2014

MgAuGa and MgAu2Ga: first representatives of the Mg-Au-Ga system

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Abstract
MgAuGa (magnesium gold gallium), the first ternary representative of the Mg-Au-Ga system, crystallizes in the space group P62m and adopts the Fe2P structure type (Pearson symbol hP9). Various phases with the general composition AB2 have been reported in the surrounding binary systems, viz. Mg2Ga (hP18), MgGa2 (hP6; CaIn2 type), AuGa2 (cF12; CaF2 type), Au2Ga (oS24; Pd2As type) and Mg2Au (oP12; Co2Si type). In principle, MgAuGa can be obtained from each of them by partial replacement of the major element with the missing element. In fact, the structure of MgAuGa closely resembles hexagonal Mg2Ga through a direct group-subgroup relationship. MgAu2Ga (magnesium digold gallium) also crystallizes hexagonally in the space group P6(3)/mmc and is isotypic with Na3As. It adopts the structure of another binary compound, viz. Mg3Au (hP8), but shows an unexpected distribution of Mg, Au, and Ga among the atomic positions of the asymmetric unit. Both MgAuGa and MgAu2Ga can be described as formally anionic Au/Ga frameworks, with pseudo-hexagonal tunnels around Mg in MgAuGa or cages in MgAu2Ga.

Keywords
Fe2P structure type, MgAu2Ga, MgAuGa, Mg-Au-Ga system, crystal structure, hexagonal Na3As structure type, ternary phase

Disciplines
Materials Chemistry | Other Chemistry | Physical Chemistry

Comments
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Acta Crystallographica Section C
Structural Chemistry
ISSN 2053-2296

MgAuGa and $MgAu_2Ga$: first representatives of the Mg–Au–Ga system

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Received 24 January 2014
Accepted 12 March 2014

MgAuGa (magnesium gold gallium), the first ternary representative of the Mg–Au–Ga system, crystallizes in the space group $P\bar{6}2m$ and adopts the Fe_2P structure type (Pearson symbol *hP*9). Various phases with the general composition AB_2 have been reported in the surrounding binary systems, *viz*. Mg_2Ga (*hP*18), $MgGa_2$ (*hP*6; $CaIn_2$ type), $AuGa_2$ (*cF*12; CaF_2 type), Au_2Ga (*oS*24; Pd_2As type) and Mg_2Au (*oP*12; Co_2Si type). In principle, MgAuGa can be obtained from each of them by partial replacement of the major element with the missing element. In fact, the structure of MgAuGa closely resembles hexagonal Mg_2Ga through a direct group–subgroup relationship. $MgAu_2Ga$ (magnesium digold gallium) also crystallizes hexagonally in the space group $P6_3/mmc$ and is isotypic with Na_3As. It adopts the structure of another binary compound, *viz*. Mg_3Au (*hP*8), but shows an unexpected distribution of Mg, Au, and Ga among the atomic positions of the asymmetric unit. Both MgAuGa and $MgAu_2Ga$ can be described as formally anionic Au/Ga frameworks, with pseudo-hexagonal tunnels around Mg in MgAuGa or cages in $MgAu_2Ga$.

Keywords: crystal structure; ternary phase; Mg–Au–Ga system; Fe_2P structure type; hexagonal Na_3As structure type; MgAuGa; $MgAu_2Ga$.

1. Introduction

Extensive synthetic explorations focusing on alkali/alkaline earth–late transition–post transition systems have revealed a variety of compounds with novel structural motifs and bonding features (Corbett, 2010). Among these combinations, systems with active metals, Au and Ga, have been our focus over the last five years, resulting in quite fruitful outcomes (Smetana, Corbett & Miller, 2012; Smetana, Lin *et al.*, 2012; Smetana, Miller & Corbett, 2012; Smetana *et al.*, 2013). These compounds exhibit polyanionic frameworks and clusters with encapsulated cations forming one-dimensional chains ($A_{0.55}Au_2Ga_2$ and AAu_2Ga_4; A = Na–Cs), two-dimensional sheets (AAu_3Ga_2; A = K–Cs) and three-dimensional cages ($Na_{13}Au_9Ga_{18}$ and $Na_{17}Au_{5.9}Ga_{46.6}$). However, the last case is better described as two interpenetrating polyanionic and polycationic networks. Moreover, the Na-containing phases, which are quasi-crystalline or its approximant, indicate significant polar–covalent Na—Au bonding.

Along these lines, Li and Mg occupy special places among the active alkali and alkaline-earth metals in their intermetallic chemistry. Their especially high electronegativities and small sizes allow these elements to be incorporated into polyanionic networks with more electronegative metals and semi-metals (Tillard-Charbonnel *et al.*, 1990; Li & Corbett, 2005). Since the Mg–Au, Mg–Ga, and Au–Ga systems contain significant numbers of binary compounds (Villars, 2013), there is an excellent opportunity to discover new ternary phases. Moreover, a large homogeneity region has been reported for MgAu (Schubert, 1966) with a maximum solubility of 13 at% Ga in Au at around 673 K (Cooke & Hume-Rothery, 1966). In spite of these reports, no compound has been reported, as yet, in the ternary Mg–Au–Ga system, so we decided to conduct a preliminary exploration.

Our initial investigations have revealed that two ternary compounds in the Mg–Au–Ga system, in particular, are derivatives of the corresponding binary systems. $MgAu_2Ga$ adopts the structure of Mg_3Au (Schubert & Anderko, 1951), with partial redistribution of all positions in the asymmetric unit and the presence of Au–Au dimers, whereas MgAuGa shows a group–subgroup relationship with Mg_2Ga (Frank & Schubert, 1970).

2. Experimental

2.1. Synthesis and crystallization

The starting materials were Mg pieces (99.98%, Alfa Aesar), Au particles (99.999%, BASF), and Ga ingots (99.999%, Alfa Aesar). Mixtures of 300–400 mg total were weighed in an N_2-filled glove-box (H_2O < 0.1 p.p.m.v.), loaded into 9 mm Ta ampoules, sealed by arc-welding under Ar and then enclosed in evacuated SiO_2 jackets. The samples were heated at 1073 K for 8 h, cooled to 623 K at a rate of 10 K h^{-1}, annealed at this temperature for 7 d and finally cooled to room temperature by switching off the furnace. Single crystals of MgAuGa and $MgAu_2Ga$ were obtained from several samples with loaded compositions of 'MgAuGa', '$MgAuGa_3$', and '$MgAu_2Ga_2$'. No homogeneity ranges were observed, in spite of frequent Au/Ga mixing in related compounds. The title compounds have a metallic luster and are stable against exposure to air or water at room temperature. Phase analyses were performed using monochromatic Cu $K\alpha_1$ radiation on a Stoe Stadi-P diffractometer.

2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. Analysis of the systematic absences for the single-crystal data of MgAuGa led to the possible space groups $P3$ (No. 143), $P\bar{3}$ (No. 147), $P\bar{3}m1$ (No. 164), $P321$ (No. 150), $P31m$ (No. 157), $P6_3/m$ (No. 176), $P6_3$

 doi:10.1107/S205322961400566X

Table 1
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	MgAuGa	$MgAu_2Ga$
M_r	291.00	487.96
Crystal system, space group	Hexagonal, $P\bar{6}2m$	Hexagonal, $P6_3/mmc$
Temperature (K)	296	297
a, c (Å)	7.3682 (5), 3.3738 (3)	4.4015 (3), 8.5398 (7)
V (Å^3)	158.63 (2)	143.28 (3)
Z	3	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	81.83	111.34
Crystal size (mm)	0.12 × 0.10 × 0.09	0.12 × 0.11 × 0.11
Data collection		
Diffractometer	Bruker SMART CCD area-detector diffractometer	Bruker SMART CCD area-detector diffractometer
Absorption correction	Empirical (using intensity measurements) (Blessing, 1995)	Empirical (using intensity measurements) (Blessing, 1995)
T_{min}, T_{max}	0.000, 0.001	0.02, 0.06
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	2837, 388, 313	1404, 129, 111
R_{int}	0.071	0.041
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.895	0.767
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.032, 0.069, 1.07	0.023, 0.054, 1.19
No. of reflections	388	129
No. of parameters	14	9
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	2.59, −2.06	2.00, −2.97
Absolute structure	Flack (1983), with 163 Friedel pairs	–
Absolute structure parameter	0.02 (5)	–

Computer programs: *SMART* (Bruker, 2001), *SAINT* (Bruker, 2001), *SHELXS97* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2008), *DIAMOND* (Brandenburg, 2006) and *publCIF* (Westrip, 2010).

(No. 173), $P\bar{6}2m$ (No. 176), and $P6_322$ (No. 166). Analysis of the systematic absences for the single-crystal data of $MgAu_2Ga$ led to the possible space groups $P\bar{3}1c$ (No. 163), $P31c$ (No. 159), $P6_3mc$ (No. 186), $P6_3/mmc$ (No. 194), and $P\bar{6}2c$ (No. 190). The space group $P\bar{6}2m$ was found to be correct for MgAuGa and $P6_3/mmc$ for $MgAu_2Ga$ during the structure refinements. The starting atomic parameters were derived *via* direct methods and the structure was refined successfully using anisotropic atomic displacement parameters for all atoms. All crystallographic positions are fully occupied. Difference Fourier synthesis exhibits almost identical residual peaks and holes of about 2.5 e Å^{-3}, which might result from insufficient data quality. However, all of these peaks and holes were found in the vicinity of Au atoms (∼1.5 Å) and could not be assigned to any new atom.

3. Results and discussion

The crystal structure of MgAuGa is best described as a ternary representative of the Fe_2P structure type (Hendricks & Kosting, 1930). Au atoms occupy the P-atom positions, whereas Mg and Ga each occupy one of two inequivalent Fe positons. No Mg/Au or Au/Ga mixing was observed in this compound. A projection of the MgAuGa polyatomic framework along the c axis is shown in Fig. 1. The Mg atoms are formally cationic in this combination, so the compound can also be represented in terms of a tunnel structure. Pentagonal Au-capped Au_4Ga_6 prisms (Fig. 2*a*) stack together, forming channels around Mg and along the c axis. The Mg—Mg distances in the chain are equivalent to the length of this axis. The Ga and Au atoms have somewhat lower coordination numbers, *viz.* 10 and 9, respectively. The coordination polyhedra of Au are two similar equatorially capped trigonal prisms with inverted locations of Ga and Mg, *i.e.* either $[Au1Ga_6Mg_3]$ or $[Au2Mg_6Ga_3]$ (Figs. 2*c* and 2*d*). All Ga—Ga and Mg—Mg bonds parallel to the c axis have lengths equal to the length of the c axis. All Mg—Ga connections within the first polyhedron are identical [3.051 (4) Å], whereas those in the second form two groups [2.981 (5) and 3.051 (4) Å]. These

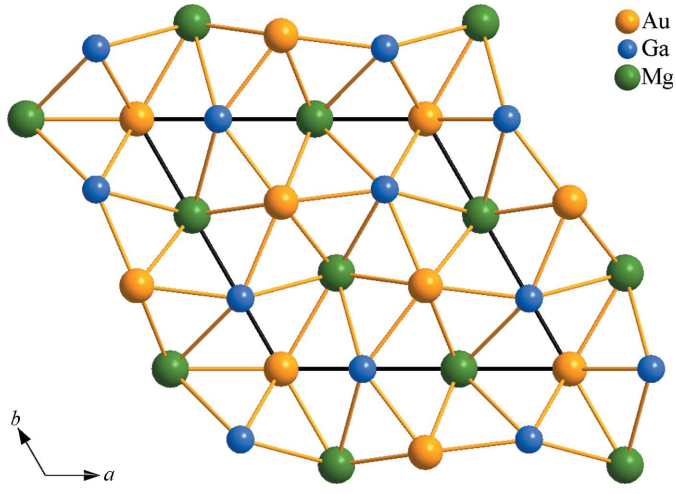

Figure 1
A projection of the MgAuGa structure along the c axis.

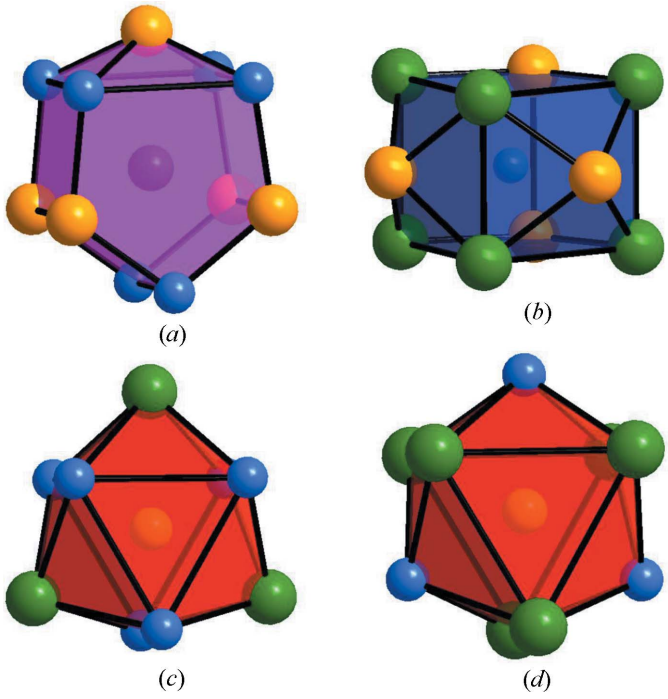

Figure 2
The coordination polyhedra of Mg, Ga, and Au in the crystal structure of MgAuGa. Au atoms are orange, Ga blue and Mg green. (*a*) The pentagonal Au-capped Au_4Ga_6 prism. (*b*) The coordination polyhedron of Ga, consisting of interpenetrating Mg_6 trigonal prisms and an Au_4 tetrahedron. (*c*) The [$Au1Ga_6Mg_3$] coordination polyhedron of Au, consisting of equatorially capped Ga_6 trigonal prisms. (*d*) The [$Au2Mg_6Ga_3$] coordination polyhedron of Au, also consisting of equatorially capped Mg_6 trigonal prisms.

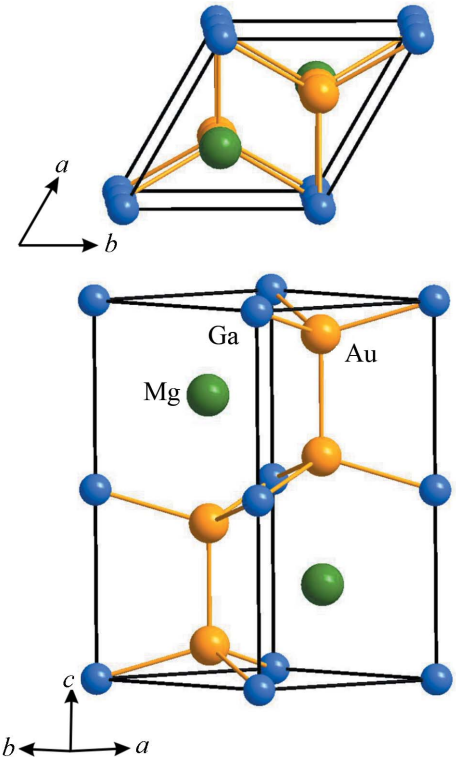

Figure 3
The crystal structure of $MgAu_2Ga$, showing views of the unit cell along two different directions.

polyhedra reveal the similar roles of Ga and Mg in this crystal structure. The coordination polyhedra of Ga consist of interpenetrating Mg_6 trigonal prisms and Au_4 tetrahedra (Fig. 2*b*), although this description is rather formal because of one short [3.3738 (3) Å] and five quite long [4.2536 (3) and 4.5759 (2) Å] Au—Au distances. The Mg—Mg and Mg—Au distances are in the ranges 3.3738 (3)–3.967 (7) and 2.835 (6)–2.844 (5) Å, respectively. This resembles the polyhedra of Au with one small exception, *i.e.* one of the equatorially capping atoms is split into two along the *c* axis.

The crystal structure of $MgAu_2Ga$ (Fig. 3), together with that of the binary compound Mg_3Au, belong to the hexagonal Na_3As structure type, although the distributions of elements in each of them are different. In Mg_3Au, the Mg and Au atoms occupy the positions of Na and As, respectively, in accordance with their electronegativities. However, the situation is slightly different in $MgAu_2Ga$, in which two Mg atoms are formally replaced by Au atoms (the 4*f* positions) and Ga replaces Au at the 2*a* positions (the sites of the As atoms in Na_3As). At first glance, this substitution pattern does not follow the relative electronegativities of Mg, Au, and Ga. However, the atomic distribution results in Au–Au dimers [2.7606 (12) Å] oriented along the *c* axis and bridged by Mg atoms [Mg—Au = 2.8896 (6) Å]. Preliminary electronic structure calculations on $MgAu_2Ga$ suggest optimum Au—Au bonding in these dimers, but further theoretical analysis is underway to identify the nature of these bonds. In fact, the three-dimensional [Au_2Ga] polyanionic network involves Au atoms four-bonded by a distorted tetrahedron of three Ga and one Au atom, and Ga atoms six-bonded by a puckered six-membered ring of Au atoms, to form a distorted close-packed environment. The Mg atoms are most closely coordinated by a trigonal prism of Ga atoms; likewise, each Ga atom is surrounded by a trigonal antiprism (distorted octahedron) of Mg atoms.

The relationship between Mg_2Ga and MgAuGa is also structurally interesting. In spite of almost identical covalent radii for Au and Mg (Cordero *et al.*, 2008), the Au atoms prefer to occupy the positions of the more electronegative Ga atoms than those of the geometrically more similar Mg atoms. As mentioned above, the same crystallographic positions are occupied by P atoms in the Fe_2P prototype, showing a strong site preference for the most electronegative element in each compound. However, Mg_2Ga deviates from the Fe_2P structure type by a doubling of the *c* axis, creating its own structure type with the space group $P\bar{6}2c$, which is a minimal non-isomorphic subgroup of $P\bar{6}2m$. MgAuGa has unit-cell parameters [a = 7.3682 (5) Å and c = 3.3738 (3) Å] that create a volume approximately one-half of that of Mg_2Ga [a = 7.794 (2) Å and c = 6.893 (1) Å]. The coordination polyhedra of Ga in Mg_2Ga remain the same tricapped trigonal prisms, but the polyhedra around the Mg atoms are significantly distorted tetragonal and pentagonal prisms. Thus, replacing Mg with Au in the structure of Mg_2Ga stimulates atomic ordering and a slight increase in symmetry. Another comparison may also come from Au_2Ga (Puselj & Schubert, 1974), which crystallizes in the ortho-

rhombic Pd_2As structure type (Baelz & Schubert, 1969). Despite the different crystallographic symmetry and no direct relation between the space groups of Au_2Ga (*Pbam*) and MgAuGa ($P\overline{6}2m$), Au_2Ga contains an ordered packing of trigonal and pentagonal prisms. Moreover, a polymorphic modification of Pd_2As (Schubert *et al.*, 1963) includes the hexagonal Fe_2P structure type. This reveals potential similarities between the Mg–Ga and Au–Ga binary systems concerning a strong structural correlation along the 33 at% Ga line, *i.e.* Mg_2Ga–MgAuGa–Au_2Ga.

This research was supported by the Office of Basic Energy Sciences, Materials Sciences Division, US Department of Energy (DOE). Ames Laboratory is operated for the DOE by Iowa State University under contract No. DE-AC02-07CH11358.

Supporting information for this paper is available from the IUCr electronic archives (Reference: KU3126).

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supplementary materials

Acta Cryst. (2014). C**70**, 355-358 [doi:10.1107/S205322961400566X]

MgAuGa and $MgAu_2Ga$: first representatives of the Mg–Au–Ga system

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Computing details

For both compounds, data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

(I) Magnesium gold gallium

Crystal data

MgAuGa
M_r = 291.00
Hexagonal, $P\bar{6}2m$
Hall symbol: P -6 -2
a = 7.3682 (5) Å
c = 3.3738 (3) Å
V = 158.63 (2) Å^3
Z = 3
F(000) = 366
D_x = 9.139 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2837 reflections
θ = 5.5–39.5°
μ = 81.83 mm^{-1}
T = 296 K
Irregular fragment, colourless
0.12 × 0.10 × 0.09 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: empirical (using intensity measurements) (Blessing, 1995)
T_{min} = 0.000, T_{max} = 0.001
2837 measured reflections
388 independent reflections
313 reflections with $I > 2\sigma(I)$
R_{int} = 0.071
θ_{max} = 39.5°, θ_{min} = 5.5°
h = −13→13
k = −12→13
l = −5→6

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.069
S = 1.07
388 reflections
14 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0308P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 2.59 e Å^{-3}
$\Delta\rho_{min}$ = −2.06 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0086 (12)
Absolute structure: Flack (1983), with 163 Friedel pairs
Absolute structure parameter: 0.02 (5)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Au1	0.0000	0.0000	0.0000	0.01147 (19)
Au2	0.3333	0.6667	0.5000	0.01267 (18)
Ga1	0.2816 (3)	0.0000	0.5000	0.0108 (3)
Mg1	0.6152 (9)	0.0000	0.0000	0.0121 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.0094 (2)	0.0094 (2)	0.0157 (4)	0.00468 (12)	0.000	0.000
Au2	0.00854 (18)	0.00854 (18)	0.0209 (4)	0.00427 (9)	0.000	0.000
Ga1	0.0080 (5)	0.0082 (7)	0.0161 (8)	0.0041 (4)	0.000	0.000
Mg1	0.010 (2)	0.014 (3)	0.014 (3)	0.0068 (13)	0.000	0.000

Geometric parameters (Å, º)

Au1—Ga1^{i}	2.6740 (15)	Au2—Au2^{ix}	3.3738 (3)
Au1—Ga1	2.6740 (15)	Ga1—Au2^{xiv}	2.6672 (12)
Au1—Ga1^{ii}	2.6740 (15)	Ga1—Au2^{xv}	2.6672 (12)
Au1—Ga1^{iii}	2.6740 (15)	Ga1—Au1^{ix}	2.6740 (15)
Au1—Ga1^{iv}	2.6740 (15)	Ga1—Mg1^{ix}	2.981 (5)
Au1—Ga1^{v}	2.6740 (15)	Ga1—Mg1	2.981 (5)
Au1—Mg1^{vi}	2.835 (6)	Ga1—Mg1^{viii}	3.051 (4)
Au1—Mg1^{vii}	2.835 (6)	Ga1—Mg1^{xiii}	3.051 (4)
Au1—Mg1^{viii}	2.835 (6)	Ga1—Mg1^{xvi}	3.051 (4)
Au1—Au1^{v}	3.3738 (3)	Ga1—Mg1^{vi}	3.051 (4)
Au1—Au1^{ix}	3.3738 (3)	Mg1—Au1^{xvii}	2.835 (6)
Au2—Ga1^{x}	2.6672 (12)	Mg1—Au2^{xv}	2.8443 (19)
Au2—Ga1^{ii}	2.6672 (12)	Mg1—Au2^{xviii}	2.8443 (19)
Au2—Ga1^{vi}	2.6672 (12)	Mg1—Au2^{xix}	2.8443 (19)
Au2—Mg1^{ii}	2.844 (5)	Mg1—Au2^{xiv}	2.8443 (19)
Au2—Mg1^{xi}	2.844 (5)	Mg1—Ga1^{v}	2.981 (5)
Au2—Mg1^{xii}	2.844 (5)	Mg1—Ga1^{xx}	3.051 (4)
Au2—Mg1^{x}	2.844 (5)	Mg1—Ga1^{xxi}	3.051 (4)
Au2—Mg1^{vi}	2.844 (5)	Mg1—Ga1^{xxii}	3.051 (4)
Au2—Mg1^{xiii}	2.844 (5)	Mg1—Ga1^{xxiii}	3.051 (4)
Au2—Au2^{v}	3.3738 (3)	Mg1—Mg1^{ix}	3.3738 (3)

Ga1^{i}—Au1—Ga1	134.346 (18)	Au2^{xiv}—Ga1—Au1	117.915 (12)
Ga1^{i}—Au1—Ga1^{ii}	134.346 (18)	Au2^{xv}—Ga1—Au1	117.915 (12)
Ga1—Au1—Ga1^{ii}	84.44 (4)	Au2^{xiv}—Ga1—Au1^{ix}	117.915 (12)
Ga1^{i}—Au1—Ga1^{iii}	78.23 (5)	Au2^{xv}—Ga1—Au1^{ix}	117.915 (12)
Ga1—Au1—Ga1^{iii}	84.44 (4)	Au1—Ga1—Au1^{ix}	78.23 (5)
Ga1^{ii}—Au1—Ga1^{iii}	84.44 (4)	Au2^{xiv}—Ga1—Mg1^{ix}	60.17 (4)
Ga1^{i}—Au1—Ga1^{iv}	84.44 (4)	Au2^{xv}—Ga1—Mg1^{ix}	60.17 (4)
Ga1—Au1—Ga1^{iv}	134.346 (18)	Au1—Ga1—Mg1^{ix}	175.35 (8)
Ga1^{ii}—Au1—Ga1^{iv}	78.23 (5)	Au1^{ix}—Ga1—Mg1^{ix}	106.43 (7)
Ga1^{iii}—Au1—Ga1^{iv}	134.346 (18)	Au2^{xiv}—Ga1—Mg1	60.17 (4)
Ga1^{i}—Au1—Ga1^{v}	84.44 (4)	Au2^{xv}—Ga1—Mg1	60.17 (4)
Ga1—Au1—Ga1^{v}	78.23 (5)	Au1—Ga1—Mg1	106.43 (7)
Ga1^{ii}—Au1—Ga1^{v}	134.346 (18)	Au1^{ix}—Ga1—Mg1	175.35 (8)
Ga1^{iii}—Au1—Ga1^{v}	134.346 (18)	Mg1^{ix}—Ga1—Mg1	68.92 (14)
Ga1^{iv}—Au1—Ga1^{v}	84.44 (4)	Au2^{xiv}—Ga1—Mg1^{viii}	59.21 (10)
Ga1^{i}—Au1—Mg1^{vi}	140.89 (3)	Au2^{xv}—Ga1—Mg1^{viii}	140.52 (4)
Ga1—Au1—Mg1^{vi}	67.173 (9)	Au1—Ga1—Mg1^{viii}	58.94 (10)
Ga1^{ii}—Au1—Mg1^{vi}	67.173 (9)	Au1^{ix}—Ga1—Mg1^{viii}	100.47 (6)
Ga1^{iii}—Au1—Mg1^{vi}	140.89 (3)	Mg1^{ix}—Ga1—Mg1^{viii}	119.37 (8)
Ga1^{iv}—Au1—Mg1^{vi}	67.173 (9)	Mg1—Ga1—Mg1^{viii}	82.23 (8)
Ga1^{v}—Au1—Mg1^{vi}	67.173 (9)	Au2^{xiv}—Ga1—Mg1^{xiii}	140.52 (4)
Ga1^{i}—Au1—Mg1^{vii}	67.173 (9)	Au2^{xv}—Ga1—Mg1^{xiii}	59.21 (10)
Ga1—Au1—Mg1^{vii}	140.89 (3)	Au1—Ga1—Mg1^{xiii}	100.47 (6)
Ga1^{ii}—Au1—Mg1^{vii}	67.173 (9)	Au1^{ix}—Ga1—Mg1^{xiii}	58.94 (10)
Ga1^{iii}—Au1—Mg1^{vii}	67.173 (9)	Mg1^{ix}—Ga1—Mg1^{xiii}	82.23 (8)
Ga1^{iv}—Au1—Mg1^{vii}	67.173 (9)	Mg1—Ga1—Mg1^{xiii}	119.37 (8)
Ga1^{v}—Au1—Mg1^{vii}	140.89 (3)	Mg1^{viii}—Ga1—Mg1^{xiii}	155.12 (17)
Mg1^{vi}—Au1—Mg1^{vii}	120.0	Au2^{xiv}—Ga1—Mg1^{xvi}	59.21 (10)
Ga1^{i}—Au1—Mg1^{viii}	67.173 (9)	Au2^{xv}—Ga1—Mg1^{xvi}	140.52 (4)
Ga1—Au1—Mg1^{viii}	67.173 (9)	Au1—Ga1—Mg1^{xvi}	100.47 (6)
Ga1^{ii}—Au1—Mg1^{viii}	140.89 (3)	Au1^{ix}—Ga1—Mg1^{xvi}	58.94 (10)
Ga1^{iii}—Au1—Mg1^{viii}	67.173 (9)	Mg1^{ix}—Ga1—Mg1^{xvi}	82.23 (8)
Ga1^{iv}—Au1—Mg1^{viii}	140.89 (3)	Mg1—Ga1—Mg1^{xvi}	119.37 (8)
Ga1^{v}—Au1—Mg1^{viii}	67.173 (9)	Mg1^{viii}—Ga1—Mg1^{xvi}	67.14 (9)
Mg1^{vi}—Au1—Mg1^{viii}	120.0	Mg1^{xiii}—Ga1—Mg1^{xvi}	107.20 (16)
Mg1^{vii}—Au1—Mg1^{viii}	120.0	Au2^{xiv}—Ga1—Mg1^{vi}	140.52 (4)
Ga1^{i}—Au1—Au1^{v}	50.89 (3)	Au2^{xv}—Ga1—Mg1^{vi}	59.21 (10)
Ga1—Au1—Au1^{v}	129.11 (3)	Au1—Ga1—Mg1^{vi}	58.94 (10)
Ga1^{ii}—Au1—Au1^{v}	129.11 (3)	Au1^{ix}—Ga1—Mg1^{vi}	100.47 (6)
Ga1^{iii}—Au1—Au1^{v}	129.11 (3)	Mg1^{ix}—Ga1—Mg1^{vi}	119.37 (8)
Ga1^{iv}—Au1—Au1^{v}	50.89 (3)	Mg1—Ga1—Mg1^{vi}	82.23 (8)
Ga1^{v}—Au1—Au1^{v}	50.89 (3)	Mg1^{viii}—Ga1—Mg1^{vi}	107.20 (16)
Mg1^{vi}—Au1—Au1^{v}	90.000 (1)	Mg1^{xiii}—Ga1—Mg1^{vi}	67.14 (9)
Mg1^{vii}—Au1—Au1^{v}	90.0	Mg1^{xvi}—Ga1—Mg1^{vi}	155.12 (17)
Mg1^{viii}—Au1—Au1^{v}	90.0	Au1^{xvii}—Mg1—Au2^{xv}	107.36 (12)
Ga1^{i}—Au1—Au1^{ix}	129.11 (3)	Au1^{xvii}—Mg1—Au2^{xviii}	107.36 (12)
Ga1—Au1—Au1^{ix}	50.89 (3)	Au2^{xv}—Mg1—Au2^{xviii}	145.3 (2)
Ga1^{ii}—Au1—Au1^{ix}	50.89 (3)	Au1^{xvii}—Mg1—Au2^{xix}	107.36 (12)
Ga1^{iii}—Au1—Au1^{ix}	50.89 (3)	Au2^{xv}—Mg1—Au2^{xix}	72.75 (6)

Ga1^{iv}—Au1—Au1^{ix}	129.11 (3)	Au2^{xviii}—Mg1—Au2^{xix}	96.80 (9)
Ga1^{v}—Au1—Au1^{ix}	129.11 (3)	Au1^{xvii}—Mg1—Au2^{xiv}	107.36 (12)
Mg1^{vi}—Au1—Au1^{ix}	90.000 (1)	Au2^{xv}—Mg1—Au2^{xiv}	96.80 (9)
Mg1^{vii}—Au1—Au1^{ix}	90.0	Au2^{xviii}—Mg1—Au2^{xiv}	72.75 (6)
Mg1^{viii}—Au1—Au1^{ix}	90.0	Au2^{xix}—Mg1—Au2^{xiv}	145.3 (2)
Au1^{v}—Au1—Au1^{ix}	180.0	Au1^{xvii}—Mg1—Ga1^{v}	145.54 (7)
Ga1^{x}—Au2—Ga1^{ii}	120.0	Au2^{xv}—Mg1—Ga1^{v}	95.14 (16)
Ga1^{x}—Au2—Ga1^{vi}	120.0	Au2^{xviii}—Mg1—Ga1^{v}	54.43 (8)
Ga1^{ii}—Au2—Ga1^{vi}	120.0	Au2^{xix}—Mg1—Ga1^{v}	54.43 (8)
Ga1^{x}—Au2—Mg1^{ii}	67.13 (12)	Au2^{xiv}—Mg1—Ga1^{v}	95.14 (16)
Ga1^{ii}—Au2—Mg1^{ii}	65.40 (11)	Au1^{xvii}—Mg1—Ga1	145.54 (7)
Ga1^{vi}—Au2—Mg1^{ii}	143.61 (3)	Au2^{xv}—Mg1—Ga1	54.43 (8)
Ga1^{x}—Au2—Mg1^{xi}	65.40 (11)	Au2^{xviii}—Mg1—Ga1	95.14 (16)
Ga1^{ii}—Au2—Mg1^{xi}	143.61 (3)	Au2^{xix}—Mg1—Ga1	95.14 (16)
Ga1^{vi}—Au2—Mg1^{xi}	67.13 (12)	Au2^{xiv}—Mg1—Ga1	54.43 (8)
Mg1^{ii}—Au2—Mg1^{xi}	132.522 (18)	Ga1^{v}—Mg1—Ga1	68.92 (14)
Ga1^{x}—Au2—Mg1^{xii}	67.13 (12)	Au1^{xvii}—Mg1—Ga1^{xx}	53.89 (10)
Ga1^{ii}—Au2—Mg1^{xii}	65.40 (11)	Au2^{xv}—Mg1—Ga1^{xx}	53.66 (4)
Ga1^{vi}—Au2—Mg1^{xii}	143.61 (3)	Au2^{xviii}—Mg1—Ga1^{xx}	160.8 (2)
Mg1^{ii}—Au2—Mg1^{xii}	72.75 (6)	Au2^{xix}—Mg1—Ga1^{xx}	93.63 (5)
Mg1^{xi}—Au2—Mg1^{xii}	88.42 (4)	Au2^{xiv}—Mg1—Ga1^{xx}	106.76 (5)
Ga1^{x}—Au2—Mg1^{x}	65.40 (11)	Ga1^{v}—Mg1—Ga1^{xx}	143.02 (9)
Ga1^{ii}—Au2—Mg1^{x}	143.61 (3)	Ga1—Mg1—Ga1^{xx}	99.96 (5)
Ga1^{vi}—Au2—Mg1^{x}	67.13 (12)	Au1^{xvii}—Mg1—Ga1^{xxi}	53.89 (10)
Mg1^{ii}—Au2—Mg1^{x}	88.42 (4)	Au2^{xv}—Mg1—Ga1^{xxi}	160.8 (2)
Mg1^{xi}—Au2—Mg1^{x}	72.75 (6)	Au2^{xviii}—Mg1—Ga1^{xxi}	53.66 (4)
Mg1^{xii}—Au2—Mg1^{x}	132.522 (18)	Au2^{xix}—Mg1—Ga1^{xxi}	106.76 (5)
Ga1^{x}—Au2—Mg1^{vi}	143.61 (3)	Au2^{xiv}—Mg1—Ga1^{xxi}	93.63 (5)
Ga1^{ii}—Au2—Mg1^{vi}	67.13 (12)	Ga1^{v}—Mg1—Ga1^{xxi}	99.96 (5)
Ga1^{vi}—Au2—Mg1^{vi}	65.40 (11)	Ga1—Mg1—Ga1^{xxi}	143.02 (9)
Mg1^{ii}—Au2—Mg1^{vi}	88.42 (4)	Ga1^{xx}—Mg1—Ga1^{xxi}	107.8 (2)
Mg1^{xi}—Au2—Mg1^{vi}	132.521 (19)	Au1^{xvii}—Mg1—Ga1^{xxii}	53.89 (10)
Mg1^{xii}—Au2—Mg1^{vi}	132.521 (19)	Au2^{xv}—Mg1—Ga1^{xxii}	106.76 (5)
Mg1^{x}—Au2—Mg1^{vi}	88.42 (4)	Au2^{xviii}—Mg1—Ga1^{xxii}	93.63 (5)
Ga1^{x}—Au2—Mg1^{xiii}	143.61 (3)	Au2^{xix}—Mg1—Ga1^{xxii}	160.8 (2)
Ga1^{ii}—Au2—Mg1^{xiii}	67.13 (12)	Au2^{xiv}—Mg1—Ga1^{xxii}	53.66 (4)
Ga1^{vi}—Au2—Mg1^{xiii}	65.40 (11)	Ga1^{v}—Mg1—Ga1^{xxii}	143.02 (9)
Mg1^{ii}—Au2—Mg1^{xiii}	132.52 (2)	Ga1—Mg1—Ga1^{xxii}	99.96 (5)
Mg1^{xi}—Au2—Mg1^{xiii}	88.42 (4)	Ga1^{xx}—Mg1—Ga1^{xxii}	72.17 (12)
Mg1^{xii}—Au2—Mg1^{xiii}	88.42 (4)	Ga1^{xxi}—Mg1—Ga1^{xxii}	67.14 (9)
Mg1^{x}—Au2—Mg1^{xiii}	132.521 (19)	Au1^{xvii}—Mg1—Ga1^{xxiii}	53.89 (10)
Mg1^{vi}—Au2—Mg1^{xiii}	72.75 (6)	Au2^{xv}—Mg1—Ga1^{xxiii}	93.63 (5)
Ga1^{x}—Au2—Au2^{v}	90.0	Au2^{xviii}—Mg1—Ga1^{xxiii}	106.76 (5)
Ga1^{ii}—Au2—Au2^{v}	90.0	Au2^{xix}—Mg1—Ga1^{xxiii}	53.66 (4)
Ga1^{vi}—Au2—Au2^{v}	90.0	Au2^{xiv}—Mg1—Ga1^{xxiii}	160.8 (2)
Mg1^{ii}—Au2—Au2^{v}	53.62 (3)	Ga1^{v}—Mg1—Ga1^{xxiii}	99.96 (5)
Mg1^{xi}—Au2—Au2^{v}	126.38 (3)	Ga1—Mg1—Ga1^{xxiii}	143.02 (9)
Mg1^{xii}—Au2—Au2^{v}	126.38 (3)	Ga1^{xx}—Mg1—Ga1^{xxiii}	67.14 (9)
Mg1^{x}—Au2—Au2^{v}	53.62 (3)	Ga1^{xxi}—Mg1—Ga1^{xxiii}	72.17 (12)

$Mg1^{vi}$—Au2—$Au2^{v}$	53.62 (3)	$Ga1^{xxii}$—Mg1—$Ga1^{xxiii}$	107.8 (2)
$Mg1^{xiii}$—Au2—$Au2^{v}$	126.38 (3)	$Au1^{xvii}$—Mg1—$Mg1^{ix}$	90.0
$Ga1^{x}$—Au2—$Au2^{ix}$	90.0	$Au2^{xv}$—Mg1—$Mg1^{ix}$	53.62 (3)
$Ga1^{ii}$—Au2—$Au2^{ix}$	90.0	$Au2^{xviii}$—Mg1—$Mg1^{ix}$	126.38 (3)
$Ga1^{vi}$—Au2—$Au2^{ix}$	90.0	$Au2^{xix}$—Mg1—$Mg1^{ix}$	126.38 (3)
$Mg1^{ii}$—Au2—$Au2^{ix}$	126.38 (3)	$Au2^{xiv}$—Mg1—$Mg1^{ix}$	53.62 (3)
$Mg1^{xi}$—Au2—$Au2^{ix}$	53.62 (3)	$Ga1^{v}$—Mg1—$Mg1^{ix}$	124.46 (7)
$Mg1^{xii}$—Au2—$Au2^{ix}$	53.62 (3)	Ga1—Mg1—$Mg1^{ix}$	55.54 (7)
$Mg1^{x}$—Au2—$Au2^{ix}$	126.38 (3)	$Ga1^{xx}$—Mg1—$Mg1^{ix}$	56.43 (5)
$Mg1^{vi}$—Au2—$Au2^{ix}$	126.38 (3)	$Ga1^{xxi}$—Mg1—$Mg1^{ix}$	123.57 (5)
$Mg1^{xiii}$—Au2—$Au2^{ix}$	53.62 (3)	$Ga1^{xxii}$—Mg1—$Mg1^{ix}$	56.43 (5)
$Au2^{v}$—Au2—$Au2^{ix}$	180.0	$Ga1^{xxiii}$—Mg1—$Mg1^{ix}$	123.57 (5)
$Au2^{xiv}$—Ga1—$Au2^{xv}$	105.78 (7)		

Symmetry codes: (i) $-x+y, -x, z-1$; (ii) $-y, x-y, z$; (iii) $-x+y, -x, z$; (iv) $-y, x-y, z-1$; (v) $x, y, z-1$; (vi) $-x+y+1, -x+1, z$; (vii) $x-1, y, z$; (viii) $-y, x-y-1, z$; (ix) $x, y, z+1$; (x) $x, y+1, z$; (xi) $x, y+1, z+1$; (xii) $-y, x-y, z+1$; (xiii) $-x+y+1, -x+1, z+1$; (xiv) $x, y-1, z$; (xv) $y, x, -z+1$; (xvi) $-y, x-y-1, z+1$; (xvii) $x+1, y, z$; (xviii) $x, y-1, z-1$; (xix) $y, x, -z$; (xx) $-y+1, x-y, z$; (xxi) $-x+y+1, -x, z-1$; (xxii) $-x+y+1, -x, z$; (xxiii) $-y+1, x-y, z-1$.

(II) Magnesium digold gallium

Crystal data

$MgAu_2Ga$
$M_r = 487.96$
Hexagonal, $P6_3/mmc$
Hall symbol: -P 6c 2c
$a = 4.4015$ (3) Å
$c = 8.5398$ (7) Å
$V = 143.28$ (3) Å^3
$Z = 2$
$F(000) = 402$
$D_x = 11.311$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1404 reflections
$\theta = 4.8$–$33.0°$
$\mu = 111.34$ mm^{-1}
$T = 297$ K
Irregular fragment, colourless
0.12 × 0.11 × 0.11 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: empirical (using intensity measurements) (Blessing, 1995)
$T_{min} = 0.02$, $T_{max} = 0.06$
1404 measured reflections
129 independent reflections
111 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 33.0°$, $\theta_{min} = 4.8°$
$h = -5\rightarrow6$
$k = -4\rightarrow6$
$l = -12\rightarrow12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.054$
$S = 1.19$
129 reflections
9 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0275P)^2 + 1.7138P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 2.00$ e Å^{-3}
$\Delta\rho_{min} = -2.97$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Au1	0.3333	0.6667	0.08837 (7)	0.0069 (2)
Mg2	0.6667	0.3333	0.2500	0.016 (2)
Ga3	0.0000	0.0000	0.0000	0.0105 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.0063 (2)	0.0063 (2)	0.0082 (3)	0.00314 (12)	0.000	0.000
Mg2	0.019 (3)	0.019 (3)	0.009 (4)	0.0097 (16)	0.000	0.000
Ga3	0.0047 (7)	0.0047 (7)	0.0221 (12)	0.0023 (4)	0.000	0.000

Geometric parameters (Å, º)

Au1—Ga3^{i}	2.6509 (2)	Mg2—Au1^{xii}	2.8919 (3)
Au1—Ga3	2.6509 (2)	Mg2—Au1^{iii}	2.8919 (3)
Au1—Ga3^{ii}	2.6509 (2)	Mg2—Ga3^{viii}	3.3190 (2)
Au1—Au1^{iii}	2.7606 (12)	Mg2—Ga3	3.3190 (2)
Au1—Mg2^{iv}	2.8896 (6)	Mg2—Ga3^{xi}	3.3190 (2)
Au1—Mg2^{i}	2.8919 (3)	Mg2—Ga3^{xiii}	3.3190 (2)
Au1—Mg2^{v}	2.8919 (3)	Ga3—Au1^{vi}	2.6509 (2)
Au1—Mg2	2.8919 (3)	Ga3—Au1^{x}	2.6509 (2)
Au1—Au1^{vi}	2.9556 (6)	Ga3—Au1^{xiv}	2.6509 (2)
Au1—Au1^{vii}	2.9556 (6)	Ga3—Au1^{iv}	2.6509 (2)
Au1—Au1^{iv}	2.9556 (6)	Ga3—Au1^{xv}	2.6509 (2)
Mg2—Au1^{viii}	2.8896 (6)	Ga3—Mg2^{xiv}	3.3190 (2)
Mg2—Au1^{iv}	2.8896 (6)	Ga3—Mg2^{xvi}	3.3190 (2)
Mg2—Au1^{ix}	2.8919 (3)	Ga3—Mg2^{v}	3.3190 (2)
Mg2—Au1^{x}	2.8919 (3)	Ga3—Mg2^{iv}	3.3190 (2)
Mg2—Au1^{xi}	2.8919 (3)	Ga3—Mg2^{xv}	3.3190 (2)
Ga3^{i}—Au1—Ga3	112.237 (10)	Au1^{x}—Mg2—Ga3	49.952 (5)
Ga3^{i}—Au1—Ga3^{ii}	112.237 (10)	Au1^{xi}—Mg2—Ga3	111.456 (11)
Ga3—Au1—Ga3^{ii}	112.237 (10)	Au1^{xii}—Mg2—Ga3	88.316 (8)
Ga3^{i}—Au1—Au1^{iii}	106.540 (12)	Au1^{iii}—Mg2—Ga3	88.316 (8)
Ga3—Au1—Au1^{iii}	106.540 (12)	Au1—Mg2—Ga3	49.952 (5)
Ga3^{ii}—Au1—Au1^{iii}	106.540 (12)	Ga3^{viii}—Mg2—Ga3	134.982 (2)
Ga3^{i}—Au1—Mg2^{iv}	73.460 (12)	Au1^{viii}—Mg2—Ga3^{xi}	130.035 (3)

Ga3—Au1—Mg2^{iv}	73.460 (12)	Au1^{iv}—Mg2—Ga3^{xi}	49.965 (3)
Ga3^{ii}—Au1—Mg2^{iv}	73.460 (12)	Au1^{ix}—Mg2—Ga3^{xi}	88.316 (8)
Au1^{iii}—Au1—Mg2^{iv}	180.0	Au1^{x}—Mg2—Ga3^{xi}	49.952 (5)
Ga3^{i}—Au1—Mg2^{i}	73.422 (3)	Au1^{xi}—Mg2—Ga3^{xi}	49.952 (5)
Ga3—Au1—Mg2^{i}	168.03 (2)	Au1^{xii}—Mg2—Ga3^{xi}	88.316 (8)
Ga3^{ii}—Au1—Mg2^{i}	73.422 (3)	Au1^{iii}—Mg2—Ga3^{xi}	168.475 (10)
Au1^{iii}—Au1—Mg2^{i}	61.491 (10)	Au1—Mg2—Ga3^{xi}	111.456 (11)
Mg2^{iv}—Au1—Mg2^{i}	118.509 (10)	Ga3^{viii}—Mg2—Ga3^{xi}	134.982 (2)
Ga3^{i}—Au1—Mg2^{v}	73.422 (3)	Ga3—Mg2—Ga3^{xi}	83.070 (5)
Ga3—Au1—Mg2^{v}	73.422 (3)	Au1^{viii}—Mg2—Ga3^{xiii}	49.965 (3)
Ga3^{ii}—Au1—Mg2^{v}	168.03 (2)	Au1^{iv}—Mg2—Ga3^{xiii}	130.035 (3)
Au1^{iii}—Au1—Mg2^{v}	61.491 (10)	Au1^{ix}—Mg2—Ga3^{xiii}	49.952 (5)
Mg2^{iv}—Au1—Mg2^{v}	118.509 (10)	Au1^{x}—Mg2—Ga3^{xiii}	88.316 (8)
Mg2^{i}—Au1—Mg2^{v}	99.107 (13)	Au1^{xi}—Mg2—Ga3^{xiii}	88.316 (8)
Ga3^{i}—Au1—Mg2	168.03 (2)	Au1^{xii}—Mg2—Ga3^{xiii}	49.952 (5)
Ga3—Au1—Mg2	73.422 (3)	Au1^{iii}—Mg2—Ga3^{xiii}	111.456 (11)
Ga3^{ii}—Au1—Mg2	73.422 (3)	Au1—Mg2—Ga3^{xiii}	168.475 (10)
Au1^{iii}—Au1—Mg2	61.491 (10)	Ga3^{viii}—Mg2—Ga3^{xiii}	83.070 (4)
Mg2^{iv}—Au1—Mg2	118.509 (10)	Ga3—Mg2—Ga3^{xiii}	134.982 (2)
Mg2^{i}—Au1—Mg2	99.107 (13)	Ga3^{xi}—Mg2—Ga3^{xiii}	80.069 (6)
Mg2^{v}—Au1—Mg2	99.107 (13)	Au1^{vi}—Ga3—Au1^{x}	180.00 (2)
Ga3^{i}—Au1—Au1^{vi}	56.118 (5)	Au1^{vi}—Ga3—Au1	67.763 (10)
Ga3—Au1—Au1^{vi}	56.118 (5)	Au1^{x}—Ga3—Au1	112.237 (10)
Ga3^{ii}—Au1—Au1^{vi}	132.75 (3)	Au1^{vi}—Ga3—Au1^{xiv}	112.237 (10)
Au1^{iii}—Au1—Au1^{vi}	120.707 (19)	Au1^{x}—Ga3—Au1^{xiv}	67.763 (10)
Mg2^{iv}—Au1—Au1^{vi}	59.293 (19)	Au1—Ga3—Au1^{xiv}	180.00 (2)
Mg2^{i}—Au1—Au1^{vi}	128.426 (2)	Au1^{vi}—Ga3—Au1^{iv}	112.237 (10)
Mg2^{v}—Au1—Au1^{vi}	59.217 (10)	Au1^{x}—Ga3—Au1^{iv}	67.763 (10)
Mg2—Au1—Au1^{vi}	128.426 (2)	Au1—Ga3—Au1^{iv}	67.763 (10)
Ga3^{i}—Au1—Au1^{vii}	56.118 (5)	Au1^{xiv}—Ga3—Au1^{iv}	112.237 (10)
Ga3—Au1—Au1^{vii}	132.75 (3)	Au1^{vi}—Ga3—Au1^{xv}	67.763 (10)
Ga3^{ii}—Au1—Au1^{vii}	56.118 (5)	Au1^{x}—Ga3—Au1^{xv}	112.237 (10)
Au1^{iii}—Au1—Au1^{vii}	120.707 (19)	Au1—Ga3—Au1^{xv}	112.237 (10)
Mg2^{iv}—Au1—Au1^{vii}	59.293 (19)	Au1^{xiv}—Ga3—Au1^{xv}	67.763 (10)
Mg2^{i}—Au1—Au1^{vii}	59.217 (10)	Au1^{iv}—Ga3—Au1^{xv}	180.00 (2)
Mg2^{v}—Au1—Au1^{vii}	128.426 (2)	Au1^{vi}—Ga3—Mg2^{xiv}	56.626 (7)
Mg2—Au1—Au1^{vii}	128.426 (2)	Au1^{x}—Ga3—Mg2^{xiv}	123.374 (7)
Au1^{vi}—Au1—Au1^{vii}	96.25 (3)	Au1—Ga3—Mg2^{xiv}	123.374 (7)
Ga3^{i}—Au1—Au1^{iv}	132.75 (3)	Au1^{xiv}—Ga3—Mg2^{xiv}	56.626 (7)
Ga3—Au1—Au1^{iv}	56.118 (5)	Au1^{iv}—Ga3—Mg2^{xiv}	123.426 (13)
Ga3^{ii}—Au1—Au1^{iv}	56.118 (5)	Au1^{xv}—Ga3—Mg2^{xiv}	56.574 (13)
Au1^{iii}—Au1—Au1^{iv}	120.707 (19)	Au1^{vi}—Ga3—Mg2	123.374 (7)
Mg2^{iv}—Au1—Au1^{iv}	59.293 (19)	Au1^{x}—Ga3—Mg2	56.626 (7)
Mg2^{i}—Au1—Au1^{iv}	128.426 (2)	Au1—Ga3—Mg2	56.626 (7)
Mg2^{v}—Au1—Au1^{iv}	128.426 (2)	Au1^{xiv}—Ga3—Mg2	123.374 (7)
Mg2—Au1—Au1^{iv}	59.217 (10)	Au1^{iv}—Ga3—Mg2	56.574 (13)
Au1^{vi}—Au1—Au1^{iv}	96.25 (3)	Au1^{xv}—Ga3—Mg2	123.426 (13)
Au1^{vii}—Au1—Au1^{iv}	96.25 (3)	Mg2^{xiv}—Ga3—Mg2	180.0
Au1^{viii}—Mg2—Au1^{iv}	180.0	Au1^{vi}—Ga3—Mg2^{xvi}	123.426 (13)

Au1^{viii}—Mg2—Au1^{ix}	61.491 (10)	Au1^{x}—Ga3—Mg2^{xvi}	56.574 (13)
Au1^{iv}—Mg2—Au1^{ix}	118.509 (10)	Au1—Ga3—Mg2^{xvi}	123.374 (7)
Au1^{viii}—Mg2—Au1^{x}	118.509 (10)	Au1^{xiv}—Ga3—Mg2^{xvi}	56.626 (7)
Au1^{iv}—Mg2—Au1^{x}	61.491 (10)	Au1^{iv}—Ga3—Mg2^{xvi}	56.626 (7)
Au1^{ix}—Mg2—Au1^{x}	127.873 (5)	Au1^{xv}—Ga3—Mg2^{xvi}	123.374 (7)
Au1^{viii}—Mg2—Au1^{xi}	118.509 (10)	Mg2^{xiv}—Ga3—Mg2^{xvi}	83.070 (5)
Au1^{iv}—Mg2—Au1^{xi}	61.491 (10)	Mg2—Ga3—Mg2^{xvi}	96.930 (4)
Au1^{ix}—Mg2—Au1^{xi}	57.02 (2)	Au1^{vi}—Ga3—Mg2^{v}	56.574 (13)
Au1^{x}—Mg2—Au1^{xi}	99.107 (13)	Au1^{x}—Ga3—Mg2^{v}	123.426 (13)
Au1^{viii}—Mg2—Au1^{xii}	61.491 (10)	Au1—Ga3—Mg2^{v}	56.626 (7)
Au1^{iv}—Mg2—Au1^{xii}	118.509 (10)	Au1^{xiv}—Ga3—Mg2^{v}	123.374 (7)
Au1^{ix}—Mg2—Au1^{xii}	99.107 (13)	Au1^{iv}—Ga3—Mg2^{v}	123.374 (7)
Au1^{x}—Mg2—Au1^{xii}	57.02 (2)	Au1^{xv}—Ga3—Mg2^{v}	56.626 (7)
Au1^{xi}—Mg2—Au1^{xii}	127.873 (5)	Mg2^{xiv}—Ga3—Mg2^{v}	96.930 (4)
Au1^{viii}—Mg2—Au1^{iii}	61.491 (10)	Mg2—Ga3—Mg2^{v}	83.070 (5)
Au1^{iv}—Mg2—Au1^{iii}	118.509 (10)	Mg2^{xvi}—Ga3—Mg2^{v}	180.0
Au1^{ix}—Mg2—Au1^{iii}	99.107 (13)	Au1^{vi}—Ga3—Mg2^{iv}	56.626 (7)
Au1^{x}—Mg2—Au1^{iii}	127.873 (5)	Au1^{x}—Ga3—Mg2^{iv}	123.374 (7)
Au1^{xi}—Mg2—Au1^{iii}	127.873 (5)	Au1—Ga3—Mg2^{iv}	56.574 (13)
Au1^{xii}—Mg2—Au1^{iii}	99.107 (13)	Au1^{xiv}—Ga3—Mg2^{iv}	123.426 (13)
Au1^{viii}—Mg2—Au1	118.509 (10)	Au1^{iv}—Ga3—Mg2^{iv}	56.626 (7)
Au1^{iv}—Mg2—Au1	61.491 (10)	Au1^{xv}—Ga3—Mg2^{iv}	123.374 (7)
Au1^{ix}—Mg2—Au1	127.873 (5)	Mg2^{xiv}—Ga3—Mg2^{iv}	83.070 (5)
Au1^{x}—Mg2—Au1	99.107 (13)	Mg2—Ga3—Mg2^{iv}	96.930 (4)
Au1^{xi}—Mg2—Au1	99.107 (13)	Mg2^{xvi}—Ga3—Mg2^{iv}	83.070 (4)
Au1^{xii}—Mg2—Au1	127.873 (5)	Mg2^{v}—Ga3—Mg2^{iv}	96.930 (4)
Au1^{iii}—Mg2—Au1	57.02 (2)	Au1^{vi}—Ga3—Mg2^{xv}	123.374 (7)
Au1^{viii}—Mg2—Ga3^{viii}	49.965 (3)	Au1^{x}—Ga3—Mg2^{xv}	56.626 (7)
Au1^{iv}—Mg2—Ga3^{viii}	130.035 (3)	Au1—Ga3—Mg2^{xv}	123.426 (13)
Au1^{ix}—Mg2—Ga3^{viii}	49.952 (5)	Au1^{xiv}—Ga3—Mg2^{xv}	56.574 (13)
Au1^{x}—Mg2—Ga3^{viii}	168.475 (10)	Au1^{iv}—Ga3—Mg2^{xv}	123.374 (7)
Au1^{xi}—Mg2—Ga3^{viii}	88.316 (8)	Au1^{xv}—Ga3—Mg2^{xv}	56.626 (7)
Au1^{xii}—Mg2—Ga3^{viii}	111.456 (11)	Mg2^{xiv}—Ga3—Mg2^{xv}	96.930 (4)
Au1^{iii}—Mg2—Ga3^{viii}	49.952 (5)	Mg2—Ga3—Mg2^{xv}	83.070 (5)
Au1—Mg2—Ga3^{viii}	88.316 (8)	Mg2^{xvi}—Ga3—Mg2^{xv}	96.930 (4)
Au1^{viii}—Mg2—Ga3	130.035 (3)	Mg2^{v}—Ga3—Mg2^{xv}	83.070 (4)
Au1^{iv}—Mg2—Ga3	49.965 (3)	Mg2^{iv}—Ga3—Mg2^{xv}	180.0
Au1^{ix}—Mg2—Ga3	168.475 (10)		

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