



Crystal structure of TiBi_2

Kei Watanabe and Hisanori Yamane*

Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577, Japan. *Correspondence e-mail: yamane@tagen.tohoku.ac.jp

Received 14 July 2016
Accepted 1 August 2016

Edited by I. D. Brown, McMaster University, Canada

Keywords: crystal structure; CuMg_2 structure type; titanium; bismuth.

CCDC reference: 1497032

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

Black granular single crystals of monotitanium dibismuth, TiBi_2 , were synthesized by slow cooling of a mixture of Bi and Ti from 693 K. The title compound is isostructural with CuMg_2 (orthorhombic $Fddd$ symmetry). Ti atoms are located in square antiprisms of Bi atoms. The network of one type of Bi atom spirals along the a -axis direction while honeycomb layers of the other type of Bi atom spreading in the ab plane interlace one another.

1. Chemical context

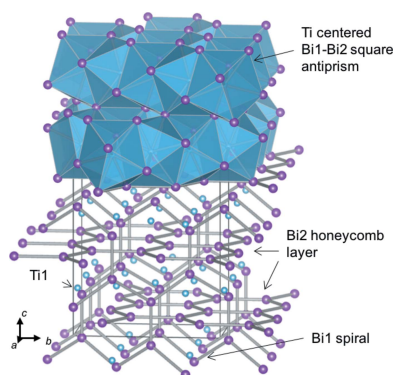
TiBi_2 was first reported in the study of the Ti–Bi binary phase diagram by Vassilev (2006). Maruyama *et al.* (2013) confirmed the presence of TiBi_2 in their phase-diagram study and showed that the powder X-ray diffraction (XRD) pattern was consistent with that of a Ti–Bi film prepared by RF sputtering (Simić & Marinković, 1990). However, the crystal system, lattice parameters and structure of TiBi_2 were not reported.

In the present study, we prepared single crystals of TiBi_2 to clarify the structure. The pellet of the starting mixture maintained the original shape after heating at 693 K. The powder XRD pattern of the sample showed that a mixture of TiBi_2 , Bi, and Ti had been obtained. Single crystals of TiBi_2 approximately 120 μm in size were picked up from the fractured sample. TiBi_2 is unstable and decomposes in air. When the mixture was heated at 703 K, the obtained sample was a mixture of Bi and Ti_8Bi_9 . This temperature was above the peritectic temperature of TiBi_2 (698 K) reported in the phase diagram by Maruyama *et al.* (2013).

2. Structural commentary

TiBi_2 is isotypic with CuMg_2 (Schubert & Anderko, 1951; Gingl *et al.*, 1993), NbSn_2 , VSn_2 , CrSn_2 (Wölpl & Jeitschko, 1994; Larsson & Lidin, 1995), and IrIn_2 (Zumdick *et al.*, 2000). TiSnSb is the only reported compound which contains Ti and crystallizes in the CuMg_2 -type structure (Malaman & Steinmetz, 1979; Dashjav & Kleinke, 2003). The crystal structure of TiSb_2 adopts the CuAl_2 type, while that of TiSn_2 is not known. TiBi_2 is the first binary compound that is composed of Ti and a group 15 element and has the CuMg_2 -type structure.

Fig. 1 shows the crystal structure of TiBi_2 while the coordination environments of the Ti1, Bi1, and Bi2 atoms are illustrated in Fig. 2. The Ti1 site is located in a square antiprism of Bi atoms. The Bi square antiprisms are aligned alternately along the $a + b$ and $a - b$ directions by sharing the square planes. Bi–Ti bond lengths in the Bi square antiprism and the Ti–Ti distance of the inter-antiprisms are 2.9382 (16)–3.0825 (6) and 2.9546 (2) Å, respectively, which are in the



OPEN ACCESS

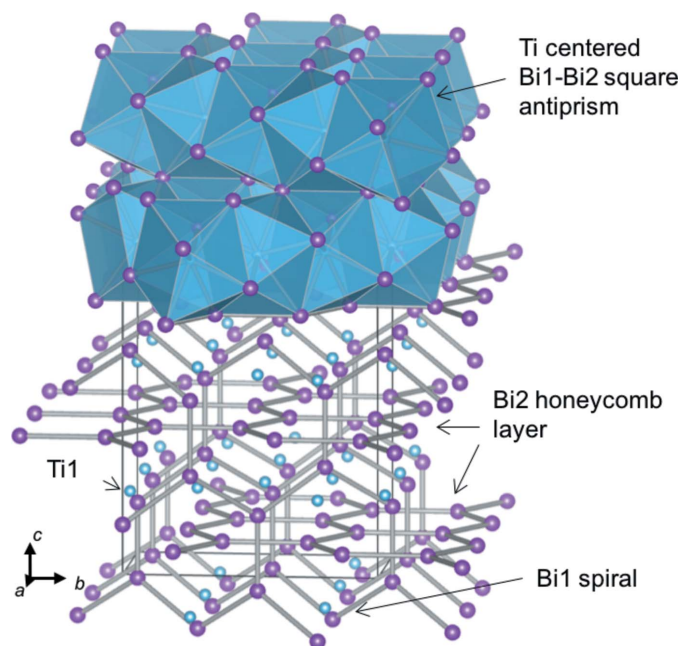


Figure 1
Crystal structure of TiBi_2 illustrated with Ti-centered Bi1–Bi2 square antiprisms and Bi1–Bi1 and Bi2–Bi2 bonds.

ranges reported for Ti_8Bi_9 [Bi–Ti = 2.818 (4)–3.144 (6) Å and Ti–Ti = 2.934 (6)–3.715 (5) Å; Richter & Jeitschko, 1997].

The Bi1–Bi1 bond lengths in the Bi1 spiral-like network are 3.0730 (8) Å in the c -axis direction and 3.4589 (4) Å in the other direction. The Bi2–Bi2 bond lengths in the Bi2 honeycomb layers in the ab plane are 3.4639 (8) Å in the b -axis direction and 3.3435 (4) Å in the other direction. The Bi–Bi bond lengths in the spiral rings and honeycomb layers in TiBi_2 are in the range of those in Bi metal (3.071 and 3.529 Å; Cucka & Barrett, 1962). The interatomic distances between the Bi atoms of the spiral network and the honey-

Table 1
Experimental details.

Crystal data	TiBi_2
Chemical formula	TiBi_2
M_r	465.86
Crystal system, space group	Orthorhombic, $Fddd$
Temperature (K)	298
a, b, c (Å)	5.7654 (4), 10.3155 (6), 19.4879 (12)
V (Å ³)	1159.00 (13)
Z	16
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	123.50
Crystal size (mm)	0.14 × 0.09 × 0.06
Data collection	
Diffractometer	Bruker D8 goniometer
Absorption correction	Numerical (<i>SADABS</i> ; Bruker, 2014)
T_{\min} , T_{\max}	0.016, 0.102
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	3881, 339, 309
R_{int}	0.048
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.024, 0.062, 1.31
No. of reflections	339
No. of parameters	17
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	2.54, -3.80

Computer programs: *Instrument Service*, *APEX2* and *SAINT-Plus* (Bruker, 2014), *SHELXL2014* (Sheldrick, 2015) and *VESTA* (Momma & Izumi, 2011).

comb layers (Bi1–Bi2) are 3.6974 (3), 3.7309 (4) and 3.7546 (4) Å, which are longer than the Bi–Bi bond lengths in Bi metal.

3. Synthesis and crystallization

Starting powders of Bi (1 mmol, Mitsuwa Chemicals Co., Ltd, 99.999%) and Ti (0.5 mmol, Mitsuwa Chemicals Co., Ltd, 99.99%) were weighed, mixed in an alumina mortar with a pestle and formed into a pellet by uniaxial pressing in an Ar gas-filled glove box (O_2 and $\text{H}_2\text{O} < 1$ p.p.m.). The pellet was put in a tantalum boat (Nilaco Corp., 99.95%). The boat was sealed in a stainless-steel (SUS 316) tube. The sample was heated to 693 K in an electric furnace with a heating rate of 3.5 K min⁻¹. This temperature was kept for 10 h, and then lowered to 473 K with a cooling rate of 5 K h⁻¹. After cooling to room temperature by shutting off the electrical power to the furnace, the stainless-steel tube was cut and opened in the glove box. To identify the crystalline phases, powder XRD (Cu $K\alpha$, Bruker, D2 phaser) was carried out for a portion of the sample which was ground in the alumina mortar and sealed under an Ar atmosphere in a holder with a kapton film window. The chemical compositions of TiBi_2 single crystals placed on a carbon tape were determined with an electron probe microanalyzer (EPMA, JEOL, JXA-8200). Bi and TiO_2 (Japan Electronics Co., Ltd) were used as standard samples. The analyzed composition ratio of Ti:Bi in the crystals was 1.0 (1):2.0 (1). A single crystal of TiBi_2 was sealed in a glass

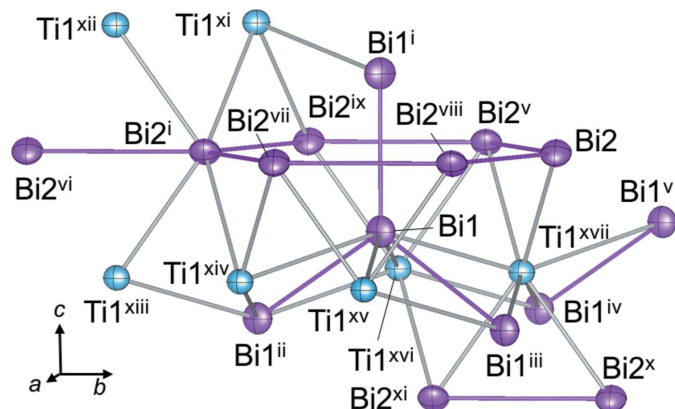


Figure 2
The atomic arrangement around Ti and Bi atoms in the structure of TiBi_2 . Displacement ellipsoids are drawn at 99% probability. [Symmetry codes: (i) $x, -y + \frac{1}{4}, -z + \frac{1}{4}$; (ii) $-x, -y, -z$; (iii) $x + \frac{1}{4}, y + \frac{1}{4}, -z$; (iv) $x - \frac{3}{4}, y + \frac{1}{4}, -z$; (v) $-x - \frac{1}{4}, -y + \frac{3}{4}, z$; (vi) $x, y - 1, z$; (vii) $-x + \frac{3}{4}, y - \frac{1}{2}, -z + \frac{1}{4}$; (viii) $-x + \frac{3}{4}, -y + \frac{3}{4}, z$; (ix) $-x - \frac{1}{4}, y - \frac{1}{2}, -z + \frac{1}{4}$; (x) $-x, -y + 1, -z$; (xi) $-x, y - \frac{1}{4}, z - \frac{1}{4}$; (xii) $x, -y - \frac{1}{4}, -z + \frac{3}{4}$; (xiii) $x, y - \frac{1}{2}, z - \frac{1}{2}$; (xiv) $x + \frac{1}{4}, y - \frac{1}{4}, -z + \frac{1}{2}$; (xv) $-x + \frac{3}{4}, -y + \frac{1}{4}, z - \frac{1}{2}$; (xvi) $-x - \frac{1}{4}, -y + \frac{1}{4}, z - \frac{1}{2}$; (xvii) $-x, -y + \frac{1}{2}, -z + \frac{1}{2}$.]

capillary with Ar gas in the glove box for the single-crystal XRD experiment.

4. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Acknowledgements

This work was supported in part by a Grant-in-Aid for Scientific Research (B) (No. 16H04494) from the Ministry of Education, Culture, Sports and Technology (MEXT), Japan.

References

Bruker (2014). *Instrument Service, APEX2, SADABS and SAINT-Plus*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cucka, P. & Barrett, C. S. (1962). *Acta Cryst.* **15**, 865–872.

Dashjav, E. & Kleinke, H. (2003). *J. Solid State Chem.* **176**, 329–337.
Gingl, F., Selvam, P. & Yvon, K. (1993). *Acta Cryst.* **B49**, 201–203.
Larsson, A. K. & Lidin, S. (1995). *J. Alloys Compd.* **221**, 136–142.
Malaman, B. & Steinmetz, J. (1979). *J. Less-Common Met.* **65**, 285–288.
Maruyama, S., Kado, Y. & Uda, T. (2013). *J. Phase Equilib. Diffus.* **34**, 289–296.
Momma, K. & Izumi, F. (2011). *J. Appl. Cryst.* **44**, 1272–1276.
Richter, C. G. & Jeitschko, W. (1997). *J. Solid State Chem.* **134**, 26–30.
Schubert, K. & Anderko, K. (1951). *Z. Metallkd.* **42**, 321–325.
Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.
Simić, V. & Marinković, Z. (1990). *Thin Solid Films*, **191**, 165–171.
Vassilev, G. P. (2006). *Cryst. Res. Technol.* **41**, 349–357.
Wölpl, T. & Jeitschko, W. (1994). *J. Alloys Compd.* **210**, 185–190.
Zumdick, M. F., Landrum, G. A., Dronskowski, R., Hoffmann, R. D. & Pöttgen, R. (2000). *J. Solid State Chem.* **150**, 19–30.

supporting information

Acta Cryst. (2016). E72, 1254-1256 [doi:10.1107/S2056989016012391]

Crystal structure of TiBi_2

Kei Watanabe and Hisanori Yamane

Computing details

Data collection: *Instrument Service* (Bruker, 2014); cell refinement: *APEX2* (Bruker, 2014); data reduction: *SAINTE-Plus* (Bruker, 2014); program(s) used to solve structure: *APEX2* (Bruker, 2014); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *VESTA* (Momma & Izumi, 2011).

Titanium dibismuth

Crystal data

TiBi_2	$D_x = 10.679 \text{ Mg m}^{-3}$
$M_r = 465.86$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Orthorhombic, $Fddd$	Cell parameters from 4528 reflections
$a = 5.7654 (4) \text{ \AA}$	$\theta = 4.2\text{--}31.4^\circ$
$b = 10.3155 (6) \text{ \AA}$	$\mu = 123.50 \text{ mm}^{-1}$
$c = 19.4879 (12) \text{ \AA}$	$T = 298 \text{ K}$
$V = 1159.00 (13) \text{ \AA}^3$	Granule, black
$Z = 16$	$0.14 \times 0.09 \times 0.06 \text{ mm}$
$F(000) = 3008$	

Data collection

Bruker D8 goniometer diffractometer	3881 measured reflections
Radiation source: micro focus sealed tube	339 independent reflections
Detector resolution: $10.4167 \text{ pixels mm}^{-1}$	309 reflections with $I > 2\sigma(I)$
ω , φ scans	$R_{\text{int}} = 0.048$
Absorption correction: numerical (SADABS; Bruker, 2014)	$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 4.2^\circ$
$T_{\text{min}} = 0.016$, $T_{\text{max}} = 0.102$	$h = -7 \rightarrow 7$
	$k = -13 \rightarrow 13$
	$l = -25 \rightarrow 25$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0275P)^2 + 47.1241P]$
$R[F^2 > 2\sigma(F^2)] = 0.024$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.062$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.31$	$\Delta\rho_{\text{max}} = 2.54 \text{ e \AA}^{-3}$
339 reflections	$\Delta\rho_{\text{min}} = -3.80 \text{ e \AA}^{-3}$
17 parameters	Extinction correction: SHELXL2014 (Sheldrick, 2015),
0 restraints	$F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
Primary atom site location: dual	Extinction coefficient: $0.00038 (3)$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Bi1	0.1250	0.1250	0.04615 (2)	0.0064 (2)
Bi2	0.1250	0.45710 (4)	0.1250	0.0066 (2)
Ti1	0.1250	0.1250	0.49898 (10)	0.0050 (4)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Bi1	0.0035 (3)	0.0076 (3)	0.0082 (3)	0.00176 (15)	0.000	0.000
Bi2	0.0058 (3)	0.0080 (3)	0.0060 (3)	0.000	-0.00212 (15)	0.000
Ti1	0.0039 (9)	0.0060 (9)	0.0051 (8)	0.0005 (8)	0.000	0.000

Geometric parameters (\AA , $^\circ$)

Ti1—Bi2 ⁱ	2.9382 (16)	Bi1—Bi2 ^{xix}	3.7546 (4)
Ti1—Bi2 ⁱⁱ	2.9382 (16)	Bi1—Bi2	3.7546 (4)
Ti1—Bi2 ⁱⁱⁱ	3.0051 (16)	Bi1—Ti1 ^{xx}	3.0257 (6)
Ti1—Bi2 ^{iv}	3.0051 (16)	Bi1—Ti1 ^{xxi}	3.0257 (6)
Ti1—Bi1 ^v	3.0257 (6)	Bi1—Ti1 ^{vii}	3.0825 (6)
Ti1—Bi1 ^{vi}	3.0257 (6)	Bi1—Ti1 ⁱ	3.0825 (6)
Ti1—Bi1 ^{vii}	3.0825 (6)	Bi1—Ti1 ^{xxii}	4.9243 (16)
Ti1—Bi1 ⁱ	3.0825 (6)	Bi1—Ti1 ^{xxiii}	4.9243 (16)
Ti1—Ti1 ^{viii}	2.9546 (2)	Bi1—Ti1 ^{xxiv}	4.9348 (16)
Ti1—Ti1 ^{ix}	2.9546 (2)	Bi1—Ti1 ^{xxv}	4.9348 (16)
Bi1—Bi1 ^x	3.0730 (8)	Bi1—Ti1 ^{xxvi}	5.1110 (4)
Bi1—Bi1 ^{xi}	3.4589 (4)	Bi2—Ti1 ⁱ	2.9382 (16)
Bi1—Bi1 ^{xii}	3.4589 (4)	Bi2—Ti1 ^{xxiv}	2.9382 (16)
Bi2—Bi2 ^{xiii}	3.3435 (4)	Bi2—Ti1 ^{xxvii}	3.0051 (16)
Bi2—Bi2 ^{xiv}	3.3435 (4)	Bi2—Ti1 ^{xxviii}	3.0051 (16)
Bi2—Bi2 ^{xv}	3.4639 (8)	Bi2—Bi1 ^{xxix}	3.6974 (3)
Bi1—Bi2 ^{xiv}	3.6974 (3)	Bi2—Bi1 ^{xxx}	3.6974 (3)
Bi1—Bi2 ^{xvi}	3.6974 (3)	Bi2—Bi1 ^{xxxi}	3.6974 (3)
Bi1—Bi2 ^{xvii}	3.6974 (3)	Bi2—Bi1 ^{xxxii}	3.6974 (3)
Bi1—Bi2 ^{xiii}	3.6974 (3)	Bi2—Bi1 ^{xii}	3.7310 (4)
Bi1—Bi2 ^{xviii}	3.7309 (4)	Ti1—Bi1 ^{xxii}	4.9242 (16)
Bi1—Bi2 ^{xii}	3.7309 (4)	Ti1—Bi1 ^{xxiii}	4.9242 (16)
Ti1 ⁱ —Bi2—Bi1 ^{xxx}	100.12 (2)	Bi2 ^{xiv} —Bi1—Ti1 ^{xxiv}	36.352 (10)
Bi1 ^{xxix} —Bi2—Bi1 ^{xii}	100.174 (6)	Bi2—Bi1—Ti1 ^{xxiv}	36.426 (10)
Bi2 ^{xvi} —Bi1—Bi2 ^{xviii}	100.175 (5)	Bi1 ^v —Ti1—Bi1 ^{xxii}	36.48 (2)

Bi1 ^{xii} —Bi1—Ti1 ^{xxii}	100.237 (12)	Bi1 ^x —Bi1—Ti1 ^{xxiv}	36.775 (14)
Bi1 ^{xii} —Bi1—Bi2 ^{xiii}	101.056 (6)	Bi2 ^{xiv} —Bi1—Ti1 ^{xxii}	37.501 (10)
Bi1 ^{xi} —Bi1—Bi2 ^{xvii}	101.056 (7)	Bi2 ⁱⁱⁱ —Ti1—Bi1 ^{xxii}	48.51 (2)
Bi2 ^{xvi} —Bi1—Bi2 ^{xvii}	102.459 (10)	Bi1 ^{xxix} —Bi2—Bi1 ^{xxx}	49.109 (12)
Bi1 ^{xxix} —Bi2—Bi1 ^{xxxii}	102.460 (10)	Ti1 ^{vii} —Bi1—Bi2 ^{xix}	49.72 (3)
Bi1 ^{xxx} —Bi2—Bi1 ^{xxxii}	102.460 (11)	Ti1 ^{xx} —Bi1—Bi2 ^{xviii}	50.23 (3)
Bi2 ^{xiii} —Bi2—Bi1 ^{xii}	102.596 (8)	Ti1 ^{vii} —Bi1—Bi2 ^{xvii}	50.37 (3)
Bi2 ^{xv} —Bi2—Bi1 ^{xii}	103.120 (6)	Ti1 ⁱ —Bi1—Bi2 ^{xviii}	51.27 (3)
Ti1 ^{xxi} —Bi1—Bi1 ^{xi}	103.83 (2)	Ti1 ^{xxi} —Bi1—Bi2 ^{xiv}	51.93 (3)
Bi1 ^{xii} —Bi1—Bi2 ^{xvii}	103.916 (6)	Ti1 ⁱ —Bi2—Bi1 ^{xii}	52.331 (19)
Bi2 ^{xiv} —Bi1—Bi2 ^{xix}	104.912 (8)	Ti1 ^{xxvii} —Bi2—Bi1 ^{xxix}	52.441 (7)
Ti1 ^{ix} —Ti1—Bi1 ^{xxii}	105.95 (7)	Ti1 ^{xxviii} —Bi2—Bi1 ^{xii}	53.148 (19)
Ti1 ^{xxiv} —Bi2—Bi2 ^{xiii}	106.077 (14)	Bi2 ^{xviii} —Bi1—Bi2 ^{xii}	53.241 (9)
Ti1 ⁱ —Bi1—Bi1 ^{xi}	106.29 (3)	Bi2 ^{xvi} —Bi1—Bi2 ^{xix}	53.310 (6)
Bi1 ^x —Bi1—Ti1 ^{vii}	106.58 (4)	Ti1 ^{xxiv} —Bi2—Bi1 ^{xxix}	53.901 (6)
Ti1 ⁱ —Bi2—Bi2 ^{xv}	106.753 (12)	Ti1 ^{vii} —Bi1—Bi1 ^{xi}	54.737 (17)
Ti1 ^{xxvii} —Bi2—Bi2 ^{xiii}	106.976 (10)	Ti1 ^{xxvii} —Bi2—Bi2 ^{xv}	54.81 (2)
Ti1 ^{xx} —Bi1—Bi1 ^x	107.69 (4)	Ti1 ⁱ —Bi2—Bi2 ^{xiii}	55.32 (2)
Bi1 ^{vi} —Ti1—Bi1 ^{xxii}	108.14 (5)	Bi1 ^{xxx} —Bi2—Bi1 ^{xii}	55.502 (6)
Ti1 ^{xxvii} —Bi2—Ti1 ^{xxviii}	109.61 (4)	Bi2 ^{xiv} —Bi1—Bi2 ^{xvii}	55.865 (12)
Ti1 ^{xx} —Bi1—Ti1 ^{vii}	111.026 (7)	Ti1 ^{xx} —Bi1—Bi1 ^{xi}	56.289 (16)
Bi1 ^{xi} —Bi1—Bi1 ^{xii}	117.32 (2)	Ti1 ^{xxi} —Bi1—Ti1 ^{vii}	57.847 (3)
Ti1 ^{ix} —Ti1—Bi1 ^v	117.43 (3)	Ti1 ^{viii} —Ti1—Bi2 ⁱⁱⁱ	59.07 (5)
Ti1 ^{xxiv} —Bi2—Bi1 ^{xii}	118.70 (2)	Ti1 ^{xxiv} —Bi2—Ti1 ^{xxvii}	59.609 (4)
Bi2 ^{xiii} —Bi2—Bi2 ^{xiv}	119.12 (2)	Ti1 ^{ix} —Ti1—Bi1 ^{vii}	60.113 (19)
Ti1 ^{ix} —Ti1—Bi2 ⁱⁱⁱ	119.48 (9)	Bi2 ⁱⁱ —Ti1—Ti1 ^{viii}	61.32 (5)
Bi2 ^{xvii} —Bi1—Ti1 ^{xxvi}	119.656 (11)	Ti1 ^{xxiii} —Bi1—Ti1 ^{xxiv}	61.418 (6)
Bi2 ^{xii} —Bi1—Ti1 ^{xxii}	119.910 (14)	Bi1 ^{xii} —Bi1—Bi2 ^{xviii}	61.757 (12)
Bi2 ⁱ —Ti1—Ti1 ^{viii}	120.13 (9)	Ti1 ^{viii} —Ti1—Bi1 ^v	62.04 (2)
Ti1 ⁱ —Bi1—Ti1 ^{xxii}	120.34 (3)	Bi2 ^{xv} —Bi2—Bi1 ^{xxix}	62.067 (6)
Bi1 ⁱ —Ti1—Bi1 ^{xxii}	120.34 (3)	Bi2 ^{xv} —Bi2—Bi1 ^{xxx}	62.067 (6)
Ti1 ^{viii} —Ti1—Bi1 ^{vii}	120.39 (3)	Bi1 ^{xi} —Bi1—Bi2 ^{xix}	62.132 (6)
Bi2 ⁱⁱ —Ti1—Bi2 ⁱⁱⁱ	120.391 (4)	Bi1 ^{xii} —Bi1—Bi2 ^{xiv}	62.742 (7)
Bi2 ^{xiii} —Bi2—Bi2 ^{xv}	120.438 (12)	Bi1 ^{xi} —Bi1—Bi2 ^{xviii}	62.826 (12)
Bi1 ^x —Bi1—Bi1 ^{xi}	121.338 (11)	Bi2 ^{xiv} —Bi2—Bi1 ^{xii}	63.380 (4)
Ti1 ^{xx} —Bi1—Ti1 ^{xxiv}	121.44 (3)	Bi2 ^{xiv} —Bi2—Bi1 ^{xxix}	64.221 (7)
Ti1 ^{vii} —Bi1—Ti1 ^{xxiv}	121.95 (3)	Bi2 ^{xiii} —Bi2—Bi1 ^{xxx}	64.221 (7)
Bi2—Bi1—Ti1 ^{xxvi}	122.061 (9)	Bi1 ^x —Bi1—Bi2 ^{xiv}	65.444 (6)
Bi1 ^{vi} —Ti1—Bi1 ^{vii}	122.154 (4)	Bi1 ^x —Bi1—Bi2 ^{xix}	65.843 (6)
Bi1 ^{xxix} —Bi2—Bi1 ^{xxx}	124.135 (12)	Bi2 ^{xix} —Bi1—Ti1 ^{xxvi}	67.048 (12)
Bi2 ^{xiv} —Bi1—Bi2 ^{xviii}	124.499 (6)	Ti1 ^{xxv} —Bi1—Ti1 ^{xxvi}	68.10 (3)
Bi2 ^{xviii} —Bi1—Bi2 ^{xix}	124.958 (7)	Bi2 ^{xviii} —Bi1—Ti1 ^{xxvi}	68.52 (2)
Ti1 ^{xxii} —Bi1—Ti1 ^{xxvi}	129.41 (3)	Bi1 ^v —Ti1—Bi1 ^{vii}	68.975 (7)
Bi1 ^{xii} —Bi1—Ti1 ^{xxvi}	129.73 (2)	Ti1 ^{xxiii} —Bi1—Ti1 ^{xxvi}	69.162 (10)
Ti1 ^{xxiv} —Bi1—Ti1 ^{xxvi}	130.440 (11)	Bi2 ⁱ —Ti1—Bi2 ⁱⁱ	69.36 (4)
Bi2 ^{xiv} —Bi1—Bi2 ^{xvi}	130.889 (12)	Bi2 ^{xiii} —Bi1—Ti1 ^{xxvi}	69.407 (12)
Bi2 ^{xix} —Bi1—Bi2	131.685 (13)	Bi2 ^{xiii} —Bi1—Ti1 ^{xxiv}	69.516 (7)
Bi1 ^{xi} —Bi1—Ti1 ^{xxii}	131.728 (9)	Bi2 ⁱⁱⁱ —Ti1—Bi2 ^{iv}	70.39 (4)

Bi2 ^{xviii} —Bi1—Ti1 ^{xxiv}	135.259 (12)	Bi2 ^{xix} —Bi1—Ti1 ^{xxii}	70.622 (7)
Bi2 ⁱⁱⁱ —Ti1—Bi1 ^{vii}	135.68 (5)	Bi2 ^{xvii} —Bi1—Ti1 ^{xxiv}	71.591 (8)
Bi2 ⁱ —Ti1—Bi1 ^v	135.83 (5)	Ti1 ^{xxii} —Bi1—Ti1 ^{xxiii}	71.66 (3)
Bi2 ^{xii} —Bi1—Ti1 ^{xxiv}	136.209 (11)	Bi1 ^{xxii} —Ti1—Bi1 ^{xxiii}	71.66 (3)
Ti1 ^{xxi} —Bi1—Ti1 ^{xxvi}	138.917 (11)	Ti1 ^{xxi} —Bi1—Ti1 ^{xxii}	71.85 (5)
Bi1 ^{xxxii} —Bi2—Bi1 ^{xii}	141.173 (9)	Ti1 ^{viii} —Ti1—Bi1 ^{xxii}	72.76 (6)
Bi2 ^{xvii} —Bi1—Bi2 ^{xviii}	141.174 (9)	Ti1 ^{xxiv} —Bi1—Ti1 ^{xxv}	73.55 (3)
Ti1 ^{xx} —Bi1—Ti1 ^{xxii}	143.52 (2)	Bi2 ^{iv} —Ti1—Bi1 ^{vii}	75.584 (18)
Bi1 ^v —Ti1—Bi1 ^{vi}	144.62 (7)	Bi2 ⁱⁱⁱ —Ti1—Bi1 ^v	75.62 (3)
Ti1 ^{xx} —Bi1—Ti1 ^{xxi}	144.63 (7)	Bi2 ⁱ —Ti1—Bi1 ^{vii}	75.73 (3)
Ti1 ⁱ —Bi2—Ti1 ^{xxiv}	146.49 (2)	Bi2 ⁱⁱ —Ti1—Bi1 ^{vii}	77.12 (3)
Ti1 ^{vii} —Bi1—Ti1 ⁱ	146.84 (7)	Bi2 ⁱⁱ —Ti1—Bi1 ^v	77.437 (16)
Bi1 ^{vii} —Ti1—Bi1 ⁱ	146.84 (7)	Bi1 ^{xii} —Bi1—Ti1 ^{xxiv}	84.563 (17)
Ti1 ⁱ —Bi2—Ti1 ^{xxvii}	146.946 (8)	Ti1 ^{vii} —Bi1—Ti1 ^{xxvi}	85.661 (13)
Bi2 ⁱ —Ti1—Bi2 ⁱⁱⁱ	146.946 (8)	Ti1 ⁱ —Bi1—Ti1 ^{xxiv}	85.87 (4)
Ti1 ⁱ —Bi2—Bi1 ^{xxix}	149.23 (2)	Ti1 ^{vii} —Bi1—Ti1 ^{xxii}	87.57 (2)
Ti1 ^{xxvii} —Bi2—Bi1 ^{xii}	149.475 (16)	Bi1 ^{vii} —Ti1—Bi1 ^{xxii}	87.57 (2)
Ti1 ^{xx} —Bi1—Bi2 ^{xiv}	150.350 (13)	Bi2 ^{xiii} —Bi1—Bi2 ^{xviii}	87.936 (5)
Ti1 ⁱ —Bi1—Bi2 ^{xvii}	151.051 (14)	Ti1 ^{xxi} —Bi1—Ti1 ^{xxiv}	88.00 (2)
Ti1 ⁱ —Bi1—Bi2 ^{xix}	151.659 (13)	Ti1 ⁱ —Bi1—Ti1 ^{xxvi}	88.706 (13)
Bi1 ^{xi} —Bi1—Bi2 ^{xiv}	152.907 (6)	Bi1 ^{xxxi} —Bi2—Bi1 ^{xii}	92.064 (5)
Bi1 ^{xii} —Bi1—Bi2 ^{xix}	153.267 (4)	Bi2 ^{xii} —Bi1—Ti1 ^{xxvi}	93.35 (2)
Bi1 ^x —Bi1—Bi2 ^{xviii}	153.380 (4)	Ti1 ^{xxviii} —Bi2—Bi1 ^{xxix}	93.992 (16)
Bi2 ^{xiii} —Bi2—Bi1 ^{xxix}	155.439 (6)	Ti1 ⁱ —Bi1—Bi2 ^{xiv}	95.236 (16)
Bi1 ^{xi} —Bi1—Ti1 ^{xxiv}	158.113 (19)	Ti1 ^{xxiv} —Bi2—Bi1 ^{xxx}	95.410 (14)
Bi2 ^{xviii} —Bi1—Ti1 ^{xxii}	161.981 (11)	Ti1 ^{xxi} —Bi1—Bi2 ^{xviii}	95.54 (4)
Bi2 ⁱ —Ti1—Bi1 ^{xxii}	162.533 (7)	Ti1 ^{vii} —Bi1—Bi2 ^{xviii}	96.63 (4)
Bi2 ^{xiv} —Bi1—Ti1 ^{xxvi}	165.35 (2)	Bi2 ^{xvi} —Bi1—Ti1 ^{xxii}	96.863 (15)
Ti1 ^{viii} —Ti1—Ti1 ^{ix}	178.47 (15)	Ti1 ^{xx} —Bi1—Bi2 ^{xix}	97.142 (14)
Ti1 ^{xx} —Bi1—Ti1 ^{xxvi}	30.870 (13)	Bi2 ^{xvi} —Bi1—Ti1 ^{xxiv}	98.027 (15)
Bi2 ^{xvi} —Bi1—Ti1 ^{xxvi}	34.47 (2)	Ti1 ^{vii} —Bi1—Bi2 ^{xiv}	98.391 (15)
Ti1 ^{xxii} —Bi1—Ti1 ^{xxiv}	34.877 (3)	Bi2 ^{xix} —Bi1—Ti1 ^{xxiv}	98.570 (15)
Bi1 ^{xi} —Bi1—Ti1 ^{xxvi}	35.089 (15)	Bi2 ^{xii} —Bi1—Bi2 ^{xix}	99.134 (9)
Bi1 ^x —Bi1—Ti1 ^{xxii}	35.832 (14)	Bi1 ^x —Bi1—Ti1 ^{xxvi}	99.91 (2)

Symmetry codes: (i) $-x, -y+1/2, -z+1/2$; (ii) $x+1/4, y-1/4, -z+1/2$; (iii) $-x+1/4, -y+3/4, z+1/2$; (iv) $x, y-1/2, z+1/2$; (v) $x+1/2, y, z+1/2$; (vi) $x-1/2, y, z+1/2$; (vii) $-x+1/2, -y, -z+1/2$; (viii) $-x+1/2, -y+1/2, -z+1$; (ix) $-x, -y, -z+1$; (x) $-x+1/4, y, -z+1/4$; (xi) $-x, -y, -z$; (xii) $-x+1/2, -y+1/2, -z$; (xiii) $-x-1/4, -y+3/4, z$; (xiv) $-x+3/4, -y+3/4, z$; (xv) $-x+1/4, -y+5/4, z$; (xvi) $x-1/2, y-1/2, z$; (xvii) $x+1/2, y-1/2, z$; (xviii) $x-1/4, y-1/4, -z$; (xix) $-x+1/4, -y+1/4, z$; (xx) $x-1/2, y, z-1/2$; (xxi) $x+1/2, y, z-1/2$; (xxii) $-x+3/4, y, -z+3/4$; (xxiii) $-x-1/4, y, -z+3/4$; (xxiv) $x+1/4, -y+1/2, z-1/4$; (xxv) $x-1/4, -y, z-1/4$; (xxvi) $-x-1/2, -y, -z+1/2$; (xxvii) $-x+1/4, y+1/2, -z+3/4$; (xxviii) $x, y+1/2, z-1/2$; (xxix) $-x+3/4, y+1/2, -z+1/4$; (xxx) $x+1/2, y+1/2, z$; (xxxii) $-x-1/4, y+1/2, -z+1/4$.