vi$     | 110.99 (5)      |
| Al$_6$—Mn$_3$—Al$_{14}vi$        | 108.13 (6)      |
| Al$_3$—Mn$_3$—Al$_{13}v$         | 72.43 (4)       |
| Al$_{12}$—Mn$_3$—Al$_{13}v$      | 65.12 (4)       |
| Al$_{12}$—Mn$_3$—Al$_{13}v$      | 128.48 (5)      |
| Al$_6$—Mn$_3$—Al$_{13}v$         | 69.36 (3)       |
| Al$_{14}vi$—Mn$_3$—Al$_{13}v$   | 106.82 (4)      |
| Al$_3$—Mn$_3$—Al$_{13}iii$       | 72.43 (4)       |
| Al$_{12}$—Mn$_3$—Al$_{13}iii$    | 128.48 (5)      |
| Al$_{12}$—Mn$_3$—Al$_{13}iii$    | 65.12 (4)       |
| Al$_6$—Mn$_3$—Al$_{13}iii$       | 69.36 (3)       |
| Al$_{14}vi$—Mn$_3$—Al$_{13}iii$ | 106.82 (4)      |
| Al$_3$—Mn$_3$—Al$_{13}iii$       | 132.84 (7)      |
| Al$_3$—Mn$_3$—Al$_{13}iii$       | 132.84 (7)      |
| Al$_3$—Mn$_3$—Al$_{13}iv$        | 106.82 (4)      |
| Al$_{13}$—Mn$_3$—Al$_{13}iv$     | 128.48 (5)      |
| Al$_{13}$—Mn$_3$—Al$_{13}iv$     | 65.12 (4)       |
| Al$_6$—Mn$_3$—Al$_{13}iv$        | 69.36 (3)       |
| Al$_{14}vi$—Mn$_3$—Al$_{13}iv$  | 106.82 (4)      |
| Al$_3$—Mn$_3$—Al$_{13}iv$        | 132.84 (7)      |
| Al$_3$—Mn$_3$—Al$_{13}iv$        | 132.84 (7)      |
| Al$_3$—Mn$_3$—Al$_{13}v$         | 106.82 (4)      |
| Al$_{13}$—Mn$_3$—Al$_{13}v$      | 132.84 (7)      |
| Al$_3$—Mn$_3$—Al$_{13}v$         | 132.84 (7)      |
| Al$_3$—Mn$_3$—Al$_{13}$i         | 128.48 (5)      |
| Al$_3$—Mn$_3$—Al$_{13}$i         | 65.12 (4)       |
| Al$_6$—Mn$_3$—Al$_{13}$i         | 69.36 (3)       |
| Al$_{14}vi$—Mn$_3$—Al$_{13}$i   | 106.82 (4)      |
| Al$_3$—Mn$_3$—Al$_{13}$i         | 132.84 (7)      |
| Al$_3$—Mn$_3$—Al$_{13}$i         | 132.84 (7)      |
### Data Reports

| Al13iv—Mn3—Al5vi | 112.78 (3) | Mn2vi—Al8—Al7Axxviii | 60.24 (7) |
| Al13iii—Mn3—Al5vi | 112.78 (3) | Mn1v—Al8—Al7Axxviii | 124.28 (6) |
| Al3—Mn3—Al11xvii | 121.85 (3) | Al7Axxv—Al8—Al7Axxviii | 96.93 (11) |
| Al12—Mn3—Al11xvii | 61.18 (4) | Mn2vi—Al8—Al6xxv | 114.85 (7) |
| Al6—Mn3—Al11xvii | 115.10 (3) | Mn1v—Al8—Al6xxv | 163.78 (10) |
| Al4vi—Mn3—Al11xvii | 58.97 (3) | Al7Axxviii—Al8—Al6xxv | 92.78 (5) |
| Al13iv—Mn3—Al11xvii | 58.86 (4) | Mn2vi—Al8—Al6xxv | 114.85 (7) |
| Al13vi—Mn3—Al11xvii | 165.67 (5) | Mn1v—Al8—Al6xxv | 58.18 (6) |
| Al5vi—Mn3—Al11xvii | 59.51 (3) | Al7Axxv—Al8—Al6xxv | 92.78 (5) |
| Al3—Mn3—Al11xvii | 121.85 (3) | Al7Axxviii—Al8—Al6xxv | 163.78 (10) |
| Al12—Mn3—Al11xvii | 116.14 (5) | Al6xxviii—Al8—Al6xxv | 75.03 (9) |
| Al12—Mn3—Al11xvii | 61.18 (4) | Mn2vi—Al8—Al9xxviii | 125.60 (11) |
| Al6—Mn3—Al11xvii | 115.10 (3) | Mn1v—Al8—Al9xxviii | 64.07 (6) |
| Al4vi—Mn3—Al11xvii | 58.97 (3) | Al7Axxv—Al8—Al9xxviii | 86.07 (8) |
| Al13iv—Mn3—Al11xvii | 165.67 (5) | Al7Axxviii—Al8—Al9xxviii | 86.07 (8) |
| Al13vi—Mn3—Al11xvii | 58.86 (4) | Al6xxviii—Al8—Al9xxviii | 107.60 (7) |
| Al5vi—Mn3—Al11xvii | 59.51 (3) | Al6xxv—Al8—Al9xxviii | 107.60 (7) |
| Al11xviii—Mn3—Al11xvii | 108.34 (5) | Mn2vi—Al8—Al13xxxiv | 52.45 (5) |
| Al3—Mn3—Al10viii | 119.02 (6) | Mn1v—Al8—Al13xxxiv | 120.86 (8) |
| Al12—Mn3—Al10viii | 114.67 (4) | Mn2vi—Al8—Al13xxxiv | 111.92 (9) |
| Al12—Mn3—Al10viii | 169.66 (5) | Al6xxvii—Al8—Al13xxxiv | 58.77 (6) |
| Al6—Mn3—Al10viii | 59.98 (4) | Al6xxviii—Al8—Al13xxxiv | 62.71 (5) |
| Al4vi—Mn3—Al10viii | 58.82 (4) | Al6xxv—Al8—Al13xxxiv | 105.49 (8) |
| Al13iv—Mn3—Al10viii | 60.10 (4) | Al9xxviii—Al8—Al13xxxiv | 141.28 (5) |
| Al13vi—Mn3—Al10viii | 114.44 (5) | Mn2vi—Al8—Al13xxxiv | 52.45 (5) |
| Al5vi—Mn3—Al10viii | 108.59 (4) | Mn1v—Al8—Al13xxxiv | 120.86 (8) |
| Al11xviii—Mn3—Al10viii | 61.50 (3) | Al7Axxv—Al8—Al13xxxvii | 58.77 (6) |
| Al11xvii—Mn3—Al10viii | 109.26 (4) | Al7Axxv—Al8—Al13xxxviii | 111.92 (9) |
| Al3—Mn3—Al10vi | 119.02 (6) | Al6xxviii—Al8—Al13xxxviii | 105.49 (8) |
| Al12—Mn3—Al10vi | 169.66 (5) | Al6xxv—Al8—Al13xxxviii | 62.71 (5) |
| Al12—Mn3—Al10vi | 114.67 (4) | Al9xxviii—Al8—Al13xxxviii | 141.28 (5) |
| Al6—Mn3—Al10vi | 59.98 (4) | Al13xxxiv—Al8—Al13xxxvii | 73.12 (7) |
| Al4vi—Mn3—Al10vi | 58.82 (4) | Mn2vi—Al8—Al10xxxv | 122.79 (6) |
| Al13iv—Mn3—Al10vi | 114.44 (5) | Mn1v—Al8—Al10xxxv | 60.78 (5) |
| Al13vi—Mn3—Al10vi | 60.10 (4) | Al7Axxv—Al8—Al10xxxv | 63.50 (5) |
| Al5vi—Mn3—Al10vi | 108.59 (4) | Al7Axxviii—Al8—Al10xxxv | 138.12 (11) |
| Al11xviii—Mn3—Al10vi | 109.26 (4) | Al6xxviii—Al8—Al10xxxv | 116.10 (9) |
| Al11xvii—Mn3—Al10vi | 61.50 (3) | Al6xxv—Al8—Al10xxxv | 58.07 (5) |
| Al10xvi—Mn3—Al10vi | 59.69 (5) | Al9xxviii—Al8—Al10xxxv | 57.55 (4) |
| Al2iii—Mn4—Al12iii | 70.30 (6) | Al13xxxiv—Al8—Al10xxxv | 161.13 (8) |
| Al2ii—Mn4—Al12xxv | 70.30 (6) | Al13xxxviii—Al8—Al10xxxv | 89.92 (4) |
| Al12—Mn4—Al12xxv | 77.24 (6) | Mn2vi—Al8—Al10xxxv | 122.79 (6) |
| Al2ii—Mn4—Al12xxv | 119.16 (6) | Mn1v—Al8—Al10xxxv | 60.78 (5) |
| Al12—Mn4—Al12xxv | 112.57 (5) | Al7Axxv—Al8—Al10xxxv | 138.12 (11) |
| Al12—Mn4—Al12xxv | 167.76 (5) | Al7Axxviii—Al8—Al10xxxv | 63.50 (5) |
| Al2ii—Mn4—Al12xvi | 119.16 (6) | Al6xxviii—Al8—Al10xxxv | 58.07 (5) |
| Al12—Mn4—Al12xvi | 167.76 (5) | Al6xxv—Al8—Al10xxxv | 116.10 (9) |
| Bond Type | Bond Length (Å) | Standard Deviation (Å) |
|-----------|-----------------|------------------------|
| Al12xix—Mn4—Al4xiii | 112.57 (5) | 3.68 |
| Al4—Mn4—Al4xiii | 56.78 (7) | 2.89 |
| Al2ii—Mn4—Al11xix | 67.93 (4) | 2.34 |
| Al12xix—Mn4—Al11xix | 130.89 (5) | 3.12 |
| Al12xix—Mn4—Al4—Al11xix | 65.30 (4) | 2.56 |
| Al4—Mn4—Al11xix | 109.69 (5) | 2.97 |
| Al4xiii—Mn4—Al11xix | 61.32 (4) | 2.15 |
| Al2ii—Mn4—Al11ii | 67.93 (4) | 2.34 |
| Al12ii—Mn4—Al11ii | 65.30 (4) | 2.56 |
| Al4—Mn4—Al11ii | 130.89 (5) | 3.12 |
| Al4xiii—Mn4—Al11ii | 61.32 (4) | 2.15 |
| Al11xix—Mn4—Al11ii | 109.69 (5) | 2.97 |
| Al11xix—Mn4—Al11 | 118.44 (6) | 2.8 |
| Al12ii—Mn4—Al11 | 125.73 (7) | 3.5 |
| Al12ii—Mn4—Al1 | 67.95 (4) | 2.34 |
| Al12xix—Mn4—Al1 | 67.95 (4) | 2.34 |
| Al4—Mn4—Al1 | 108.06 (4) | 2.8 |
| Al4xiii—Mn4—Al1 | 108.06 (4) | 2.8 |
| Al11xix—Mn4—Al1 | 120.10 (3) | 2.4 |
| Al11ii—Mn4—Al1 | 120.10 (3) | 2.4 |
| Al2ii—Mn4—Al5 | 121.80 (3) | 2.5 |
| Al12ii—Mn4—Al5 | 62.05 (4) | 2.6 |
| Al12xix—Mn4—Al5 | 124.60 (5) | 3.5 |
| Al4—Mn4—Al5 | 58.77 (5) | 2.9 |
| Al4xiii—Mn4—Al5 | 105.73 (4) | 2.8 |
| Al11xix—Mn4—Al5 | 167.00 (5) | 3.5 |
| Al11ii—Mn4—Al5 | 63.11 (4) | 2.4 |
| Al1—Mn4—Al5 | 62.93 (4) | 2.5 |
| Al2ii—Mn4—Al5xiii | 121.80 (3) | 2.4 |
| Al12ii—Mn4—Al5xiii | 124.60 (5) | 3.5 |
| Al12xix—Mn4—Al5xiii | 62.05 (4) | 2.6 |
| Al4—Mn4—Al5xiii | 105.73 (4) | 2.8 |
| Al4xiii—Mn4—Al5xiii | 58.77 (5) | 2.9 |
| Al11xix—Mn4—Al5xiii | 63.11 (4) | 2.4 |
| Al11ii—Mn4—Al5xiii | 167.00 (5) | 3.5 |
| Al1—Mn4—Al5xiii | 62.93 (4) | 2.5 |
| Al2ii—Mn4—Al9iii | 65.12 (7) | 2.7 |
| Al12ii—Mn4—Al9iii | 119.85 (5) | 3.5 |
| Al12xix—Mn4—Al9iii | 119.85 (5) | 3.5 |
| Al4—Mn4—Al9iii | 62.64 (4) | 2.6 |
| Al4xiii—Mn4—Al9iii | 62.64 (4) | 2.6 |
| Al11xix—Mn4—Al9iii | 61.75 (3) | 2.3 |
| Al11ii—Mn4—Al9iii | 61.75 (3) | 2.3 |
| Al1—Mn4—Al9iii | 169.14 (6) | 3.6 |
| Al5—Mn4—Al9iii | 112.73 (4) | 2.9 |
| Al5xiii—Mn4—Al9iii | 112.73 (4) | 2.9 |
| Al1—Mn4—Mn4iv | 175.64 (6) | 3.8 |
| Al10xiii—Al9—Al4xiii | 96.50 (4) | 2.9 |
| Al10xiii—Al9—Al4x | 55.13 (5) | 3.0 |
| Al11—Al9—Al4x | 99.98 (7) | 3.2 |
| Al11—Al9—Al4xii | 57.08 (4) | 2.9 |
| Al11—Al9—Al4xx | 96.50 (4) | 2.9 |
| Al11—Al9—Al4xii | 148.15 (4) | 3.1 |
| Al11—Al9—Al4xii | 57.08 (4) | 2.9 |
| Al11—Al9—Al4xii | 99.98 (7) | 3.2 |
| Compound                          | Charge | Bond Angle | Error | Bond Angle | Error | Bond Angle | Error |
|----------------------------------|--------|------------|-------|------------|-------|------------|-------|
| Al12<sub>iii</sub>—Mn4—Mn4<sup>xiv</sup> | 112.93 (3) | Al4<sup>xi</sup>—Al9—Al4<sup>xi</sup> | 52.11 (7) |
| Al12<sub>iv</sub>—Mn4—Mn4<sup>xiv</sup> | 112.93 (3) | Ni1—Al9—Al2 | 82.51 (4) |
| Al4—Mn4—Mn4<sup>xiv</sup> | 57.21 (3) | Ni1<sup>xi</sup>—Al9—Al2 | 82.51 (4) |
| Al4<sup>xiv</sup>—Mn4—Mn4<sup>xiv</sup> | 57.21 (3) | Al10<sup>xi</sup>—Al9—Al2 | 123.19 (4) |
| Al11<sup>xi</sup>—Mn4—Mn4<sup>xiv</sup> | 110.38 (3) | Al10<sup>ii</sup>—Al9—Al2 | 123.19 (4) |
| Al11<sup>ii</sup>—Mn4—Mn4<sup>xiv</sup> | 110.38 (3) | Al9<sup>ix</sup>—Al9—Al2 | 60.21 (4) |
| Al1—Mn4—Mn4<sup>xiv</sup> | 58.63 (3) | Mn4<sup>iii</sup>—Al9—Al2 | 50.30 (4) |
| Al5—Mn4—Mn4<sup>xiv</sup> | 59.23 (2) | Al11—Al9—Al2 | 60.52 (4) |
| Al5<sup>xii</sup>—Mn4—Mn4<sup>xiv</sup> | 59.23 (2) | Al11<sup>xi</sup>—Al9—Al2 | 60.52 (4) |
| Al9<sup>xii</sup>—Mn4—Mn4<sup>xiv</sup> | 110.52 (4) | Al4<sup>xi</sup>—Al9—Al2 | 99.67 (6) |
| Mn2—Al1—Mn4 | 148.62 (3) | Ni1—Al9—Mn1<sup>iii</sup> | 111.21 (4) |
| Mn2—Al1—Mn4<sup>xiv</sup> | 148.63 (3) | Ni1<sup>xi</sup>—Al9—Mn1<sup>iii</sup> | 111.21 (4) |
| Mn4—Al1—Mn4<sup>xiv</sup> | 62.75 (6) | Al10<sup>xi</sup>—Al9—Mn1<sup>iii</sup> | 111.21 (4) |
| Mn2—Al1—Al5 | 126.65 (5) | Al10<sup>ii</sup>—Al9—Mn1<sup>iii</sup> | 58.46 (4) |
| Mn4—Al1—Al5 | 59.36 (5) | Al9<sup>ix</sup>—Al9—Mn1<sup>iii</sup> | 58.46 (4) |
| Mn4<sup>xiv</sup>—Al1—Al5<sup>iii</sup> | 106.69 (10) | Mn4<sup>iii</sup>—Al9—Mn1<sup>iii</sup> | 147.96 (4) |
| Mn2—Al1—Al5<sup>iii</sup> | 102.72 (5) | Al11—Al9—Mn1<sup>iii</sup> | 106.89 (5) |
| Mn4—Al1—Al5<sup>iii</sup> | 59.36 (5) | Al11<sup>xi</sup>—Al9—Mn1<sup>iii</sup> | 106.89 (5) |
| Mn4<sup>xiv</sup>—Al1—Al5<sup>iii</sup> | 59.36 (5) | Al4<sup>xi</sup>—Al9—Mn1<sup>iii</sup> | 55.61 (5) |
| Al5—Al1—Al5<sup>iii</sup> | 106.69 (10) | A14<sup>xi</sup>—Al9—Mn1<sup>iii</sup> | 55.61 (5) |
| Mn2—Al1—Al12<sup>xv</sup> | 102.72 (5) | Al4—Al10—Al6<sup>xii</sup> | 123.31 (5) |
| Mn4—Al1—Al12<sup>xv</sup> | 52.13 (3) | Al4—Al10—Al6<sup>xii</sup> | 98.33 (5) |
| Mn4<sup>xiv</sup>—Al1—Al12<sup>xv</sup> | 103.75 (7) | Al6<sup>xi</sup>—Al10—Al6<sup>xii</sup> | 78.80 (7) |
| Al5—Al1—Al12<sup>xv</sup> | 56.09 (3) | Ni1<sup>ii</sup>—Al10—Mn1 | 122.22 (5) |
| Al5<sup>xiv</sup>—Al1—Al12<sup>xv</sup> | 107.16 (6) | Al4—Al10—Mn1 | 58.18 (5) |
| Al12<sup>vi</sup>—Al1—Al12<sup>xv</sup> | 154.55 (10) | Al6<sup>xi</sup>—Al10—Mn1 | 55.26 (5) |
| Mn2—Al1—Al12<sup>vi</sup> | 102.72 (5) | Al6<sup>xii</sup>—Al10—Mn1 | 114.14 (5) |
| Mn4—Al1—Al12<sup>vi</sup> | 52.13 (3) | Ni1<sup>ii</sup>—Al10—Al9<sup>iii</sup> | 61.91 (5) |
| Mn4<sup>xiv</sup>—Al1—Al12<sup>vi</sup> | 103.75 (7) | Al4—Al10—Al9<sup>iii</sup> | 62.38 (5) |
| Al5—Al1—Al12<sup>vi</sup> | 56.09 (3) | Al6<sup>ix</sup>—Al10—Al9<sup>iii</sup> | 109.94 (6) |
| Al5<sup>xiv</sup>—Al1—Al12<sup>vi</sup> | 107.16 (6) | Al6<sup>xi</sup>—Al10—Al9<sup>iii</sup> | 159.88 (7) |
| Al12<sup>vi</sup>—Al1—Al12<sup>vi</sup> | 64.22 (5) | Mn1—Al10—Al9<sup>iii</sup> | 62.12 (4) |
| Al12<sup>ii</sup>—Al1—Al12<sup>vi</sup> | 109.74 (6) | Ni1<sup>ii</sup>—Al10—Al13<sup>xvi</sup> | 62.42 (4) |
| Mn2—Al1—Al12<sup>ii</sup> | 102.72 (5) | Al4—Al10—Al13<sup>xvi</sup> | 98.14 (6) |
| Mn4—Al1—Al12<sup>ii</sup> | 52.13 (3) | Al6<sup>ii</sup>—Al10—Al13<sup>xvi</sup> | 138.97 (6) |
| Mn4<sup>xiv</sup>—Al1—Al12<sup>ii</sup> | 103.75 (7) | Al6<sup>xi</sup>—Al10—Al13<sup>xvi</sup> | 63.76 (5) |
| Al5—Al1—Al12<sup>ii</sup> | 107.16 (6) | Mn1—Al10—Al13<sup>xvi</sup> | 156.23 (6) |
| Al5<sup>xiv</sup>—Al1—Al12<sup>ii</sup> | 52.13 (3) | Al9<sup>iii</sup>—Al10—Al13<sup>xvi</sup> | 110.94 (6) |
| Al12<sup>ii</sup>—Al1—Al12<sup>ii</sup> | 109.74 (6) | Ni1<sup>ii</sup>—Al10—Al17B<sup>xli</sup> | 49.73 (5) |
| Al12<sup>iv</sup>—Al1—Al12<sup>ii</sup> | 64.22 (5) | Al4—Al10—Al17B<sup>xli</sup> | 155.17 (5) |
| Al12<sup>iv</sup>—Al1—Al12<sup>ii</sup> | 154.55 (10) | Al6<sup>ii</sup>—Al10—Al17B<sup>xli</sup> | 97.94 (4) |
| Mn2—Al1—Al13 | 49.10 (4) | Al6<sup>xii</sup>—Al10—Al17B<sup>xli</sup> | 97.86 (4) |
| Mn4—Al1—Al13 | 107.71 (3) | Mn1—Al10—Al17B<sup>xli</sup> | 129.61 (5) |
| Angle     | Edge 1 | Edge 2 | Edge 3 | Weight |
|-----------|--------|--------|--------|--------|
| Mn⁴v—Alı—Alı3 | 144.48 (4) | Alı9—Alı0—Alı7Bvli | 98.73 (5) |
| Al5—Alı—Alı3 | 85.93 (4) | Alı13xxxvi—Alı0—Alı7Bvli | 72.59 (4) |
| Alı5viii—Alı—Alı3 | 148.52 (3) | Niı iv—Alı0—Alı8x | 88.21 (6) |
| Alı12v—Alı—Alı3 | 148.29 (8) | Alı4—Alı0—Alı8x | 103.25 (6) |
| Alı12iv—Alı—Alı3 | 55.78 (3) | Alı6vii—Alı0—Alı8x | 57.93 (6) |
| Alı12v—Alı—Alı3 | 103.80 (4) | Alı6viii—Alı0—Alı8x | 134.91 (7) |
| Alı12viii—Alı—Alı3 | 92.86 (4) | Mnı—Alı0—Alı8x | 51.89 (5) |
| Mnı—Alı1—Alı3v | 49.10 (4) | Alı9vii—Alı0—Alı8x | 60.42 (5) |
| Mnıv—Alı1—Alı3v | 144.49 (4) | Alı13xxxvii—Alı0—Alı8x | 147.50 (8) |
| Mnıv—Alı1—Alı13v | 107.71 (3) | Niı iv—Alı0—Alı10v | 161.38 (3) |
| Alı5—Alı1—Alı13v | 85.93 (4) | Alı4—Alı0—Alı10v | 57.62 (3) |
| Alı5viii—Alı1—Alı13v | 148.52 (3) | Alı6vii—Alı0—Alı10v | 57.93 (9) |
| Alı12v—Alı1—Alı13v | 92.86 (4) | Alı6vii—Alı0—Alı10v | 58.04 (3) |
| Alı12iv—Alı1—Alı13v | 103.80 (4) | Mnı—Alı0—Alı10v | 58.05 (3) |
| Alı12iv—Alı1—Alı13v | 55.79 (3) | Alı9vii—Alı0—Alı10v | 110.28 (4) |
| Alı12viii—Alı1—Alı13v | 148.29 (8) | Alı13xxxvii—Alı0—Alı10v | 109.46 (4) |
| Alı13—Alı1—Alı13v | 58.63 (6) | Alı8x—Alı0—Alı10v | 102.64 (6) |
| Mnı—Alı1—Alı13viii | 49.10 (4) | Niı iv—Alı0—Alı17Avd | 53.82 (5) |
| Mnıv—Alı1—Alı13viii | 107.71 (3) | Alı4—Alı0—Alı17Avd | 144.61 (7) |
| Mnıv—Alı1—Alı13xiii | 144.49 (4) | Alı6vii—Alı0—Alı17Avd | 86.56 (5) |
| Alı5—Alı1—Alı13xiii | 148.52 (3) | Alı6vii—Alı0—Alı17Avd | 116.97 (7) |
| Alı5viii—Alı1—Alı13xiii | 85.93 (4) | Mnı—Alı0—Alı17Avd | 105.45 (6) |
| Alı12v—Alı1—Alı13xiii | 103.80 (4) | Alı9vii—Alı0—Alı17Avd | 82.25 (7) |
| Alı12iv—Alı1—Alı13xiii | 92.86 (4) | Alı13xxxvii—Alı0—Alı17Avd | 95.49 (6) |
| Alı12v—Alı1—Alı13xiii | 55.79 (3) | Alı8x—Alı0—Alı17Avd | 53.56 (7) |
| Alı12v—Alı1—Alı13xiii | 148.29 (8) | Alı10v—Alı0—Alı17Avd | 144.48 (4) |
| Alı13—Alı1—Alı13xiii | 70.31 (7) | Niı iv—Alı0—Alı17Avd | 104.59 (4) |
| Alı13—Alı1—Alı13xviii | 98.19 (9) | Alı4—Alı0—Alı17Avd | 54.15 (4) |
| Mnıv—Alı2—Mnıv | 171.29 (12) | Alı6vii—Alı0—Mnıvxxiii | 115.15 (5) |
| Mnıv—Alı2—Alı12 | 117.15 (7) | Alı6vii—Alı0—Mnıvxxiii | 52.92 (4) |
| Mnıv—Alı2—Alı12 | 56.15 (4) | Mnı—Alı0—Mnıvxxiii | 104.50 (4) |
| Mnıv—Alı2—Alı12v | 56.15 (4) | Alı9vii—Alı0—Mnıvxxiii | 107.56 (5) |
| Mnıv—Alı2—Alı12v | 117.15 (7) | Alı13xxxvii—Alı0—Mnıvxxiii | 54.12 (4) |
| Alı12—Alı2—Alı12v | 61.08 (6) | Alı8x—Alı0—Mnıvxxiii | 156.03 (6) |
| Mnıv—Alı2—Alı12vii | 56.15 (4) | Alı10v—Alı0—Mnıvxxiii | 60.16 (2) |
| Mnıv—Alı2—Alı12vii | 117.15 (7) | Alı17Avd—Alı0—Mnıvxxiii | 149.60 (6) |
| Alı12—Alı2—Alı2v | 97.05 (9) | Niı—Alı1—Mnıv | 120.04 (5) |
| Alı12—Alı2—Alı2vii | 66.82 (7) | Niı—Alı1—Alı4vi | 105.21 (5) |
| Mnıv—Alı2—Alı12xx | 117.15 (7) | Mnıv—Alı1—Alı4vi | 58.05 (5) |
| Mnıv—Alı2—Alı12xx | 56.15 (4) | Niı—Alı1—Alı13vi | 63.18 (4) |
| Alı12—Alı2—Alı2xx | 66.82 (7) | Mnıv—Alı1—Alı13vi | 157.51 (6) |
| Alı2—Alı2—Alı2xx | 97.05 (9) | Alı4vi—Alı1—Alı13vi | 99.47 (6) |
| Alı12—Alı2—Alı12xx | 61.08 (6) | Niı—Alı1—Alı12viii | 120.70 (5) |
| Mnıv—Alı2—Alı12vii | 64.57 (5) | Mnıv—Alı1—Alı12viii | 118.86 (5) |
| Mnıv—Alı2—Alı12vii | 124.14 (9) | Alı4vi—Alı1—Alı12viii | 99.45 (6) |
| Alı12—Alı2—Alı12vi | 145.81 (4) | Alı11—Alı1—Alı12viii | 60.03 (4) |
| Alı2—Alı2—Alı12vi | 108.81 (4) | Niı—Alı1—Alı12 | 140.58 (6) |
| Alı12—Alı2—Alı12vi | 108.81 (4) | Mnıv—Alı1—Alı12 | 53.81 (4) |
| Bond | Angle |
|------|-------|
| Al12−Al2−Al9 | 145.82 (4) |
| Mn4−Al2−Al9 | 124.14 (9) |
| Mn4−Al2−Al9 | 64.57 (5) |
| Al12−Al2−Al9 | 108.81 (4) |
| Al12−Al2−Al9 | 145.81 (4) |
| Al12−Al2−Al9 | 108.81 (4) |
| Al9−Al2−Al9 | 59.57 (9) |
| Mn4−Al2−Al11 | 122.17 (3) |
| Mn4−Al2−Al11 | 60.75 (3) |
| Al12−Al2−Al11 | 112.13 (4) |
| Al12−Al2−Al11 | 153.77 (8) |
| Al12−Al2−Al11 | 90.36 (4) |
| Al12−Al2−Al11 | 90.36 (4) |
| Al12−Al2−Al11 | 59.07 (3) |
| Al12−Al2−Al11 | 112.13 (4) |
| Al12−Al2−Al11 | 153.77 (8) |
| Al9−Al2−Al11 | 90.19 (6) |
| Al11−Al2−Al11 | 146.39 (10) |
| Mn4−Al2−Al11 | 60.75 (3) |
| Mn4−Al2−Al11 | 122.17 (3) |
| Al12−Al2−Al11 | 153.77 (8) |
| Al12−Al2−Al11 | 112.13 (4) |
| Al12−Al2−Al11 | 90.36 (4) |
| Al9−Al2−Al11 | 90.19 (6) |
| Al11−Al2−Al11 | 61.59 (5) |
| Al11−Al2−Al11 | 107.97 (6) |
| Mn4−Al2−Al11 | 122.17 (3) |
| Mn4−Al2−Al11 | 60.75 (3) |
| Al12−Al2−Al11 | 59.07 (3) |
| Al12−Al2−Al11 | 90.36 (4) |
| Al12−Al2−Al11 | 153.77 (8) |
| Al12−Al2−Al11 | 112.13 (4) |
| Al9−Al2−Al11 | 90.19 (6) |
| Al11−Al2−Al11 | 59.65 (4) |
| Mn3−Al3−Al6 | 174.83 (12) |
| Mn3−Al3−Al6 | 128.61 (10) |
Mn$_3$—Al$_3$—Al$_6$  56.56 (5)  Al$_{12}$—Al$_{11}$—Al$_{10}$  156.83 (6)  
Mn$_3$—Al$_3$—Al$_6$  56.56 (5)  Al$_9$—Al$_{11}$—Al$_{10}$  56.86 (4)  
Mn$_3$—Al$_3$—Al$_6$  128.61 (10)  Al$_2$—Al$_{11}$—Al$_{10}$  115.42 (6)  
Al$_6$—Al$_3$—Al$_6$  72.05 (9)  Al$_{15}$—Al$_{11}$—Al$_{10}$  106.83 (5)  
Mn$_3$—Al$_3$—Al$_{12}$  120.36 (8)  Mn$_{3,vi}$—Al$_{11}$—Al$_{10}$  59.38 (4)  
Mn$_3$—Al$_3$—Al$_{12}$  55.46 (4)  Al$_{11}$—Al$_{11}$—Al$_{10}$  107.73 (3)  
Al$_6$—Al$_3$—Al$_{12}$  103.70 (4)  Mn$_{4,vi}$—Al$_{12}$—Mn$_3$  161.15 (6)  
Al$_6$—Al$_3$—Al$_{12}$  150.24 (3)  Mn$_{4,vi}$—Al$_{12}$—Al$_{15}$  64.16 (5)  
Mn$_3$—Al$_3$—Al$_{12,vii}$  120.36 (8)  Mn$_3$—Al$_{12}$—Al$_{15}$  133.76 (6)  
Mn$_3$—Al$_3$—Al$_{12,vii}$  55.46 (4)  Mn$_{4,vi}$—Al$_{12}$—Al$_{13}$  122.41 (6)  
Al$_6$—Al$_3$—Al$_{12,vii}$  103.70 (4)  Mn$_3$—Al$_{12}$—Al$_{13}$  58.70 (4)  
Al$_6$—Al$_3$—Al$_{12,vii}$  150.24 (3)  Al$_{15}$—Al$_{12}$—Al$_{13}$  93.09 (6)  
Al$_{12,vi}$—Al$_3$—Al$_{12,vii}$  59.39 (6)  Mn$_{4,vi}$—Al$_{12}$—Al$_{11}$  131.84 (6)  
Mn$_3$—Al$_3$—Al$_{12}$  55.46 (4)  Mn$_3$—Al$_{12}$—Al$_{11}$  66.33 (4)  
Mn$_3$—Al$_3$—Al$_{12}$  120.35 (8)  Al$_{15}$—Al$_{12}$—Al$_{11}$  67.68 (5)  
Al$_6$—Al$_3$—Al$_{12}$  150.24 (3)  Al$_{13}$—Al$_{12}$—Al$_{11}$  58.79 (4)  
Al$_6$—Al$_3$—Al$_{12}$  103.70 (4)  Mn$_{4,vi}$—Al$_{12}$—Al$_{11}$  60.89 (4)  
Mn$_3$—Al$_3$—Al$_{12}$  64.92 (6)  Mn$_3$—Al$_{12}$—Al$_{11}$  128.46 (6)  
Mn$_3$—Al$_3$—Al$_{12}$  93.84 (8)  Mn$_3$—Al$_{12}$—Al$_{11}$  152.13 (6)  
Mn$_3$—Al$_3$—Al$_{12}$  93.84 (8)  Mn$_3$—Al$_{12}$—Al$_{11}$  97.38 (5)  
Mn$_3$—Al$_3$—Al$_{12}$  93.84 (8)  Mn$_3$—Al$_{12}$—Al$_{11}$  53.54 (3)  
Mn$_3$—Al$_3$—Al$_{12}$  113.47 (5)  Mn$_3$—Al$_{12}$—Al$_2$  111.47 (5)  
Mn$_3$—Al$_3$—Al$_{12}$  109.70 (6)  Mn$_3$—Al$_{12}$—Al$_{12}$  145.60 (6)  
Al$_6$—Al$_3$—Al$_{12}$  150.24 (3)  Mn$_3$—Al$_{12}$—Al$_{12}$  153.67 (6)  
Al$_6$—Al$_3$—Al$_{12}$  103.70 (4)  Al$_{11}$—Al$_{12}$—Al$_{12}$  61.18 (5)  
Al$_6$—Al$_3$—Al$_{12}$  64.92 (6)  Al$_{11}$—Al$_{12}$—Al$_{12}$  125.99 (6)  
Al$_6$—Al$_3$—Al$_{12}$  93.84 (8)  Al$_{11}$—Al$_{12}$—Al$_{12}$  63.87 (4)  
Al$_6$—Al$_3$—Al$_{12}$  55.87 (3)  Al$_{13}$—Al$_{12}$—Al$_{12}$  108.09 (6)  
Al$_6$—Al$_3$—Al$_{12}$  125.40 (3)  Mn$_{4,vi}$—Al$_{12}$—Al$_{12}$  60.97 (4)  
Al$_6$—Al$_3$—Al$_{12}$  99.90 (7)  Mn$_3$—Al$_{12}$—Al$_{12}$  65.61 (5)  
Al$_6$—Al$_3$—Al$_{12}$  60.04 (4)  Mn$_3$—Al$_{12}$—Al$_{12}$  94.51 (5)  
Al$_6$—Al$_3$—Al$_{12}$  147.01 (8)  Mn$_3$—Al$_{12}$—Al$_{12}$  112.93 (3)  
Al$_6$—Al$_3$—Al$_{12}$  92.89 (4)  Mn$_3$—Al$_{12}$—Al$_{12}$  55.32 (3)  
Al$_6$—Al$_3$—Al$_{12}$  103.07 (5)  Al$_{15}$—Al$_{12}$—Al$_{12}$  152.94 (4)  
Al$_6$—Al$_3$—Al$_{12}$  55.79 (3)  Al$_{15}$—Al$_{12}$—Al$_{12}$  110.01 (4)  
Al$_6$—Al$_3$—Al$_{12}$  103.07 (5)  Al$_{15}$—Al$_{12}$—Al$_{12}$  109.41 (4)  
Al$_6$—Al$_3$—Al$_{12}$  147.01 (8)  Al$_{15}$—Al$_{12}$—Al$_{12}$  90.65 (4)  
Al$_6$—Al$_3$—Al$_{12}$  92.89 (4)  Al$_{15}$—Al$_{12}$—Al$_{12}$  59.46 (3)  
Al$_6$—Al$_3$—Al$_{12}$  103.07 (5)  Al$_{15}$—Al$_{12}$—Al$_{12}$  59.92 (3)  
Al$_6$—Al$_3$—Al$_{12}$  156.64 (10)  Mn$_{4,vi}$—Al$_{12}$—Al$_{3}$  108.70 (5)  
Al$_6$—Al$_3$—Al$_{12}$  125.40 (3)  Mn$_3$—Al$_{12}$—Al$_{3}$  53.43 (4)  
Al$_6$—Al$_3$—Al$_{12}$  55.87 (3)  Al$_{15}$—Al$_{12}$—Al$_{3}$  148.34 (6)  
Al$_6$—Al$_3$—Al$_{12}$  60.04 (4)  Al$_{13}$—Al$_{12}$—Al$_{3}$  63.77 (5)  
Al$_6$—Al$_3$—Al$_{12}$  99.90 (7)  Al$_{11}$—Al$_{12}$—Al$_{3}$  111.56 (5)  
Al$_6$—Al$_3$—Al$_{12}$  103.07 (5)  Al$_{11}$—Al$_{12}$—Al$_{3}$  143.97 (6)
| Bond                  | Angle (°) (°) | Bond                  | Angle (°) (°) |
|----------------------|--------------|----------------------|--------------|
| Al12v—Al3—Al13xii    | 55.79 (3)    | Al2—Al12—Al3         | 84.56 (6)    |
| Al12v—Al3—Al13xii    | 92.89 (4)    | Al5vi—Al12—Al3       | 109.80 (5)   |
| Al12—Al3—Al13xii     | 147.01 (8)   | Al12v—Al12—Al3       | 60.31 (3)    |
| Al13v—Al3—Al13xii    | 69.61 (5)    | Al12v—Al12—Al3       | 59.92 (5)    |
| Al13xv—Al3—Al13xii   | 105.46 (6)   | Mn4iii—Al12—Al1ii    | 119.49 (6)   |
| Mn3—Al3—Al13xii      | 55.87 (3)    | Al5vi—Al12—Al1ii     | 61.05 (5)    |
| Mn3xv—Al3—Al13xii    | 125.40 (3)   | Al13ii—Al12—Al1ii    | 62.78 (6)    |
| Al6xv—Al3—Al13xii    | 99.90 (7)    | Al11viii—Al12—Al1ii  | 95.91 (5)    |
| Al6—Al3—Al13xii      | 60.04 (4)    | Al11—Al12—Al1ii      | 110.32 (6)   |
| Al12xv—Al3—Al13xii   | 92.89 (4)    | Al2—Al12—Al1ii       | 105.59 (5)   |
| Al12ii—Al3—Al13xii   | 147.01 (8)   | Al5vi—Al12—Al1ii     | 154.32 (5)   |
| Al12v—Al3—Al13xii    | 103.07 (5)   | Al12v—Al12—Al1ii     | 144.87 (3)   |
| Al12—Al3—Al13xii     | 55.79 (3)    | Al3—Al12—Al1ii       | 88.24 (5)    |
| Al13v—Al3—Al13xii    | 105.46 (6)   | Mn2—Al13—Mn3iii      | 149.28 (6)   |
| Al13xv—Al3—Al13xii   | 69.61 (5)    | Mn2—Al13—Al17A       | 59.00 (7)    |
| Al13xviii—Al3—Al13xii| 156.64 (10)  | Mn3iii—Al13—Al17A    | 134.09 (6)   |
| Al4xviii—Al4—Mn3xviii| 179.94 (4)   | Mn2—Al13—Al11xiii    | 140.75 (7)   |
| Al4xviii—Al4—Mn4xvi  | 61.61 (4)    | Mn3iii—Al13—Al11xiii | 66.42 (4)    |
| Mn3xviii—Al4—Mn4xvi  | 118.34 (5)   | Al7A—Al13—Al11xiii   | 113.16 (8)   |
| Al4xviii—Al4—Mn4     | 61.61 (4)    | Mn2—Al13—Ni1xiii     | 102.62 (5)   |
| Mn3xviii—Al4—Mn4     | 118.34 (5)   | Mn3iii—Al13—Ni1xiii  | 107.22 (5)   |
| Mn4xiv—Al4—Mn4       | 65.57 (5)    | Al7A—Al13—Ni1xiii    | 58.62 (6)    |
| Al4xviii—Al4—Mn1     | 61.94 (4)    | Al11xiii—Al13—Ni1xiii| 54.73 (4)    |
| Mn3xviii—Al4—Mn1     | 118.11 (6)   | Mn2—Al13—Al12ii      | 117.03 (7)   |
| Mn4xiv—Al4—Mn1       | 112.85 (5)   | Mn3iii—Al13—Al12ii   | 56.18 (4)    |
| Mn4—Al4—Mn1          | 112.85 (5)   | Al17A—Al13—Al12ii    | 167.20 (7)   |
| Al4xviii—Al4—Al5     | 113.51 (5)   | Al11xiii—Al13—Al12ii | 61.18 (4)    |
| Mn3xviii—Al4—Al5     | 66.43 (6)    | Ni1xiii—Al13—Al12ii  | 113.74 (5)   |
| Mn4—Al4—Al5          | 63.50 (5)    | Mn2—Al13—Al10xxxvi   | 130.87 (7)   |
| Mn4—Al4—Al5          | 63.50 (5)    | Mn3iii—Al13—Al10xxxvi| 65.78 (4)    |
| Mn1—Al4—Al5          | 175.45 (8)   | Al17A—Al13—Al10xxxvi | 72.73 (6)    |
| Al4xviii—Al4—Al10    | 113.02 (4)   | Al11xiii—Al13—Al10xxxvi| 65.72 (4) |
| Mn3xviii—Al4—Al10    | 67.03 (5)    | Ni1xiii—Al13—Al10xxxvi| 53.97 (4) |
| Mn4xiv—Al4—Al10      | 174.21 (8)   | Al12ii—Al13—Al10xxxvi| 110.08 (6) |
| Mn4—Al4—Al10         | 114.51 (3)   | Mn2—Al13—Al8vii      | 52.37 (6)    |
| Mn1—Al4—Al10         | 61.53 (4)    | Mn3iii—Al13—Al8vii   | 107.45 (7)   |
| Al5—Al4—Al10         | 122.04 (7)   | Al7A—Al13—Al8vii     | 56.17 (7)    |
| Al4xviii—Al4—Al10v   | 113.02 (4)   | Al11xiii—Al13—Al8vii | 159.89 (6)   |
| Mn3xviii—Al4—Al10v   | 67.03 (5)    | Ni1xiii—Al13—Al8vii  | 113.35 (6)   |
| Mn4xiv—Al4—Al10v     | 114.51 (3)   | Al12ii—Al13—Al8vii   | 132.88 (7)   |
| Mn4—Al4—Al10v        | 174.21 (8)   | Al10xxxvi—Al13—Al8vii| 94.20 (5)    |
| Mn1—Al4—Al10v        | 61.53 (4)    | Mn2—Al13—Al13v       | 51.85 (3)    |
| Al5—Al4—Al10v        | 122.04 (7)   | Mn3iii—Al13—Al13v    | 156.42 (3)   |
| Al10—Al4—Al10v       | 64.76 (6)    | Al7A—Al13—Al13v      | 57.51 (4)    |
| Al4xviii—Al4—Al11ii  | 113.18 (4)   | Al11xiii—Al13—Al13v  | 90.35 (4)    |
| Mn3xviii—Al4—Al11ii  | 66.80 (4)    | Ni1xiii—Al13—Al13v   | 58.13 (3)    |
| Mn4xiv—Al4—Al11ii    | 116.83 (6)   | Al12ii—Al13—Al13v    | 110.01 (4)   |
| Mn4—Al4—Al11ii       | 60.63 (3)    | Al10xxxvi—Al13—Al13v | 109.45 (4)   |
| Symmetry          | Mn1—Al4—Al11 iii | Al5—Al4—Al11 iii | Al10—Al4—Al11 iii | Al10 vii—Al4—Al11 iii | Al10 viii—Al4—Al11 iii | Al10 vii—Al4—Al11 iii | Al10 viii—Al4—Al11 iii | Al10 vi—Al4—Al11 iv | Al1 viii—Al4—Al11 iv | Al1 vi—Al4—Al11 iv | Al4 vii—Al4—Al19 v | Mn3 vii—Al4—Al19 v | Mn4 viii—Al4—Al19 v | Mn1—Al4—Al11 iv | Al5—Al4—Al11 iv | Al10—Al4—Al11 iv | Al10 vii—Al4—Al11 iv | Al10 viii—Al4—Al11 iv | Al10 vi—Al4—Al11 iv | Al1 viii—Al4—Al11 iv | Al1 vi—Al4—Al11 iv |
|------------------|------------------|------------------|-------------------|------------------------|------------------------|------------------------|------------------------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|
|                  | 116.63 (4)       | 64.51 (4)        | 66.64 (4)         | 122.34 (7)           | 113.18 (4)            | 66.80 (4)              | 60.63 (3)              | 116.83 (6)          | 116.63 (4)          | 64.51 (4)           | 66.64 (4)           | 122.34 (7)          | 60.63 (3)           | 116.83 (6)         | 64.51 (4)        | 66.64 (4)        | 122.34 (7)        | 60.63 (3)         | 116.83 (6)        | 64.51 (4)        | 66.64 (4)        | 122.34 (7)        | 60.63 (3)         | 116.83 (6)        |
| Symmetry codes: | (i) x, y+1/2, z; | (ii) −x, −y+2, −z+1; (iii) −x+1/2, −y+3/2, −z+1; (iv) x+1/2, −y+3/2, −z+1; (v) −x, y, z; (vi) x, y, z−1; (vii) −x, y, −z+1/2; | (viii) −x, y, z+1; (ix) x−1/2, −y+1/2, z+1/2; (x) x−1/2, −y+1/2, −z−1/2; (xi) −x, −y+1, z+1/2; (xii) −x, −y+1, −z+1; (xiii) x, y, −z+3/2; (xiv) −x, y, −z+3/2; | (xv) x−1/2, −y+3/2, z+1/2; (xvi) x, −y+1, z+1/2; (xvii) x−1/2, −y+3/2, −z; (xviii) −x+1/2, −y+3/2, −z; (xix) −x+1/2, −y+3/2, z+1/2; (xx) x, y, −z+1/2; (xxi) −x+1/2, −y+3/2, z+1/2; (xxii) x−1/2, −y+3/2, z+1/2; (xxiii) x, y, z+1; (xxiv) −x, y, z+1; (xxv) −x+1/2, y+1/2, −z−1/2; (xxvi) x−1/2, y+1/2, z; (xxvii) x−1/2, −y+1/2, z; (xxviii) −x+1/2, y+1/2, z−1; (xxix) x−1/2, −y+1/2, z+1; (xxx) x, −y+1, z; (xxx) −x−1/2, −y+1, −z+1/2; (xxxii) −x+1/2, −y+1, z; (xxxvii) −x+1/2, −y+1, −z+1; (xxxviii) −x+1/2, −y+1, z; (xxxix) −x+1/2, −y+1, −z+1; (xl) x+1/2, y+1/2, z; (xli) x+1/2, y+1/2, z; (xlii) x+1/2, y+1/2, z; (xliii) x, −y+1, −z+1/2; (xliv) x, −y+1, −z+1/2; (xlv) −x, −y+1, −z+1/2; (xlvi) −x, −y+1, −z+1/2; |