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Titanium vanadium nickel, $TiV_{0.08}Ni_{0.92}$

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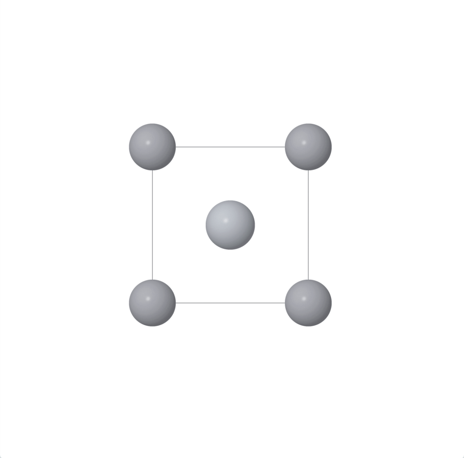
A single-crystal of the intermetallic phase $TiV_{0.08}Ni_{0.92}$ was obtained by the high-temperature sintering of a mixture of nominal composition $Ti_{0.9}V_{0.1}Ni$. The title compound adopts the CsCl structure type with one site solely occupied by Ti and the other by V and Ni with a ratio of 0.08 (7):0.92 (7).

3D view



Structure description

The Ti–V–Ni alloy system has been widely studied for its excellent hydrogen-storage properties. For example, the structure of the $Ti_{1.4}V_{0.6}Ni$ alloy was studied by powder X-ray diffraction, which identified an icosahedral quasicrystal phase (I-phase), fcc-Ti_2Ni-type phase and bcc-V-based solid-solution phase. The TEM patterns of the I-phase along the fivefold and twofold symmetry axes have been reported (Sun *et al.*, 2015). Anahara *et al.* (2003) synthesized the $Ti_{0.73}V_{1.4}Ni_{0.27}$ alloy, in which Ti was partially replaced by Ni to compare with the parent $TiV_{1.4}$ phase. The PXRD peaks of the $Ti_{0.73}V_{1.4}Ni_{0.27}$ alloy after heat treatment can be indexed as a b.c.c. solid solution of vanadium and the Ti_2Ni phase. Iwakura *et al.* (2000) synthesized $TiV_{0.9}Ni_{0.5}$, which is composed of 'black' and 'white' phases as characterized by X-ray diffraction and electron probe analysis. The black phase is the V-based solid solution, the white phase is a TiNi-based solid solution along with traces of TiNi or Ti_2Ni-based alloys. The existence of the $Ni_3(Ti_xV_{1-x})$ long-period structure was confirmed by electron diffraction and high-resolution lattice imaging (Zhang *et al.*, 1984). $V_{85}Ni_{15}$ was obtained by dissolving Ni atoms into a vanadium-atom matrix to form a single supersaturated solid solution and $V_{85}Ni_{10}Ti_5$ was obtained by replacing Ni with 5 at% Ti (Jiang *et al.*, 2020). Souvatzis *et al.* (2010) prepared the TiNi cubic phase known as the B2 or β phase with space group $Pm\overline{3}m$. It can be seen from the literature and databases that previous research on the Ti–V–Ni system only indicated the existence of the bcc structure without any refined structure models.

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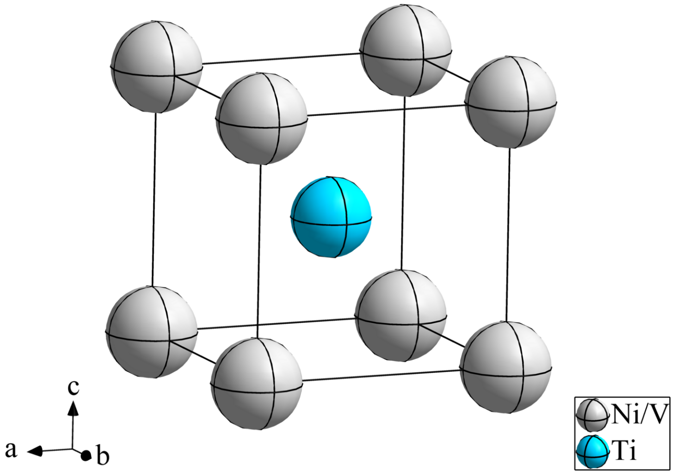

Figure 1
The crystal structure of $TiV_{0.08}Ni_{0.92}$, with displacement ellipsoids at the 95% probability level.

The structure of the title alloy, $TiV_{0.08}Ni_{0.92}$, revealed that one site is co-occupied by V and Ni compared with TiNi phase in space-group type $Pm\bar{3}m$. Fig. 1 shows the overall atomic distribution in the unit cell of $TiV_{0.08}Ni_{0.92}$. Each Ni1/V1 atom is located at a dodecahedron (Wyckoff 1*a* site), being surrounded by six Ni1/V1 atoms and eight Ti1 atoms (Fig. 2). The Ti1 atom (1*b* site) is surrounded by six Ti1 atoms and eight Ni1/V1 atoms, defining the centre of its dodecahedron (Fig. 3). The shortest Ni1/V1 to Ti1 separation is 2.5890 (5) Å and the shortest Ni1/V1 to Ni1/V1 separation is 2.9895 (6) Å.

Synthesis and crystallization

High-purity titanium powder (indicated purity 99.5%, 0.4043 g), vanadium powder (indicated purity 99.9%, 0.0565 g) and nickel powder (indicated purity 99.9%, 0.5501 g) were mixed in the atomic ratio 0.9:0.1:1 and fully ground in an agate mortar. The mixture was placed into a 5 mm cemented carbide grinding mould and pressed into a tablet at about 6 MPa for 2 min to obtain a cylindrical block without deformations or cracks. The detailed description of the high-pressure sintering experiment using a six-anvil high-temperature and high-pressure apparatus can be found elsewhere (Liu & Fan, 2018). The sample was pressurized up to 6 GPa and heated to 1623 K for 20 min, cooled to 1173 K and held at that temperature for 1 h. Finally, the furnace power was turned off to rapidly cool to room temperature. Two phases were isolated from two samples from the same batch. According to the complementary EDX results, the chemical composition was refined to be exactly $TiV_{0.08}Ni_{0.92}$ originated from sample 1 (see Table S1 of the electronic supporting information, ESI). Another phase of $TiV_{0.07}Ni_{0.93}$ with very similar refined composition, was isolated from sample 2, its composition is in accordance with the complementary EDX results also (see Table S2 of the ESI). Different options of refinements for the two phases $TiV_{\delta}Ni_{1-\delta}$ (δ = 0.07, 0.08) are listed in Table S3 of the ESI. The crystal structures of $TiV_{0.08}Ni_{0.92}$ and $TiV_{0.07}Ni_{0.93}$ are very similar, differing only in atomic

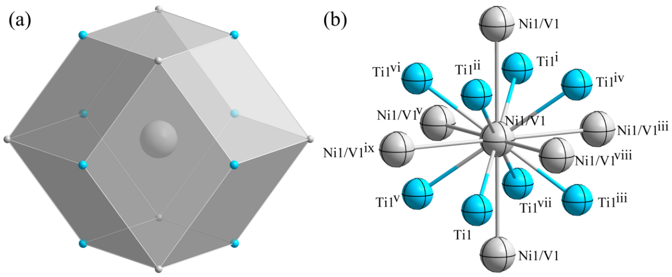

Figure 2
(*a*) The dodecahedron formed around the Ni1/V1 atom at the 1*a* Wyckoff site; (*b*) the environment of the Ni1/V1 atom with displacement ellipsoids given at the 95% probability level. [Symmetry codes: (i) $x - 1, y - 1, z - 1$; (ii) $x - 1, y, z$; (iii) $x, y - 1, z$; (iv) $x - 1, y - 1, z$; (v) $x, y, z - 1$; (vi) $x - 1, y, z - 1$; (vii) $x, y - 1, z - 1$; (viii) $x, y, z + 1$; (ix) $x, y + 1, z$.]

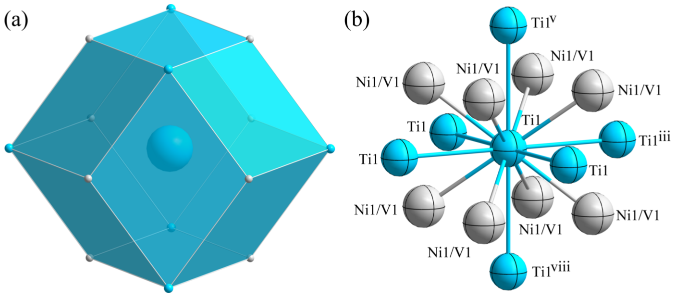

Figure 3
(*a*) The dodecahedron formed around the Ti1 atom at the 1*b* site; (*b*) the environment of the Ti1 atom with displacement ellipsoids given at the 95% probability level. [Symmetry codes: (iii) $x, y - 1, z$; (v) $x, y, z - 1$; (viii) $x, y, z + 1$.]

Table 1
Experimental details.

Crystal data	
Chemical formula	$TiV_{0.08}Ni_{0.92}$
M_r	105.96
Crystal system, space group	Cubic, $Pm\bar{3}m$
Temperature (K)	296
a (Å)	2.9895 (6)
V (Å^3)	26.72 (2)
Z	1
Radiation type	Mo $K\alpha$
μ (mm^{-1})	23.34
Crystal size (mm)	0.10 × 0.08 × 0.06
Data collection	
Diffractometer	Bruker D8 Venture Photon 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.394, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	774, 14, 12
R_{int}	0.058
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.626
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.022, 0.039, 1.39
No. of reflections	14
No. of parameters	4
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.20

Computer programs: *APEX3* and *SAINT* (Bruker, 2015), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2016/6* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2017) and *publCIF* (Westrip, 2010).

proportions at the (Ni/V) site, so the $TiV_{0.08}Ni_{0.92}$ phase was selected for the current report. The structure data of $TiV_{0.07}Ni_{0.93}$ are summarized in Table S4 of the ESI.

Refinement

Crystal data, data collection and structure refinement details of $TiV_{0.08}Ni_{0.92}$ are summarized in Table 1. Only one site is co-occupied by Ni and V atoms (Ni1/V1). Site occupation factor (s. o. f.) were refined to 0.08 (7) for V1 and 0.92 (7) for Ni1, assuming full occupancy for each site. Atoms sharing the same site were constrained to have the same coordinates and displacement parameters. The maximum and minimum residual electron densities in the final difference map are located 0.00 Å and 0.78 Å from the atom V1.

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full crystallographic data

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Titanium vanadium nickel, $TiV_{0.08}Ni_{0.92}$

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Titanium vanadium nickel

Crystal data

$TiV_{0.08}Ni_{0.92}$
$M_r = 105.96$
Cubic, $Pm\overline{3}m$
$a = 2.9895$ (6) Å
$V = 26.72$ (2) Å^3
$Z = 1$
$F(000) = 50$
$D_x = 6.585$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 433 reflections
$\theta = 6.8$–26.4°
$\mu = 23.34$ mm^{-1}
$T = 296$ K
Lump, gray
0.10 × 0.08 × 0.06 mm

Data collection

Bruker D8 Venture Photon 100 CMOS diffractometer
phi and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
$T_{min} = 0.394$, $T_{max} = 0.746$
774 measured reflections
14 independent reflections
12 reflections with $I > 2\sigma(I)$
$R_{int} = 0.058$
$\theta_{max} = 26.4°$, $\theta_{min} = 6.8°$
$h = -3 \rightarrow 3$
$k = -3 \rightarrow 3$
$l = -3 \rightarrow 3$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.022$
$wR(F^2) = 0.039$
$S = 1.39$
14 reflections
4 parameters
0 restraints
$w = 1/[\sigma^2(F_o^2) + 0.1191P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ni1	0.000000	0.000000	0.000000	0.0332 (12)	0.92 (7)
V1	0.000000	0.000000	0.000000	0.0332 (12)	0.08 (7)
Ti1	0.500000	0.500000	0.500000	0.0257 (14)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0332 (12)	0.0332 (12)	0.0332 (12)	0.000	0.000	0.000
V1	0.0332 (12)	0.0332 (12)	0.0332 (12)	0.000	0.000	0.000
Ti1	0.0257 (14)	0.0257 (14)	0.0257 (14)	0.000	0.000	0.000

Geometric parameters (Å, º)

Ni1—Ti1^{i}	2.5890 (5)	V1—Ti1^{i}	2.5890 (5)
Ni1—Ti1	2.5890 (5)	V1—Ti1	2.5890 (5)
Ni1—Ti1^{ii}	2.5890 (5)	V1—Ti1^{ii}	2.5890 (5)
Ni1—Ti1^{iii}	2.5890 (5)	V1—Ti1^{vii}	2.5890 (5)
Ni1—Ti1^{iv}	2.5890 (5)	V1—Ti1^{vi}	2.5890 (5)
Ni1—Ti1^{v}	2.5890 (5)	V1—Ti1^{v}	2.5890 (5)
Ni1—Ti1^{vi}	2.5890 (5)	V1—Ti1^{iv}	2.5890 (5)
Ni1—Ti1^{vii}	2.5890 (5)	V1—Ti1^{iii}	2.5890 (5)
Ni1—Ni1^{iii}	2.9895 (6)	Ti1—Ti1^{viii}	2.9895 (6)
Ni1—Ni1^{v}	2.9895 (6)	Ti1—Ti1^{v}	2.9895 (6)
Ni1—Ni1^{viii}	2.9895 (6)	Ti1—Ti1^{iii}	2.9895 (6)
Ni1—Ni1^{ix}	2.9895 (6)		

Ti1^{i}—Ni1—Ti1	180.0	Ti1^{vii}—V1—Ti1^{vi}	109.5
Ti1^{i}—Ni1—Ti1^{ii}	109.5	Ti1^{i}—V1—Ti1^{v}	109.5
Ti1—Ni1—Ti1^{ii}	70.5	Ti1—V1—Ti1^{v}	70.5
Ti1^{i}—Ni1—Ti1^{iii}	109.5	Ti1^{ii}—V1—Ti1^{v}	109.5
Ti1—Ni1—Ti1^{iii}	70.5	Ti1^{vii}—V1—Ti1^{v}	70.5
Ti1^{ii}—Ni1—Ti1^{iii}	109.5	Ti1^{vi}—V1—Ti1^{v}	70.5
Ti1^{i}—Ni1—Ti1^{iv}	70.5	Ti1^{i}—V1—Ti1^{iv}	70.5
Ti1—Ni1—Ti1^{iv}	109.5	Ti1—V1—Ti1^{iv}	109.5
Ti1^{ii}—Ni1—Ti1^{iv}	70.5	Ti1^{ii}—V1—Ti1^{iv}	70.5
Ti1^{iii}—Ni1—Ti1^{iv}	70.5	Ti1^{vii}—V1—Ti1^{iv}	109.5
Ti1^{i}—Ni1—Ti1^{v}	109.5	Ti1^{vi}—V1—Ti1^{iv}	109.5
Ti1—Ni1—Ti1^{v}	70.5	Ti1^{v}—V1—Ti1^{iv}	180.0
Ti1^{ii}—Ni1—Ti1^{v}	109.5	Ti1^{i}—V1—Ti1^{iii}	109.5
Ti1^{iii}—Ni1—Ti1^{v}	109.5	Ti1—V1—Ti1^{iii}	70.5
Ti1^{iv}—Ni1—Ti1^{v}	180.0	Ti1^{ii}—V1—Ti1^{iii}	109.5
Ti1^{i}—Ni1—Ti1^{vi}	70.5	Ti1^{vii}—V1—Ti1^{iii}	70.5
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Ti1^{iii}—Ni1—Ti1^{vi}	180.0	Ti1^{iv}—V1—Ti1^{iii}	70.5
Ti1^{iv}—Ni1—Ti1^{vi}	109.5	Ni1^{x}—Ti1—Ni1	180.0
Ti1^{v}—Ni1—Ti1^{vi}	70.5	Ni1^{x}—Ti1—Ni1^{xi}	109.5
Ti1^{i}—Ni1—Ti1^{vii}	70.5	Ni1—Ti1—Ni1^{xi}	70.5
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Ti1^{iii}—Ni1—Ti1^{vii}	70.5	Ni1^{xi}—Ti1—Ni1^{ix}	109.5
Ti1^{iv}—Ni1—Ti1^{vii}	109.5	Ni1^{x}—Ti1—Ni1^{xii}	70.5

Ti1^{v}—Ni1—Ti1^{vii}	70.5	Ni1—Ti1—Ni1^{xii}	109.5
Ti1^{vi}—Ni1—Ti1^{vii}	109.5	Ni1^{xi}—Ti1—Ni1^{xii}	70.5
Ti1^{i}—Ni1—Ni1^{iii}	54.7	Ni1^{ix}—Ti1—Ni1^{xii}	70.5
Ti1—Ni1—Ni1^{iii}	125.3	Ni1^{x}—Ti1—Ni1^{viii}	109.5
Ti1^{ii}—Ni1—Ni1^{iii}	125.3	Ni1—Ti1—Ni1^{viii}	70.529 (1)
Ti1^{iii}—Ni1—Ni1^{iii}	54.7	Ni1^{xi}—Ti1—Ni1^{viii}	109.5
Ti1^{iv}—Ni1—Ni1^{iii}	54.7	Ni1^{ix}—Ti1—Ni1^{viii}	109.5
Ti1^{v}—Ni1—Ni1^{iii}	125.3	Ni1^{xii}—Ti1—Ni1^{viii}	180.0
Ti1^{vi}—Ni1—Ni1^{iii}	125.3	Ni1^{x}—Ti1—Ni1^{xiii}	70.5
Ti1^{vii}—Ni1—Ni1^{iii}	54.7	Ni1—Ti1—Ni1^{xiii}	109.5
Ti1^{i}—Ni1—Ni1^{v}	54.7	Ni1^{xi}—Ti1—Ni1^{xiii}	70.5
Ti1—Ni1—Ni1^{v}	125.3	Ni1^{ix}—Ti1—Ni1^{xiii}	180.0
Ti1^{ii}—Ni1—Ni1^{v}	125.3	Ni1^{xii}—Ti1—Ni1^{xiii}	109.5
Ti1^{iii}—Ni1—Ni1^{v}	125.3	Ni1^{viii}—Ti1—Ni1^{xiii}	70.5
Ti1^{iv}—Ni1—Ni1^{v}	125.3	Ni1^{x}—Ti1—Ni1^{xiv}	70.5
Ti1^{v}—Ni1—Ni1^{v}	54.7	Ni1—Ti1—Ni1^{xiv}	109.5
Ti1^{vi}—Ni1—Ni1^{v}	54.7	Ni1^{xi}—Ti1—Ni1^{xiv}	180.0
Ti1^{vii}—Ni1—Ni1^{v}	54.7	Ni1^{ix}—Ti1—Ni1^{xiv}	70.5
Ni1^{iii}—Ni1—Ni1^{v}	90.0	Ni1^{xii}—Ti1—Ni1^{xiv}	109.5
Ti1^{i}—Ni1—Ni1^{viii}	125.3	Ni1^{viii}—Ti1—Ni1^{xiv}	70.5
Ti1—Ni1—Ni1^{viii}	54.7	Ni1^{xiii}—Ti1—Ni1^{xiv}	109.5
Ti1^{ii}—Ni1—Ni1^{viii}	54.7	Ni1^{x}—Ti1—Ti1^{viii}	54.7
Ti1^{iii}—Ni1—Ni1^{viii}	54.7	Ni1—Ti1—Ti1^{viii}	125.3
Ti1^{iv}—Ni1—Ni1^{viii}	54.7	V1—Ti1—Ti1^{viii}	125.3
Ti1^{v}—Ni1—Ni1^{viii}	125.3	Ni1^{xi}—Ti1—Ti1^{viii}	125.3
Ti1^{vi}—Ni1—Ni1^{viii}	125.3	Ni1^{ix}—Ti1—Ti1^{viii}	125.3
Ti1^{vii}—Ni1—Ni1^{viii}	125.3	Ni1^{xii}—Ti1—Ti1^{viii}	125.3
Ni1^{iii}—Ni1—Ni1^{viii}	90.0	Ni1^{viii}—Ti1—Ti1^{viii}	54.7
Ni1^{v}—Ni1—Ni1^{viii}	180.0	Ni1^{xiii}—Ti1—Ti1^{viii}	54.7
Ti1^{i}—Ni1—Ni1^{ix}	125.3	Ni1^{xiv}—Ti1—Ti1^{viii}	54.7
Ti1—Ni1—Ni1^{ix}	54.7	Ni1^{x}—Ti1—Ti1^{v}	125.3
Ti1^{ii}—Ni1—Ni1^{ix}	54.7	Ni1—Ti1—Ti1^{v}	54.7
Ti1^{iii}—Ni1—Ni1^{ix}	125.3	Ni1^{xi}—Ti1—Ti1^{v}	54.7
Ti1^{iv}—Ni1—Ni1^{ix}	125.3	Ni1^{ix}—Ti1—Ti1^{v}	54.7
Ti1^{v}—Ni1—Ni1^{ix}	54.7	Ni1^{xii}—Ti1—Ti1^{v}	54.7
Ti1^{vi}—Ni1—Ni1^{ix}	54.7	Ni1^{viii}—Ti1—Ti1^{v}	125.3
Ti1^{vii}—Ni1—Ni1^{ix}	125.3	Ni1^{xiii}—Ti1—Ti1^{v}	125.3
Ni1^{iii}—Ni1—Ni1^{ix}	180.0	Ni1^{xiv}—Ti1—Ti1^{v}	125.3
Ni1^{v}—Ni1—Ni1^{ix}	90.0	Ti1^{viii}—Ti1—Ti1^{v}	180.0
Ni1^{viii}—Ni1—Ni1^{ix}	90.0	Ni1^{x}—Ti1—Ti1^{iii}	125.3
Ti1^{i}—V1—Ti1	180.0	Ni1—Ti1—Ti1^{iii}	54.7
Ti1^{i}—V1—Ti1^{ii}	109.5	Ni1^{xi}—Ti1—Ti1^{iii}	54.7
Ti1—V1—Ti1^{ii}	70.5	Ni1^{ix}—Ti1—Ti1^{iii}	125.3
Ti1^{i}—V1—Ti1^{vii}	70.5	Ni1^{xii}—Ti1—Ti1^{iii}	125.3
Ti1—V1—Ti1^{vii}	109.5	Ni1^{viii}—Ti1—Ti1^{iii}	54.7
Ti1^{ii}—V1—Ti1^{vii}	180.0	Ni1^{xiii}—Ti1—Ti1^{iii}	54.7
Ti1^{i}—V1—Ti1^{vi}	70.5	Ni1^{xiv}—Ti1—Ti1^{iii}	125.3

Ti1—V1—Ti1^{vi}	109.5	Ti1^{viii}—Ti1—Ti1^{iii}	90.0
Ti1^{ii}—V1—Ti1^{vi}	70.5	Ti1^{v}—Ti1—Ti1^{iii}	90.0

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