STRUCTURAL CHEMISTRY

ISSN 2053-2296

Single-crystal structure determination of two new ternary bismuthides: $Rh_6Mn_5Bi_{18}$ and $RhMnBi_3$

Peter Kainzbauer,[a] Klaus W. Richter,[a]* Herta Silvia Effenberger,[b] Martin C. J. Marker[a] and Herbert Ipser[a]*

[a]Department of Inorganic Chemistry – Functional Materials, University of Vienna, Faculty of Chemistry, Althanstrasse 14, Vienna 1090, Austria, and [b]Institute of Mineralogy and Crystallography, University of Vienna, Althanstrasse 14, Vienna 1090, Austria. *Correspondence e-mail: klaus.richter@univie.ac.at, herbert.ipser@univie.ac.at

Received 18 April 2018
Accepted 21 June 2018

Edited by A. L. Spek, Utrecht University, The Netherlands

Keywords: $Rh_6Mn_5Bi_{18}$; $RhMnBi_3$; crystal structure; Rh-Mn-Bi phase diagram; ternary bismuthide; intermetallic; pnictide.

CCDC references: 1850893; 1850892

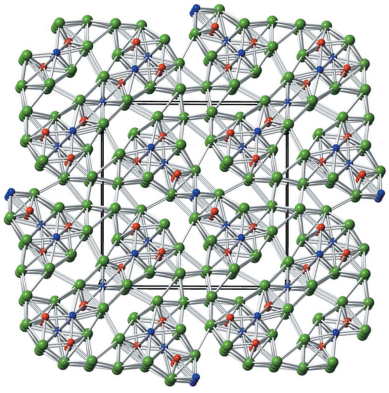
Supporting information: this article has supporting information at journals.iucr.org/c

A study of the ternary Rh–Mn–Bi phase diagram revealed the existence of two new ternary bismuthides, *viz.* hexarhodium pentamanganese octadecabismuthide ($Rh_6Mn_5Bi_{18}$) and rhodium manganese tribismuthide ($RhMnBi_3$). Their crystal structures represent new structure types. $Rh_6Mn_5Bi_{18}$, with a Wyckoff sequence *a f*2 *g*2 *i*5, crystallizes in the tetragonal system (space group $P4_2/mnm$; Pearson symbol *tP*58), and $RhMnBi_3$, with a Wyckoff sequence *a c g i q*, crystallizes in the orthorhombic system (*Cmmm*; *oS*20). In the $Rh_6Mn_5Bi_{18}$ structure, the transition metal atoms are linked into ribbon-like structural units aligned along the [001] direction, whereas planar sheets are formed in $RhMnBi_3$. In both crystal structures, the units formed by the transition metal atoms are enveloped by Bi atoms, which themselves form a loosely bound network. The linkage results in a layer structure for $RhMnBi_3$, while in the case of $Rh_6Mn_5Bi_{18}$, a three-dimensional network is formed; the latter, however, contains several areas where Bi···Bi distances suggest van der Waals interactions. Both phases under discussion have analogous structural motifs.

1. Introduction

For decades, there has been an ongoing search for ferromagnetic materials free of rare earth elements. One promising candidate is the intermetallic phase α-BiMn; unfortunately, it has not been possible to synthesize this phase as a single-phase bulk material in spite of intensive research (*e.g.* Liu *et al.*, 2004; Rama Rao *et al.*, 2013; Cui *et al.*, 2014; Chen *et al.*, 2015; Marker *et al.*, 2018). A possible approach to circumvent these problems was considered to be the addition of a third component, *e.g.* Rh, which forms an intermetallic phase with Bi that is isotypic with α-BiMn (Ross & Hume-Rothery, 1962; Kainzbauer *et al.*, 2018).

Street *et al.* (1974) identified a ferromagnetic compound, *i.e.* $Mn_5Rh_2Bi_4$ (cubic, $Fm\bar{3}m$), with a Curie temperature of 266 K. A similar observation was made by Taufour *et al.* (2015), who described the ferromagnetic compound $Mn_{1.05}Rh_{0.02}Bi$, with a Curie temperature below 416 K. Furthermore, Suits (1975) discovered ferromagnetism in Bi-substituted RhMn with the composition $RhMn_{0.8}Bi_{0.2}$. Based on these observations, a systematic study of the ternary Rh–Mn–Bi system at different temperatures was considered of interest, with the focus on finding additional intermetallic phases which might possibly exhibit ferromagnetism. The synthesized samples were checked by powder X-ray diffraction (PXRD) investigations. As a result of this ongoing research, the phases hexarhodium pentamanganese octadecabismuthide ($Rh_6Mn_5Bi_{18}$) and rhodium manganese tribismuthide ($RhMnBi_3$) were detected; admittedly, they are not ferromagnetic.



OPEN ACCESS

Table 1
Experimental details.

	$Rh_6Mn_5Bi_{18}$	$RhMnBi_3$
Crystal data		
Chemical formula	$Rh_6Mn_5Bi_{18}$	$RhMnBi_3$
M_r	4653.80	784.79
Crystal system, space group	Tetragonal, $P4_2/mnm$	Orthorhombic, $Cmmm$
Temperature (K)	293	293
a, b, c (Å)	18.526 (3), 18.526 (3), 4.1722 (11)	8.885 (3), 13.696 (6), 4.1310 (12)
α, β, γ (°)	90, 90, 90	90, 90, 90
V (Å^3)	1432.0 (6)	502.7 (3)
Z	2	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	115.57	110.13
Crystal size (mm)	0.16 × 0.03 × 0.02	0.10 × 0.05 × 0.03
Data collection		
Diffractometer	Nonius KappaCCD	Nonius KappaCCD
Absorption correction	Multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)	Multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)
T_{min}, T_{max}	0.009, 0.011	0.003, 0.005
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	21380, 1784, 1297	3699, 667, 522
R_{int}	0.169	0.141
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.803	0.806
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.088, 1.05	0.094, 0.257, 1.19
No. of reflections	1784	667
No. of parameters	50	21
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	4.24, −3.66	11.68, −8.87

Computer programs: *COLLECT* (Hooft, 1999), *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *CrystalMaker* (CrystalMaker, 2009).

A literature survey of the ternary Rh–*M*–Bi systems (*M* = 3*d* transition metal) shows that they are relatively unexplored. Except for the aforementioned phases, only a handful of compounds are known. Examples are $RhNiBi_2$ (Zhuravlev *et al.*, 1962) and $RhNiBi_6$ (Fjellvåg & Furuseth, 1987). It may be of particular interest that $Rh_6Mn_5Bi_{18}$ is probably one of the first reported ternary manganese pnictide phases, with a network formed by Bi atoms where alkaline or rare earth metal elements are absent. Further examples are known to crystallize in the cubic structure type $Cu_4Mn_3Bi_4$ (Street *et al.*, 1974; Szytula *et al.*, 1981).

2. Experimental

2.1. Synthesis and crystallization

Bulk samples were prepared from pure element pieces of Bi (99.999%, ASARCO, New Jersey, USA) and Mn (99.95%, Alfa Aesar, Johnson Matthey Chemicals, Karlsruhe, Germany), and from Rh powder (99.95% ÖGUSSA, Austria). Except for Rh, the metals were pulverized manually and sieved (grain size <0.09 mm). For the $Rh_6Mn_5Bi_{18}$ phase, 76.40 mg Rh, 33.81 mg Mn and 389.26 mg Bi in powder form were mixed, and for $RhMnBi_3$, the amounts were 95.14 mg Rh, 67.50 mg Mn and 838.14 mg Bi; in both cases, the powder mixtures were pressed into pellets in a 5 mm pressing cylinder under a load of 20–25 kN. The bulk samples for the $Rh_6Mn_5Bi_{18}$ phase were sealed in an evacuated silica-glass tube and melted over an oxyhydrogen flame under shaking, with optical control of the melting process. For the alloying process, the samples were heated quickly to 1373 K, cooled over a period of 5 d to 613 K and annealed at this temperature for two weeks. The bulk samples for the $RhMnBi_3$ phase were prepared as sinter pellets. The pellet was sealed in an evacuated silica-glass tube with a small alumina plate at the bottom and covered with an inverted closed silica-glass tube to reduce the gas volume (annealing time of four months). After the annealing process at 613 K in a muffle furnace (Nabertherm, Germany, temperature accuracy ±5 K), all samples were quenched in cold water.

Small single crystals of $Rh_6Mn_5Bi_{18}$ and $RhMnBi_3$ were obtained in several inhomogeneous bulk samples. The target compounds had a metallic luster and were selected manually using an optical stereomicroscope. Adherent bismuth was removed with a scalpel. The entire preparation process was performed in an Ar-filled glove-box (Labmaster SP MBraun, H_2O and O_2 levels below 0.1 ppm). Differential thermal analysis was performed on a DSC 404F1 Pegasus (Netzsch, Selb, Germany) and showed that the $Rh_6Mn_5Bi_{18}$ compound is stable up to 730 K. Phase identification was performed under ambient conditions by PXRD on a Bruker D8 Advance diffractometer in Bragg–Brentano pseudo-focusing geometry, using Cu $K\alpha$ radiation and a LynxEye® one-dimensional silicon strip detector. Energy-dispersive X-ray spectroscopy analyses on a scanning electron microscope (Zeiss Supra 55 VP) confirmed that the elemental compositions corresponded to those from the single-crystal X-ray structure determination. Morphologically, both new bismuthides are acicular and flaky.

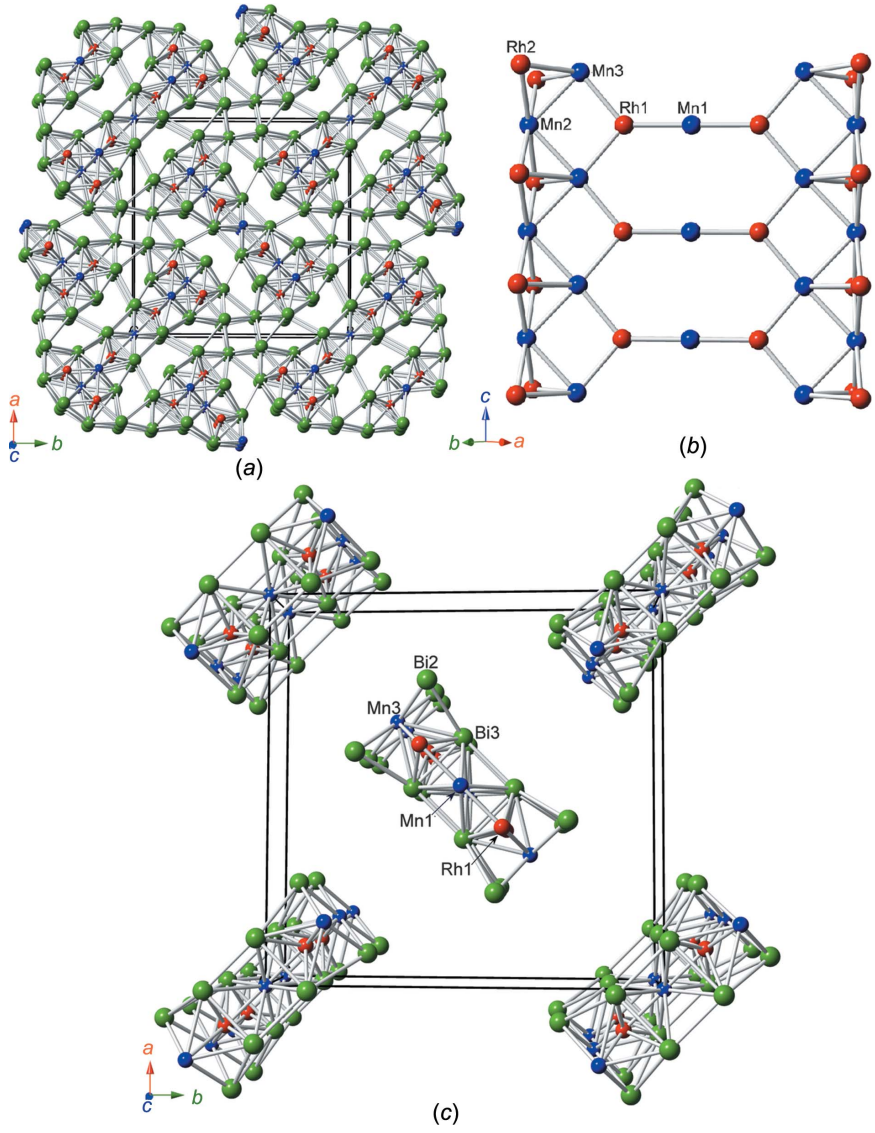


Figure 1
(*a*) The crystal structure of $Rh_6Mn_5Bi_{18}$; the view is slightly inclined to the [001] direction. (*b*) The Rh_6Mn_5 ribbons (distances and angles are listed in Table 3). (*c*) A clinographic projection of the central parts of the ribbons (atoms Bi2, Bi3, Rh1, Mn1 and Mn3). Colour code: green represents Bi, blue Mn and red Rh atoms.

2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. A number of crystal chips were checked for their scattering behaviour and, in particular, to exclude admixtures as adherent bismuth. Crystals of sufficient quality were used for collection of the intensity data in the full reciprocal sphere. To minimize absorption effects, the crystals were mounted approximately parallel to the φ axes with their longest extension. As the crystal structures are composed of structural units only bonded by weak Bi—Bi bonds, extensive cleavage of the crystals is evident. As a consequence of this behaviour, only a crystal of limited quality could be found for $Rh_6Mn_5Bi_{18}$, even though a large number of crystals was checked by single-crystal X-ray diffraction; thus, the R_{int} value and, consequently, the structure refinements remained poor. Nevertheless, the structure type could be clearly established.

A careful inspection of the reciprocal space gave no evidence for any superstructure reflections; twinning was not recognized. As mixed occupation of individual atom positions was not evident and the anisotropic displacement parameters were not conspicuous, a violation of centrosymmetry can be excluded within the accuracy of the structure refinements. Due to the high mosaicity of both samples, their extinction is negligible. Complex neutral atomic scattering functions were applied (Prince, 2006). The program *STRUCTURE TIDY* (Gelato & Parthé, 1987) was used to standardize all atomic coordinates.

3. Results and discussion

As mentioned above, only a few pnictides are known with Rh and a second 3*d* transition metal as constituents (Street *et al.*, 1974; Szytula *et al.*, 1981; Huang *et al.*, 2015). The title phases

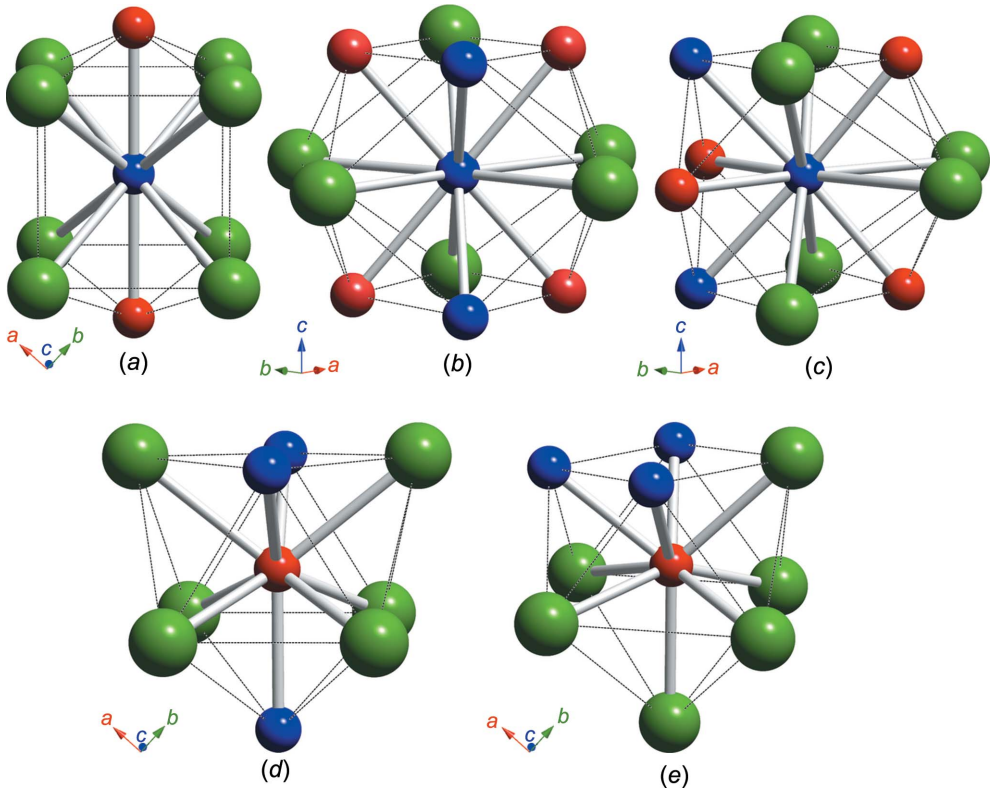


Figure 2
A schematic representation of the distinct atomic coordination spheres in the $Rh_6Mn_5Bi_{18}$ structure. All neighbours within 3.2 Å are shown. (*a*) The bicapped square prism around the Mn1 atom [CN (coordination number) = 10]. (*b*) The distorted cuboctahedron around the Mn2 atom (CN = 12). (*c*) The distorted cuboctahedron around the Mn3 atom (CN = 12). (*d*) The tricapped trigonal prism (alternatively monocapped tetragonal antiprism) around the Rh1 atom (CN = 9). (*e*) The capped square antiprism (alternatively tricapped trigonal prism) around the Rh2 atom (CN = 9). The colour coding is as in Fig. 1.

are probably also the only reported ternary bismuthides containing a platinum group element and Mn, which adopt new structure types.

$Rh_6Mn_5Bi_{18}$ crystallizes in the tetragonal space group $P4_2/mnm$ (Pearson symbol *tP*58). The asymmetric unit contains ten atoms, which are listed together with their Wyckoff letters and site symmetries in Table 2. Fig. 1 shows the whole crystal structure and the main structural element of $Rh_6Mn_5Bi_{18}$ formed by extensive linkage of the Mn and Rh atoms. It is characterized by double chains running parallel to [001], each with the formal composition Rh_3Mn_2. They are linked by an additional Mn1 atom to form ribbons with a linear Rh1—Mn1—Rh1 configuration. The central part of the chains consists of the atoms Rh2, Mn2 and Mn3, the Rh1 atom points towards the linking atom Mn1, and the Mn1 atom itself is surrounded in a bicapped square-prismatic coordination (CN = 10, position 2*a*) (see Fig. 2*a* and Table 3). The ribbons are surrounded by Bi atoms, with Rh/Mn—Bi bond distances > 2.814 Å. All Bi atoms are exclusively bonded to one Rh_3Mn_2—Mn1—Rh_3Mn_2 ribbon. The Bi atoms themselves form an extended three-dimensional anionic network. The Bi—Bi bonds are longer than 3.316 Å; although Bi—Bi distances in the network were found up to 3.5808 (12) Å, which is slightly longer than the interlayer Bi—Bi distance in native Bi under ambient conditions (3.529 Å; Donohue, 1974), bonding interactions are still implicated. In addition to the interatomic bonds, weak van der Waals Bi4···Bi4 [3.920 (2) Å] and Bi2···Bi5 [3.848 (1) Å] interactions contribute to the cohesion of the network. These longer distances are not shown in Fig. 1(*a*). The coordination spheres around all the transition-metal positions are depicted in Fig. 2.

A characteristic feature of the ribbons are eight-membered rings formed by two Mn1 and two Mn3 atoms, as well as four Rh1 atoms. In addition, four-membered rings are built by two Mn3, one Mn2 and one Rh1 atom. These two kinds of rings are planar by space-group symmetry. Only the Rh2 atoms are, respectively, above and below the layers; see Fig. 1(*b*). These structural units are the common structural motif of the two

Table 2
Fractional atomic coordinates, Wyckoff letter and site symmetry of $Rh_6Mn_5Bi_{18}$.

	Wyckoff letter	Site symmetry	*x*	*y*	*z*
Bi1	4*g*	*m*.2*m*	0.17112 (3)	0.82888 (3)	0
Bi2	8*i*	*m*..	0.08340 (3)	0.25924 (3)	0
Bi3	8*i*	*m*..	0.37210 (3)	0.50115 (3)	0
Bi4	8*i*	*m*..	0.08560 (4)	0.56218 (4)	0
Bi5	8*i*	*m*..	0.20740 (4)	0.41210 (4)	0
Rh1	4*f*	*m*.2*m*	0.10090 (7)	0.10090 (7)	0
Rh2	8*i*	*m*..	0.18578 (7)	0.67667 (7)	0
Mn1	2*a*	*m*.*mm*	0	0	0
Mn2	4*f*	*m*.2*m*	0.24406 (14)	0.24406 (14)	0
Mn3	4*g*	*m*.2*m*	0.33193 (14)	0.66807 (14)	0

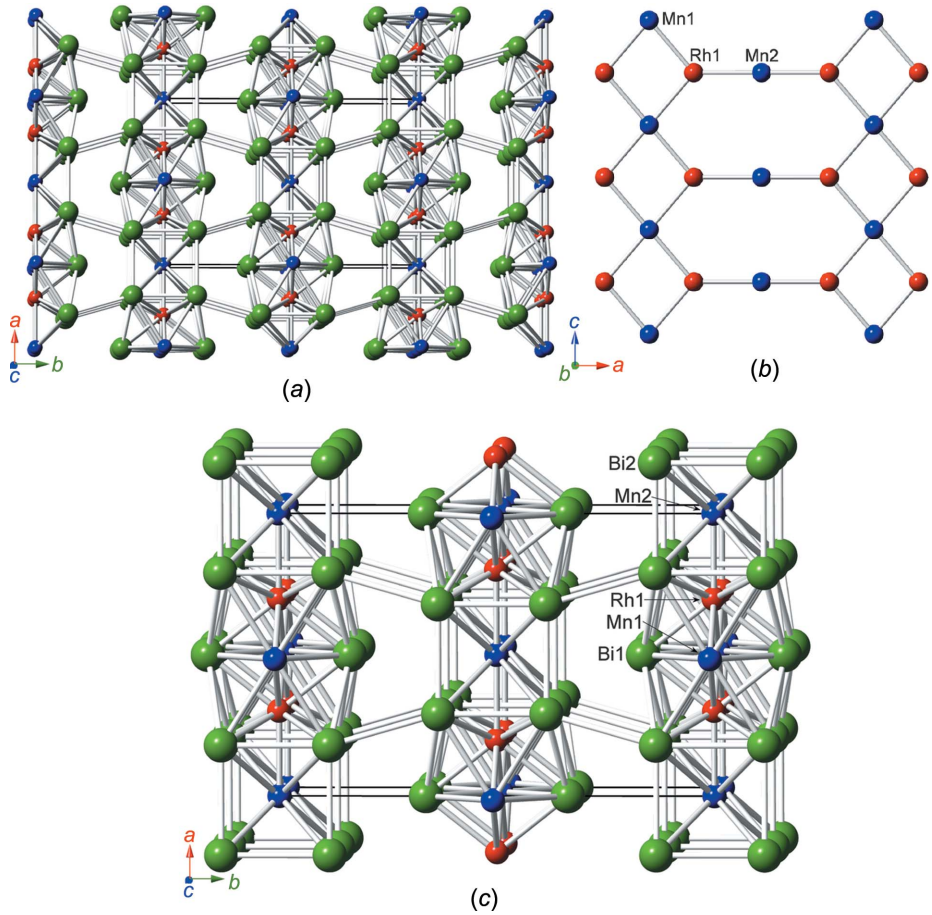


Figure 3
(*a*) The crystal structure of $RhMnBi_3$, viewed approximately parallel to [001]. (*b*) The exactly planar Mn–Rh nets; the view is slightly inclined to the *b* direction (distances and angles are listed in Table 5). (*c*) A clinographic projection of the main structural elements parallel to [001]. The colour coding is as in Fig. 1.

title compounds. However, tetragonal symmetry causes a herring-bone pattern of these one-dimensional structural units along [001] in $Rh_6Mn_5Bi_{18}$, whereas they are linked into a two-dimensional arrangement in $RhMnBi_3$ (see below).

$RhMnBi_3$ crystallizes in the orthorhombic space group *Cmmm* (Pearson symbol *oS*20). Like $Rh_6Mn_5Bi_{18}$, $RhMnBi_3$ represents a new structure type and exhibits a layer structure consisting of planar Mn–Rh sheets parallel to (010) surrounded by Bi atoms, as presented in detail in Fig. 3. Fig. 3(*a*) shows the crystal structure along *c*, clearly indicating the layering. Bi—Bi bond distances between the layers are mainly in the range of van der Waals interactions, except for the Bi2···Bi2 distances of 3.590 (3) Å, which are slightly longer than the interlayer distance in native Bi (3.529 Å), but are still assumed to exhibit weak bonding interactions. The planar nets formed by the transition metals shown in Fig. 3(*b*) consist of eight-membered rings of alternating Mn and Rh atoms, similar to the motif shown in Fig. 1(*b*). The coordination spheres around all the transition-metal positions are depicted in Fig. 4.

The asymmetric unit of the structure of $RhMnBi_3$ itself contains five atoms, which are listed together with their Wyckoff letters and site symmetries in Table 4.

Finally, Fig. 5 illustrates clearly the relationship between the structures of $Rh_6Mn_5Bi_{18}$ and $RhMnBi_3$.

Table 3
Selected geometric parameters (Å, °) for $Rh_6Mn_5Bi_{18}$.

Rh1—Mn1	2.6435 (19)	Rh2—Mn2^{ii}	2.7568 (10)
Rh1—Mn3^{i}	2.729 (3)	Mn2—Mn3^{iii}	2.884 (4)
Rh2—Mn3	2.712 (3)		
Mn1—Rh1—Mn3^{iii}	130.15 (6)	Rh2^{v}—Mn3—Mn2^{ii}	58.93 (7)
Mn3^{i}—Rh1—Mn3^{iii}	99.69 (13)	Rh1^{ii}—Mn3—Mn2^{ii}	83.82 (7)
Rh1—Mn1—Rh1^{iv}	180.00 (8)	Rh1^{vi}—Mn3—Mn2^{ii}	176.49 (13)
Rh2^{v}—Mn3—Rh2	83.27 (12)	Rh1^{vi}—Mn3—Mn2^{vi}	83.82 (7)
Rh2^{v}—Mn3—Rh1^{ii}	118.81 (3)	Mn2^{ii}—Mn3—Mn2^{vi}	92.67 (15)
Rh1^{ii}—Mn3—Rh1^{vi}	99.69 (13)		

Symmetry codes: (i) $y-\frac{1}{2}, -x+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-y+\frac{1}{2}, x+\frac{1}{2}, z+\frac{1}{2}$; (iii) $y-\frac{1}{2}, -x+\frac{1}{2}, -z-\frac{1}{2}$; (iv) $-x, -y, -z$; (v) $-y+1, -x+1, z$; (vi) $-y+\frac{1}{2}, x+\frac{1}{2}, z-\frac{1}{2}$.

Table 4
Fractional atomic coordinates, Wyckoff letter and site symmetry of $RhMnBi_3$.

	Wyckoff letter	Site symmetry	*x*	*y*	*z*
Bi1	4*i*	*m*2*m*	0	0.33689 (14)	0
Bi2	8*q*	..*m*	0.19449 (14)	0.12399 (10)	$\frac{1}{2}$
Mn1	2*c*	*mmm*	$\frac{1}{2}$	0	$\frac{1}{2}$
Mn2	2*a*	*mmm*	0	0	0
Rh1	4*g*	2*mm*	0.3016 (4)	0	0

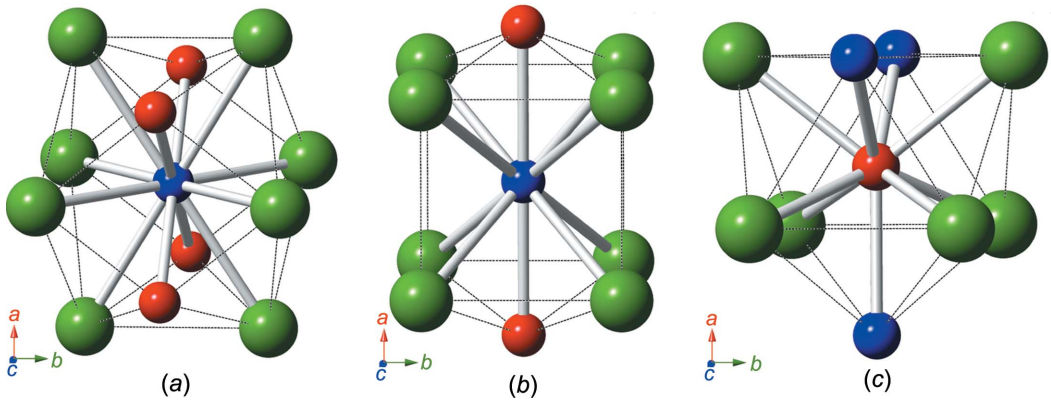


Figure 4
A schematic representation of different atomic coordination spheres in the $RhMnBi_3$ structure, showing all neighbouring atoms up to a distance of 3.3 Å. (*a*) The monocapped square antiprism around the Rh1 atom (CN = 9). (*b*) The distorted cuboctahedron around the Mn1 atom (CN = 12). (*c*) The bicapped square prism around the Mn2 atom (CN = 10). The colour coding is as in Fig. 1.

Table 5
Selected geometric parameters (Å, °) for $RhMnBi_3$.

Mn1—Rh1	2.715 (2)	Mn2—Rh1	2.680 (4)
$Rh1^{i}$—Mn1—$Rh1^{ii}$	99.05 (12)	$Rh1^{ii}$—Mn1—Rh1	80.95 (12)
$Rh1^{i}$—Mn1—$Rh1^{iii}$	80.95 (12)	Mn2—Rh1—Mn1	130.48 (6)
$Rh1^{i}$—Mn1—Rh1	180.0		

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x+1, -y, -z$; (iii) $x, y, z+1$.

Acknowledgements

We thank Dr Stephan Puchegger from the Center for Nano Structure Research, University of Vienna, for support with the SEM/EDX measurements.

Funding information

Funding for this research was provided by: Austrian Science Fund (FWF) (project No. P 26023); University of Vienna (open-access funding).

References

Chen, Y., Gregori, G., Leineweber, A., Qu, F., Chen, C., Tietze, T., Kronmüller, H., Schütz, G. & Goering, E. (2015). *Scripta Mater.* **107**, 131–135.

CrystalMaker (2009). *CrystalMaker*. CrystalMaker Software Ltd, Bicester, England. http://crystalmaker.com/.

Cui, J., Choi, J.-P., Polikarpov, E., Bowden, M. E., Xie, W., Li, G., Nie, Z., Zarkevich, N., Kramer, M. J. & Johnson, D. (2014). *Acta Mater.* **79**, 374–381.

Donohue, J. (1974). *The Structures of the Elements*, p. 454. New York: Wiley.

Fjellvåg, H. & Furuseth, S. (1987). *J. Less-Common Met.* **128**, 177–183.

Gelato, L. M. & Parthé, E. (1987). *J. Appl. Cryst.* **20**, 139–143.

Hooft, R. W. W. (1999). *COLLECT*. Nonius BV, Delft, The Netherlands.

Huang, W., Wang, X., Chen, X., Lu, W., Damewood, L. & Fong, C. Y. (2015). *J. Magn. Magn. Mater.* **377**, 252–258.

Kainzbauer, P., Richter, K. W. & Ipser, H. (2018). *J. Phase Equilibria Diffus.* **39**, 17–34.

Liu, Y., Zhang, J., Jia, G., Zhang, Y., Ren, Z., Li, X., Jing, Ch., Cao, S. & Deng, K. (2004). *Phys. Rev. B*, **70**, 184424.

Marker, M. C. J., Terzieff, P., Kainzbauer, P., Bobnar, M., Richter, K. W. & Ipser, H. (2018). *J. Alloys Compd*, **741**, 682–688.

Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.

Prince, E. (2006). Editor. *International Tables for Crystallography*, Vol. C, *Mathematical, physical and chemical tables*, 3rd ed. Chester: International Union of Crystallography.

Rama Rao, N. V., Gabay, A. M. & Hadjipanayis, G. C. (2013). *J. Phys. D*, **46**, 062001.

Ross, R. G. & Hume-Rothery, W. (1962). *J. Less-Common Met.* **4**, 454–459.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.

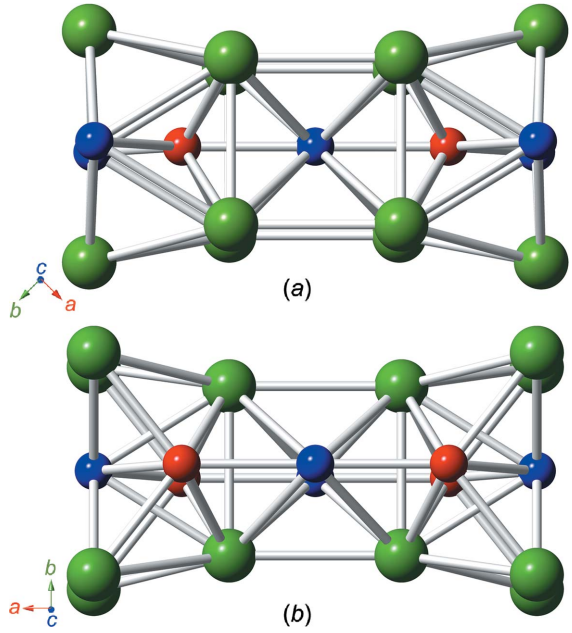


Figure 5
Comparison of the similar structural motif in the two new bismuthides under discussion. (*a*) In $Rh_6Mn_5Bi_{18}$, the motif consists of Bi2, Bi3, Mn2, Mn3 and Rh1 atoms. (*b*) In $RhMnBi_3$, all distinct atom positions listed in Table 4 are included, and the motif is repeated infinitely forming two-dimensional layers (*cf.* Fig. 3). The colour coding is as in Fig. 1.

Street, G. B., Suits, J. C. & Lee, K. (1974). *Solid State Commun.* **14**, 33–36.
Suits, J. C. (1975). *IBM J. Res. Dev.* **19**, 422–423.
Szytula, A., Bińszycka, H. & Todorović, J. (1981). *Solid State Commun.* **38**, 41–43.
Taufour, V., Thimmaiah, S., March, S., Saunders, S., Sun, K., Lamichhane, T. N., Kramer, M. J., Bud'ko, S. L. & Canfield, P. C. (2015). *Phys. Rev. Appl.* **4**, 014021.
Zhuravlev, N. N., Zhdanov, G. S. & Smirnova, E. M. (1962). *Fiz. Met. Metalloved.* **13**, 62–70.

supporting information

Acta Cryst. (2018). C**74**, 863-869 [https://doi.org/10.1107/S2053229618009087]

Single-crystal structure determination of two new ternary bismuthides: $Rh_6Mn_5Bi_{18}$ and $RhMnBi_3$

Peter Kainzbauer, Klaus W. Richter, Herta Silvia Effenberger, Martin C. J. Marker and Herbert Ipser

Computing details

For both structures, data collection: *COLLECT* (Hooft, 1999); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997; data reduction: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *CrystalMaker* (*CrystalMaker*, 2009); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015).

Hexarhodium pentamanganese octadecabismuthide (Rh6Mn5Bi18)

Crystal data

$Rh_6Mn_5Bi_{18}$
M_r = 4653.80
Tetragonal, $P4_2/mnm$
a = 18.526 (3) Å
c = 4.1722 (11) Å
V = 1432.0 (6) Å^3
Z = 2
F(000) = 3778
D_x = 10.793 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 21380 reflections
θ = 3–34.8°
μ = 115.57 mm^{-1}
T = 293 K
Needle like crystal, gray
0.16 × 0.03 × 0.02 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: Nonius
ω scans
Absorption correction: multi-scan
T_{min} = 0.009, T_{max} = 0.011
21380 measured reflections
1784 independent reflections
1297 reflections with $I > 2\sigma(I)$
R_{int} = 0.169
θ_{max} = 34.8°, θ_{min} = 3.1°
h = −29→29
k = −29→29
l = −6→6

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.088
S = 1.05
1784 reflections
50 parameters
0 restraints
$w = 1/[\sigma^2(F_o^2) + (0.013P)^2 + 93.P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 4.24 e Å^{-3}
$\Delta\rho_{min}$ = −3.66 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Bi1	0.17112 (3)	0.82888 (3)	0.0000	0.0212 (2)
Bi2	0.08340 (3)	0.25924 (3)	0.0000	0.01802 (14)
Bi3	0.37210 (3)	0.50115 (3)	0.0000	0.01935 (14)
Bi4	0.08560 (4)	0.56218 (4)	0.0000	0.02587 (17)
Bi5	0.20740 (4)	0.41210 (4)	0.0000	0.02015 (15)
Rh1	0.10090 (7)	0.10090 (7)	0.0000	0.0195 (4)
Rh2	0.18578 (7)	0.67667 (7)	0.0000	0.0187 (3)
Mn1	0.0000	0.0000	0.0000	0.0261 (12)
Mn2	0.24406 (14)	0.24406 (14)	0.0000	0.0177 (7)
Mn3	0.33193 (14)	0.66807 (14)	0.0000	0.0182 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Bi1	0.0180 (2)	0.0180 (2)	0.0277 (5)	0.0010 (3)	0.000	0.000
Bi2	0.0156 (3)	0.0175 (3)	0.0209 (3)	−0.0003 (2)	0.000	0.000
Bi3	0.0178 (3)	0.0173 (3)	0.0230 (3)	−0.0002 (2)	0.000	0.000
Bi4	0.0241 (3)	0.0236 (3)	0.0298 (4)	−0.0041 (3)	0.000	0.000
Bi5	0.0215 (3)	0.0172 (3)	0.0217 (3)	−0.0024 (2)	0.000	0.000
Rh1	0.0188 (5)	0.0188 (5)	0.0208 (10)	−0.0030 (6)	0.000	0.000
Rh2	0.0166 (5)	0.0198 (6)	0.0198 (7)	0.0014 (5)	0.000	0.000
Mn1	0.0257 (16)	0.0257 (16)	0.027 (3)	−0.008 (2)	0.000	0.000
Mn2	0.0187 (10)	0.0187 (10)	0.0157 (18)	0.0027 (13)	0.000	0.000
Mn3	0.0168 (10)	0.0168 (10)	0.021 (2)	0.0017 (13)	0.000	0.000

Geometric parameters (Å, º)

Bi1—Rh2	2.8329 (16)	Bi5—Bi1^{vii}	3.4341 (7)
Bi1—Rh2^{i}	2.8329 (16)	Rh1—Mn1	2.6435 (19)
Bi1—Mn2^{ii}	3.048 (3)	Rh1—Mn3^{vi}	2.729 (3)
Bi1—Mn2^{iii}	3.048 (3)	Rh1—Mn3^{vii}	2.729 (3)
Bi1—Bi5^{iii}	3.4342 (7)	Rh1—Bi3^{ix}	2.8315 (9)
Bi1—Bi5^{iv}	3.4342 (7)	Rh1—Bi3^{vii}	2.8315 (9)
Bi1—Bi5^{ii}	3.4342 (7)	Rh1—Bi3^{x}	2.8315 (9)
Bi1—Bi5^{v}	3.4342 (7)	Rh1—Bi3^{vi}	2.8315 (9)
Bi2—Rh2^{vi}	2.8939 (11)	Rh1—Bi2^{viii}	2.9513 (14)
Bi2—Rh2^{vii}	2.8939 (11)	Rh2—Mn3	2.712 (3)
Bi2—Rh1	2.9513 (14)	Rh2—Mn2^{ii}	2.7568 (10)
Bi2—Mn2	2.990 (2)	Rh2—Mn2^{iii}	2.7568 (10)

Bi2—Mn3^{vi}	3.1089 (7)	Rh2—Bi5^{iii}	2.8220 (11)
Bi2—Mn3^{vii}	3.1089 (7)	Rh2—Bi5^{ii}	2.8220 (11)
Bi2—Bi3^{vii}	3.5489 (9)	Rh2—Bi2^{iii}	2.8939 (11)
Bi2—Bi3^{vi}	3.5489 (9)	Rh2—Bi2^{ii}	2.8939 (11)
Bi2—Bi4^{vi}	3.5733 (9)	Mn1—Rh1^{xi}	2.6435 (19)
Bi2—Bi4^{vii}	3.5733 (9)	Mn1—Bi3^{xii}	3.1570 (7)
Bi2—Bi5	3.6465 (11)	Mn1—Bi3^{xiii}	3.1570 (7)
Bi3—Rh1^{ii}	2.8315 (9)	Mn1—Bi3^{x}	3.1570 (7)
Bi3—Rh1^{iii}	2.8315 (9)	Mn1—Bi3^{vi}	3.1570 (7)
Bi3—Mn1^{ii}	3.1569 (7)	Mn1—Bi3^{xiv}	3.1570 (7)
Bi3—Mn1^{iii}	3.1569 (7)	Mn1—Bi3^{ix}	3.1570 (7)
Bi3—Mn3	3.181 (3)	Mn1—Bi3^{vii}	3.1570 (7)
Bi3—Bi3^{i}	3.3209 (14)	Mn1—Bi3^{xv}	3.1570 (7)
Bi3—Bi3^{viii}	3.3809 (14)	Mn2—Rh2^{vi}	2.7568 (10)
Bi3—Bi5	3.4687 (11)	Mn2—Rh2^{vii}	2.7568 (10)
Bi3—Bi2^{iii}	3.5489 (9)	Mn2—Rh2^{x}	2.7568 (10)
Bi3—Bi2^{ii}	3.5489 (9)	Mn2—Rh2^{ix}	2.7568 (10)
Bi4—Rh2	2.8184 (16)	Mn2—Mn3^{vii}	2.884 (4)
Bi4—Bi5^{ii}	3.4046 (9)	Mn2—Mn3^{vi}	2.884 (4)
Bi4—Bi5^{iii}	3.4046 (9)	Mn2—Bi2^{viii}	2.990 (2)
Bi4—Bi4^{vii}	3.4692 (10)	Mn2—Bi1^{vi}	3.048 (3)
Bi4—Bi4^{vi}	3.4692 (10)	Mn2—Bi1^{vii}	3.048 (3)
Bi4—Bi4^{iii}	3.4693 (9)	Mn2—Bi5^{viii}	3.186 (2)
Bi4—Bi4^{ii}	3.4693 (10)	Mn3—Rh2^{i}	2.712 (3)
Bi4—Bi2^{ii}	3.5734 (9)	Mn3—Rh1^{ii}	2.729 (3)
Bi4—Bi2^{iii}	3.5734 (9)	Mn3—Rh1^{iii}	2.729 (3)
Bi4—Bi5	3.5808 (12)	Mn3—Mn2^{ii}	2.884 (4)
Bi5—Rh2^{vii}	2.8221 (11)	Mn3—Mn2^{iii}	2.884 (4)
Bi5—Rh2^{vi}	2.8221 (11)	Mn3—Bi2^{iv}	3.1089 (7)
Bi5—Mn2	3.186 (2)	Mn3—Bi2^{iii}	3.1089 (7)
Bi5—Bi4^{vii}	3.4047 (9)	Mn3—Bi2^{v}	3.1089 (7)
Bi5—Bi4^{vi}	3.4046 (9)	Mn3—Bi2^{ii}	3.1089 (7)
Bi5—Bi1^{vi}	3.4341 (7)	Mn3—Bi3^{i}	3.181 (3)

Rh2—Bi1—Rh2^{i}	79.00 (6)	Mn3^{vi}—Rh1—Bi3^{vi}	69.75 (5)
Rh2—Bi1—Mn2^{ii}	55.77 (4)	Mn3^{vii}—Rh1—Bi3^{vi}	141.27 (4)
Rh2^{i}—Bi1—Mn2^{ii}	55.77 (4)	Bi3^{ix}—Rh1—Bi3^{vi}	140.66 (8)
Rh2—Bi1—Mn2^{iii}	55.77 (4)	Bi3^{vii}—Rh1—Bi3^{vi}	94.91 (4)
Rh2^{i}—Bi1—Mn2^{iii}	55.77 (4)	Bi3^{x}—Rh1—Bi3^{vi}	71.81 (3)
Mn2^{ii}—Bi1—Mn2^{iii}	86.39 (10)	Mn1—Rh1—Bi2^{viii}	128.69 (3)
Rh2—Bi1—Bi5^{iii}	52.46 (2)	Mn3^{vi}—Rh1—Bi2^{viii}	66.23 (4)
Rh2^{i}—Bi1—Bi5^{iii}	112.58 (3)	Mn3^{vii}—Rh1—Bi2^{viii}	66.23 (4)
Mn2^{ii}—Bi1—Bi5^{iii}	108.02 (4)	Bi3^{ix}—Rh1—Bi2^{viii}	75.682 (17)
Mn2^{iii}—Bi1—Bi5^{iii}	58.52 (2)	Bi3^{vii}—Rh1—Bi2^{viii}	131.92 (3)
Rh2—Bi1—Bi5^{iv}	112.58 (3)	Bi3^{x}—Rh1—Bi2^{viii}	75.682 (17)
Rh2^{i}—Bi1—Bi5^{iv}	52.46 (2)	Bi3^{vi}—Rh1—Bi2^{viii}	131.92 (3)
Mn2^{ii}—Bi1—Bi5^{iv}	58.52 (2)	Mn1—Rh1—Bi2	128.69 (3)
Mn2^{iii}—Bi1—Bi5^{iv}	108.02 (4)	Mn3^{vi}—Rh1—Bi2	66.23 (4)

Bi5^{iii}—Bi1—Bi5^{iv}	163.22 (4)	Mn3^{vii}—Rh1—Bi2	66.23 (4)
Rh2—Bi1—Bi5^{ii}	52.46 (2)	Bi3^{ix}—Rh1—Bi2	131.92 (3)
Rh2^{i}—Bi1—Bi5^{ii}	112.58 (3)	Bi3^{vii}—Rh1—Bi2	75.682 (17)
Mn2^{ii}—Bi1—Bi5^{ii}	58.52 (2)	Bi3^{x}—Rh1—Bi2	131.92 (3)
Mn2^{iii}—Bi1—Bi5^{ii}	108.02 (4)	Bi3^{vi}—Rh1—Bi2	75.682 (17)
Bi5^{iii}—Bi1—Bi5^{ii}	74.81 (2)	Bi2^{viii}—Rh1—Bi2	102.61 (6)
Bi5^{iv}—Bi1—Bi5^{ii}	102.67 (2)	Mn3—Rh2—Mn2^{ii}	63.64 (8)
Rh2—Bi1—Bi5^{v}	112.58 (3)	Mn3—Rh2—Mn2^{iii}	63.64 (7)
Rh2^{i}—Bi1—Bi5^{v}	52.46 (2)	Mn2^{ii}—Rh2—Mn2^{iii}	98.35 (5)
Mn2^{ii}—Bi1—Bi5^{v}	108.02 (4)	Mn3—Rh2—Bi4	127.82 (7)
Mn2^{iii}—Bi1—Bi5^{v}	58.52 (2)	Mn2^{ii}—Rh2—Bi4	130.64 (2)
Bi5^{iii}—Bi1—Bi5^{v}	102.67 (2)	Mn2^{iii}—Rh2—Bi4	130.64 (2)
Bi5^{iv}—Bi1—Bi5^{v}	74.81 (2)	Mn3—Rh2—Bi5^{iii}	130.79 (3)
Bi5^{ii}—Bi1—Bi5^{v}	163.22 (4)	Mn2^{ii}—Rh2—Bi5^{iii}	140.44 (9)
Rh2^{vi}—Bi2—Rh2^{vii}	92.25 (5)	Mn2^{iii}—Rh2—Bi5^{iii}	69.65 (5)
Rh2^{vi}—Bi2—Rh1	106.51 (4)	Bi4—Rh2—Bi5^{iii}	74.26 (3)
Rh2^{vii}—Bi2—Rh1	106.51 (4)	Mn3—Rh2—Bi5^{ii}	130.79 (3)
Rh2^{vi}—Bi2—Mn2	55.85 (4)	Mn2^{ii}—Rh2—Bi5^{ii}	69.65 (5)
Rh2^{vii}—Bi2—Mn2	55.85 (4)	Mn2^{iii}—Rh2—Bi5^{ii}	140.44 (9)
Rh1—Bi2—Mn2	78.30 (7)	Bi4—Rh2—Bi5^{ii}	74.26 (3)
Rh2^{vi}—Bi2—Mn3^{vi}	53.57 (6)	Bi5^{iii}—Rh2—Bi5^{ii}	95.33 (5)
Rh2^{vii}—Bi2—Mn3^{vi}	111.94 (6)	Mn3—Rh2—Bi1	98.87 (7)
Rh1—Bi2—Mn3^{vi}	53.46 (5)	Mn2^{ii}—Rh2—Bi1	66.07 (7)
Mn2—Bi2—Mn3^{vi}	56.40 (6)	Mn2^{iii}—Rh2—Bi1	66.07 (7)
Rh2^{vi}—Bi2—Mn3^{vii}	111.94 (6)	Bi4—Rh2—Bi1	133.31 (5)
Rh2^{vii}—Bi2—Mn3^{vii}	53.57 (6)	Bi5^{iii}—Rh2—Bi1	74.79 (3)
Rh1—Bi2—Mn3^{vii}	53.46 (5)	Bi5^{ii}—Rh2—Bi1	74.79 (3)
Mn2—Bi2—Mn3^{vii}	56.40 (6)	Mn3—Rh2—Bi2^{iii}	67.27 (4)
Mn3^{vi}—Bi2—Mn3^{vii}	84.29 (2)	Mn2^{ii}—Rh2—Bi2^{iii}	130.54 (9)
Rh2^{vi}—Bi2—Bi3^{vii}	157.13 (3)	Mn2^{iii}—Rh2—Bi2^{iii}	63.83 (6)
Rh2^{vii}—Bi2—Bi3^{vii}	94.24 (3)	Bi4—Rh2—Bi2^{iii}	77.43 (3)
Rh1—Bi2—Bi3^{vii}	50.63 (2)	Bi5^{iii}—Rh2—Bi2^{iii}	79.26 (2)
Mn2—Bi2—Bi3^{vii}	111.28 (5)	Bi5^{ii}—Rh2—Bi2^{iii}	151.58 (6)
Mn3^{vi}—Bi2—Bi3^{vii}	103.80 (6)	Bi1—Rh2—Bi2^{iii}	128.91 (3)
Mn3^{vii}—Bi2—Bi3^{vii}	56.62 (6)	Mn3—Rh2—Bi2^{ii}	67.27 (4)
Rh2^{vi}—Bi2—Bi3^{vi}	94.24 (3)	Mn2^{ii}—Rh2—Bi2^{ii}	63.83 (6)
Rh2^{vii}—Bi2—Bi3^{vi}	157.13 (3)	Mn2^{iii}—Rh2—Bi2^{ii}	130.54 (9)
Rh1—Bi2—Bi3^{vi}	50.63 (2)	Bi4—Rh2—Bi2^{ii}	77.43 (3)
Mn2—Bi2—Bi3^{vi}	111.28 (5)	Bi5^{iii}—Rh2—Bi2^{ii}	151.58 (6)
Mn3^{vi}—Bi2—Bi3^{vi}	56.62 (6)	Bi5^{ii}—Rh2—Bi2^{ii}	79.26 (2)
Mn3^{vii}—Bi2—Bi3^{vi}	103.80 (6)	Bi1—Rh2—Bi2^{ii}	128.91 (3)
Bi3^{vii}—Bi2—Bi3^{vi}	72.01 (2)	Bi2^{iii}—Rh2—Bi2^{ii}	92.25 (5)
Rh2^{vi}—Bi2—Bi4^{vi}	50.34 (3)	Rh1—Mn1—Rh1^{xi}	180.00 (8)
Rh2^{vii}—Bi2—Bi4^{vi}	101.74 (3)	Rh1—Mn1—Bi3^{xii}	122.375 (12)
Rh1—Bi2—Bi4^{vi}	144.255 (12)	Rh1^{xi}—Mn1—Bi3^{xii}	57.625 (12)
Mn2—Bi2—Bi4^{vi}	100.67 (5)	Rh1—Mn1—Bi3^{xiii}	122.375 (12)
Mn3^{vi}—Bi2—Bi4^{vi}	95.78 (4)	Rh1^{xi}—Mn1—Bi3^{xiii}	57.625 (12)
Mn3^{vii}—Bi2—Bi4^{vi}	152.16 (7)	Bi3^{xii}—Mn1—Bi3^{xiii}	63.47 (2)

Bi3^{vii}—Bi2—Bi4^{vi}	147.94 (2)	Rh1—Mn1—Bi3^{x}	57.625 (12)
Bi3^{vi}—Bi2—Bi4^{vi}	99.273 (19)	Rh1^{xi}—Mn1—Bi3^{x}	122.375 (12)
Rh2^{vi}—Bi2—Bi4^{vii}	101.74 (3)	Bi3^{xii}—Mn1—Bi3^{x}	116.53 (2)
Rh2^{vii}—Bi2—Bi4^{vii}	50.34 (3)	Bi3^{xiii}—Mn1—Bi3^{x}	180.00 (3)
Rh1—Bi2—Bi4^{vii}	144.255 (13)	Rh1—Mn1—Bi3^{vi}	57.625 (12)
Mn2—Bi2—Bi4^{vii}	100.67 (5)	Rh1^{xi}—Mn1—Bi3^{vi}	122.375 (12)
Mn3^{vi}—Bi2—Bi4^{vii}	152.16 (7)	Bi3^{xii}—Mn1—Bi3^{vi}	180.00 (3)
Mn3^{vii}—Bi2—Bi4^{vii}	95.78 (4)	Bi3^{xiii}—Mn1—Bi3^{vi}	116.53 (2)
Bi3^{vii}—Bi2—Bi4^{vii}	99.273 (19)	Bi3^{x}—Mn1—Bi3^{vi}	63.47 (2)
Bi3^{vi}—Bi2—Bi4^{vii}	147.94 (2)	Rh1—Mn1—Bi3^{xiv}	122.375 (12)
Bi4^{vi}—Bi2—Bi4^{vii}	71.44 (2)	Rh1^{xi}—Mn1—Bi3^{xiv}	57.625 (11)
Rh2^{vi}—Bi2—Bi5	49.50 (2)	Bi3^{xii}—Mn1—Bi3^{xiv}	82.72 (2)
Rh2^{vii}—Bi2—Bi5	49.50 (2)	Bi3^{xiii}—Mn1—Bi3^{xiv}	115.25 (2)
Rh1—Bi2—Bi5	134.64 (4)	Bi3^{x}—Mn1—Bi3^{xiv}	64.75 (2)
Mn2—Bi2—Bi5	56.35 (6)	Bi3^{vi}—Mn1—Bi3^{xiv}	97.28 (2)
Mn3^{vi}—Bi2—Bi5	95.97 (7)	Rh1—Mn1—Bi3^{ix}	57.625 (11)
Mn3^{vii}—Bi2—Bi5	95.97 (7)	Rh1^{xi}—Mn1—Bi3^{ix}	122.375 (12)
Bi3^{vii}—Bi2—Bi5	143.415 (13)	Bi3^{xii}—Mn1—Bi3^{ix}	64.75 (2)
Bi3^{vi}—Bi2—Bi5	143.415 (13)	Bi3^{xiii}—Mn1—Bi3^{ix}	97.28 (2)
Bi4^{vi}—Bi2—Bi5	56.262 (17)	Bi3^{x}—Mn1—Bi3^{ix}	82.72 (2)
Bi4^{vii}—Bi2—Bi5	56.262 (16)	Bi3^{vi}—Mn1—Bi3^{ix}	115.25 (2)
Rh1^{ii}—Bi3—Rh1^{iii}	94.91 (4)	Bi3^{xiv}—Mn1—Bi3^{ix}	116.53 (2)
Rh1^{ii}—Bi3—Mn1^{ii}	52.05 (4)	Rh1—Mn1—Bi3^{vii}	57.625 (12)
Rh1^{iii}—Bi3—Mn1^{ii}	111.02 (3)	Rh1^{xi}—Mn1—Bi3^{vii}	122.375 (12)
Rh1^{ii}—Bi3—Mn1^{iii}	111.02 (3)	Bi3^{xii}—Mn1—Bi3^{vii}	97.28 (2)
Rh1^{iii}—Bi3—Mn1^{iii}	52.05 (4)	Bi3^{xiii}—Mn1—Bi3^{vii}	64.75 (2)
Mn1^{ii}—Bi3—Mn1^{iii}	82.72 (2)	Bi3^{x}—Mn1—Bi3^{vii}	115.25 (2)
Rh1^{ii}—Bi3—Mn3	53.61 (4)	Bi3^{vi}—Mn1—Bi3^{vii}	82.72 (2)
Rh1^{iii}—Bi3—Mn3	53.61 (4)	Bi3^{xiv}—Mn1—Bi3^{vii}	180.000 (15)
Mn1^{ii}—Bi3—Mn3	100.50 (3)	Bi3^{ix}—Mn1—Bi3^{vii}	63.47 (2)
Mn1^{iii}—Bi3—Mn3	100.50 (3)	Rh1—Mn1—Bi3^{xv}	122.375 (12)
Rh1^{ii}—Bi3—Bi3^{i}	54.097 (16)	Rh1^{xi}—Mn1—Bi3^{xv}	57.625 (11)
Rh1^{iii}—Bi3—Bi3^{i}	54.097 (16)	Bi3^{xii}—Mn1—Bi3^{xv}	115.25 (2)
Mn1^{ii}—Bi3—Bi3^{i}	58.268 (12)	Bi3^{xiii}—Mn1—Bi3^{xv}	82.72 (2)
Mn1^{iii}—Bi3—Bi3^{i}	58.268 (12)	Bi3^{x}—Mn1—Bi3^{xv}	97.28 (2)
Mn3—Bi3—Bi3^{i}	58.53 (4)	Bi3^{vi}—Mn1—Bi3^{xv}	64.75 (2)
Rh1^{ii}—Bi3—Bi3^{viii}	109.67 (4)	Bi3^{xiv}—Mn1—Bi3^{xv}	63.47 (2)
Rh1^{iii}—Bi3—Bi3^{viii}	109.67 (4)	Bi3^{ix}—Mn1—Bi3^{xv}	180.00 (3)
Mn1^{ii}—Bi3—Bi3^{viii}	57.625 (11)	Bi3^{vii}—Mn1—Bi3^{xv}	116.53 (2)
Mn1^{iii}—Bi3—Bi3^{viii}	57.625 (11)	Rh2^{vi}—Mn2—Rh2^{vii}	98.35 (5)
Mn3—Bi3—Bi3^{viii}	148.53 (4)	Rh2^{vi}—Mn2—Rh2^{x}	81.63 (5)
Bi3^{i}—Bi3—Bi3^{viii}	90.0	Rh2^{vii}—Mn2—Rh2^{x}	178.50 (17)
Rh1^{ii}—Bi3—Bi5	117.76 (2)	Rh2^{vi}—Mn2—Rh2^{ix}	178.50 (17)
Rh1^{iii}—Bi3—Bi5	117.76 (2)	Rh2^{vii}—Mn2—Rh2^{ix}	81.63 (5)
Mn1^{ii}—Bi3—Bi5	131.073 (15)	Rh2^{x}—Mn2—Rh2^{ix}	98.35 (5)
Mn1^{iii}—Bi3—Bi5	131.073 (15)	Rh2^{vi}—Mn2—Mn3^{vii}	123.81 (11)
Mn3—Bi3—Bi5	104.87 (4)	Rh2^{vii}—Mn2—Mn3^{vii}	57.43 (5)
Bi3^{i}—Bi3—Bi5	163.398 (15)	Rh2^{x}—Mn2—Mn3^{vii}	123.81 (11)

Bi3^{viii}—Bi3—Bi5	106.601 (15)	Rh2^{ix}—Mn2—Mn3^{vii}	57.43 (5)
Rh1^{ii}—Bi3—Bi2^{iii}	105.90 (4)	Rh2^{vi}—Mn2—Mn3^{vi}	57.43 (5)
Rh1^{iii}—Bi3—Bi2^{iii}	53.69 (3)	Rh2^{vii}—Mn2—Mn3^{vi}	123.81 (11)
Mn1^{ii}—Bi3—Bi2^{iii}	154.95 (2)	Rh2^{x}—Mn2—Mn3^{vi}	57.43 (5)
Mn1^{iii}—Bi3—Bi2^{iii}	97.415 (18)	Rh2^{ix}—Mn2—Mn3^{vi}	123.81 (11)
Mn3—Bi3—Bi2^{iii}	54.70 (3)	Mn3^{vii}—Mn2—Mn3^{vi}	92.68 (15)
Bi3^{i}—Bi3—Bi2^{iii}	100.440 (14)	Rh2^{vi}—Mn2—Bi2^{viii}	120.79 (9)
Bi3^{viii}—Bi3—Bi2^{iii}	142.039 (13)	Rh2^{vii}—Mn2—Bi2^{viii}	120.79 (9)
Bi5—Bi3—Bi2^{iii}	66.489 (17)	Rh2^{x}—Mn2—Bi2^{viii}	60.31 (4)
Rh1^{ii}—Bi3—Bi2^{ii}	53.69 (3)	Rh2^{ix}—Mn2—Bi2^{viii}	60.31 (4)
Rh1^{iii}—Bi3—Bi2^{ii}	105.90 (4)	Mn3^{vii}—Mn2—Bi2^{viii}	63.89 (7)
Mn1^{ii}—Bi3—Bi2^{ii}	97.415 (18)	Mn3^{vi}—Mn2—Bi2^{viii}	63.89 (7)
Mn1^{iii}—Bi3—Bi2^{ii}	154.95 (2)	Rh2^{vi}—Mn2—Bi2	60.31 (4)
Mn3—Bi3—Bi2^{ii}	54.70 (3)	Rh2^{vii}—Mn2—Bi2	60.31 (4)
Bi3^{i}—Bi3—Bi2^{ii}	100.440 (14)	Rh2^{x}—Mn2—Bi2	120.79 (9)
Bi3^{viii}—Bi3—Bi2^{ii}	142.039 (13)	Rh2^{ix}—Mn2—Bi2	120.79 (9)
Bi5—Bi3—Bi2^{ii}	66.489 (17)	Mn3^{vii}—Mn2—Bi2	63.89 (7)
Bi2^{iii}—Bi3—Bi2^{ii}	72.00 (2)	Mn3^{vi}—Mn2—Bi2	63.89 (7)
Rh2—Bi4—Bi5^{ii}	52.92 (2)	Bi2^{viii}—Mn2—Bi2	100.79 (11)
Rh2—Bi4—Bi5^{iii}	52.92 (2)	Rh2^{vi}—Mn2—Bi1^{vi}	58.16 (5)
Bi5^{ii}—Bi4—Bi5^{iii}	75.57 (3)	Rh2^{vii}—Mn2—Bi1^{vi}	120.56 (10)
Rh2—Bi4—Bi4^{vii}	132.55 (3)	Rh2^{x}—Mn2—Bi1^{vi}	58.16 (5)
Bi5^{ii}—Bi4—Bi4^{vii}	173.51 (3)	Rh2^{ix}—Mn2—Bi1^{vi}	120.56 (10)
Bi5^{iii}—Bi4—Bi4^{vii}	104.875 (19)	Mn3^{vii}—Mn2—Bi1^{vi}	176.85 (12)
Rh2—Bi4—Bi4^{vi}	132.55 (3)	Mn3^{vi}—Mn2—Bi1^{vi}	90.47 (6)
Bi5^{ii}—Bi4—Bi4^{vi}	104.875 (19)	Bi2^{viii}—Mn2—Bi1^{vi}	117.694 (15)
Bi5^{iii}—Bi4—Bi4^{vi}	173.51 (3)	Bi2—Mn2—Bi1^{vi}	117.694 (15)
Bi4^{vii}—Bi4—Bi4^{vi}	73.93 (3)	Rh2^{vi}—Mn2—Bi1^{vii}	120.56 (10)
Rh2—Bi4—Bi4^{iii}	115.18 (3)	Rh2^{vii}—Mn2—Bi1^{vii}	58.16 (5)
Bi5^{ii}—Bi4—Bi4^{iii}	106.23 (3)	Rh2^{x}—Mn2—Bi1^{vii}	120.56 (10)
Bi5^{iii}—Bi4—Bi4^{iii}	62.78 (2)	Rh2^{ix}—Mn2—Bi1^{vii}	58.16 (5)
Bi4^{vii}—Bi4—Bi4^{iii}	68.803 (14)	Mn3^{vii}—Mn2—Bi1^{vii}	90.47 (6)
Bi4^{vi}—Bi4—Bi4^{iii}	111.197 (14)	Mn3^{vi}—Mn2—Bi1^{vii}	176.85 (12)
Rh2—Bi4—Bi4^{ii}	115.18 (3)	Bi2^{viii}—Mn2—Bi1^{vii}	117.694 (15)
Bi5^{ii}—Bi4—Bi4^{ii}	62.78 (2)	Bi2—Mn2—Bi1^{vii}	117.694 (15)
Bi5^{iii}—Bi4—Bi4^{ii}	106.23 (3)	Bi1^{vi}—Mn2—Bi1^{vii}	86.39 (10)
Bi4^{vii}—Bi4—Bi4^{ii}	111.197 (14)	Rh2^{vi}—Mn2—Bi5^{viii}	122.89 (8)
Bi4^{vi}—Bi4—Bi4^{ii}	68.803 (14)	Rh2^{vii}—Mn2—Bi5^{viii}	122.89 (8)
Bi4^{iii}—Bi4—Bi4^{ii}	73.93 (3)	Rh2^{x}—Mn2—Bi5^{viii}	56.14 (4)
Rh2—Bi4—Bi2^{ii}	52.23 (2)	Rh2^{ix}—Mn2—Bi5^{viii}	56.14 (4)
Bi5^{ii}—Bi4—Bi2^{ii}	62.953 (18)	Mn3^{vii}—Mn2—Bi5^{viii}	111.89 (3)
Bi5^{iii}—Bi4—Bi2^{ii}	105.11 (3)	Mn3^{vi}—Mn2—Bi5^{viii}	111.89 (3)
Bi4^{vii}—Bi4—Bi2^{ii}	122.58 (3)	Bi2^{viii}—Mn2—Bi5^{viii}	72.295 (17)
Bi4^{vi}—Bi4—Bi2^{ii}	80.58 (2)	Bi2—Mn2—Bi5^{viii}	173.09 (11)
Bi4^{iii}—Bi4—Bi2^{ii}	166.43 (3)	Bi1^{vi}—Mn2—Bi5^{viii}	66.81 (6)
Bi4^{ii}—Bi4—Bi2^{ii}	105.67 (2)	Bi1^{vii}—Mn2—Bi5^{viii}	66.81 (6)
Rh2—Bi4—Bi2^{iii}	52.23 (2)	Rh2^{vi}—Mn2—Bi5	56.14 (4)
Bi5^{ii}—Bi4—Bi2^{iii}	105.11 (3)	Rh2^{vii}—Mn2—Bi5	56.14 (4)

Bi5^{iii}—Bi4—Bi2^{iii}	62.953 (18)	Rh2^{x}—Mn2—Bi5	122.89 (8)
Bi4^{vii}—Bi4—Bi2^{iii}	80.58 (2)	Rh2^{ix}—Mn2—Bi5	122.89 (8)
Bi4^{vi}—Bi4—Bi2^{iii}	122.58 (3)	Mn3^{vii}—Mn2—Bi5	111.89 (3)
Bi4^{iii}—Bi4—Bi2^{iii}	105.67 (2)	Mn3^{vi}—Mn2—Bi5	111.89 (3)
Bi4^{ii}—Bi4—Bi2^{iii}	166.43 (3)	Bi2^{viii}—Mn2—Bi5	173.09 (11)
Bi2^{ii}—Bi4—Bi2^{iii}	71.44 (2)	Bi2—Mn2—Bi5	72.295 (17)
Rh2—Bi4—Bi5	99.75 (4)	Bi1^{vi}—Mn2—Bi5	66.81 (6)
Bi5^{ii}—Bi4—Bi5	127.277 (17)	Bi1^{vii}—Mn2—Bi5	66.81 (6)
Bi5^{iii}—Bi4—Bi5	127.277 (17)	Bi5^{viii}—Mn2—Bi5	114.62 (12)
Bi4^{vii}—Bi4—Bi5	57.73 (2)	Rh2^{i}—Mn3—Rh2	83.27 (12)
Bi4^{vi}—Bi4—Bi5	57.73 (2)	Rh2^{i}—Mn3—Rh1^{ii}	118.81 (3)
Bi4^{iii}—Bi4—Bi5	126.471 (17)	Rh2—Mn3—Rh1^{ii}	118.81 (3)
Bi4^{ii}—Bi4—Bi5	126.471 (17)	Rh2^{i}—Mn3—Rh1^{iii}	118.81 (3)
Bi2^{ii}—Bi4—Bi5	65.072 (17)	Rh2—Mn3—Rh1^{iii}	118.81 (3)
Bi2^{iii}—Bi4—Bi5	65.072 (17)	Rh1^{ii}—Mn3—Rh1^{iii}	99.69 (13)
Rh2^{vii}—Bi5—Rh2^{vi}	95.33 (5)	Rh2^{i}—Mn3—Mn2^{ii}	58.93 (7)
Rh2^{vii}—Bi5—Mn2	54.21 (3)	Rh2—Mn3—Mn2^{ii}	58.94 (7)
Rh2^{vi}—Bi5—Mn2	54.21 (4)	Rh1^{ii}—Mn3—Mn2^{ii}	83.82 (7)
Rh2^{vii}—Bi5—Bi4^{vii}	52.82 (3)	Rh1^{iii}—Mn3—Mn2^{ii}	176.49 (13)
Rh2^{vi}—Bi5—Bi4^{vii}	107.55 (4)	Rh2^{i}—Mn3—Mn2^{iii}	58.93 (7)
Mn2—Bi5—Bi4^{vii}	100.41 (5)	Rh2—Mn3—Mn2^{iii}	58.93 (7)
Rh2^{vii}—Bi5—Bi4^{vi}	107.55 (4)	Rh1^{ii}—Mn3—Mn2^{iii}	176.49 (13)
Rh2^{vi}—Bi5—Bi4^{vi}	52.82 (3)	Rh1^{iii}—Mn3—Mn2^{iii}	83.82 (7)
Mn2—Bi5—Bi4^{vi}	100.41 (5)	Mn2^{ii}—Mn3—Mn2^{iii}	92.67 (15)
Bi4^{vii}—Bi5—Bi4^{vi}	75.57 (3)	Rh2^{i}—Mn3—Bi2^{iv}	59.16 (3)
Rh2^{vii}—Bi5—Bi1^{vi}	107.02 (3)	Rh2—Mn3—Bi2^{iv}	118.15 (9)
Rh2^{vi}—Bi5—Bi1^{vi}	52.75 (3)	Rh1^{ii}—Mn3—Bi2^{iv}	60.31 (3)
Mn2—Bi5—Bi1^{vi}	54.67 (4)	Rh1^{iii}—Mn3—Bi2^{iv}	122.04 (8)
Bi4^{vii}—Bi5—Bi1^{vi}	153.59 (3)	Mn2^{ii}—Mn3—Bi2^{iv}	59.72 (4)
Bi4^{vi}—Bi5—Bi1^{vi}	98.70 (2)	Mn2^{iii}—Mn3—Bi2^{iv}	117.81 (9)
Rh2^{vii}—Bi5—Bi1^{vii}	52.75 (3)	Rh2^{i}—Mn3—Bi2^{iii}	118.15 (9)
Rh2^{vi}—Bi5—Bi1^{vii}	107.02 (3)	Rh2—Mn3—Bi2^{iii}	59.16 (3)
Mn2—Bi5—Bi1^{vii}	54.67 (4)	Rh1^{ii}—Mn3—Bi2^{iii}	122.04 (8)
Bi4^{vii}—Bi5—Bi1^{vii}	98.70 (2)	Rh1^{iii}—Mn3—Bi2^{iii}	60.31 (3)
Bi4^{vi}—Bi5—Bi1^{vii}	153.59 (3)	Mn2^{ii}—Mn3—Bi2^{iii}	117.81 (9)
Bi1^{vi}—Bi5—Bi1^{vii}	74.81 (2)	Mn2^{iii}—Mn3—Bi2^{iii}	59.72 (4)
Rh2^{vii}—Bi5—Bi3	118.89 (3)	Bi2^{iv}—Mn3—Bi2^{iii}	176.87 (14)
Rh2^{vi}—Bi5—Bi3	118.89 (3)	Rh2^{i}—Mn3—Bi2^{v}	59.16 (3)
Mn2—Bi5—Bi3	106.09 (6)	Rh2—Mn3—Bi2^{v}	118.15 (9)
Bi4^{vii}—Bi5—Bi3	133.563 (18)	Rh1^{ii}—Mn3—Bi2^{v}	122.04 (8)
Bi4^{vi}—Bi5—Bi3	133.563 (18)	Rh1^{iii}—Mn3—Bi2^{v}	60.31 (3)
Bi1^{vi}—Bi5—Bi3	68.72 (2)	Mn2^{ii}—Mn3—Bi2^{v}	117.81 (9)
Bi1^{vii}—Bi5—Bi3	68.72 (2)	Mn2^{iii}—Mn3—Bi2^{v}	59.72 (4)
Rh2^{vii}—Bi5—Bi4	111.83 (3)	Bi2^{iv}—Mn3—Bi2^{v}	84.29 (2)
Rh2^{vi}—Bi5—Bi4	111.83 (3)	Bi2^{iii}—Mn3—Bi2^{v}	95.62 (2)
Mn2—Bi5—Bi4	153.25 (6)	Rh2^{i}—Mn3—Bi2^{ii}	118.15 (9)
Bi4^{vii}—Bi5—Bi4	59.49 (2)	Rh2—Mn3—Bi2^{ii}	59.16 (3)
Bi4^{vi}—Bi5—Bi4	59.49 (2)	Rh1^{ii}—Mn3—Bi2^{ii}	60.31 (3)

Bi1^{vi}—Bi5—Bi4	139.601 (14)	Rh1^{iii}—Mn3—Bi2^{ii}	122.04 (8)
Bi1^{vii}—Bi5—Bi4	139.601 (14)	Mn2^{ii}—Mn3—Bi2^{ii}	59.72 (4)
Bi3—Bi5—Bi4	100.66 (2)	Mn2^{iii}—Mn3—Bi2^{ii}	117.81 (9)
Rh2^{vii}—Bi5—Bi2	51.24 (3)	Bi2^{iv}—Mn3—Bi2^{ii}	95.62 (2)
Rh2^{vi}—Bi5—Bi2	51.24 (3)	Bi2^{iii}—Mn3—Bi2^{ii}	84.29 (2)
Mn2—Bi5—Bi2	51.36 (6)	Bi2^{v}—Mn3—Bi2^{ii}	176.87 (14)
Bi4^{vii}—Bi5—Bi2	60.784 (18)	Rh2^{i}—Mn3—Bi3	169.83 (9)
Bi4^{vi}—Bi5—Bi2	60.784 (18)	Rh2—Mn3—Bi3	106.90 (4)
Bi1^{vi}—Bi5—Bi2	93.68 (2)	Rh1^{ii}—Mn3—Bi3	56.63 (6)
Bi1^{vii}—Bi5—Bi2	93.68 (2)	Rh1^{iii}—Mn3—Bi3	56.63 (6)
Bi3—Bi5—Bi2	157.45 (3)	Mn2^{ii}—Mn3—Bi3	126.08 (5)
Bi4—Bi5—Bi2	101.89 (2)	Mn2^{iii}—Mn3—Bi3	126.08 (5)
Mn1—Rh1—Mn3^{vi}	130.15 (6)	Bi2^{iv}—Mn3—Bi3	114.21 (9)
Mn1—Rh1—Mn3^{vii}	130.15 (6)	Bi2^{iii}—Mn3—Bi3	68.69 (4)
Mn3^{vi}—Rh1—Mn3^{vii}	99.69 (13)	Bi2^{v}—Mn3—Bi3	114.21 (9)
Mn1—Rh1—Bi3^{ix}	70.33 (4)	Bi2^{ii}—Mn3—Bi3	68.69 (4)
Mn3^{vi}—Rh1—Bi3^{ix}	141.27 (4)	Rh2^{i}—Mn3—Bi3^{i}	106.90 (4)
Mn3^{vii}—Rh1—Bi3^{ix}	69.75 (5)	Rh2—Mn3—Bi3^{i}	169.83 (9)
Mn1—Rh1—Bi3^{vii}	70.33 (4)	Rh1^{ii}—Mn3—Bi3^{i}	56.63 (6)
Mn3^{vi}—Rh1—Bi3^{vii}	141.27 (4)	Rh1^{iii}—Mn3—Bi3^{i}	56.63 (6)
Mn3^{vii}—Rh1—Bi3^{vii}	69.75 (5)	Mn2^{ii}—Mn3—Bi3^{i}	126.08 (5)
Bi3^{ix}—Rh1—Bi3^{vii}	71.81 (3)	Mn2^{iii}—Mn3—Bi3^{i}	126.08 (5)
Mn1—Rh1—Bi3^{x}	70.33 (4)	Bi2^{iv}—Mn3—Bi3^{i}	68.69 (4)
Mn3^{vi}—Rh1—Bi3^{x}	69.75 (5)	Bi2^{iii}—Mn3—Bi3^{i}	114.21 (9)
Mn3^{vii}—Rh1—Bi3^{x}	141.27 (4)	Bi2^{v}—Mn3—Bi3^{i}	68.69 (4)
Bi3^{ix}—Rh1—Bi3^{x}	94.91 (4)	Bi2^{ii}—Mn3—Bi3^{i}	114.21 (9)
Bi3^{vii}—Rh1—Bi3^{x}	140.66 (8)	Bi3—Mn3—Bi3^{i}	62.94 (7)
Mn1—Rh1—Bi3^{vi}	70.33 (4)		

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

Rhodium manganese tribismuthide (RhMnBi3)

Crystal data

$RhMnBi_3$	D_x = 10.369 Mg m^{-3}
M_r = 784.79	Mo $K\alpha$ radiation, λ = 0.71073 Å
Orthorhombic, *Cmmm*	Cell parameters from 3699 reflections
a = 8.885 (3) Å	θ = 3–34.9°
b = 13.696 (6) Å	μ = 110.13 mm^{-1}
c = 4.1310 (12) Å	*T* = 293 K
V = 502.7 (3) Å^3	Irregular, gray
Z = 4	0.10 × 0.05 × 0.03 mm
F(000) = 1276	

Data collection

Nonius KappaCCD diffractometer	T_{min} = 0.003, T_{max} = 0.005
Radiation source: Nonius	3699 measured reflections
ω scans	667 independent reflections
Absorption correction: multi-scan	522 reflections with $I > 2\sigma(I)$
	R_{int} = 0.141

θ_{max} = 35.0°, θ_{min} = 2.7°
h = −14→14
k = −22→21
l = −6→6

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.094
$wR(F^2)$ = 0.257
S = 1.19
667 reflections
21 parameters
0 restraints
$w = 1/[\sigma^2(F_o^2) + (0.150P)^2 + 14.P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 11.68 e Å^{-3}
$\Delta\rho_{min}$ = −8.87 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Bi1	0.0000	0.33689 (14)	0.0000	0.0279 (5)
Bi2	0.19449 (14)	0.12399 (10)	0.5000	0.0263 (4)
Mn1	0.5000	0.0000	0.5000	0.026 (2)
Mn2	0.0000	0.0000	0.0000	0.033 (2)
Rh1	0.3016 (4)	0.0000	0.0000	0.0240 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Bi1	0.0201 (8)	0.0243 (9)	0.0393 (10)	0.000	0.000	0.000
Bi2	0.0223 (7)	0.0263 (7)	0.0302 (7)	0.0019 (4)	0.000	0.000
Mn1	0.007 (3)	0.045 (6)	0.027 (5)	0.000	0.000	0.000
Mn2	0.025 (5)	0.034 (6)	0.039 (6)	0.000	0.000	0.000
Rh1	0.0172 (15)	0.0288 (18)	0.0260 (16)	0.000	0.000	0.000

Geometric parameters (Å, º)

Bi1—Rh1^{i}	2.846 (3)	Mn1—Bi1^{xii}	3.0426 (16)
Bi1—Rh1^{ii}	2.846 (3)	Mn1—Bi1^{iv}	3.0426 (16)
Bi1—Mn1^{ii}	3.0425 (16)	Mn1—Bi1^{xiii}	3.0426 (16)
Bi1—Mn1^{iii}	3.0425 (16)	Mn1—Bi1^{i}	3.0426 (16)
Bi1—Bi2^{iv}	3.4527 (13)	Mn1—Bi2^{xiv}	3.2018 (15)
Bi1—Bi2^{v}	3.4527 (13)	Mn1—Bi2^{viii}	3.2018 (15)
Bi1—Bi2^{i}	3.4527 (13)	Mn1—Bi2^{x}	3.2018 (15)
Bi1—Bi2^{vi}	3.4527 (13)	Mn2—Rh1	2.680 (4)
Bi2—Rh1	2.8383 (16)	Mn2—Rh1^{xv}	2.680 (4)
Bi2—Rh1^{vii}	2.8383 (16)	Mn2—Bi2^{xv}	3.1837 (12)
Bi2—Mn2	3.1837 (12)	Mn2—Bi2^{viii}	3.1837 (12)
Bi2—Mn2^{vii}	3.1837 (12)	Mn2—Bi2^{xvi}	3.1837 (12)

Bi2—Mn1	3.2018 (15)	Mn2—Bi2^{xvii}	3.1837 (12)
Bi2—Bi2^{viii}	3.396 (3)	Mn2—Bi2^{ix}	3.1837 (12)
Bi2—Bi1^{iv}	3.4528 (13)	Mn2—Bi2^{xviii}	3.1837 (12)
Bi2—Bi1^{i}	3.4528 (13)	Mn2—Bi2^{xix}	3.1837 (12)
Bi2—Bi2^{ix}	3.456 (3)	Rh1—Mn1^{xviii}	2.715 (2)
Bi2—Bi2^{iv}	3.590 (3)	Rh1—Bi2^{xvii}	2.8383 (16)
Mn1—Rh1^{x}	2.715 (2)	Rh1—Bi2^{xviii}	2.8383 (16)
Mn1—Rh1^{xi}	2.715 (2)	Rh1—Bi2^{viii}	2.8383 (16)
Mn1—Rh1^{vii}	2.715 (2)	Rh1—Bi1^{i}	2.846 (3)
Mn1—Rh1	2.715 (2)	Rh1—Bi1^{xii}	2.846 (3)

Rh1^{i}—Bi1—Rh1^{ii}	76.55 (12)	Rh1^{xi}—Mn1—Bi2^{viii}	123.39 (5)
Rh1^{i}—Bi1—Mn1^{ii}	54.80 (5)	Rh1^{vii}—Mn1—Bi2^{viii}	56.61 (5)
Rh1^{ii}—Bi1—Mn1^{ii}	54.80 (5)	Rh1—Mn1—Bi2^{viii}	56.61 (5)
Rh1^{i}—Bi1—Mn1^{iii}	54.80 (5)	Bi1^{xii}—Mn1—Bi2^{viii}	67.08 (2)
Rh1^{ii}—Bi1—Mn1^{iii}	54.80 (5)	Bi1^{iv}—Mn1—Bi2^{viii}	112.92 (2)
Mn1^{ii}—Bi1—Mn1^{iii}	85.51 (6)	Bi1^{xiii}—Mn1—Bi2^{viii}	67.08 (2)
Rh1^{i}—Bi1—Bi2^{iv}	52.50 (5)	Bi1^{i}—Mn1—Bi2^{viii}	112.92 (2)
Rh1^{ii}—Bi1—Bi2^{iv}	111.41 (7)	Bi2^{xiv}—Mn1—Bi2^{viii}	180.00 (4)
Mn1^{ii}—Bi1—Bi2^{iv}	58.66 (3)	Rh1^{x}—Mn1—Bi2^{x}	56.61 (5)
Mn1^{iii}—Bi1—Bi2^{iv}	106.99 (5)	Rh1^{xi}—Mn1—Bi2^{x}	56.61 (5)
Rh1^{i}—Bi1—Bi2^{v}	111.41 (7)	Rh1^{vii}—Mn1—Bi2^{x}	123.39 (5)
Rh1^{ii}—Bi1—Bi2^{v}	52.50 (5)	Rh1—Mn1—Bi2^{x}	123.39 (5)
Mn1^{ii}—Bi1—Bi2^{v}	106.99 (5)	Bi1^{xii}—Mn1—Bi2^{x}	67.08 (2)
Mn1^{iii}—Bi1—Bi2^{v}	58.66 (3)	Bi1^{iv}—Mn1—Bi2^{x}	112.92 (2)
Bi2^{iv}—Bi1—Bi2^{v}	162.14 (8)	Bi1^{xiii}—Mn1—Bi2^{x}	67.08 (2)
Rh1^{i}—Bi1—Bi2^{i}	52.50 (5)	Bi1^{i}—Mn1—Bi2^{x}	112.92 (2)
Rh1^{ii}—Bi1—Bi2^{i}	111.41 (7)	Bi2^{xiv}—Mn1—Bi2^{x}	64.06 (6)
Mn1^{ii}—Bi1—Bi2^{i}	106.99 (5)	Bi2^{viii}—Mn1—Bi2^{x}	115.94 (6)
Mn1^{iii}—Bi1—Bi2^{i}	58.66 (3)	Rh1^{x}—Mn1—Bi2	123.39 (5)
Bi2^{iv}—Bi1—Bi2^{i}	73.48 (3)	Rh1^{xi}—Mn1—Bi2	123.39 (5)
Bi2^{v}—Bi1—Bi2^{i}	103.66 (4)	Rh1^{vii}—Mn1—Bi2	56.61 (5)
Rh1^{i}—Bi1—Bi2^{vi}	111.41 (7)	Rh1—Mn1—Bi2	56.61 (5)
Rh1^{ii}—Bi1—Bi2^{vi}	52.50 (5)	Bi1^{xii}—Mn1—Bi2	112.92 (2)
Mn1^{ii}—Bi1—Bi2^{vi}	58.66 (3)	Bi1^{iv}—Mn1—Bi2	67.08 (2)
Mn1^{iii}—Bi1—Bi2^{vi}	106.99 (5)	Bi1^{xiii}—Mn1—Bi2	112.92 (2)
Bi2^{iv}—Bi1—Bi2^{vi}	103.66 (4)	Bi1^{i}—Mn1—Bi2	67.08 (2)
Bi2^{v}—Bi1—Bi2^{vi}	73.48 (4)	Bi2^{xiv}—Mn1—Bi2	115.94 (6)
Bi2^{i}—Bi1—Bi2^{vi}	162.14 (8)	Bi2^{viii}—Mn1—Bi2	64.06 (6)
Rh1—Bi2—Rh1^{vii}	93.39 (7)	Bi2^{x}—Mn1—Bi2	180.0
Rh1—Bi2—Mn2	52.47 (7)	Rh1—Mn2—Rh1^{xv}	180.0
Rh1^{vii}—Bi2—Mn2	109.57 (6)	Rh1—Mn2—Bi2^{xv}	122.87 (2)
Rh1—Bi2—Mn2^{vii}	109.57 (6)	Rh1^{xv}—Mn2—Bi2^{xv}	57.13 (2)
Rh1^{vii}—Bi2—Mn2^{vii}	52.47 (7)	Rh1—Mn2—Bi2^{viii}	57.13 (2)
Mn2—Bi2—Mn2^{vii}	80.90 (4)	Rh1^{xv}—Mn2—Bi2^{viii}	122.87 (2)
Rh1—Bi2—Mn1	53.01 (6)	Bi2^{xv}—Mn2—Bi2^{viii}	115.53 (5)
Rh1^{vii}—Bi2—Mn1	53.01 (6)	Rh1—Mn2—Bi2^{xvi}	122.87 (2)
Mn2—Bi2—Mn1	100.21 (4)	Rh1^{xv}—Mn2—Bi2^{xvi}	57.13 (2)

Mn2^{vii}—Bi2—Mn1	100.21 (4)	Bi2^{xv}—Mn2—Bi2^{xvi}	64.47 (5)
Rh1—Bi2—Bi2^{viii}	53.25 (3)	Bi2^{viii}—Mn2—Bi2^{xvi}	180.00 (4)
Rh1^{vii}—Bi2—Bi2^{viii}	53.25 (3)	Rh1—Mn2—Bi2^{xvii}	57.13 (2)
Mn2—Bi2—Bi2^{viii}	57.77 (2)	Rh1^{xv}—Mn2—Bi2^{xvii}	122.87 (2)
Mn2^{vii}—Bi2—Bi2^{viii}	57.77 (2)	Bi2^{xv}—Mn2—Bi2^{xvii}	65.75 (5)
Mn1—Bi2—Bi2^{viii}	57.97 (3)	Bi2^{viii}—Mn2—Bi2^{xvii}	80.90 (4)
Rh1—Bi2—Bi1^{iv}	105.34 (8)	Bi2^{xvi}—Mn2—Bi2^{xvii}	99.10 (4)
Rh1^{vii}—Bi2—Bi1^{iv}	52.69 (6)	Rh1—Mn2—Bi2^{ix}	122.87 (2)
Mn2—Bi2—Bi1^{iv}	153.84 (5)	Rh1^{xv}—Mn2—Bi2^{ix}	57.13 (2)
Mn2^{vii}—Bi2—Bi1^{iv}	96.97 (3)	Bi2^{xv}—Mn2—Bi2^{ix}	114.25 (5)
Mn1—Bi2—Bi1^{iv}	54.26 (3)	Bi2^{viii}—Mn2—Bi2^{ix}	99.10 (4)
Bi2^{viii}—Bi2—Bi1^{iv}	98.93 (4)	Bi2^{xvi}—Mn2—Bi2^{ix}	80.90 (4)
Rh1—Bi2—Bi1^{i}	52.69 (6)	Bi2^{xvii}—Mn2—Bi2^{ix}	180.00 (6)
Rh1^{vii}—Bi2—Bi1^{i}	105.34 (8)	Rh1—Mn2—Bi2^{xviii}	57.13 (2)
Mn2—Bi2—Bi1^{i}	96.97 (3)	Rh1^{xv}—Mn2—Bi2^{xviii}	122.87 (2)
Mn2^{vii}—Bi2—Bi1^{i}	153.84 (5)	Bi2^{xv}—Mn2—Bi2^{xviii}	99.10 (4)
Mn1—Bi2—Bi1^{i}	54.26 (3)	Bi2^{viii}—Mn2—Bi2^{xviii}	114.25 (5)
Bi2^{viii}—Bi2—Bi1^{i}	98.93 (4)	Bi2^{xvi}—Mn2—Bi2^{xviii}	65.75 (5)
Bi1^{iv}—Bi2—Bi1^{i}	73.48 (4)	Bi2^{xvii}—Mn2—Bi2^{xviii}	64.47 (5)
Rh1—Bi2—Bi2^{ix}	109.59 (7)	Bi2^{ix}—Mn2—Bi2^{xviii}	115.53 (5)
Rh1^{vii}—Bi2—Bi2^{ix}	109.59 (7)	Rh1—Mn2—Bi2^{xix}	122.87 (2)
Mn2—Bi2—Bi2^{ix}	57.13 (2)	Rh1^{xv}—Mn2—Bi2^{xix}	57.13 (2)
Mn2^{vii}—Bi2—Bi2^{ix}	57.13 (2)	Bi2^{xv}—Mn2—Bi2^{xix}	80.90 (4)
Mn1—Bi2—Bi2^{ix}	147.97 (3)	Bi2^{viii}—Mn2—Bi2^{xix}	65.75 (5)
Bi2^{viii}—Bi2—Bi2^{ix}	90.000 (1)	Bi2^{xvi}—Mn2—Bi2^{xix}	114.25 (5)
Bi1^{iv}—Bi2—Bi2^{ix}	141.828 (19)	Bi2^{xvii}—Mn2—Bi2^{xix}	115.53 (5)
Bi1^{i}—Bi2—Bi2^{ix}	141.828 (19)	Bi2^{ix}—Mn2—Bi2^{xix}	64.47 (5)
Rh1—Bi2—Bi2^{iv}	118.89 (5)	Bi2^{xviii}—Mn2—Bi2^{xix}	180.00 (4)
Rh1^{vii}—Bi2—Bi2^{iv}	118.89 (5)	Rh1—Mn2—Bi2	57.13 (2)
Mn2—Bi2—Bi2^{iv}	131.45 (3)	Rh1^{xv}—Mn2—Bi2	122.87 (2)
Mn2^{vii}—Bi2—Bi2^{iv}	131.45 (3)	Bi2^{xv}—Mn2—Bi2	180.0
Mn1—Bi2—Bi2^{iv}	106.08 (5)	Bi2^{viii}—Mn2—Bi2	64.47 (5)
Bi2^{viii}—Bi2—Bi2^{iv}	164.05 (4)	Bi2^{xvi}—Mn2—Bi2	115.53 (5)
Bi1^{iv}—Bi2—Bi2^{iv}	68.58 (4)	Bi2^{xvii}—Mn2—Bi2	114.25 (5)
Bi1^{i}—Bi2—Bi2^{iv}	68.58 (4)	Bi2^{ix}—Mn2—Bi2	65.75 (5)
Bi2^{ix}—Bi2—Bi2^{iv}	105.95 (4)	Bi2^{xviii}—Mn2—Bi2	80.90 (4)
Rh1^{x}—Mn1—Rh1^{xi}	99.05 (12)	Bi2^{xix}—Mn2—Bi2	99.10 (4)
Rh1^{x}—Mn1—Rh1^{vii}	80.95 (12)	Mn2—Rh1—Mn1	130.48 (6)
Rh1^{xi}—Mn1—Rh1^{vii}	180.0	Mn2—Rh1—Mn1^{xviii}	130.48 (6)
Rh1^{x}—Mn1—Rh1	180.0	Mn1—Rh1—Mn1^{xviii}	99.05 (12)
Rh1^{xi}—Mn1—Rh1	80.95 (12)	Mn2—Rh1—Bi2^{xvii}	70.41 (7)
Rh1^{vii}—Mn1—Rh1	99.05 (12)	Mn1—Rh1—Bi2^{xvii}	140.47 (7)
Rh1^{x}—Mn1—Bi1^{xii}	121.09 (4)	Mn1^{xviii}—Rh1—Bi2^{xvii}	70.37 (3)
Rh1^{xi}—Mn1—Bi1^{xii}	58.91 (4)	Mn2—Rh1—Bi2^{xviii}	70.41 (7)
Rh1^{vii}—Mn1—Bi1^{xii}	121.09 (4)	Mn1—Rh1—Bi2^{xviii}	140.47 (7)
Rh1—Mn1—Bi1^{xii}	58.91 (4)	Mn1^{xviii}—Rh1—Bi2^{xviii}	70.37 (3)
Rh1^{x}—Mn1—Bi1^{iv}	58.91 (4)	Bi2^{xvii}—Rh1—Bi2^{xviii}	73.50 (6)
Rh1^{xi}—Mn1—Bi1^{iv}	121.09 (4)	Mn2—Rh1—Bi2^{viii}	70.41 (7)

Rh1^{vii}—Mn1—Bi1^{iv}	58.91 (4)	Mn1—Rh1—Bi2^{viii}	70.37 (3)
Rh1—Mn1—Bi1^{iv}	121.09 (4)	Mn1^{xviii}—Rh1—Bi2^{viii}	140.47 (7)
Bi1^{xii}—Mn1—Bi1^{iv}	180.0	Bi2^{xvii}—Rh1—Bi2^{viii}	93.39 (7)
Rh1^{x}—Mn1—Bi1^{xiii}	58.91 (4)	Bi2^{xviii}—Rh1—Bi2^{viii}	140.81 (14)
Rh1^{xi}—Mn1—Bi1^{xiii}	121.09 (4)	Mn2—Rh1—Bi2	70.41 (7)
Rh1^{vii}—Mn1—Bi1^{xiii}	58.91 (4)	Mn1—Rh1—Bi2	70.37 (3)
Rh1—Mn1—Bi1^{xiii}	121.09 (4)	Mn1^{xviii}—Rh1—Bi2	140.47 (7)
Bi1^{xii}—Mn1—Bi1^{xiii}	85.51 (6)	Bi2^{xvii}—Rh1—Bi2	140.81 (14)
Bi1^{iv}—Mn1—Bi1^{xiii}	94.49 (6)	Bi2^{xviii}—Rh1—Bi2	93.39 (7)
Rh1^{x}—Mn1—Bi1^{i}	121.09 (4)	Bi2^{viii}—Rh1—Bi2	73.50 (6)
Rh1^{xi}—Mn1—Bi1^{i}	58.91 (4)	Mn2—Rh1—Bi1^{i}	128.27 (6)
Rh1^{vii}—Mn1—Bi1^{i}	121.09 (4)	Mn1—Rh1—Bi1^{i}	66.29 (6)
Rh1—Mn1—Bi1^{i}	58.91 (4)	Mn1^{xviii}—Rh1—Bi1^{i}	66.29 (6)
Bi1^{xii}—Mn1—Bi1^{i}	94.49 (6)	Bi2^{xvii}—Rh1—Bi1^{i}	132.64 (5)
Bi1^{iv}—Mn1—Bi1^{i}	85.51 (6)	Bi2^{xviii}—Rh1—Bi1^{i}	74.81 (4)
Bi1^{xiii}—Mn1—Bi1^{i}	180.0	Bi2^{viii}—Rh1—Bi1^{i}	132.64 (5)
Rh1^{x}—Mn1—Bi2^{xiv}	56.61 (5)	Bi2—Rh1—Bi1^{i}	74.81 (4)
Rh1^{xi}—Mn1—Bi2^{xiv}	56.61 (5)	Mn2—Rh1—Bi1^{xii}	128.27 (6)
Rh1^{vii}—Mn1—Bi2^{xiv}	123.39 (5)	Mn1—Rh1—Bi1^{xii}	66.29 (6)
Rh1—Mn1—Bi2^{xiv}	123.39 (5)	Mn1^{xviii}—Rh1—Bi1^{xii}	66.29 (6)
Bi1^{xii}—Mn1—Bi2^{xiv}	112.92 (2)	Bi2^{xvii}—Rh1—Bi1^{xii}	74.81 (4)
Bi1^{iv}—Mn1—Bi2^{xiv}	67.08 (2)	Bi2^{xviii}—Rh1—Bi1^{xii}	132.64 (5)
Bi1^{xiii}—Mn1—Bi2^{xiv}	112.92 (2)	Bi2^{viii}—Rh1—Bi1^{xii}	74.81 (4)
Bi1^{i}—Mn1—Bi2^{xiv}	67.08 (2)	Bi2—Rh1—Bi1^{xii}	132.64 (5)
Rh1^{x}—Mn1—Bi2^{viii}	123.39 (5)	Bi1^{i}—Rh1—Bi1^{xii}	103.45 (12)

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