IUCrData

ISSN 2414-3146

# The $Al_{61.49}Mn_{11.35}Ni_4$ phase in the Al–Mn–Ni system

Qifa Hu, Bin Wen and Changzeng Fan*

State Key Laboratory of Metastable Materials Science and Technology, Yanshan University, Qinhuangdao 066004, People's Republic of China. *Correspondence e-mail: chzfan@ysu.edu.cn

Received 29 November 2021
Accepted 11 January 2022

Edited by M. Weil, Vienna University of Technology, Austria

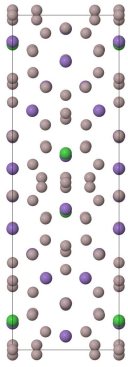
**Keywords:** crystal structure; high-temperature sintering; *R*-phase; Al–Mn–Ni system..

**CCDC reference**: 2141311

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

An intermetallic phase in the Al–Mn–Ni system crystallizing in space group *Cmcm* (No. 63) and refined formula $Al_{61.49}Mn_{11.35}Ni_4$ (called the $R'$ phase) has been synthesized by high-temperature sintering of a mixture with initial chemical composition $Al_{60}Mn_7Ni_3$. In comparison with the structure model of the previously reported *R* phase with composition $Al_{60}Mn_{11}Ni_4$ [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 $R'$ phase.

**3D view**



## 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 $Al_{60}Mn_{11}Ni_4$ was reported as thermodynamically stable, crystallizing in space group *Bbmm* (non-conventional setting of space group *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 $Al_{80.0}Mn_{14.7}Ni_{5.3}$ 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 $Al_{20}Mn_3Cu_2$ phase (Damjanovic, 1961). It is interesting to note that the orthorhombic phase in the Al–Mn system is isostructural with

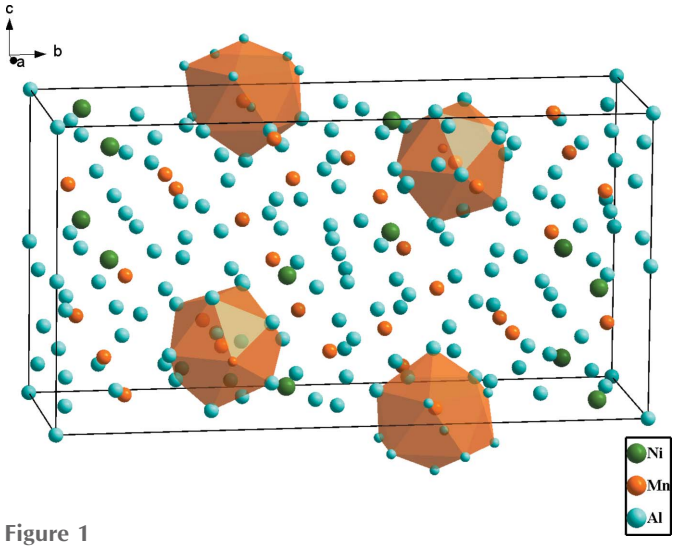



**Figure 1**
The crystal structure of $Al_{61.49}Mn_{11.35}Ni_4$ with two Mn3 atoms and two Mn4 atoms displayed with their coordination environments as polyhedra.

the *R* phase and in coexistence with the decagonal quasicrystal in a rapidly solidified Al–Mn alloy, implying it is inseparable from the formation of quasicrystals (Li & Kuo, 1992).

In the present study, a slightly different crystal-structure model for the *R* phase in the Al–Mn–Ni system has been refined on basis of single-crystal X-ray diffraction data. This phase has similar unit-cell parameters to the previously reported *R* phase (Table 1, using the conventional setting *Cmcm*). Its chemical composition was refined to be $Al_{61.49}Mn_{11.35}Ni_4$, in accordance with complementary SEM/EDX results (see Fig. S1 and Table S1 of the supporting information).

In comparison with the *R* phase, the *R*′ phase has a slightly higher Al and Mn content. A detailed comparison of the atomic labelling and coordinates between these two structure models along with the transformation matrix that transforms the original non-conventional setting to the current standard setting can be found in Table S2 of the supporting information. The *R*′ phase has two reversed sites compared to the original *R* phase whereby Mn4 in the original model becomes Ni1 in the current 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 $Al_{61.49}Mn_{11.35}Ni_4$ with four distorted icosahedra illustrated for simplicity. The environments of the Mn3 and Mn4 sites are shown in Fig. 2*a* and 2*b*, respectively. The icosahedron centered at Mn3 is surrounded solely by Al atoms (Al3, Al4, Al5, Al6, Al10, Al11, Al12 and Al13) while that centered at Mn4 atom is composed by 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. 3*a*. The environments of Al3 are displayed in Fig. 3*b*, 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

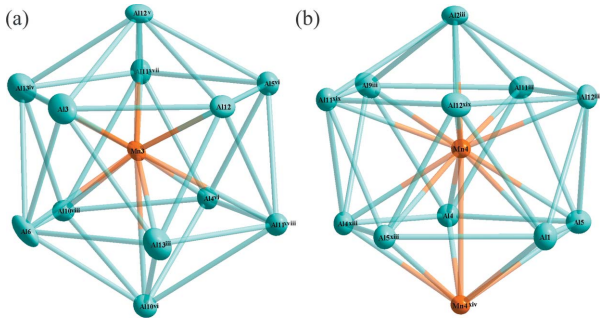



**Figure 2**
(*a*) The environment of the Mn3 atom at the 8*f* site; (*b*) the environment of the Mn4 atom at the 8*g* site with displacement ellipsoids given at the 90% probability level. [Symmetry codes: (iii) $-x+1/2, -y+\frac{3}{2}, -z+1$; (iv) $x-\frac{1}{2}, -y+\frac{3}{2}, -z+1$; (v) $-x, y, z$; (vi) $x, y, z-1$; (viii) $-x, y, z-1$; (xiii) $x, y, -z+\frac{3}{2}$; (xiv) $-x, y, -z+\frac{3}{2}$; (xvii) $x-\frac{1}{2}, -y+\frac{3}{2}, -z$; (xviii) $-x+\frac{1}{2}, -y+\frac{3}{2}, -z$; (xix) $-x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$.]

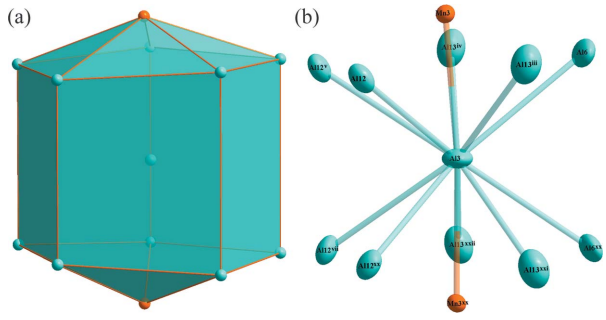



**Figure 3**
(*a*) The polyhedron formed around the Al3 atom at the 4*c* site; (*b*) the environment of the Al3 atom with displacement ellipsoids given at the 90% probability level. [Symmetry codes: (iii) $-x+\frac{1}{2}, -y+\frac{3}{2}, -z+1$; (iv) $x-\frac{1}{2}, -y+\frac{3}{2}, -z+1$; (v) $-x, y, z$; (vii) $-x, y, -z+\frac{1}{2}$; (xx) $x, y, -z+\frac{1}{2}$; (xxi) $-x+\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (xxii) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$.]

**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) |
| $V$ (Å$^3$) | 2276.93 (18) |
| $Z$ | 2 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (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) |
| $T_{min}$, $T_{max}$ | 0.648, 0.746 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 40442, 1584, 1269 |
| $R_{int}$ | 0.090 |
| (sin $\theta/\lambda)_{max}$ (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 |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 1.85, −1.03 |

Computer programs: *APEX3* and *SAINT* (Bruker, 2015), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *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 Al7*A* and Al7*B*, 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 Al7*A*, respectively.

## Funding information

Funding for this research was provided by: The National Natural Science Foundation of China (grant No. 52173231 and 51771165).

## References

Brandenburg, K. & Putz, H. (2017). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2015). *APEX3* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Damjanovic, A. (1961). *Acta Cryst.* **14**, 982–987.
Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.
Li, X. & Kuo, K. (1992). *Philos. Mag. B*, **65**, 525–533.
Raynor, G. V. (1944). *J. Inst. Met.* **70**, 507.
Robinson, K. (1954). *Acta Cryst.* **7**, 494–497.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

# full crystallographic data

*IUCrData* (2022). **7**, x220038 [https://doi.org/10.1107/S2414314622000384]

## The $Al_{61.49}Mn_{11.35}Ni_4$ phase in the Al–Mn–Ni system

**Qifa Hu, Bin Wen and Changzeng Fan**

**(I)**

*Crystal data*

$Al_{61.49}Mn_{11.35}Ni_4$
$M_r$ = 2517.49
Orthorhombic, *Cmcm*
$a$ = 7.6135 (3) Å
$b$ = 23.9582 (11) Å
$c$ = 12.4828 (6) Å
$V$ = 2276.93 (18) Å$^3$
$Z$ = 2
$F$(000) = 2390
$D_x$ = 3.672 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 8707 reflections
$\theta$ = 2.4–30.6°
$\mu$ = 5.85 mm$^{-1}$
$T$ = 296 K
Fragment, metallic
0.10 × 0.10 × 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)
$T_{min}$ = 0.648, $T_{max}$ = 0.746
40442 measured reflections
1584 independent reflections
1269 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.090
$\theta_{max}$ = 28.3°, $\theta_{min}$ = 2.4°
$h$ = −10→10
$k$ = −31→31
$l$ = −16→16

*Refinement*

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
1584 reflections
114 parameters
0 restraints
$w = 1/[\sigma^2(F_o^2) + (0.0463P)^2 + 17.4467P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.85 e Å$^{-3}$
$\Delta\rho_{min}$ = −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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ | 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) | |

| | | | | | |
|---|---|---|---|---|---|
| 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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, º)*

| | | | |
|---|---|---|---|
| Ni1—Al7B$^{i}$ | 2.2523 (7) | Al2—Al9$^{vii}$ | 2.829 (3) |
| Ni1—Al7A$^{ii}$ | 2.468 (2) | Al2—Al9 | 2.829 (3) |
| Ni1—Al10$^{iii}$ | 2.4921 (12) | Al2—Al11$^{xx}$ | 2.8490 (13) |
| Ni1—Al10$^{iv}$ | 2.4921 (12) | Al2—Al11$^{v}$ | 2.8490 (13) |
| Ni1—Al11 | 2.4989 (13) | Al2—Al11$^{vii}$ | 2.8490 (13) |

| | | | |
|---|---|---|---|
| Ni1—Al11$^{v}$ | 2.4989 (13) | Al2—Al11 | 2.8490 (13) |
| Ni1—Al7A$^{vi}$ | 2.652 (3) | Al3—Al6$^{xx}$ | 2.819 (3) |
| Ni1—Al9 | 2.7106 (12) | Al3—Al6 | 2.819 (3) |
| Ni1—Al9$^{vii}$ | 2.7107 (12) | Al3—Al12$^{xx}$ | 2.881 (2) |
| Ni1—Al13$^{viii}$ | 2.7315 (15) | Al3—Al12$^{vii}$ | 2.881 (2) |
| Ni1—Al13$^{vi}$ | 2.7315 (15) | Al3—Al12$^{v}$ | 2.881 (2) |
| Mn1—Al8$^{ix}$ | 2.462 (2) | Al3—Al12 | 2.881 (2) |
| Mn1—Al8$^{x}$ | 2.462 (2) | Al3—Al13$^{iv}$ | 2.9714 (14) |
| Mn1—Al6$^{xi}$ | 2.5310 (19) | Al3—Al13$^{xxi}$ | 2.9714 (14) |
| Mn1—Al6$^{xii}$ | 2.5310 (19) | Al3—Al13$^{xxii}$ | 2.9714 (14) |
| Mn1—Al4 | 2.6399 (19) | Al3—Al13$^{iii}$ | 2.9714 (14) |
| Mn1—Al4$^{xiii}$ | 2.6400 (19) | Al4—Al4$^{xiii}$ | 2.483 (3) |
| Mn1—Al10$^{xiv}$ | 2.7312 (12) | Al4—Al5 | 2.641 (2) |
| Mn1—Al10$^{v}$ | 2.7312 (12) | Al4—Al10 | 2.6985 (18) |
| Mn1—Al10$^{xiii}$ | 2.7312 (12) | Al4—Al10$^{v}$ | 2.6985 (18) |
| Mn1—Al10 | 2.7312 (12) | Al4—Al11$^{iii}$ | 2.7001 (15) |
| Mn1—Al9$^{iii}$ | 2.8328 (18) | Al4—Al11$^{iv}$ | 2.7001 (14) |
| Mn1—Al9$^{xv}$ | 2.8328 (18) | Al4—Al9$^{xv}$ | 2.8270 (18) |
| Mn2—Al8$^{xvi}$ | 2.333 (2) | Al4—Al9$^{iii}$ | 2.8270 (18) |
| Mn2—Al8$^{xii}$ | 2.333 (2) | Al5—Al12$^{iii}$ | 2.7131 (15) |
| Mn2—Al13$^{xiv}$ | 2.3349 (14) | Al5—Al12$^{iv}$ | 2.7131 (15) |
| Mn2—Al13$^{xiii}$ | 2.3349 (14) | Al5—Al12$^{xxiii}$ | 2.8480 (18) |
| Mn2—Al13$^{v}$ | 2.3349 (14) | Al5—Al12$^{xxiv}$ | 2.8480 (18) |
| Mn2—Al13 | 2.3349 (14) | Al5—Al11$^{iv}$ | 2.8510 (15) |
| Mn2—Al7A$^{xiii}$ | 2.491 (3) | Al5—Al11$^{iii}$ | 2.8510 (15) |
| Mn2—Al7A | 2.491 (3) | Al6—Al8$^{xxv}$ | 2.722 (2) |
| Mn2—Al1 | 2.633 (3) | Al6—Al8$^{xxvi}$ | 2.722 (2) |
| Mn3—Al3 | 2.4459 (8) | Al6—Al10$^{xii}$ | 2.7266 (19) |
| Mn3—Al12$^{v}$ | 2.5085 (13) | Al6—Al10$^{xxvii}$ | 2.7266 (19) |
| Mn3—Al12 | 2.5086 (13) | Al6—Al10$^{viii}$ | 2.7300 (19) |
| Mn3—Al6 | 2.5162 (19) | Al6—Al10$^{vi}$ | 2.7300 (19) |
| Mn3—Al4$^{vi}$ | 2.5563 (18) | Al6—Al13$^{iii}$ | 2.9000 (16) |
| Mn3—Al13$^{iv}$ | 2.5800 (14) | Al6—Al13$^{iv}$ | 2.9000 (16) |
| Mn3—Al13$^{iii}$ | 2.5800 (14) | Al7A—Al7A$^{xxviii}$ | 2.442 (5) |
| Mn3—Al5$^{vi}$ | 2.8481 (18) | Al7A—Al8$^{xii}$ | 2.608 (3) |
| Mn3—Al11$^{xvii}$ | 2.8962 (13) | Al7A—Al8$^{xvi}$ | 2.608 (3) |
| Mn3—Al11$^{xviii}$ | 2.8962 (13) | Al7A—Al13$^{v}$ | 2.685 (2) |
| Mn3—Al10$^{viii}$ | 2.9039 (13) | Al7A—Al13 | 2.685 (2) |
| Mn3—Al10$^{vi}$ | 2.9039 (13) | Al7A—Al10$^{xxix}$ | 2.9016 (17) |
| Mn4—Al2$^{iii}$ | 2.3996 (9) | Al7A—Al10$^{xxvi}$ | 2.9016 (17) |
| Mn4—Al12$^{iii}$ | 2.4779 (13) | Al7B—Al10$^{xxx}$ | 2.8166 (12) |
| Mn4—Al12$^{xix}$ | 2.4779 (13) | Al7B—Al10$^{xxxi}$ | 2.8166 (12) |
| Mn4—Al4 | 2.6116 (15) | Al7B—Al10$^{xxxii}$ | 2.8166 (12) |
| Mn4—Al4$^{xiii}$ | 2.6116 (15) | Al7B—Al10$^{x}$ | 2.8166 (12) |
| Mn4—Al11$^{xix}$ | 2.6823 (12) | Al8—Al9$^{xxxiii}$ | 2.843 (3) |
| Mn4—Al11$^{iii}$ | 2.6823 (12) | Al8—Al13$^{xxxiv}$ | 2.847 (2) |
| Mn4—Al1 | 2.716 (2) | Al8—Al13$^{xxvii}$ | 2.847 (2) |
| Mn4—Al5 | 2.7642 (15) | Al8—Al10$^{x}$ | 2.8874 (16) |

| | | | |
|---|---|---|---|
| Mn4—Al5$^{xiii}$ | 2.7642 (15) | Al8—Al10$^{xxxv}$ | 2.8874 (16) |
| Mn4—Al9$^{iii}$ | 2.8163 (19) | Al9—Al10$^{xxi}$ | 2.7591 (15) |
| Mn4—Mn4$^{xiv}$ | 2.8282 (17) | Al9—Al10$^{iii}$ | 2.7591 (15) |
| Al1—Al5 | 2.861 (2) | Al9—Al9$^{vii}$ | 2.811 (4) |
| Al1—Al5$^{xiii}$ | 2.861 (2) | Al9—Al11 | 2.8242 (15) |
| Al1—Al12$^{xv}$ | 2.9093 (14) | Al9—Al11$^{xx}$ | 2.8242 (15) |
| Al1—Al12$^{iii}$ | 2.9093 (14) | Al10—Al13$^{xxxvi}$ | 2.7603 (17) |
| Al1—Al12$^{iv}$ | 2.9093 (14) | Al10—Al10$^{v}$ | 2.890 (2) |
| Al1—Al12$^{xix}$ | 2.9093 (14) | Al11—Al13$^{vi}$ | 2.7046 (17) |
| Al1—Al13 | 2.946 (2) | Al11—Al12$^{xviii}$ | 2.7705 (16) |
| Al1—Al13$^{v}$ | 2.946 (2) | Al11—Al12 | 2.7891 (16) |
| Al1—Al13$^{xiii}$ | 2.946 (2) | Al11—Al11$^{v}$ | 2.917 (2) |
| Al2—Al12 | 2.809 (2) | Al12—Al13$^{iii}$ | 2.7393 (17) |
| Al2—Al12$^{v}$ | 2.809 (2) | Al12—Al12$^{v}$ | 2.855 (3) |
| Al2—Al12$^{vii}$ | 2.809 (2) | Al13—Al13$^{v}$ | 2.884 (3) |
| Al2—Al12$^{xx}$ | 2.809 (2) | | |

| | | | |
|---|---|---|---|
| Al7A$^{ii}$—Ni1—Al10$^{iii}$ | 71.59 (3) | Al11$^{iv}$—Al4—Al9$^{iii}$ | 177.12 (7) |
| Al7A$^{ii}$—Ni1—Al10$^{iv}$ | 71.59 (3) | Al9$^{xv}$—Al4—Al9$^{iii}$ | 116.30 (7) |
| Al10$^{iii}$—Ni1—Al10$^{iv}$ | 142.75 (6) | Al4—Al5—Al12$^{iii}$ | 104.51 (5) |
| Al7B$^{i}$—Ni1—Al11 | 138.65 (3) | Al4—Al5—Al12$^{iv}$ | 104.51 (5) |
| Al7A$^{ii}$—Ni1—Al11 | 143.68 (3) | Al12$^{iii}$—Al5—Al12$^{iv}$ | 122.57 (8) |
| Al10$^{iii}$—Ni1—Al11 | 72.91 (4) | Al4—Al5—Mn4 | 57.73 (5) |
| Al10$^{iv}$—Ni1—Al11 | 144.33 (5) | Al12$^{iii}$—Al5—Mn4 | 53.78 (4) |
| Al7A$^{ii}$—Ni1—Al11$^{v}$ | 143.68 (3) | Al12$^{iv}$—Al5—Mn4 | 107.85 (6) |
| Al10$^{iii}$—Ni1—Al11$^{v}$ | 144.33 (5) | Al4—Al5—Mn4$^{xiv}$ | 57.73 (5) |
| Al10$^{iv}$—Ni1—Al11$^{v}$ | 72.91 (4) | Al12$^{iii}$—Al5—Mn4$^{xiv}$ | 107.85 (6) |
| Al11—Ni1—Al11$^{v}$ | 71.42 (6) | Al12$^{iv}$—Al5—Mn4$^{xiv}$ | 53.78 (4) |
| Al7A$^{ii}$—Ni1—Al7A$^{vi}$ | 56.83 (10) | Mn4—Al5—Mn4$^{xiv}$ | 61.54 (5) |
| Al10$^{iii}$—Ni1—Al7A$^{vi}$ | 77.70 (3) | Al4—Al5—Al12$^{xxiii}$ | 98.93 (6) |
| Al10$^{iv}$—Ni1—Al7A$^{vi}$ | 77.70 (3) | Al12$^{iii}$—Al5—Al12$^{xxiii}$ | 82.56 (4) |
| Al11—Ni1—Al7A$^{vi}$ | 121.67 (5) | Al12$^{iv}$—Al5—Al12$^{xxiii}$ | 138.55 (6) |
| Al11$^{v}$—Ni1—Al7A$^{vi}$ | 121.67 (5) | Mn4—Al5—Al12$^{xxiii}$ | 113.56 (4) |
| Al7B$^{i}$—Ni1—Al9 | 116.69 (4) | Mn4$^{xiv}$—Al5—Al12$^{xxiii}$ | 155.84 (7) |
| Al7A$^{ii}$—Ni1—Al9 | 91.85 (7) | Al4—Al5—Al12$^{xxiv}$ | 98.93 (6) |
| Al10$^{iii}$—Ni1—Al9 | 63.89 (4) | Al12$^{iii}$—Al5—Al12$^{xxiv}$ | 138.55 (6) |
| Al10$^{iv}$—Ni1—Al9 | 122.86 (5) | Al12$^{iv}$—Al5—Al12$^{xxiv}$ | 82.56 (4) |
| Al11—Ni1—Al9 | 65.51 (4) | Mn4—Al5—Al12$^{xxiv}$ | 155.84 (7) |
| Al11$^{v}$—Ni1—Al9 | 101.00 (5) | Mn4$^{xiv}$—Al5—Al12$^{xxiv}$ | 113.56 (4) |
| Al7A$^{vi}$—Ni1—Al9 | 137.13 (5) | Al12$^{xxiii}$—Al5—Al12$^{xxiv}$ | 60.15 (6) |
| Al7A$^{ii}$—Ni1—Al9$^{vii}$ | 91.85 (7) | Al4—Al5—Mn3$^{xxiii}$ | 55.36 (5) |
| Al10$^{iii}$—Ni1—Al9$^{vii}$ | 122.86 (5) | Al12$^{iii}$—Al5—Mn3$^{xxiii}$ | 118.66 (4) |
| Al10$^{iv}$—Ni1—Al9$^{vii}$ | 63.89 (4) | Al12$^{iv}$—Al5—Mn3$^{xxiii}$ | 118.66 (4) |
| Al11—Ni1—Al9$^{vii}$ | 100.99 (5) | Mn4—Al5—Mn3$^{xxiii}$ | 104.50 (5) |
| Al11$^{v}$—Ni1—Al9$^{vii}$ | 65.51 (4) | Mn4$^{xiv}$—Al5—Mn3$^{xxiii}$ | 104.50 (5) |
| Al7A$^{vi}$—Ni1—Al9$^{vii}$ | 137.13 (5) | Al12$^{xxiii}$—Al5—Mn3$^{xxiii}$ | 52.26 (4) |
| Al9—Ni1—Al9$^{vii}$ | 62.46 (7) | Al12$^{xxiv}$—Al5—Mn3$^{xxiii}$ | 52.26 (4) |
| Al7A$^{ii}$—Ni1—Al13$^{viii}$ | 107.32 (6) | Al4—Al5—Al11$^{iv}$ | 58.75 (4) |

| | | | |
|---|---|---|---|
| Al10$^{iii}$—Ni1—Al13$^{viii}$ | 123.79 (5) | Al12$^{iii}$—Al5—Al11$^{iv}$ | 161.14 (7) |
| Al10$^{iv}$—Ni1—Al13$^{viii}$ | 63.61 (4) | Al12$^{iv}$—Al5—Al11$^{iv}$ | 60.11 (4) |
| Al11—Ni1—Al13$^{viii}$ | 98.53 (4) | Mn4—Al5—Al11$^{iv}$ | 107.38 (6) |
| Al11$^{v}$—Ni1—Al13$^{viii}$ | 62.09 (4) | Mn4$^{xiv}$—Al5—Al11$^{iv}$ | 57.04 (3) |
| Al7A$^{vi}$—Ni1—Al13$^{viii}$ | 59.81 (5) | Al12$^{xxiii}$—Al5—Al11$^{iv}$ | 107.35 (6) |
| Al9—Ni1—Al13$^{viii}$ | 160.69 (5) | Al12$^{xxiv}$—Al5—Al11$^{iv}$ | 58.17 (4) |
| Al9$^{vii}$—Ni1—Al13$^{viii}$ | 113.34 (4) | Mn3$^{xxiii}$—Al5—Al11$^{iv}$ | 61.09 (4) |
| Al7A$^{ii}$—Ni1—Al13$^{vi}$ | 107.32 (6) | Al4—Al5—Al11$^{iii}$ | 58.75 (4) |
| Al10$^{iii}$—Ni1—Al13$^{vi}$ | 63.61 (4) | Al12$^{iii}$—Al5—Al11$^{iii}$ | 60.11 (4) |
| Al10$^{iv}$—Ni1—Al13$^{vi}$ | 123.79 (5) | Al12$^{iv}$—Al5—Al11$^{iii}$ | 161.14 (7) |
| Al11—Ni1—Al13$^{vi}$ | 62.09 (4) | Mn4—Al5—Al11$^{iii}$ | 57.04 (3) |
| Al11$^{v}$—Ni1—Al13$^{vi}$ | 98.53 (4) | Mn4$^{xiv}$—Al5—Al11$^{iii}$ | 107.38 (6) |
| Al7A$^{vi}$—Ni1—Al13$^{vi}$ | 59.81 (5) | Al12$^{xxiii}$—Al5—Al11$^{iii}$ | 58.17 (4) |
| Al9—Ni1—Al13$^{vi}$ | 113.34 (4) | Al12$^{xxiv}$—Al5—Al11$^{iii}$ | 107.35 (6) |
| Al9$^{vii}$—Ni1—Al13$^{vi}$ | 160.69 (5) | Mn3$^{xxiii}$—Al5—Al11$^{iii}$ | 61.09 (4) |
| Al13$^{viii}$—Ni1—Al13$^{vi}$ | 63.74 (6) | Al11$^{iv}$—Al5—Al11$^{iii}$ | 110.89 (7) |
| Al8$^{ix}$—Mn1—Al8$^{x}$ | 115.05 (12) | Al4—Al5—Al1 | 103.14 (8) |
| Al8$^{ix}$—Mn1—Al6$^{xi}$ | 66.07 (5) | Al12$^{iii}$—Al5—Al1 | 62.86 (4) |
| Al8$^{x}$—Mn1—Al6$^{xi}$ | 66.07 (5) | Al12$^{iv}$—Al5—Al1 | 62.86 (4) |
| Al8$^{ix}$—Mn1—Al6$^{xii}$ | 66.07 (5) | Mn4—Al5—Al1 | 57.71 (5) |
| Al8$^{x}$—Mn1—Al6$^{xii}$ | 66.07 (5) | Mn4$^{xiv}$—Al5—Al1 | 57.71 (5) |
| Al6$^{xi}$—Mn1—Al6$^{xii}$ | 81.85 (9) | Al12$^{xxiii}$—Al5—Al1 | 142.53 (5) |
| Al8$^{ix}$—Mn1—Al4 | 118.28 (5) | Al12$^{xxiv}$—Al5—Al1 | 142.53 (5) |
| Al8$^{x}$—Mn1—Al4 | 118.28 (5) | Mn3$^{xxiii}$—Al5—Al1 | 158.50 (8) |
| Al6$^{xi}$—Mn1—Al4 | 167.13 (6) | Al11$^{iv}$—Al5—Al1 | 109.95 (5) |
| Al6$^{xii}$—Mn1—Al4 | 111.02 (5) | Al11$^{iii}$—Al5—Al1 | 109.95 (5) |
| Al8$^{ix}$—Mn1—Al4$^{xiii}$ | 118.28 (5) | Mn3—Al6—Mn1$^{xii}$ | 157.26 (8) |
| Al8$^{x}$—Mn1—Al4$^{xiii}$ | 118.28 (5) | Mn3—Al6—Al8$^{xxv}$ | 113.33 (6) |
| Al6$^{xi}$—Mn1—Al4$^{xiii}$ | 111.02 (5) | Mn1$^{xii}$—Al6—Al8$^{xxv}$ | 55.75 (5) |
| Al6$^{xii}$—Mn1—Al4$^{xiii}$ | 167.13 (6) | Mn3—Al6—Al8$^{xxvi}$ | 113.33 (6) |
| Al4—Mn1—Al4$^{xiii}$ | 56.11 (7) | Mn1$^{xii}$—Al6—Al8$^{xxvi}$ | 55.75 (5) |
| Al8$^{ix}$—Mn1—Al10$^{xiv}$ | 67.33 (3) | Al8$^{xxv}$—Al6—Al8$^{xxvi}$ | 99.45 (9) |
| Al8$^{x}$—Mn1—Al10$^{xiv}$ | 120.48 (3) | Mn3—Al6—Al10$^{xii}$ | 134.52 (6) |
| Al6$^{xi}$—Mn1—Al10$^{xiv}$ | 62.28 (4) | Mn1$^{xii}$—Al6—Al10$^{xii}$ | 62.46 (4) |
| Al6$^{xii}$—Mn1—Al10$^{xiv}$ | 129.53 (5) | Al8$^{xxv}$—Al6—Al10$^{xii}$ | 111.74 (7) |
| Al4—Mn1—Al10$^{xiv}$ | 107.18 (5) | Al8$^{xxvi}$—Al6—Al10$^{xii}$ | 64.00 (5) |
| Al4$^{xiii}$—Mn1—Al10$^{xiv}$ | 60.29 (4) | Mn3—Al6—Al10$^{xxvii}$ | 134.52 (6) |
| Al8$^{ix}$—Mn1—Al10$^{v}$ | 67.33 (3) | Mn1$^{xii}$—Al6—Al10$^{xxvii}$ | 62.46 (4) |
| Al8$^{x}$—Mn1—Al10$^{v}$ | 120.48 (3) | Al8$^{xxv}$—Al6—Al10$^{xxvii}$ | 64.00 (5) |
| Al6$^{xi}$—Mn1—Al10$^{v}$ | 129.53 (5) | Al8$^{xxvi}$—Al6—Al10$^{xxvii}$ | 111.74 (7) |
| Al6$^{xii}$—Mn1—Al10$^{v}$ | 62.28 (4) | Al10$^{xii}$—Al6—Al10$^{xxvii}$ | 64.01 (6) |
| Al4—Mn1—Al10$^{v}$ | 60.29 (4) | Mn3—Al6—Al10$^{viii}$ | 67.07 (5) |
| Al4$^{xiii}$—Mn1—Al10$^{v}$ | 107.18 (5) | Mn1$^{xii}$—Al6—Al10$^{viii}$ | 130.58 (6) |
| Al10$^{xiv}$—Mn1—Al10$^{v}$ | 114.48 (5) | Al8$^{xxv}$—Al6—Al10$^{viii}$ | 160.60 (7) |
| Al8$^{ix}$—Mn1—Al10$^{xiii}$ | 120.48 (3) | Al8$^{xxvi}$—Al6—Al10$^{viii}$ | 97.78 (4) |
| Al8$^{x}$—Mn1—Al10$^{xiii}$ | 67.33 (3) | Al10$^{xii}$—Al6—Al10$^{viii}$ | 68.47 (6) |
| Al6$^{xi}$—Mn1—Al10$^{xiii}$ | 62.28 (4) | Al10$^{xxvii}$—Al6—Al10$^{viii}$ | 101.20 (7) |
| Al6$^{xii}$—Mn1—Al10$^{xiii}$ | 129.53 (5) | Mn3—Al6—Al10$^{vi}$ | 67.07 (5) |

| | | | |
|---|---|---|---|
| Al4—Mn1—Al10$^{xiii}$ | 107.18 (5) | Mn1$^{xii}$—Al6—Al10$^{vi}$ | 130.58 (6) |
| Al4$^{xiii}$—Mn1—Al10$^{xiii}$ | 60.29 (4) | Al8$^{xxv}$—Al6—Al10$^{vi}$ | 97.78 (4) |
| Al10$^{xiv}$—Mn1—Al10$^{xiii}$ | 63.89 (5) | Al8$^{xxvi}$—Al6—Al10$^{vi}$ | 160.60 (7) |
| Al10$^{v}$—Mn1—Al10$^{xiii}$ | 166.98 (7) | Al10$^{xii}$—Al6—Al10$^{vi}$ | 101.20 (7) |
| Al8$^{ix}$—Mn1—Al10 | 120.48 (3) | Al10$^{xxvii}$—Al6—Al10$^{vi}$ | 68.47 (6) |
| Al8$^{x}$—Mn1—Al10 | 67.33 (3) | Al10$^{viii}$—Al6—Al10$^{vi}$ | 63.92 (6) |
| Al6$^{xi}$—Mn1—Al10 | 129.54 (5) | Mn3—Al6—Al3 | 54.21 (5) |
| Al6$^{xii}$—Mn1—Al10 | 62.28 (4) | Mn1$^{xii}$—Al6—Al3 | 103.05 (7) |
| Al4—Mn1—Al10 | 60.29 (4) | Al8$^{xxv}$—Al6—Al3 | 79.47 (6) |
| Al4$^{xiii}$—Mn1—Al10 | 107.18 (5) | Al8$^{xxvi}$—Al6—Al3 | 79.47 (6) |
| Al10$^{xiv}$—Mn1—Al10 | 166.98 (7) | Al10$^{xii}$—Al6—Al3 | 142.84 (5) |
| Al10$^{v}$—Mn1—Al10 | 63.89 (5) | Al10$^{xxvii}$—Al6—Al3 | 142.84 (5) |
| Al10$^{xiii}$—Mn1—Al10 | 114.48 (5) | Al10$^{viii}$—Al6—Al3 | 112.56 (6) |
| Al8$^{ix}$—Mn1—Al9$^{iii}$ | 179.56 (8) | Al10$^{vi}$—Al6—Al3 | 112.56 (6) |
| Al8$^{x}$—Mn1—Al9$^{iii}$ | 64.51 (6) | Mn3—Al6—Al13$^{iii}$ | 56.36 (4) |
| Al6$^{xi}$—Mn1—Al9$^{iii}$ | 113.63 (3) | Mn1$^{xii}$—Al6—Al13$^{iii}$ | 116.48 (5) |
| Al6$^{xii}$—Mn1—Al9$^{iii}$ | 113.63 (3) | Al8$^{xxv}$—Al6—Al13$^{iii}$ | 60.75 (5) |
| Al4—Mn1—Al9$^{iii}$ | 62.08 (4) | Al8$^{xxvi}$—Al6—Al13$^{iii}$ | 139.08 (8) |
| Al4$^{xiii}$—Mn1—Al9$^{iii}$ | 62.09 (4) | Al10$^{xii}$—Al6—Al13$^{iii}$ | 154.26 (6) |
| Al10$^{xiv}$—Mn1—Al9$^{iii}$ | 112.85 (4) | Al10$^{xxvii}$—Al6—Al13$^{iii}$ | 92.09 (4) |
| Al10$^{v}$—Mn1—Al9$^{iii}$ | 112.85 (4) | Al10$^{viii}$—Al6—Al13$^{iii}$ | 110.04 (7) |
| Al10$^{xiii}$—Mn1—Al9$^{iii}$ | 59.42 (3) | Al10$^{vi}$—Al6—Al13$^{iii}$ | 58.63 (4) |
| Al10—Mn1—Al9$^{iii}$ | 59.42 (3) | Al3—Al6—Al13$^{iii}$ | 62.59 (4) |
| Al8$^{ix}$—Mn1—Al9$^{xv}$ | 64.51 (6) | Mn3—Al6—Al13$^{iv}$ | 56.36 (4) |
| Al8$^{x}$—Mn1—Al9$^{xv}$ | 179.56 (8) | Mn1$^{xii}$—Al6—Al13$^{iv}$ | 116.48 (5) |
| Al6$^{xi}$—Mn1—Al9$^{xv}$ | 113.63 (3) | Al8$^{xxv}$—Al6—Al13$^{iv}$ | 139.08 (8) |
| Al6$^{xii}$—Mn1—Al9$^{xv}$ | 113.63 (3) | Al8$^{xxvi}$—Al6—Al13$^{iv}$ | 60.75 (5) |
| Al4—Mn1—Al9$^{xv}$ | 62.09 (4) | Al10$^{xii}$—Al6—Al13$^{iv}$ | 92.09 (4) |
| Al4$^{xiii}$—Mn1—Al9$^{xv}$ | 62.09 (4) | Al10$^{xxvii}$—Al6—Al13$^{iv}$ | 154.26 (6) |
| Al10$^{xiv}$—Mn1—Al9$^{xv}$ | 59.42 (3) | Al10$^{viii}$—Al6—Al13$^{iv}$ | 58.63 (4) |
| Al10$^{v}$—Mn1—Al9$^{xv}$ | 59.42 (3) | Al10$^{vi}$—Al6—Al13$^{iv}$ | 110.04 (7) |
| Al10$^{xiii}$—Mn1—Al9$^{xv}$ | 112.85 (4) | Al3—Al6—Al13$^{iv}$ | 62.59 (4) |
| Al10—Mn1—Al9$^{xv}$ | 112.85 (4) | Al13$^{iii}$—Al6—Al13$^{iv}$ | 109.24 (7) |
| Al9$^{iii}$—Mn1—Al9$^{xv}$ | 115.92 (8) | Al7A$^{xxviii}$—Al7A—Ni1$^{ii}$ | 65.38 (9) |
| Al8$^{xvi}$—Mn2—Al8$^{xii}$ | 95.71 (13) | Al7A$^{xxviii}$—Al7A—Mn2 | 158.53 (16) |
| Al8$^{xvi}$—Mn2—Al13$^{xiv}$ | 131.32 (5) | Ni1$^{ii}$—Al7A—Mn2 | 136.09 (12) |
| Al8$^{xii}$—Mn2—Al13$^{xiv}$ | 75.18 (5) | Al7A$^{xxviii}$—Al7A—Al8$^{xii}$ | 135.57 (7) |
| Al8$^{xvi}$—Mn2—Al13$^{xiii}$ | 75.18 (5) | Ni1$^{ii}$—Al7A—Al8$^{xii}$ | 95.36 (8) |
| Al8$^{xii}$—Mn2—Al13$^{xiii}$ | 131.32 (5) | Mn2—Al7A—Al8$^{xii}$ | 54.39 (7) |
| Al13$^{xiv}$—Mn2—Al13$^{xiii}$ | 76.30 (7) | Al7A$^{xxviii}$—Al7A—Al8$^{xvi}$ | 135.57 (7) |
| Al8$^{xvi}$—Mn2—Al13$^{v}$ | 131.32 (5) | Ni1$^{ii}$—Al7A—Al8$^{xvi}$ | 95.36 (8) |
| Al8$^{xii}$—Mn2—Al13$^{v}$ | 75.18 (5) | Mn2—Al7A—Al8$^{xvi}$ | 54.39 (7) |
| Al13$^{xiv}$—Mn2—Al13$^{v}$ | 93.17 (7) | Al8$^{xii}$—Al7A—Al8$^{xvi}$ | 83.07 (11) |
| Al13$^{xiii}$—Mn2—Al13$^{v}$ | 144.92 (10) | Al7A$^{xxviii}$—Al7A—Ni1$^{xxiii}$ | 57.79 (10) |
| Al8$^{xvi}$—Mn2—Al13 | 75.18 (5) | Ni1$^{ii}$—Al7A—Ni1$^{xxiii}$ | 123.17 (10) |
| Al8$^{xii}$—Mn2—Al13 | 131.32 (5) | Mn2—Al7A—Ni1$^{xxiii}$ | 100.74 (8) |
| Al13$^{xiv}$—Mn2—Al13 | 144.91 (10) | Al8$^{xii}$—Al7A—Ni1$^{xxiii}$ | 124.80 (8) |
| Al13$^{xiii}$—Mn2—Al13 | 93.16 (7) | Al8$^{xvi}$—Al7A—Ni1$^{xxiii}$ | 124.80 (8) |

| | | | |
|---|---|---|---|
| Al13$^{v}$—Mn2—Al13 | 76.30 (7) | Al7A$^{xxviii}$—Al7A—Al13$^{v}$ | 109.59 (12) |
| Al8$^{xvi}$—Mn2—Al7A$^{xiii}$ | 65.38 (5) | Ni1$^{ii}$—Al7A—Al13$^{v}$ | 147.49 (4) |
| Al8$^{xii}$—Mn2—Al7A$^{xiii}$ | 65.38 (5) | Mn2—Al7A—Al13$^{v}$ | 53.47 (6) |
| Al13$^{xiv}$—Mn2—Al7A$^{xiii}$ | 67.53 (5) | Al8$^{xii}$—Al7A—Al13$^{v}$ | 65.06 (7) |
| Al13$^{xiii}$—Mn2—Al7A$^{xiii}$ | 67.53 (5) | Al8$^{xvi}$—Al7A—Al13$^{v}$ | 106.89 (10) |
| Al13$^{v}$—Mn2—Al7A$^{xiii}$ | 139.16 (5) | Ni1$^{xxiii}$—Al7A—Al13$^{v}$ | 61.56 (6) |
| Al13—Mn2—Al7A$^{xiii}$ | 139.16 (5) | Al7A$^{xxviii}$—Al7A—Al13 | 109.59 (12) |
| Al8$^{xvi}$—Mn2—Al7A | 65.38 (6) | Ni1$^{ii}$—Al7A—Al13 | 147.49 (4) |
| Al8$^{xii}$—Mn2—Al7A | 65.38 (5) | Mn2—Al7A—Al13 | 53.47 (6) |
| Al13$^{xiv}$—Mn2—Al7A | 139.16 (5) | Al8$^{xii}$—Al7A—Al13 | 106.89 (10) |
| Al13$^{xiii}$—Mn2—Al7A | 139.16 (5) | Al8$^{xvi}$—Al7A—Al13 | 65.06 (7) |
| Al13$^{v}$—Mn2—Al7A | 67.53 (5) | Ni1$^{xxiii}$—Al7A—Al13 | 61.56 (6) |
| Al13—Mn2—Al7A | 67.53 (5) | Al13$^{v}$—Al7A—Al13 | 64.98 (7) |
| Al7A$^{xiii}$—Mn2—Al7A | 103.23 (13) | Al7A$^{xxviii}$—Al7A—Al10$^{xxix}$ | 73.80 (7) |
| Al8$^{xvi}$—Mn2—Al1 | 132.14 (7) | Ni1$^{ii}$—Al7A—Al10$^{xxix}$ | 54.58 (4) |
| Al8$^{xii}$—Mn2—Al1 | 132.14 (7) | Mn2—Al7A—Al10$^{xxix}$ | 116.50 (6) |
| Al13$^{xiv}$—Mn2—Al1 | 72.46 (5) | Al8$^{xii}$—Al7A—Al10$^{xxix}$ | 128.64 (11) |
| Al13$^{xiii}$—Mn2—Al1 | 72.46 (5) | Al8$^{xvi}$—Al7A—Al10$^{xxix}$ | 62.94 (5) |
| Al13$^{v}$—Mn2—Al1 | 72.46 (5) | Ni1$^{xxiii}$—Al7A—Al10$^{xxix}$ | 106.41 (7) |
| Al13—Mn2—Al1 | 72.46 (5) | Al13$^{v}$—Al7A—Al10$^{xxix}$ | 157.69 (7) |
| Al7A$^{xiii}$—Mn2—Al1 | 128.38 (6) | Al13—Al7A—Al10$^{xxix}$ | 92.91 (4) |
| Al7A—Mn2—Al1 | 128.38 (6) | Al7A$^{xxviii}$—Al7A—Al10$^{xxvi}$ | 73.80 (7) |
| Al3—Mn3—Al12$^{v}$ | 71.11 (6) | Ni1$^{ii}$—Al7A—Al10$^{xxvi}$ | 54.58 (4) |
| Al3—Mn3—Al12 | 71.11 (6) | Mn2—Al7A—Al10$^{xxvi}$ | 116.50 (6) |
| Al12$^{v}$—Mn3—Al12 | 69.36 (6) | Al8$^{xii}$—Al7A—Al10$^{xxvi}$ | 62.94 (5) |
| Al3—Mn3—Al6 | 69.22 (7) | Al8$^{xvi}$—Al7A—Al10$^{xxvi}$ | 128.64 (11) |
| Al12$^{v}$—Mn3—Al6 | 126.30 (5) | Ni1$^{xxiii}$—Al7A—Al10$^{xxvi}$ | 106.41 (7) |
| Al12—Mn3—Al6 | 126.30 (5) | Al13$^{v}$—Al7A—Al10$^{xxvi}$ | 92.91 (4) |
| Al3—Mn3—Al4$^{vi}$ | 177.36 (8) | Al13—Al7A—Al10$^{xxvi}$ | 157.69 (7) |
| Al12$^{v}$—Mn3—Al4$^{vi}$ | 110.99 (5) | Al10$^{xxix}$—Al7A—Al10$^{xxvi}$ | 108.96 (8) |
| Al12—Mn3—Al4$^{vi}$ | 110.99 (5) | Ni1$^{xxxvii}$—Al7B—Ni1$^{xxxiii}$ | 180.00 (4) |
| Al6—Mn3—Al4$^{vi}$ | 108.13 (6) | Ni1$^{xxxvii}$—Al7B—Al10$^{xxx}$ | 57.62 (2) |
| Al3—Mn3—Al13$^{iv}$ | 72.43 (4) | Ni1$^{xxxiii}$—Al7B—Al10$^{xxx}$ | 122.38 (2) |
| Al12$^{v}$—Mn3—Al13$^{iv}$ | 65.12 (4) | Ni1$^{xxxvii}$—Al7B—Al10$^{xxxi}$ | 122.38 (2) |
| Al12—Mn3—Al13$^{iv}$ | 128.48 (5) | Ni1$^{xxxiii}$—Al7B—Al10$^{xxxi}$ | 57.62 (2) |
| Al6—Mn3—Al13$^{iv}$ | 69.36 (3) | Al10$^{xxx}$—Al7B—Al10$^{xxxi}$ | 180.00 (6) |
| Al4$^{vi}$—Mn3—Al13$^{iv}$ | 106.82 (4) | Ni1$^{xxxvii}$—Al7B—Al10$^{xxxii}$ | 57.62 (2) |
| Al3—Mn3—Al13$^{iii}$ | 72.43 (4) | Ni1$^{xxxiii}$—Al7B—Al10$^{xxxii}$ | 122.38 (2) |
| Al12$^{v}$—Mn3—Al13$^{iii}$ | 128.48 (5) | Al10$^{xxx}$—Al7B—Al10$^{xxxii}$ | 113.96 (5) |
| Al12—Mn3—Al13$^{iii}$ | 65.12 (4) | Al10$^{xxxi}$—Al7B—Al10$^{xxxii}$ | 66.04 (5) |
| Al6—Mn3—Al13$^{iii}$ | 69.36 (3) | Ni1$^{xxxvii}$—Al7B—Al10$^{x}$ | 122.38 (2) |
| Al4$^{vi}$—Mn3—Al13$^{iii}$ | 106.82 (4) | Ni1$^{xxxiii}$—Al7B—Al10$^{x}$ | 57.62 (2) |
| Al13$^{iv}$—Mn3—Al13$^{iii}$ | 132.84 (7) | Al10$^{xxx}$—Al7B—Al10$^{x}$ | 66.04 (5) |
| Al3—Mn3—Al5$^{vi}$ | 124.43 (8) | Al10$^{xxxi}$—Al7B—Al10$^{x}$ | 113.96 (5) |
| Al12$^{v}$—Mn3—Al5$^{vi}$ | 63.87 (4) | Al10$^{xxxii}$—Al7B—Al10$^{x}$ | 180.00 (6) |
| Al12—Mn3—Al5$^{vi}$ | 63.87 (4) | Mn2$^{xii}$—Al8—Mn1$^{x}$ | 170.33 (12) |
| Al6—Mn3—Al5$^{vi}$ | 166.34 (6) | Mn2$^{xii}$—Al8—Al7A$^{xii}$ | 60.24 (7) |
| Al4$^{vi}$—Mn3—Al5$^{vi}$ | 58.21 (5) | Mn1$^{x}$—Al8—Al7A$^{xii}$ | 124.28 (6) |

| | | | |
|---|---|---|---|
| Al13$^{iv}$—Mn3—Al5$^{vi}$ | 112.78 (3) | Mn2$^{xii}$—Al8—Al7A$^{xxxviii}$ | 60.24 (7) |
| Al13$^{iii}$—Mn3—Al5$^{vi}$ | 112.78 (3) | Mn1$^{x}$—Al8—Al7A$^{xxxviii}$ | 124.28 (6) |
| Al3—Mn3—Al11$^{xvii}$ | 121.85 (3) | Al7A$^{xii}$—Al8—Al7A$^{xxxviii}$ | 96.93 (11) |
| Al12$^{v}$—Mn3—Al11$^{xvii}$ | 61.18 (4) | Mn2$^{xii}$—Al8—Al6$^{xxxix}$ | 114.85 (7) |
| Al12—Mn3—Al11$^{xvii}$ | 116.13 (5) | Mn1$^{x}$—Al8—Al6$^{xxxix}$ | 58.18 (6) |
| Al6—Mn3—Al11$^{xvii}$ | 115.10 (3) | Al7A$^{xii}$—Al8—Al6$^{xxxix}$ | 163.78 (10) |
| Al4$^{vi}$—Mn3—Al11$^{xvii}$ | 58.97 (3) | Al7A$^{xxxviii}$—Al8—Al6$^{xxxix}$ | 92.78 (5) |
| Al13$^{iv}$—Mn3—Al11$^{xvii}$ | 58.86 (4) | Mn2$^{xii}$—Al8—Al6$^{xl}$ | 114.85 (7) |
| Al13$^{iii}$—Mn3—Al11$^{xvii}$ | 165.67 (5) | Mn1$^{x}$—Al8—Al6$^{xl}$ | 58.18 (6) |
| Al5$^{vi}$—Mn3—Al11$^{xvii}$ | 59.51 (3) | Al7A$^{xii}$—Al8—Al6$^{xl}$ | 92.78 (5) |
| Al3—Mn3—Al11$^{xviii}$ | 121.85 (3) | Al7A$^{xxxviii}$—Al8—Al6$^{xl}$ | 163.78 (10) |
| Al12$^{v}$—Mn3—Al11$^{xviii}$ | 116.14 (5) | Al6$^{xxxix}$—Al8—Al6$^{xl}$ | 75.03 (9) |
| Al12—Mn3—Al11$^{xviii}$ | 61.18 (4) | Mn2$^{xii}$—Al8—Al9$^{xxxiii}$ | 125.60 (11) |
| Al6—Mn3—Al11$^{xviii}$ | 115.10 (3) | Mn1$^{x}$—Al8—Al9$^{xxxiii}$ | 64.07 (6) |
| Al4$^{vi}$—Mn3—Al11$^{xviii}$ | 58.97 (3) | Al7A$^{xii}$—Al8—Al9$^{xxxiii}$ | 86.07 (8) |
| Al13$^{iv}$—Mn3—Al11$^{xviii}$ | 165.67 (5) | Al7A$^{xxxviii}$—Al8—Al9$^{xxxiii}$ | 86.07 (8) |
| Al13$^{iii}$—Mn3—Al11$^{xviii}$ | 58.86 (4) | Al6$^{xxxix}$—Al8—Al9$^{xxxiii}$ | 107.60 (7) |
| Al5$^{vi}$—Mn3—Al11$^{xviii}$ | 59.51 (3) | Al6$^{xl}$—Al8—Al9$^{xxxiii}$ | 107.60 (7) |
| Al11$^{xvii}$—Mn3—Al11$^{xviii}$ | 108.34 (5) | Mn2$^{xii}$—Al8—Al13$^{xxxiv}$ | 52.45 (5) |
| Al3—Mn3—Al10$^{viii}$ | 119.02 (6) | Mn1$^{x}$—Al8—Al13$^{xxxiv}$ | 120.86 (8) |
| Al12$^{v}$—Mn3—Al10$^{viii}$ | 114.67 (4) | Al7A$^{xii}$—Al8—Al13$^{xxxiv}$ | 111.92 (9) |
| Al12—Mn3—Al10$^{viii}$ | 169.66 (5) | Al7A$^{xxxviii}$—Al8—Al13$^{xxxiv}$ | 58.77 (6) |
| Al6—Mn3—Al10$^{viii}$ | 59.98 (4) | Al6$^{xxxix}$—Al8—Al13$^{xxxiv}$ | 62.71 (5) |
| Al4$^{vi}$—Mn3—Al10$^{viii}$ | 58.82 (4) | Al6$^{xl}$—Al8—Al13$^{xxxiv}$ | 105.48 (9) |
| Al13$^{iv}$—Mn3—Al10$^{viii}$ | 60.10 (4) | Al9$^{xxxiii}$—Al8—Al13$^{xxxiv}$ | 141.28 (5) |
| Al13$^{iii}$—Mn3—Al10$^{viii}$ | 114.44 (5) | Mn2$^{xii}$—Al8—Al13$^{xxvii}$ | 52.45 (5) |
| Al5$^{vi}$—Mn3—Al10$^{viii}$ | 108.59 (4) | Mn1$^{x}$—Al8—Al13$^{xxvii}$ | 120.86 (8) |
| Al11$^{xvii}$—Mn3—Al10$^{viii}$ | 61.50 (3) | Al7A$^{xii}$—Al8—Al13$^{xxvii}$ | 58.77 (6) |
| Al11$^{xviii}$—Mn3—Al10$^{viii}$ | 109.26 (4) | Al7A$^{xxxviii}$—Al8—Al13$^{xxvii}$ | 111.92 (9) |
| Al3—Mn3—Al10$^{vi}$ | 119.02 (6) | Al6$^{xxxix}$—Al8—Al13$^{xxvii}$ | 105.48 (9) |
| Al12$^{v}$—Mn3—Al10$^{vi}$ | 169.66 (5) | Al6$^{xl}$—Al8—Al13$^{xxvii}$ | 62.71 (5) |
| Al12—Mn3—Al10$^{vi}$ | 114.67 (4) | Al9$^{xxxiii}$—Al8—Al13$^{xxvii}$ | 141.28 (5) |
| Al6—Mn3—Al10$^{vi}$ | 59.98 (4) | Al13$^{xxxiv}$—Al8—Al13$^{xxvii}$ | 73.12 (7) |
| Al4$^{vi}$—Mn3—Al10$^{vi}$ | 58.82 (4) | Mn2$^{xii}$—Al8—Al10$^{x}$ | 122.79 (6) |
| Al13$^{iv}$—Mn3—Al10$^{vi}$ | 114.44 (5) | Mn1$^{x}$—Al8—Al10$^{x}$ | 60.78 (5) |
| Al13$^{iii}$—Mn3—Al10$^{vi}$ | 60.10 (4) | Al7A$^{xii}$—Al8—Al10$^{x}$ | 63.50 (5) |
| Al5$^{vi}$—Mn3—Al10$^{vi}$ | 108.59 (4) | Al7A$^{xxxviii}$—Al8—Al10$^{x}$ | 138.12 (11) |
| Al11$^{xvii}$—Mn3—Al10$^{vi}$ | 109.26 (4) | Al6$^{xxxix}$—Al8—Al10$^{x}$ | 116.10 (9) |
| Al11$^{xviii}$—Mn3—Al10$^{vi}$ | 61.50 (3) | Al6$^{xl}$—Al8—Al10$^{x}$ | 58.07 (5) |
| Al10$^{viii}$—Mn3—Al10$^{vi}$ | 59.69 (5) | Al9$^{xxxiii}$—Al8—Al10$^{x}$ | 57.55 (4) |
| Al2$^{iii}$—Mn4—Al12$^{iii}$ | 70.30 (6) | Al13$^{xxxiv}$—Al8—Al10$^{x}$ | 161.13 (8) |
| Al2$^{iii}$—Mn4—Al12$^{xix}$ | 70.30 (6) | Al13$^{xxvii}$—Al8—Al10$^{x}$ | 89.92 (4) |
| Al12$^{iii}$—Mn4—Al12$^{xix}$ | 77.24 (6) | Mn2$^{xii}$—Al8—Al10$^{xxxv}$ | 122.79 (6) |
| Al2$^{iii}$—Mn4—Al4 | 119.16 (6) | Mn1$^{x}$—Al8—Al10$^{xxxv}$ | 60.78 (5) |
| Al12$^{iii}$—Mn4—Al4 | 112.57 (5) | Al7A$^{xii}$—Al8—Al10$^{xxxv}$ | 138.12 (11) |
| Al12$^{xix}$—Mn4—Al4 | 167.76 (5) | Al7A$^{xxxviii}$—Al8—Al10$^{xxxv}$ | 63.50 (5) |
| Al2$^{iii}$—Mn4—Al4$^{xiii}$ | 119.16 (6) | Al6$^{xxxix}$—Al8—Al10$^{xxxv}$ | 58.07 (5) |
| Al12$^{iii}$—Mn4—Al4$^{xiii}$ | 167.76 (5) | Al6$^{xl}$—Al8—Al10$^{xxxv}$ | 116.10 (9) |

| | | | |
|---|---|---|---|
| Al12$^{xix}$—Mn4—Al4$^{xiii}$ | 112.57 (5) | Al9$^{xxxiii}$—Al8—Al10$^{xxxv}$ | 57.55 (4) |
| Al4—Mn4—Al4$^{xiii}$ | 56.78 (7) | Al13$^{xxxiv}$—Al8—Al10$^{xxxv}$ | 89.92 (4) |
| Al2$^{iii}$—Mn4—Al11$^{xix}$ | 67.93 (4) | Al13$^{xxvii}$—Al8—Al10$^{xxxv}$ | 161.13 (8) |
| Al12$^{iii}$—Mn4—Al11$^{xix}$ | 130.89 (5) | Al10$^{x}$—Al8—Al10$^{xxxv}$ | 105.39 (8) |
| Al12$^{xix}$—Mn4—Al11$^{xix}$ | 65.30 (4) | Ni1—Al9—Ni1$^{xx}$ | 114.80 (7) |
| Al4—Mn4—Al11$^{xix}$ | 109.69 (5) | Ni1—Al9—Al10$^{xxi}$ | 144.85 (7) |
| Al4$^{xiii}$—Mn4—Al11$^{xix}$ | 61.32 (4) | Ni1$^{xx}$—Al9—Al10$^{xxi}$ | 54.20 (3) |
| Al2$^{iii}$—Mn4—Al11$^{iii}$ | 67.93 (4) | Ni1—Al9—Al10$^{iii}$ | 54.20 (3) |
| Al12$^{iii}$—Mn4—Al11$^{iii}$ | 65.30 (4) | Ni1$^{xx}$—Al9—Al10$^{iii}$ | 144.85 (7) |
| Al12$^{xix}$—Mn4—Al11$^{iii}$ | 130.89 (5) | Al10$^{xxi}$—Al9—Al10$^{iii}$ | 112.70 (8) |
| Al4—Mn4—Al11$^{iii}$ | 61.32 (4) | Ni1—Al9—Al9$^{vii}$ | 58.77 (3) |
| Al4$^{xiii}$—Mn4—Al11$^{iii}$ | 109.69 (5) | Ni1$^{xx}$—Al9—Al9$^{vii}$ | 58.77 (3) |
| Al11$^{xix}$—Mn4—Al11$^{iii}$ | 118.44 (6) | Al10$^{xxi}$—Al9—Al9$^{vii}$ | 110.28 (4) |
| Al2$^{iii}$—Mn4—Al1 | 125.73 (7) | Al10$^{iii}$—Al9—Al9$^{vii}$ | 110.28 (4) |
| Al12$^{iii}$—Mn4—Al1 | 67.95 (4) | Ni1—Al9—Mn4$^{iii}$ | 108.60 (4) |
| Al12$^{xix}$—Mn4—Al1 | 67.95 (4) | Ni1$^{xx}$—Al9—Mn4$^{iii}$ | 108.60 (4) |
| Al4—Mn4—Al1 | 108.06 (4) | Al10$^{xxi}$—Al9—Mn4$^{iii}$ | 106.47 (5) |
| Al4$^{xiii}$—Mn4—Al1 | 108.06 (4) | Al10$^{iii}$—Al9—Mn4$^{iii}$ | 106.47 (5) |
| Al11$^{xix}$—Mn4—Al1 | 120.10 (3) | Al9$^{vii}$—Al9—Mn4$^{iii}$ | 110.52 (4) |
| Al11$^{iii}$—Mn4—Al1 | 120.10 (3) | Ni1—Al9—Al11 | 53.63 (3) |
| Al2$^{iii}$—Mn4—Al5 | 121.80 (3) | Ni1$^{xx}$—Al9—Al11 | 141.43 (7) |
| Al12$^{iii}$—Mn4—Al5 | 62.05 (4) | Al10$^{xxi}$—Al9—Al11 | 157.30 (8) |
| Al12$^{xix}$—Mn4—Al5 | 124.60 (5) | Al10$^{iii}$—Al9—Al11 | 64.15 (3) |
| Al4—Mn4—Al5 | 58.77 (5) | Al9$^{vii}$—Al9—Al11 | 91.08 (4) |
| Al4$^{xiii}$—Mn4—Al5 | 105.73 (4) | Mn4$^{iii}$—Al9—Al11 | 56.79 (4) |
| Al11$^{xix}$—Mn4—Al5 | 167.00 (5) | Ni1—Al9—Al11$^{xx}$ | 141.43 (7) |
| Al11$^{iii}$—Mn4—Al5 | 63.11 (4) | Ni1$^{xx}$—Al9—Al11$^{xx}$ | 53.63 (3) |
| Al1—Mn4—Al5 | 62.93 (4) | Al10$^{xxi}$—Al9—Al11$^{xx}$ | 64.16 (3) |
| Al2$^{iii}$—Mn4—Al5$^{xiii}$ | 121.80 (3) | Al10$^{iii}$—Al9—Al11$^{xx}$ | 157.30 (8) |
| Al12$^{iii}$—Mn4—Al5$^{xiii}$ | 124.60 (5) | Al9$^{vii}$—Al9—Al11$^{xx}$ | 91.08 (4) |
| Al12$^{xix}$—Mn4—Al5$^{xiii}$ | 62.05 (4) | Mn4$^{iii}$—Al9—Al11$^{xx}$ | 56.79 (4) |
| Al4—Mn4—Al5$^{xiii}$ | 105.73 (4) | Al11—Al9—Al11$^{xx}$ | 109.37 (7) |
| Al4$^{xiii}$—Mn4—Al5$^{xiii}$ | 58.77 (5) | Ni1—Al9—Al4$^{xxi}$ | 148.57 (6) |
| Al11$^{xix}$—Mn4—Al5$^{xiii}$ | 63.11 (4) | Ni1$^{xx}$—Al9—Al4$^{xxi}$ | 96.50 (4) |
| Al11$^{iii}$—Mn4—Al5$^{xiii}$ | 167.00 (5) | Al10$^{xxi}$—Al9—Al4$^{xxi}$ | 57.76 (5) |
| Al1—Mn4—Al5$^{xiii}$ | 62.93 (4) | Al10$^{iii}$—Al9—Al4$^{xxi}$ | 101.40 (7) |
| Al5—Mn4—Al5$^{xiii}$ | 112.26 (5) | Al9$^{vii}$—Al9—Al4$^{xxi}$ | 148.15 (4) |
| Al2$^{iii}$—Mn4—Al9$^{iii}$ | 65.12 (7) | Mn4$^{iii}$—Al9—Al4$^{xxi}$ | 55.13 (5) |
| Al12$^{iii}$—Mn4—Al9$^{iii}$ | 119.85 (5) | Al11—Al9—Al4$^{xxi}$ | 99.98 (7) |
| Al12$^{xix}$—Mn4—Al9$^{iii}$ | 119.85 (5) | Al11$^{xx}$—Al9—Al4$^{xxi}$ | 57.08 (4) |
| Al4—Mn4—Al9$^{iii}$ | 62.64 (4) | Ni1—Al9—Al4$^{iii}$ | 96.50 (4) |
| Al4$^{xiii}$—Mn4—Al9$^{iii}$ | 62.64 (4) | Ni1$^{xx}$—Al9—Al4$^{iii}$ | 148.57 (6) |
| Al11$^{xix}$—Mn4—Al9$^{iii}$ | 61.75 (3) | Al10$^{xxi}$—Al9—Al4$^{iii}$ | 101.40 (7) |
| Al11$^{iii}$—Mn4—Al9$^{iii}$ | 61.75 (3) | Al10$^{iii}$—Al9—Al4$^{iii}$ | 57.76 (5) |
| Al1—Mn4—Al9$^{iii}$ | 169.14 (6) | Al9$^{vii}$—Al9—Al4$^{iii}$ | 148.15 (4) |
| Al5—Mn4—Al9$^{iii}$ | 112.73 (4) | Mn4$^{iii}$—Al9—Al4$^{iii}$ | 55.13 (5) |
| Al5$^{xiii}$—Mn4—Al9$^{iii}$ | 112.73 (4) | Al11—Al9—Al4$^{iii}$ | 57.08 (4) |
| Al2$^{iii}$—Mn4—Mn4$^{xiv}$ | 175.64 (6) | Al11$^{xx}$—Al9—Al4$^{iii}$ | 99.98 (7) |

| | | | |
|---|---|---|---|
| Al12$^{iii}$—Mn4—Mn4$^{xiv}$ | 112.93 (3) | Al4$^{xxi}$—Al9—Al4$^{iii}$ | 52.11 (7) |
| Al12$^{xix}$—Mn4—Mn4$^{xiv}$ | 112.93 (3) | Ni1—Al9—Al2 | 82.51 (4) |
| Al4—Mn4—Mn4$^{xiv}$ | 57.21 (3) | Ni1$^{xx}$—Al9—Al2 | 82.51 (4) |
| Al4$^{xiii}$—Mn4—Mn4$^{xiv}$ | 57.21 (3) | Al10$^{xxi}$—Al9—Al2 | 123.19 (4) |
| Al11$^{xix}$—Mn4—Mn4$^{xiv}$ | 110.38 (3) | Al10$^{iii}$—Al9—Al2 | 123.19 (4) |
| Al11$^{iii}$—Mn4—Mn4$^{xiv}$ | 110.38 (3) | Al9$^{vii}$—Al9—Al2 | 60.21 (4) |
| Al1—Mn4—Mn4$^{xiv}$ | 58.63 (3) | Mn4$^{iii}$—Al9—Al2 | 50.30 (4) |
| Al5—Mn4—Mn4$^{xiv}$ | 59.23 (2) | Al11—Al9—Al2 | 60.52 (4) |
| Al5$^{xiii}$—Mn4—Mn4$^{xiv}$ | 59.23 (2) | Al11$^{xx}$—Al9—Al2 | 60.52 (4) |
| Al9$^{iii}$—Mn4—Mn4$^{xiv}$ | 110.52 (4) | Al4$^{xxi}$—Al9—Al2 | 99.67 (6) |
| Mn2—Al1—Mn4 | 148.62 (3) | Al4$^{iii}$—Al9—Al2 | 99.67 (6) |
| Mn2—Al1—Mn4$^{xiv}$ | 148.63 (3) | Ni1—Al9—Mn1$^{iii}$ | 111.21 (4) |
| Mn4—Al1—Mn4$^{xiv}$ | 62.75 (6) | Ni1$^{xx}$—Al9—Mn1$^{iii}$ | 111.21 (4) |
| Mn2—Al1—Al5 | 126.65 (5) | Al10$^{xxi}$—Al9—Mn1$^{iii}$ | 58.46 (4) |
| Mn4—Al1—Al5 | 59.36 (5) | Al10$^{iii}$—Al9—Mn1$^{iii}$ | 58.46 (4) |
| Mn4$^{xiv}$—Al1—Al5 | 59.36 (5) | Al9$^{vii}$—Al9—Mn1$^{iii}$ | 147.96 (4) |
| Mn2—Al1—Al5$^{xiii}$ | 126.65 (5) | Mn4$^{iii}$—Al9—Mn1$^{iii}$ | 101.52 (6) |
| Mn4—Al1—Al5$^{xiii}$ | 59.36 (5) | Al11—Al9—Mn1$^{iii}$ | 106.89 (5) |
| Mn4$^{xiv}$—Al1—Al5$^{xiii}$ | 59.36 (5) | Al11$^{xx}$—Al9—Mn1$^{iii}$ | 106.89 (5) |
| Al5—Al1—Al5$^{xiii}$ | 106.69 (10) | Al4$^{xxi}$—Al9—Mn1$^{iii}$ | 55.61 (5) |
| Mn2—Al1—Al12$^{xv}$ | 102.72 (5) | Al4$^{iii}$—Al9—Mn1$^{iii}$ | 55.61 (5) |
| Mn4—Al1—Al12$^{xv}$ | 103.75 (7) | Al2—Al9—Mn1$^{iii}$ | 151.82 (8) |
| Mn4$^{xiv}$—Al1—Al12$^{xv}$ | 52.13 (3) | Ni1$^{iii}$—Al10—Al4 | 105.45 (5) |
| Al5—Al1—Al12$^{xv}$ | 107.16 (6) | Ni1$^{iii}$—Al10—Al6$^{xii}$ | 139.58 (5) |
| Al5$^{xiii}$—Al1—Al12$^{xv}$ | 56.09 (3) | Al4—Al10—Al6$^{xii}$ | 103.57 (5) |
| Mn2—Al1—Al12$^{iii}$ | 102.72 (5) | Ni1$^{iii}$—Al10—Al6$^{xxiii}$ | 123.31 (5) |
| Mn4—Al1—Al12$^{iii}$ | 52.13 (3) | Al4—Al10—Al6$^{xxiii}$ | 98.33 (5) |
| Mn4$^{xiv}$—Al1—Al12$^{iii}$ | 103.75 (7) | Al6$^{xii}$—Al10—Al6$^{xxiii}$ | 78.80 (7) |
| Al5—Al1—Al12$^{iii}$ | 56.09 (3) | Ni1$^{iii}$—Al10—Mn1 | 122.22 (5) |
| Al5$^{xiii}$—Al1—Al12$^{iii}$ | 107.16 (6) | Al4—Al10—Mn1 | 58.18 (5) |
| Al12$^{xv}$—Al1—Al12$^{iii}$ | 154.55 (10) | Al6$^{xii}$—Al10—Mn1 | 55.26 (5) |
| Mn2—Al1—Al12$^{iv}$ | 102.72 (5) | Al6$^{xxiii}$—Al10—Mn1 | 114.14 (5) |
| Mn4—Al1—Al12$^{iv}$ | 103.75 (7) | Ni1$^{iii}$—Al10—Al9$^{iii}$ | 61.91 (5) |
| Mn4$^{xiv}$—Al1—Al12$^{iv}$ | 52.13 (3) | Al4—Al10—Al9$^{iii}$ | 62.38 (5) |
| Al5—Al1—Al12$^{iv}$ | 56.09 (3) | Al6$^{xii}$—Al10—Al9$^{iii}$ | 109.94 (6) |
| Al5$^{xiii}$—Al1—Al12$^{iv}$ | 107.16 (6) | Al6$^{xxiii}$—Al10—Al9$^{iii}$ | 159.88 (7) |
| Al12$^{xv}$—Al1—Al12$^{iv}$ | 64.22 (5) | Mn1—Al10—Al9$^{iii}$ | 62.12 (4) |
| Al12$^{iii}$—Al1—Al12$^{iv}$ | 109.74 (6) | Ni1$^{iii}$—Al10—Al13$^{xxxvi}$ | 62.42 (4) |
| Mn2—Al1—Al12$^{xix}$ | 102.72 (5) | Al4—Al10—Al13$^{xxxvi}$ | 98.14 (6) |
| Mn4—Al1—Al12$^{xix}$ | 52.13 (3) | Al6$^{xii}$—Al10—Al13$^{xxxvi}$ | 138.97 (6) |
| Mn4$^{xiv}$—Al1—Al12$^{xix}$ | 103.75 (7) | Al6$^{xxiii}$—Al10—Al13$^{xxxvi}$ | 63.76 (5) |
| Al5—Al1—Al12$^{xix}$ | 107.16 (6) | Mn1—Al10—Al13$^{xxxvi}$ | 156.23 (6) |
| Al5$^{xiii}$—Al1—Al12$^{xix}$ | 56.09 (3) | Al9$^{iii}$—Al10—Al13$^{xxxvi}$ | 110.94 (6) |
| Al12$^{xv}$—Al1—Al12$^{xix}$ | 109.74 (6) | Ni1$^{iii}$—Al10—Al7B$^{xli}$ | 49.75 (3) |
| Al12$^{iii}$—Al1—Al12$^{xix}$ | 64.22 (5) | Al4—Al10—Al7B$^{xli}$ | 155.17 (5) |
| Al12$^{iv}$—Al1—Al12$^{xix}$ | 154.55 (10) | Al6$^{xii}$—Al10—Al7B$^{xli}$ | 97.94 (4) |
| Mn2—Al1—Al13 | 49.10 (4) | Al6$^{xxiii}$—Al10—Al7B$^{xli}$ | 97.86 (4) |
| Mn4—Al1—Al13 | 107.71 (3) | Mn1—Al10—Al7B$^{xli}$ | 129.61 (5) |

| | | | |
|---|---|---|---|
| Mn4$^{xiv}$—Al1—Al13 | 144.48 (4) | Al9$^{iii}$—Al10—Al7B$^{xli}$ | 98.73 (5) |
| Al5—Al1—Al13 | 85.93 (4) | Al13$^{xxxvi}$—Al10—Al7B$^{xli}$ | 72.59 (4) |
| Al5$^{xiii}$—Al1—Al13 | 148.52 (3) | Ni1$^{iii}$—Al10—Al8$^{x}$ | 88.21 (6) |
| Al12$^{xv}$—Al1—Al13 | 148.29 (8) | Al4—Al10—Al8$^{x}$ | 103.25 (6) |
| Al12$^{iii}$—Al1—Al13 | 55.78 (3) | Al6$^{xii}$—Al10—Al8$^{x}$ | 57.93 (6) |
| Al12$^{iv}$—Al1—Al13 | 103.80 (4) | Al6$^{xxiii}$—Al10—Al8$^{x}$ | 134.91 (7) |
| Al12$^{xix}$—Al1—Al13 | 92.86 (4) | Mn1—Al10—Al8$^{x}$ | 51.89 (5) |
| Mn2—Al1—Al13$^{v}$ | 49.10 (4) | Al9$^{iii}$—Al10—Al8$^{x}$ | 60.42 (5) |
| Mn4—Al1—Al13$^{v}$ | 144.49 (4) | Al13$^{xxxvi}$—Al10—Al8$^{x}$ | 147.50 (8) |
| Mn4$^{xiv}$—Al1—Al13$^{v}$ | 107.71 (3) | Ni1$^{iii}$—Al10—Al10$^{v}$ | 161.38 (3) |
| Al5—Al1—Al13$^{v}$ | 85.93 (4) | Al4—Al10—Al10$^{v}$ | 57.62 (3) |
| Al5$^{xiii}$—Al1—Al13$^{v}$ | 148.52 (3) | Al6$^{xii}$—Al10—Al10$^{v}$ | 57.99 (3) |
| Al12$^{xv}$—Al1—Al13$^{v}$ | 92.86 (4) | Al6$^{xxiii}$—Al10—Al10$^{v}$ | 58.04 (3) |
| Al12$^{iii}$—Al1—Al13$^{v}$ | 103.80 (4) | Mn1—Al10—Al10$^{v}$ | 58.05 (3) |
| Al12$^{iv}$—Al1—Al13$^{v}$ | 55.79 (3) | Al9$^{iii}$—Al10—Al10$^{v}$ | 110.28 (4) |
| Al12$^{xix}$—Al1—Al13$^{v}$ | 148.29 (8) | Al13$^{xxxvi}$—Al10—Al10$^{v}$ | 109.46 (4) |
| Al13—Al1—Al13$^{v}$ | 58.63 (6) | Al8$^{x}$—Al10—Al10$^{v}$ | 102.64 (6) |
| Mn2—Al1—Al13$^{xiii}$ | 49.10 (4) | Ni1$^{iii}$—Al10—Al7A$^{xl}$ | 53.82 (5) |
| Mn4—Al1—Al13$^{xiii}$ | 107.71 (3) | Al4—Al10—Al7A$^{xl}$ | 144.61 (7) |
| Mn4$^{xiv}$—Al1—Al13$^{xiii}$ | 144.49 (4) | Al6$^{xii}$—Al10—Al7A$^{xl}$ | 86.56 (5) |
| Al5—Al1—Al13$^{xiii}$ | 148.52 (3) | Al6$^{xxiii}$—Al10—Al7A$^{xl}$ | 116.97 (7) |
| Al5$^{xiii}$—Al1—Al13$^{xiii}$ | 85.93 (4) | Mn1—Al10—Al7A$^{xl}$ | 105.45 (6) |
| Al12$^{xv}$—Al1—Al13$^{xiii}$ | 103.80 (4) | Al9$^{iii}$—Al10—Al7A$^{xl}$ | 82.25 (7) |
| Al12$^{iii}$—Al1—Al13$^{xiii}$ | 92.86 (4) | Al13$^{xxxvi}$—Al10—Al7A$^{xl}$ | 95.49 (6) |
| Al12$^{iv}$—Al1—Al13$^{xiii}$ | 148.29 (8) | Al8$^{x}$—Al10—Al7A$^{xl}$ | 53.56 (7) |
| Al12$^{xix}$—Al1—Al13$^{xiii}$ | 55.79 (3) | Al10$^{v}$—Al10—Al7A$^{xl}$ | 144.48 (4) |
| Al13—Al1—Al13$^{xiii}$ | 70.31 (7) | Ni1$^{iii}$—Al10—Mn3$^{xxiii}$ | 104.59 (4) |
| Al13$^{v}$—Al1—Al13$^{xiii}$ | 98.19 (9) | Al4—Al10—Mn3$^{xxiii}$ | 54.15 (4) |
| Mn4$^{xxii}$—Al2—Mn4$^{iii}$ | 171.29 (12) | Al6$^{xii}$—Al10—Mn3$^{xxiii}$ | 115.15 (5) |
| Mn4$^{xxii}$—Al2—Al12 | 117.15 (7) | Al6$^{xxiii}$—Al10—Mn3$^{xxiii}$ | 52.94 (4) |
| Mn4$^{iii}$—Al2—Al12 | 56.15 (4) | Mn1—Al10—Mn3$^{xxiii}$ | 104.50 (4) |
| Mn4$^{xxii}$—Al2—Al12$^{v}$ | 56.15 (4) | Al9$^{iii}$—Al10—Mn3$^{xxiii}$ | 107.56 (5) |
| Mn4$^{iii}$—Al2—Al12$^{v}$ | 117.15 (7) | Al13$^{xxxvi}$—Al10—Mn3$^{xxiii}$ | 54.12 (4) |
| Al12—Al2—Al12$^{v}$ | 61.08 (6) | Al8$^{x}$—Al10—Mn3$^{xxiii}$ | 156.03 (6) |
| Mn4$^{xxii}$—Al2—Al12$^{vii}$ | 56.15 (4) | Al10$^{v}$—Al10—Mn3$^{xxiii}$ | 60.16 (2) |
| Mn4$^{iii}$—Al2—Al12$^{vii}$ | 117.15 (7) | Al7A$^{xl}$—Al10—Mn3$^{xxiii}$ | 149.60 (6) |
| Al12—Al2—Al12$^{vii}$ | 97.05 (9) | Ni1—Al11—Mn4$^{iii}$ | 120.04 (5) |
| Al12$^{v}$—Al2—Al12$^{vii}$ | 66.82 (7) | Ni1—Al11—Al4$^{iii}$ | 105.21 (5) |
| Mn4$^{xxii}$—Al2—Al12$^{xx}$ | 117.15 (7) | Mn4$^{iii}$—Al11—Al4$^{iii}$ | 58.05 (5) |
| Mn4$^{iii}$—Al2—Al12$^{xx}$ | 56.15 (4) | Ni1—Al11—Al13$^{vi}$ | 63.18 (4) |
| Al12—Al2—Al12$^{xx}$ | 66.82 (7) | Mn4$^{iii}$—Al11—Al13$^{vi}$ | 157.51 (6) |
| Al12$^{v}$—Al2—Al12$^{xx}$ | 97.05 (9) | Al4$^{iii}$—Al11—Al13$^{vi}$ | 99.47 (6) |
| Al12$^{vii}$—Al2—Al12$^{xx}$ | 61.08 (6) | Ni1—Al11—Al12$^{xviii}$ | 120.70 (5) |
| Mn4$^{xxii}$—Al2—Al9$^{vii}$ | 64.57 (5) | Mn4$^{iii}$—Al11—Al12$^{xviii}$ | 118.86 (5) |
| Mn4$^{iii}$—Al2—Al9$^{vii}$ | 124.14 (9) | Al4$^{iii}$—Al11—Al12$^{xviii}$ | 99.45 (6) |
| Al12—Al2—Al9$^{vii}$ | 145.81 (4) | Al13$^{vi}$—Al11—Al12$^{xviii}$ | 60.03 (4) |
| Al12$^{v}$—Al2—Al9$^{vii}$ | 108.81 (4) | Ni1—Al11—Al12 | 140.58 (6) |
| Al12$^{vii}$—Al2—Al9$^{vii}$ | 108.81 (4) | Mn4$^{iii}$—Al11—Al12 | 53.81 (4) |

| | | | |
|---|---|---|---|
| Al12$^{xx}$—Al2—Al9$^{vii}$ | 145.82 (4) | Al4$^{iii}$—Al11—Al12 | 100.93 (6) |
| Mn4$^{xxii}$—Al2—Al9 | 124.14 (9) | Al13$^{vi}$—Al11—Al12 | 139.80 (6) |
| Mn4$^{iii}$—Al2—Al9 | 64.57 (5) | Al12$^{xviii}$—Al11—Al12 | 82.62 (5) |
| Al12—Al2—Al9 | 108.81 (4) | Ni1—Al11—Al9 | 60.86 (4) |
| Al12$^{v}$—Al2—Al9 | 145.81 (4) | Mn4$^{iii}$—Al11—Al9 | 61.46 (4) |
| Al12$^{vii}$—Al2—Al9 | 145.81 (4) | Al4$^{iii}$—Al11—Al9 | 61.51 (5) |
| Al12$^{xx}$—Al2—Al9 | 108.81 (4) | Al13$^{vi}$—Al11—Al9 | 110.64 (6) |
| Al9$^{vii}$—Al2—Al9 | 59.57 (9) | Al12$^{xviii}$—Al11—Al9 | 158.50 (6) |
| Mn4$^{xxii}$—Al2—Al11$^{xx}$ | 122.17 (3) | Al12—Al11—Al9 | 109.52 (5) |
| Mn4$^{iii}$—Al2—Al11$^{xx}$ | 60.75 (3) | Ni1—Al11—Al2 | 85.94 (6) |
| Al12—Al2—Al11$^{xx}$ | 112.13 (4) | Mn4$^{iii}$—Al11—Al2 | 51.31 (3) |
| Al12$^{v}$—Al2—Al11$^{xx}$ | 153.77 (8) | Al4$^{iii}$—Al11—Al2 | 102.30 (5) |
| Al12$^{vii}$—Al2—Al11$^{xx}$ | 90.36 (4) | Al13$^{vi}$—Al11—Al2 | 145.99 (6) |
| Al12$^{xx}$—Al2—Al11$^{xx}$ | 59.07 (3) | Al12$^{xviii}$—Al11—Al2 | 139.28 (7) |
| Al9$^{vii}$—Al2—Al11$^{xx}$ | 90.20 (6) | Al12—Al11—Al2 | 59.75 (6) |
| Al9—Al2—Al11$^{xx}$ | 59.65 (4) | Al9—Al11—Al2 | 59.83 (6) |
| Mn4$^{xxii}$—Al2—Al11$^{v}$ | 60.75 (3) | Ni1—Al11—Al5$^{iii}$ | 160.26 (6) |
| Mn4$^{iii}$—Al2—Al11$^{v}$ | 122.17 (3) | Mn4$^{iii}$—Al11—Al5$^{iii}$ | 59.85 (4) |
| Al12—Al2—Al11$^{v}$ | 90.36 (4) | Al4$^{iii}$—Al11—Al5$^{iii}$ | 56.74 (5) |
| Al12$^{v}$—Al2—Al11$^{v}$ | 59.07 (3) | Al13$^{vi}$—Al11—Al5$^{iii}$ | 108.98 (6) |
| Al12$^{vii}$—Al2—Al11$^{v}$ | 112.13 (4) | Al12$^{xviii}$—Al11—Al5$^{iii}$ | 60.86 (5) |
| Al12$^{xx}$—Al2—Al11$^{v}$ | 153.77 (8) | Al12—Al11—Al5$^{iii}$ | 57.49 (4) |
| Al9$^{vii}$—Al2—Al11$^{v}$ | 59.65 (4) | Al9—Al11—Al5$^{iii}$ | 109.91 (6) |
| Al9—Al2—Al11$^{v}$ | 90.19 (6) | Al2—Al11—Al5$^{iii}$ | 104.78 (6) |
| Al11$^{xx}$—Al2—Al11$^{v}$ | 146.39 (10) | Ni1—Al11—Mn3$^{xviii}$ | 104.64 (4) |
| Mn4$^{xxii}$—Al2—Al11$^{vii}$ | 60.75 (3) | Mn4$^{iii}$—Al11—Mn3$^{xviii}$ | 105.35 (5) |
| Mn4$^{iii}$—Al2—Al11$^{vii}$ | 122.17 (3) | Al4$^{iii}$—Al11—Mn3$^{xviii}$ | 54.22 (4) |
| Al12—Al2—Al11$^{vii}$ | 153.77 (8) | Al13$^{vi}$—Al11—Mn3$^{xviii}$ | 54.73 (4) |
| Al12$^{v}$—Al2—Al11$^{vii}$ | 112.13 (4) | Al12$^{xviii}$—Al11—Mn3$^{xviii}$ | 52.49 (4) |
| Al12$^{vii}$—Al2—Al11$^{vii}$ | 59.07 (3) | Al12—Al11—Mn3$^{xviii}$ | 114.57 (5) |
| Al12$^{xx}$—Al2—Al11$^{vii}$ | 90.36 (4) | Al9—Al11—Mn3$^{xviii}$ | 106.02 (5) |
| Al9$^{vii}$—Al2—Al11$^{vii}$ | 59.65 (4) | Al2—Al11—Mn3$^{xviii}$ | 155.83 (5) |
| Al9—Al2—Al11$^{vii}$ | 90.19 (6) | Al5$^{iii}$—Al11—Mn3$^{xviii}$ | 59.41 (4) |
| Al11$^{xx}$—Al2—Al11$^{vii}$ | 61.59 (5) | Ni1—Al11—Al11$^{v}$ | 54.29 (3) |
| Al11$^{v}$—Al2—Al11$^{vii}$ | 107.97 (6) | Mn4$^{iii}$—Al11—Al11$^{v}$ | 110.38 (3) |
| Mn4$^{xxii}$—Al2—Al11 | 122.17 (3) | Al4$^{iii}$—Al11—Al11$^{v}$ | 150.42 (4) |
| Mn4$^{iii}$—Al2—Al11 | 60.75 (3) | Al13$^{vi}$—Al11—Al11$^{v}$ | 89.65 (4) |
| Al12—Al2—Al11 | 59.07 (3) | Al12$^{xviii}$—Al11—Al11$^{v}$ | 109.41 (4) |
| Al12$^{v}$—Al2—Al11 | 90.36 (4) | Al12—Al11—Al11$^{v}$ | 89.35 (4) |
| Al12$^{vii}$—Al2—Al11 | 153.77 (8) | Al9—Al11—Al11$^{v}$ | 88.92 (4) |
| Al12$^{xx}$—Al2—Al11 | 112.13 (4) | Al2—Al11—Al11$^{v}$ | 59.20 (3) |
| Al9$^{vii}$—Al2—Al11 | 90.19 (6) | Al5$^{iii}$—Al11—Al11$^{v}$ | 145.45 (4) |
| Al9—Al2—Al11 | 59.65 (4) | Mn3$^{xviii}$—Al11—Al11$^{v}$ | 144.17 (3) |
| Al11$^{xx}$—Al2—Al11 | 107.97 (6) | Ni1—Al11—Al10$^{iii}$ | 53.44 (3) |
| Al11$^{v}$—Al2—Al11 | 61.59 (5) | Mn4$^{iii}$—Al11—Al10$^{iii}$ | 104.42 (5) |
| Al11$^{vii}$—Al2—Al11 | 146.39 (10) | Al4$^{iii}$—Al11—Al10$^{iii}$ | 56.65 (5) |
| Mn3—Al3—Mn3$^{xx}$ | 174.83 (12) | Al13$^{vi}$—Al11—Al10$^{iii}$ | 58.05 (4) |
| Mn3—Al3—Al6$^{xx}$ | 128.61 (10) | Al12$^{xviii}$—Al11—Al10$^{iii}$ | 105.30 (5) |

| | | | |
|---|---|---|---|
| Mn3$^{xx}$—Al3—Al6$^{xx}$ | 56.56 (5) | Al12—Al11—Al10$^{iii}$ | 156.83 (6) |
| Mn3—Al3—Al6 | 56.56 (5) | Al9—Al11—Al10$^{iii}$ | 56.86 (4) |
| Mn3$^{xx}$—Al3—Al6 | 128.61 (10) | Al2—Al11—Al10$^{iii}$ | 115.42 (6) |
| Al6$^{xx}$—Al3—Al6 | 72.05 (9) | Al5$^{iii}$—Al11—Al10$^{iii}$ | 106.83 (5) |
| Mn3—Al3—Al12$^{xx}$ | 120.36 (8) | Mn3$^{xviii}$—Al11—Al10$^{iii}$ | 59.38 (4) |
| Mn3$^{xx}$—Al3—Al12$^{xx}$ | 55.46 (4) | Al11$^{v}$—Al11—Al10$^{iii}$ | 107.73 (3) |
| Al6$^{xx}$—Al3—Al12$^{xx}$ | 103.70 (4) | Mn4$^{iii}$—Al12—Mn3 | 161.15 (6) |
| Al6—Al3—Al12$^{xx}$ | 150.24 (3) | Mn4$^{iii}$—Al12—Al5$^{iii}$ | 64.16 (5) |
| Mn3—Al3—Al12$^{vii}$ | 120.36 (8) | Mn3—Al12—Al5$^{iii}$ | 133.76 (6) |
| Mn3$^{xx}$—Al3—Al12$^{vii}$ | 55.46 (4) | Mn4$^{iii}$—Al12—Al13$^{iii}$ | 122.41 (6) |
| Al6$^{xx}$—Al3—Al12$^{vii}$ | 103.70 (4) | Mn3—Al12—Al13$^{iii}$ | 58.70 (4) |
| Al6—Al3—Al12$^{vii}$ | 150.24 (3) | Al5$^{iii}$—Al12—Al13$^{iii}$ | 93.09 (6) |
| Al12$^{xx}$—Al3—Al12$^{vii}$ | 59.39 (6) | Mn4$^{iii}$—Al12—Al11$^{xviii}$ | 131.84 (6) |
| Mn3—Al3—Al12$^{v}$ | 55.46 (4) | Mn3—Al12—Al11$^{xviii}$ | 66.33 (4) |
| Mn3$^{xx}$—Al3—Al12$^{v}$ | 120.35 (8) | Al5$^{iii}$—Al12—Al11$^{xviii}$ | 67.68 (5) |
| Al6$^{xx}$—Al3—Al12$^{v}$ | 150.24 (3) | Al13$^{iii}$—Al12—Al11$^{xviii}$ | 58.79 (4) |
| Al6—Al3—Al12$^{v}$ | 103.70 (4) | Mn4$^{iii}$—Al12—Al11 | 60.89 (4) |
| Al12$^{xx}$—Al3—Al12$^{v}$ | 93.84 (8) | Mn3—Al12—Al11 | 128.46 (6) |
| Al12$^{vii}$—Al3—Al12$^{v}$ | 64.92 (6) | Al5$^{iii}$—Al12—Al11 | 62.40 (5) |
| Mn3—Al3—Al12 | 55.46 (4) | Al13$^{iii}$—Al12—Al11 | 152.13 (6) |
| Mn3$^{xx}$—Al3—Al12 | 120.35 (8) | Al11$^{xviii}$—Al12—Al11 | 97.38 (5) |
| Al6$^{xx}$—Al3—Al12 | 150.24 (3) | Mn4$^{iii}$—Al12—Al2 | 53.54 (3) |
| Al6—Al3—Al12 | 103.70 (4) | Mn3—Al12—Al2 | 113.47 (5) |
| Al12$^{xx}$—Al3—Al12 | 64.92 (6) | Al5$^{iii}$—Al12—Al2 | 109.70 (6) |
| Al12$^{vii}$—Al3—Al12 | 93.84 (8) | Al13$^{iii}$—Al12—Al2 | 145.60 (6) |
| Al12$^{v}$—Al3—Al12 | 59.38 (6) | Al11$^{xviii}$—Al12—Al2 | 153.67 (6) |
| Mn3—Al3—Al13$^{iv}$ | 55.87 (3) | Al11—Al12—Al2 | 61.18 (5) |
| Mn3$^{xx}$—Al3—Al13$^{iv}$ | 125.40 (3) | Mn4$^{iii}$—Al12—Al5$^{vi}$ | 125.99 (6) |
| Al6$^{xx}$—Al3—Al13$^{iv}$ | 99.90 (7) | Mn3—Al12—Al5$^{vi}$ | 63.87 (4) |
| Al6—Al3—Al13$^{iv}$ | 60.04 (4) | Al5$^{iii}$—Al12—Al5$^{vi}$ | 97.44 (4) |
| Al12$^{xx}$—Al3—Al13$^{iv}$ | 147.01 (8) | Al13$^{iii}$—Al12—Al5$^{vi}$ | 108.09 (6) |
| Al12$^{vii}$—Al3—Al13$^{iv}$ | 92.89 (4) | Al11$^{xviii}$—Al12—Al5$^{vi}$ | 60.97 (4) |
| Al12$^{v}$—Al3—Al13$^{iv}$ | 55.79 (3) | Al11—Al12—Al5$^{vi}$ | 65.61 (5) |
| Al12—Al3—Al13$^{iv}$ | 103.07 (5) | Al2—Al12—Al5$^{vi}$ | 94.51 (5) |
| Mn3—Al3—Al13$^{xxi}$ | 125.40 (3) | Mn4$^{iii}$—Al12—Al12$^{v}$ | 112.93 (3) |
| Mn3$^{xx}$—Al3—Al13$^{xxi}$ | 55.87 (3) | Mn3—Al12—Al12$^{v}$ | 55.32 (3) |
| Al6$^{xx}$—Al3—Al13$^{xxi}$ | 60.04 (4) | Al5$^{iii}$—Al12—Al12$^{v}$ | 151.29 (4) |
| Al6—Al3—Al13$^{xxi}$ | 99.90 (7) | Al13$^{iii}$—Al12—Al12$^{v}$ | 110.01 (4) |
| Al12$^{xx}$—Al3—Al13$^{xxi}$ | 55.79 (3) | Al11$^{xviii}$—Al12—Al12$^{v}$ | 109.41 (4) |
| Al12$^{vii}$—Al3—Al13$^{xxi}$ | 103.07 (5) | Al11—Al12—Al12$^{v}$ | 90.65 (4) |
| Al12$^{v}$—Al3—Al13$^{xxi}$ | 147.01 (8) | Al2—Al12—Al12$^{v}$ | 59.46 (3) |
| Al12—Al3—Al13$^{xxi}$ | 92.89 (4) | Al5$^{vi}$—Al12—Al12$^{v}$ | 59.92 (3) |
| Al13$^{iv}$—Al3—Al13$^{xxi}$ | 156.64 (10) | Mn4$^{iii}$—Al12—Al3 | 108.70 (5) |
| Mn3—Al3—Al13$^{xxii}$ | 125.40 (3) | Mn3—Al12—Al3 | 53.43 (4) |
| Mn3$^{xx}$—Al3—Al13$^{xxii}$ | 55.87 (3) | Al5$^{iii}$—Al12—Al3 | 148.34 (6) |
| Al6$^{xx}$—Al3—Al13$^{xxii}$ | 60.04 (4) | Al13$^{iii}$—Al12—Al3 | 63.77 (5) |
| Al6—Al3—Al13$^{xxii}$ | 99.90 (7) | Al11$^{xviii}$—Al12—Al3 | 111.56 (5) |
| Al12$^{xx}$—Al3—Al13$^{xxii}$ | 103.07 (5) | Al11—Al12—Al3 | 143.97 (6) |

| | | | |
|---|---|---|---|
| Al12$^{vii}$—Al3—Al13$^{xxii}$ | 55.79 (3) | Al2—Al12—Al3 | 84.56 (6) |
| Al12$^{v}$—Al3—Al13$^{xxii}$ | 92.89 (4) | Al5$^{vi}$—Al12—Al3 | 109.80 (5) |
| Al12—Al3—Al13$^{xxii}$ | 147.01 (8) | Al12$^{v}$—Al12—Al3 | 60.31 (3) |
| Al13$^{iv}$—Al3—Al13$^{xxii}$ | 69.61 (5) | Mn4$^{iii}$—Al12—Al1$^{iii}$ | 59.92 (5) |
| Al13$^{xxi}$—Al3—Al13$^{xxii}$ | 105.46 (6) | Mn3—Al12—Al1$^{iii}$ | 119.49 (6) |
| Mn3—Al3—Al13$^{iii}$ | 55.87 (3) | Al5$^{iii}$—Al12—Al1$^{iii}$ | 61.05 (5) |
| Mn3$^{xx}$—Al3—Al13$^{iii}$ | 125.40 (3) | Al13$^{iii}$—Al12—Al1$^{iii}$ | 62.78 (6) |
| Al6$^{xx}$—Al3—Al13$^{iii}$ | 99.90 (7) | Al11$^{xviii}$—Al12—Al1$^{iii}$ | 95.91 (5) |
| Al6—Al3—Al13$^{iii}$ | 60.04 (4) | Al11—Al12—Al1$^{iii}$ | 110.32 (6) |
| Al12$^{xx}$—Al3—Al13$^{iii}$ | 92.89 (4) | Al2—Al12—Al1$^{iii}$ | 105.59 (5) |
| Al12$^{vii}$—Al3—Al13$^{iii}$ | 147.01 (8) | Al5$^{vi}$—Al12—Al1$^{iii}$ | 154.32 (5) |
| Al12$^{v}$—Al3—Al13$^{iii}$ | 103.07 (5) | Al12$^{v}$—Al12—Al1$^{iii}$ | 144.87 (3) |
| Al12—Al3—Al13$^{iii}$ | 55.79 (3) | Al3—Al12—Al1$^{iii}$ | 88.24 (5) |
| Al13$^{iv}$—Al3—Al13$^{iii}$ | 105.46 (6) | Mn2—Al13—Mn3$^{iii}$ | 149.28 (6) |
| Al13$^{xxi}$—Al3—Al13$^{iii}$ | 69.61 (5) | Mn2—Al13—Al7A | 59.00 (7) |
| Al13$^{xxii}$—Al3—Al13$^{iii}$ | 156.64 (10) | Mn3$^{iii}$—Al13—Al7A | 134.09 (6) |
| Al4$^{xiii}$—Al4—Mn3$^{xxiii}$ | 179.94 (4) | Mn2—Al13—Al11$^{xxiii}$ | 140.75 (7) |
| Al4$^{xiii}$—Al4—Mn4$^{xiv}$ | 61.61 (4) | Mn3$^{iii}$—Al13—Al11$^{xxiii}$ | 66.42 (4) |
| Mn3$^{xxiii}$—Al4—Mn4$^{xiv}$ | 118.34 (5) | Al7A—Al13—Al11$^{xxiii}$ | 113.16 (8) |
| Al4$^{xiii}$—Al4—Mn4 | 61.61 (4) | Mn2—Al13—Ni1$^{xxiii}$ | 102.62 (5) |
| Mn3$^{xxiii}$—Al4—Mn4 | 118.34 (5) | Mn3$^{iii}$—Al13—Ni1$^{xxiii}$ | 107.22 (5) |
| Mn4$^{xiv}$—Al4—Mn4 | 65.57 (5) | Al7A—Al13—Ni1$^{xxiii}$ | 58.62 (6) |
| Al4$^{xiii}$—Al4—Mn1 | 61.94 (4) | Al11$^{xxiii}$—Al13—Ni1$^{xxiii}$ | 54.73 (4) |
| Mn3$^{xxiii}$—Al4—Mn1 | 118.11 (6) | Mn2—Al13—Al12$^{iii}$ | 117.03 (7) |
| Mn4$^{xiv}$—Al4—Mn1 | 112.85 (5) | Mn3$^{iii}$—Al13—Al12$^{iii}$ | 56.18 (4) |
| Mn4—Al4—Mn1 | 112.85 (5) | Al7A—Al13—Al12$^{iii}$ | 167.20 (7) |
| Al4$^{xiii}$—Al4—Al5 | 113.51 (5) | Al11$^{xxiii}$—Al13—Al12$^{iii}$ | 61.18 (4) |
| Mn3$^{xxiii}$—Al4—Al5 | 66.43 (6) | Ni1$^{xxiii}$—Al13—Al12$^{iii}$ | 113.74 (5) |
| Mn4$^{xiv}$—Al4—Al5 | 63.50 (5) | Mn2—Al13—Al10$^{xxxvi}$ | 130.87 (7) |
| Mn4—Al4—Al5 | 63.50 (5) | Mn3$^{iii}$—Al13—Al10$^{xxxvi}$ | 65.78 (4) |
| Mn1—Al4—Al5 | 175.45 (8) | Al7A—Al13—Al10$^{xxxvi}$ | 72.73 (6) |
| Al4$^{xiii}$—Al4—Al10 | 113.02 (4) | Al11$^{xxiii}$—Al13—Al10$^{xxxvi}$ | 65.72 (4) |
| Mn3$^{xxiii}$—Al4—Al10 | 67.03 (5) | Ni1$^{xxiii}$—Al13—Al10$^{xxxvi}$ | 53.97 (4) |
| Mn4$^{xiv}$—Al4—Al10 | 174.21 (8) | Al12$^{iii}$—Al13—Al10$^{xxxvi}$ | 112.08 (6) |
| Mn4—Al4—Al10 | 114.51 (3) | Mn2—Al13—Al8$^{xvi}$ | 52.37 (6) |
| Mn1—Al4—Al10 | 61.53 (4) | Mn3$^{iii}$—Al13—Al8$^{xvi}$ | 107.45 (7) |
| Al5—Al4—Al10 | 122.04 (7) | Al7A—Al13—Al8$^{xvi}$ | 56.17 (7) |
| Al4$^{xiii}$—Al4—Al10$^{v}$ | 113.02 (4) | Al11$^{xxiii}$—Al13—Al8$^{xvi}$ | 159.89 (6) |
| Mn3$^{xxiii}$—Al4—Al10$^{v}$ | 67.03 (5) | Ni1$^{xxiii}$—Al13—Al8$^{xvi}$ | 113.35 (6) |
| Mn4$^{xiv}$—Al4—Al10$^{v}$ | 114.51 (3) | Al12$^{iii}$—Al13—Al8$^{xvi}$ | 132.88 (7) |
| Mn4—Al4—Al10$^{v}$ | 174.21 (8) | Al10$^{xxxvi}$—Al13—Al8$^{xvi}$ | 94.20 (5) |
| Mn1—Al4—Al10$^{v}$ | 61.53 (4) | Mn2—Al13—Al13$^{v}$ | 51.85 (3) |
| Al5—Al4—Al10$^{v}$ | 122.04 (7) | Mn3$^{iii}$—Al13—Al13$^{v}$ | 156.42 (3) |
| Al10—Al4—Al10$^{v}$ | 64.76 (6) | Al7A—Al13—Al13$^{v}$ | 57.51 (4) |
| Al4$^{xiii}$—Al4—Al11$^{iii}$ | 113.18 (4) | Al11$^{xxiii}$—Al13—Al13$^{v}$ | 90.35 (4) |
| Mn3$^{xxiii}$—Al4—Al11$^{iii}$ | 66.80 (4) | Ni1$^{xxiii}$—Al13—Al13$^{v}$ | 58.13 (3) |
| Mn4$^{xiv}$—Al4—Al11$^{iii}$ | 116.83 (6) | Al12$^{iii}$—Al13—Al13$^{v}$ | 110.01 (4) |
| Mn4—Al4—Al11$^{iii}$ | 60.63 (3) | Al10$^{xxxvi}$—Al13—Al13$^{v}$ | 109.45 (4) |

| | | | |
|---|---|---|---|
| Mn1—Al4—Al11$^{iii}$ | 116.63 (4) | Al8$^{xvi}$—Al13—Al13$^{v}$ | 95.79 (6) |
| Al5—Al4—Al11$^{iii}$ | 64.51 (4) | Mn2—Al13—Al6$^{iii}$ | 108.64 (6) |
| Al10—Al4—Al11$^{iii}$ | 66.64 (4) | Mn3$^{iii}$—Al13—Al6$^{iii}$ | 54.29 (4) |
| Al10$^{v}$—Al4—Al11$^{iii}$ | 122.34 (7) | Al7A—Al13—Al6$^{iii}$ | 87.37 (5) |
| Al4$^{xiii}$—Al4—Al11$^{iv}$ | 113.18 (4) | Al11$^{xxiii}$—Al13—Al6$^{iii}$ | 109.27 (6) |
| Mn3$^{xxiii}$—Al4—Al11$^{iv}$ | 66.80 (4) | Ni1$^{xxiii}$—Al13—Al6$^{iii}$ | 109.41 (5) |
| Mn4$^{xiv}$—Al4—Al11$^{iv}$ | 60.63 (3) | Al12$^{iii}$—Al13—Al6$^{iii}$ | 105.27 (6) |
| Mn4—Al4—Al11$^{iv}$ | 116.83 (6) | Al10$^{xxxvi}$—Al13—Al6$^{iii}$ | 57.61 (5) |
| Mn1—Al4—Al11$^{iv}$ | 116.63 (4) | Al8$^{xvi}$—Al13—Al6$^{iii}$ | 56.54 (6) |
| Al5—Al4—Al11$^{iv}$ | 64.51 (4) | Al13$^{v}$—Al13—Al6$^{iii}$ | 144.62 (4) |
| Al10—Al4—Al11$^{iv}$ | 122.34 (7) | Mn2—Al13—Al1 | 58.45 (6) |
| Al10$^{v}$—Al4—Al11$^{iv}$ | 66.64 (4) | Mn3$^{iii}$—Al13—Al1 | 115.78 (6) |
| Al11$^{iii}$—Al4—Al11$^{iv}$ | 120.83 (8) | Al7A—Al13—Al1 | 109.92 (7) |
| Al4$^{xiii}$—Al4—Al9$^{xv}$ | 63.95 (3) | Al11$^{xxiii}$—Al13—Al1 | 96.52 (5) |
| Mn3$^{xxiii}$—Al4—Al9$^{xv}$ | 116.07 (4) | Ni1$^{xxiii}$—Al13—Al1 | 109.98 (4) |
| Mn4$^{xiv}$—Al4—Al9$^{xv}$ | 62.23 (4) | Al12$^{iii}$—Al13—Al1 | 61.44 (5) |
| Mn4—Al4—Al9$^{xv}$ | 117.00 (6) | Al10$^{xxxvi}$—Al13—Al1 | 160.56 (6) |
| Mn1—Al4—Al9$^{xv}$ | 62.31 (4) | Al8$^{xvi}$—Al13—Al1 | 103.19 (6) |
| Al5—Al4—Al9$^{xv}$ | 116.32 (5) | Al13$^{v}$—Al13—Al1 | 60.68 (3) |
| Al10—Al4—Al9$^{xv}$ | 114.06 (7) | Al6$^{iii}$—Al13—Al1 | 140.42 (6) |
| Al10$^{v}$—Al4—Al9$^{xv}$ | 59.86 (4) | Mn2—Al13—Al3$^{iii}$ | 97.93 (5) |
| Al11$^{iii}$—Al4—Al9$^{xv}$ | 177.12 (7) | Mn3$^{iii}$—Al13—Al3$^{iii}$ | 51.70 (3) |
| Al11$^{iv}$—Al4—Al9$^{xv}$ | 61.41 (4) | Al7A—Al13—Al3$^{iii}$ | 130.66 (8) |
| Al4$^{xiii}$—Al4—Al9$^{iii}$ | 63.95 (3) | Al11$^{xxiii}$—Al13—Al3$^{iii}$ | 110.78 (6) |
| Mn3$^{xxiii}$—Al4—Al9$^{iii}$ | 116.07 (4) | Ni1$^{xxiii}$—Al13—Al3$^{iii}$ | 158.58 (5) |
| Mn4$^{xiv}$—Al4—Al9$^{iii}$ | 117.00 (6) | Al12$^{iii}$—Al13—Al3$^{iii}$ | 60.44 (6) |
| Mn4—Al4—Al9$^{iii}$ | 62.23 (4) | Al10$^{xxxvi}$—Al13—Al3$^{iii}$ | 107.22 (5) |
| Mn1—Al4—Al9$^{iii}$ | 62.31 (4) | Al8$^{xvi}$—Al13—Al3$^{iii}$ | 74.99 (7) |
| Al5—Al4—Al9$^{iii}$ | 116.32 (5) | Al13$^{v}$—Al13—Al3$^{iii}$ | 142.73 (3) |
| Al10—Al4—Al9$^{iii}$ | 59.86 (4) | Al6$^{iii}$—Al13—Al3$^{iii}$ | 57.38 (6) |
| Al10$^{v}$—Al4—Al9$^{iii}$ | 114.06 (7) | Al1—Al13—Al3$^{iii}$ | 85.90 (5) |
| Al11$^{iii}$—Al4—Al9$^{iii}$ | 61.41 (4) | | |

Symmetry codes: (i) $x$, $y$+1, $z$; (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; (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) $x$, −$y$+1, −$z$+1; (xxviii) −$x$, −$y$+2, −$z$+2; (xxix) −$x$+1/2, $y$+1/2, $z$; (xxx) −$x$+1/2, $y$−1/2, $z$−1; (xxxi) $x$−1/2, −$y$+1/2, −$z$+1; (xxxii) $x$−1/2, $y$−1/2, $z$−1; (xxxiii) $x$, $y$−1, $z$; (xxxiv) $x$, −$y$+1, $z$−1/2; (xxxv) −$x$+1/2, −$y$+1/2, $z$−1/2; (xxxvi) −$x$+1/2, −$y$+3/2, −$z$+2; (xxxvii) −$x$, −$y$+1, −$z$; (xxxviii) −$x$, −$y$+1, $z$−1/2; (xxxix) $x$+1/2, $y$−1/2, −$z$+1/2; (xl) $x$+1/2, $y$−1/2, $z$; (xli) $x$+1/2, $y$+1/2, $z$+1.