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Crystal structure of Ti_4Ni_2C

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Single crystals of the intermetallic phase with composition Ti_4Ni_2C were serendipitously obtained by high-pressure sintering of a mixture with initial chemical composition Ti_2Ni. The Ti_4Ni_2C phase crystallizes in the $Fd\overline{3}m$ space group and can be considered as a partially filled Ti_2Ni structure with the C atom occupying an octahedral void. Ti_4Ni_2C is isotypic with Ti_4Ni_2O, Nb_4Ni_2C and Ta_4Ni_2C, all of which were studied previously by means of powder diffraction.

Structure description

A large number of intermetallic phases can be grouped into classes of compounds based on structural or chemical similarities. For example, Mueller & Knott (1963) investigated the related crystal structures of Ti_2Cu, Ti_2Ni, Ti_4Ni_2O and Ti_4Cu_2O by X-ray and neutron powder diffraction. They determined that the Ti_2Ni phase crystallizes in the $Fd\overline{3}m$ space group, with cell parameter a = 11.3193 (2) Å and with 96 atoms per unit cell; the Ti_4Ni_2O (Ti_4Cu_2O) phase also crystallizes in the $Fd\overline{3}m$ space group, with cell parameter a = 11.3279 (1) Å [a = 11.4353 (2) Å] and with 112 atoms per unit cell. The latter phases can be considered as partially filled Ti_2Ni variants with the additional oxygen atom occupying an octahedral position. Holleck & Thummler (1967) studied a series of carbides, nitrides and oxides in ternary systems and reported that Nb_4Ni_2C (a = 11.64 Å) and Ta_4Ni_2C (a = 11.61 Å) crystallize in the same partially filled Ti_2Ni structure. Sadrnezhaad *et al.* (2009) and Shigeo *et al.* (1993) have confirmed the existence of the Ti_4Ni_2C phase. However, no detailed study has been performed so far with respect to the determination of its crystal structure.

In the present study, the crystal structure model of Ti_4Ni_2C has been refined on the basis of single-crystal X-ray diffraction data. The lattice parameter a is similar to those of previously reported isotypic phases (see above), and its chemical composition was refined to be exactly Ti_4Ni_2C in accordance with the EDX results (see Fig. S1 and Table S1 in the supporting information). Carbon present in the crystal structure most likely originated from the graphite crucible used during high pressure sintering (HPS).

Ti_4Ni_2C crystallizes isotypically with other Ti_4Ni_2X compounds (X = C, N, O) with a partially filled Ti_2Ni structure in space group type $Fd\overline{3}m$. Fig. 1 shows the distribution of the atoms in the unit cell of Ti_4Ni_2C. The environments of the Ti1 and C1 sites are shown in Figs. 2 and 3, respectively. The Ti1 atom is situated at a position with site symmetry $.\overline{3}m$ (multiplicity 16, Wyckoff letter c). It is surrounded by six Ti2 atoms (2.mm, 48f) and six Ni1 atoms (.3m; 32e), defining the center of an icosahedron. The C1 atom occupies a position with site symmetry $.\overline{3}m$ (16d) and centers an octahedron defined by six Ti2 atoms. The shortest Ti1···Ti2 separation is 2.9415 (9) Å and the shortest Ti1···Ni1 separation is 2.4750 (4) Å; the C1—Ti2 bond length is 2.1127 (4) Å.

Synthesis and crystallization

The high-purity elements Ti (indicated purity 99.5%; 0.6291 g) and Ni (indicated purity 99.9%; 0.3869 g) were mixed uniformly in the stoichiometric ratio 2:1 and thoroughly ground in an agate mortar. The blended powders were then placed in a cemented carbide grinding mould of 5 mm diameter, and pressed into a tablet at about 4 MPa for 1 min. A

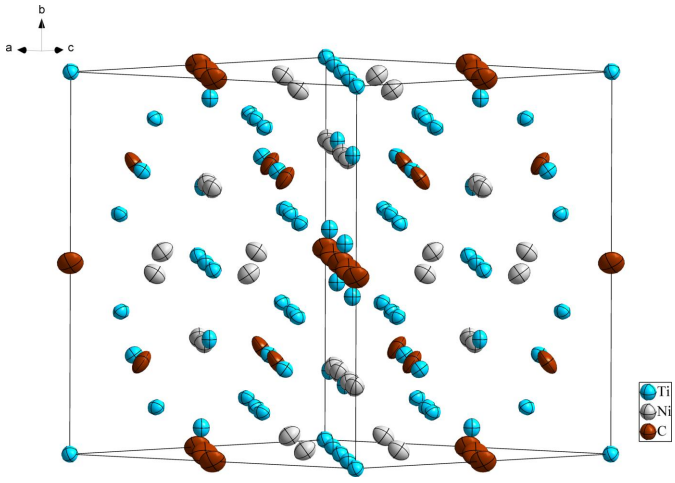

Figure 1
The crystal structure of Ti_4Ni_2C (one unit cell), with displacement ellipsoids drawn at the 99% probability level.

cylindrical block was obtained without deformations or cracks. Details of the high-pressure sintering experiment using a six-anvil high-temperature high-pressure apparatus can be found elsewhere (Liu & Fan, 2018). The samples were pressurized up to 6 GPa and heated to 1573 K for 40 min, and then rapidly cooled to room temperature by turning off the furnace power. A piece of a single-crystal ($0.06\times0.06\times0.04$ mm^3) was selected and mounted on a glass fibre for SXRD measurements.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. For better comparison, the labeling scheme and atomic coordinates of Ti_4Ni_2C were adapted from Nb_4Ni_2C and Ta_4Ni_2C (Holleck & Thuemmler, 1967). The maximum and minimum residual electron densities in the final difference map are located 1.10 Å from site Ni1 and 0.17 Å from Ti2, respectively.

Table 1
Experimental details.

Crystal data	
Chemical formula	Ti_4Ni_2C
M_r	320.87
Crystal system, space group	Cubic, $Fd\overline{3}m$
Temperature (K)	296
a (Å)	11.3235 (8)
V (Å^3)	1451.9 (3)
Z	16
Radiation type	Mo $K\alpha$
μ (mm^{-1})	18.28
Crystal size (mm)	0.06 × 0.06 × 0.04
Data collection	
Diffractometer	Bruker D8 Venture Photon 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.520, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12231, 105, 97
R_{int}	0.091
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.024, 0.051, 1.22
No. of reflections	105
No. of parameters	12
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.48, −0.70

Computer programs: *APEX3* (Bruker, 2015), *SAINT* (Bruker, 2015), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2017) and *publCIF* (Westrip, 2010).

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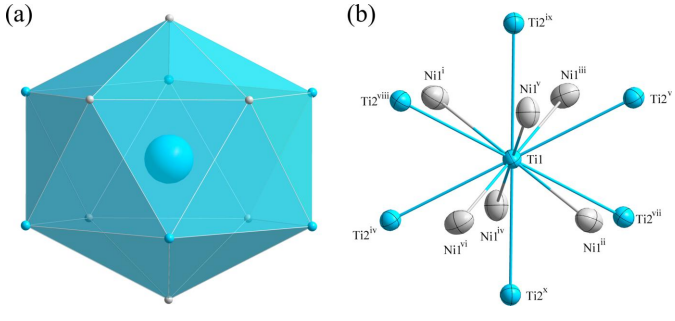

Figure 2
(*a*) The icosahedron formed around the Ti1 atom at the 16 *c* site; (*b*) the environment of the Ti1 atom with displacement ellipsoids given at the 99% probability level. [Symmetry codes: (i) $x-\frac{1}{4}, -y, z-\frac{1}{4}$; (ii) $-x+\frac{1}{4}, y, -z+\frac{1}{4}$; (iii) $-x, y-\frac{1}{4}, z-\frac{1}{4}$; (iv) $x-\frac{1}{4}, y-\frac{1}{4}, -z$; (v) $-x+\frac{1}{4}, -y+\frac{1}{4}, z$; (vi) $x, -y+\frac{1}{4}, -z+\frac{1}{4}$; (vii) $-z, x-\frac{1}{4}, y-\frac{1}{4}$; (viii) $z, -x+\frac{1}{4}, -y+\frac{1}{4}$; (ix) $y-\frac{1}{4}, -z, x-\frac{1}{4}$; (*x*) $-y+\frac{1}{4}, z, -x+\frac{1}{4}$.]

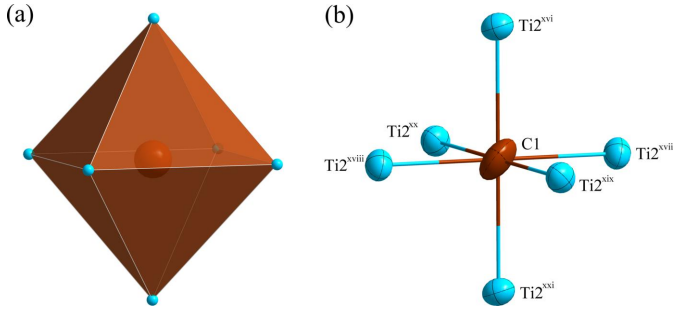

Figure 3
(*a*) The octahedron formed around the C1 atom at the 16 *d* site; (*b*) the environment of the C1 atom with displacement ellipsoids given at the 99% probability level. [Symmetry codes:·(xvi) $-y+\frac{1}{2}, -z+\frac{1}{2}, -x+1$; (xvii) $x, y+\frac{1}{2}, z+\frac{1}{2}$; (xviii) $-x+1, -y+\frac{1}{2}, -z+\frac{1}{2}$; (xix) $z+\frac{1}{2}, x, y+\frac{1}{2}$; (xx) $-z+\frac{1}{2}, -x+1, -y+\frac{1}{2}$; (xxi) $y+\frac{1}{2}, z+\frac{1}{2}, x$.]

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full crystallographic data

IUCrData (2024). **9**, x240043 [https://doi.org/10.1107/S2414314624000439]

Crystal structure of Ti_4Ni_2C

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Tetratitanium dinickel carbide

Crystal data

Ti_4Ni_2C
M_r = 320.87
Cubic, $Fd\overline{3}m$
a = 11.3235 (8) Å
V = 1451.9 (3) Å^3
Z = 16
$F(000)$ = 2400
D_x = 5.875 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3145 reflections
θ = 3.1–27.5°
μ = 18.28 mm^{-1}
T = 296 K
Lump, gray
0.06 × 0.06 × 0.04 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} = 0.520, T_{max} = 0.746
12231 measured reflections
105 independent reflections
97 reflections with $I > 2\sigma(I)$
R_{int} = 0.091
θ_{max} = 27.5°, θ_{min} = 3.1°
h = −14→14
k = −14→14
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.051
S = 1.22
105 reflections
12 parameters
0 restraints
$w = 1/[\sigma^2(F_o^2) + (0.0226P)^2 + 31.699P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.70 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}
Ti1	0.000000	0.000000	0.000000	0.0054 (5)
Ni1	0.21179 (6)	0.21179 (6)	0.21179 (6)	0.0080 (3)
Ti2	0.44034 (11)	0.125000	0.125000	0.0052 (3)

C1	0.500000	0.500000	0.500000	0.010 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ti1	0.0054 (5)	0.0054 (5)	0.0054 (5)	0.0004 (5)	0.0004 (5)	0.0004 (5)
Ni1	0.0080 (3)	0.0080 (3)	0.0080 (3)	0.0011 (2)	0.0011 (2)	0.0011 (2)
Ti2	0.0063 (6)	0.0046 (4)	0.0046 (4)	0.000	0.000	−0.0005 (4)
C1	0.010 (3)	0.010 (3)	0.010 (3)	−0.003 (3)	−0.003 (3)	−0.003 (3)

Geometric parameters (Å, º)

Ti1—Ni1^{i}	2.4750 (4)	Ni1—Ti2^{xiii}	2.6249 (9)
Ti1—Ni1^{ii}	2.4750 (4)	Ni1—Ni1^{v}	2.7797 (18)
Ti1—Ni1^{iii}	2.4750 (4)	Ni1—Ni1^{vi}	2.7797 (18)
Ti1—Ni1^{iv}	2.4750 (4)	Ni1—Ni1^{ii}	2.7797 (18)
Ti1—Ni1^{v}	2.4750 (4)	Ni1—Ti2^{xiv}	2.9376 (11)
Ti1—Ni1^{vi}	2.4750 (4)	Ni1—Ti2^{xv}	2.9376 (11)
Ti1—Ti2^{vii}	2.9415 (9)	Ni1—Ti2	2.9376 (11)
Ti1—Ti2^{viii}	2.9415 (9)	Ti2—C1^{xvi}	2.1127 (4)
Ti1—Ti2^{ix}	2.9415 (9)	Ti2—C1^{xvii}	2.1127 (4)
Ti1—Ti2^{iv}	2.9415 (9)	Ti2—Ti2^{xviii}	2.9571 (17)
Ti1—Ti2^{v}	2.9415 (9)	Ti2—Ti2^{xix}	2.9571 (17)
Ti1—Ti2^{x}	2.9415 (9)	Ti2—Ti2^{xx}	2.9571 (17)
Ni1—Ti2^{xi}	2.6249 (9)	Ti2—Ti2^{xxi}	2.9571 (17)
Ni1—Ti2^{xii}	2.6249 (9)		
Ni1^{i}—Ti1—Ni1^{ii}	180.00 (4)	Ti2^{xiii}—Ni1—Ti2^{xiv}	65.437 (12)
Ni1^{i}—Ti1—Ni1^{iii}	68.33 (4)	Ni1^{v}—Ni1—Ti2^{xiv}	61.76 (2)
Ni1^{ii}—Ti1—Ni1^{iii}	111.67 (4)	Ni1^{vi}—Ni1—Ti2^{xiv}	112.73 (2)
Ni1^{i}—Ti1—Ni1^{iv}	68.33 (4)	Ni1^{ii}—Ni1—Ti2^{xiv}	112.73 (2)
Ni1^{ii}—Ti1—Ni1^{iv}	111.67 (4)	Ti1^{vi}—Ni1—Ti2^{xv}	65.185 (5)
Ni1^{iii}—Ti1—Ni1^{iv}	68.33 (4)	Ti1^{v}—Ni1—Ti2^{xv}	65.185 (5)
Ni1^{i}—Ti1—Ni1^{v}	111.67 (4)	Ti1^{ii}—Ni1—Ti2^{xv}	166.08 (5)
Ni1^{ii}—Ti1—Ni1^{v}	68.33 (4)	Ti2^{xi}—Ni1—Ti2^{xv}	65.437 (12)
Ni1^{iii}—Ti1—Ni1^{v}	111.67 (4)	Ti2^{xii}—Ni1—Ti2^{xv}	123.55 (5)
Ni1^{iv}—Ti1—Ni1^{v}	180.00 (6)	Ti2^{xiii}—Ni1—Ti2^{xv}	65.437 (12)
Ni1^{i}—Ti1—Ni1^{vi}	111.67 (4)	Ni1^{v}—Ni1—Ti2^{xv}	112.73 (2)
Ni1^{ii}—Ti1—Ni1^{vi}	68.33 (4)	Ni1^{vi}—Ni1—Ti2^{xv}	112.73 (2)
Ni1^{iii}—Ti1—Ni1^{vi}	180.0	Ni1^{ii}—Ni1—Ti2^{xv}	61.76 (2)
Ni1^{iv}—Ti1—Ni1^{vi}	111.67 (4)	Ti2^{xiv}—Ni1—Ti2^{xv}	118.526 (10)
Ni1^{v}—Ti1—Ni1^{vi}	68.33 (4)	Ti1^{vi}—Ni1—Ti2	166.08 (5)
Ni1^{i}—Ti1—Ti2^{vii}	122.80 (3)	Ti1^{v}—Ni1—Ti2	65.185 (5)
Ni1^{ii}—Ti1—Ti2^{vii}	57.20 (3)	Ti1^{ii}—Ni1—Ti2	65.185 (5)
Ni1^{iii}—Ti1—Ti2^{vii}	65.020 (15)	Ti2^{xi}—Ni1—Ti2	65.437 (12)
Ni1^{iv}—Ti1—Ti2^{vii}	65.020 (15)	Ti2^{xii}—Ni1—Ti2	65.437 (12)
Ni1^{v}—Ti1—Ti2^{vii}	114.980 (15)	Ti2^{xiii}—Ni1—Ti2	123.55 (5)
Ni1^{vi}—Ti1—Ti2^{vii}	114.980 (15)	Ni1^{v}—Ni1—Ti2	112.73 (2)

Ni1^{i}—Ti1—Ti2^{viii}	57.20 (3)	Ni1^{vi}—Ni1—Ti2	61.76 (2)
Ni1^{ii}—Ti1—Ti2^{viii}	122.80 (3)	Ni1^{ii}—Ni1—Ti2	112.73 (2)
Ni1^{iii}—Ti1—Ti2^{viii}	114.980 (15)	Ti2^{xiv}—Ni1—Ti2	118.525 (10)
Ni1^{iv}—Ti1—Ti2^{viii}	114.980 (15)	Ti2^{xv}—Ni1—Ti2	118.525 (10)
Ni1^{v}—Ti1—Ti2^{viii}	65.020 (15)	C1^{xvi}—Ti2—C1^{xvii}	142.70 (6)
Ni1^{vi}—Ti1—Ti2^{viii}	65.020 (15)	C1^{xvi}—Ti2—Ni1^{xxii}	88.304 (12)
Ti2^{vii}—Ti1—Ti2^{viii}	180.00 (3)	C1^{xvii}—Ti2—Ni1^{xxii}	88.304 (12)
Ni1^{i}—Ti1—Ti2^{ix}	65.020 (15)	C1^{xvi}—Ti2—Ni1^{xxiii}	88.304 (12)
Ni1^{ii}—Ti1—Ti2^{ix}	114.980 (15)	C1^{xvii}—Ti2—Ni1^{xxiii}	88.304 (12)
Ni1^{iii}—Ti1—Ti2^{ix}	65.020 (15)	Ni1^{xxii}—Ti2—Ni1^{xxiii}	169.38 (6)
Ni1^{iv}—Ti1—Ti2^{ix}	122.80 (3)	C1^{xvi}—Ti2—Ni1^{vi}	136.89 (5)
Ni1^{v}—Ti1—Ti2^{ix}	57.20 (3)	C1^{xvii}—Ti2—Ni1^{vi}	80.41 (3)
Ni1^{vi}—Ti1—Ti2^{ix}	114.980 (15)	Ni1^{xxii}—Ti2—Ni1^{vi}	94.68 (3)
Ti2^{vii}—Ti1—Ti2^{ix}	118.270 (7)	Ni1^{xxiii}—Ti2—Ni1^{vi}	94.68 (3)
Ti2^{viii}—Ti1—Ti2^{ix}	61.730 (7)	C1^{xvi}—Ti2—Ni1	80.41 (3)
Ni1^{i}—Ti1—Ti2^{iv}	65.020 (15)	C1^{xvii}—Ti2—Ni1	136.89 (5)
Ni1^{ii}—Ti1—Ti2^{iv}	114.980 (15)	Ni1^{xxii}—Ti2—Ni1	94.68 (3)
Ni1^{iii}—Ti1—Ti2^{iv}	122.80 (3)	Ni1^{xxiii}—Ti2—Ni1	94.68 (3)
Ni1^{iv}—Ti1—Ti2^{iv}	65.020 (15)	Ni1^{vi}—Ti2—Ni1	56.48 (5)
Ni1^{v}—Ti1—Ti2^{iv}	114.980 (15)	C1^{xvi}—Ti2—Ti1^{ii}	103.550 (18)
Ni1^{vi}—Ti1—Ti2^{iv}	57.20 (3)	C1^{xvii}—Ti2—Ti1^{ii}	103.550 (18)
Ti2^{vii}—Ti1—Ti2^{iv}	118.270 (7)	Ni1^{xxii}—Ti2—Ti1^{ii}	138.19 (4)
Ti2^{viii}—Ti1—Ti2^{iv}	61.730 (7)	Ni1^{xxiii}—Ti2—Ti1^{ii}	52.426 (19)
Ti2^{ix}—Ti1—Ti2^{iv}	118.270 (7)	Ni1^{vi}—Ti2—Ti1^{ii}	49.79 (2)
Ni1^{i}—Ti1—Ti2^{v}	114.980 (15)	Ni1—Ti2—Ti1^{ii}	49.79 (2)
Ni1^{ii}—Ti1—Ti2^{v}	65.020 (15)	C1^{xvi}—Ti2—Ti1^{v}	103.550 (18)
Ni1^{iii}—Ti1—Ti2^{v}	57.20 (3)	C1^{xvii}—Ti2—Ti1^{v}	103.550 (18)
Ni1^{iv}—Ti1—Ti2^{v}	114.980 (15)	Ni1^{xxii}—Ti2—Ti1^{v}	52.426 (19)
Ni1^{v}—Ti1—Ti2^{v}	65.020 (15)	Ni1^{xxiii}—Ti2—Ti1^{v}	138.19 (4)
Ni1^{vi}—Ti1—Ti2^{v}	122.80 (3)	Ni1^{vi}—Ti2—Ti1^{v}	49.79 (2)
Ti2^{vii}—Ti1—Ti2^{v}	61.730 (7)	Ni1—Ti2—Ti1^{v}	49.79 (2)
Ti2^{viii}—Ti1—Ti2^{v}	118.270 (7)	Ti1^{ii}—Ti2—Ti1^{v}	85.77 (3)
Ti2^{ix}—Ti1—Ti2^{v}	61.730 (7)	C1^{xvi}—Ti2—Ti2^{xviii}	45.58 (2)
Ti2^{iv}—Ti1—Ti2^{v}	180.00 (3)	C1^{xvii}—Ti2—Ti2^{xviii}	104.34 (3)
Ni1^{i}—Ti1—Ti2^{x}	114.980 (15)	Ni1^{xxii}—Ti2—Ti2^{xviii}	115.62 (3)
Ni1^{ii}—Ti1—Ti2^{x}	65.020 (15)	Ni1^{xxiii}—Ti2—Ti2^{xviii}	55.72 (2)
Ni1^{iii}—Ti1—Ti2^{x}	114.980 (15)	Ni1^{vi}—Ti2—Ti2^{xviii}	149.263 (5)
Ni1^{iv}—Ti1—Ti2^{x}	57.20 (3)	Ni1—Ti2—Ti2^{xviii}	112.73 (2)
Ni1^{v}—Ti1—Ti2^{x}	122.80 (3)	Ti1^{ii}—Ti2—Ti2^{xviii}	100.245 (14)
Ni1^{vi}—Ti1—Ti2^{x}	65.020 (15)	Ti1^{v}—Ti2—Ti2^{xviii}	149.135 (4)
Ti2^{vii}—Ti1—Ti2^{x}	61.730 (7)	C1^{xvi}—Ti2—Ti2^{xix}	45.58 (2)
Ti2^{viii}—Ti1—Ti2^{x}	118.270 (7)	C1^{xvii}—Ti2—Ti2^{xix}	104.34 (3)
Ti2^{ix}—Ti1—Ti2^{x}	180.0	Ni1^{xxii}—Ti2—Ti2^{xix}	55.72 (2)
Ti2^{iv}—Ti1—Ti2^{x}	61.730 (7)	Ni1^{xxiii}—Ti2—Ti2^{xix}	115.62 (3)
Ti2^{v}—Ti1—Ti2^{x}	118.270 (7)	Ni1^{vi}—Ti2—Ti2^{xix}	149.263 (5)
Ti1^{vi}—Ni1—Ti1^{v}	107.95 (2)	Ni1—Ti2—Ti2^{xix}	112.73 (2)
Ti1^{vi}—Ni1—Ti1^{ii}	107.95 (2)	Ti1^{ii}—Ti2—Ti2^{xix}	149.135 (4)
Ti1^{v}—Ni1—Ti1^{ii}	107.95 (2)	Ti1^{v}—Ti2—Ti2^{xix}	100.245 (14)

Ti1^{vi}—Ni1—Ti2^{xi}	125.12 (2)	Ti2^{xviii}—Ti2—Ti2^{xix}	60.0
Ti1^{v}—Ni1—Ti2^{xi}	70.38 (3)	C1^{xvi}—Ti2—Ti2^{xx}	104.34 (3)
Ti1^{ii}—Ni1—Ti2^{xi}	125.12 (2)	C1^{xvii}—Ti2—Ti2^{xx}	45.58 (2)
Ti1^{vi}—Ni1—Ti2^{xii}	125.12 (2)	Ni1^{xxii}—Ti2—Ti2^{xx}	115.62 (3)
Ti1^{v}—Ni1—Ti2^{xii}	125.12 (2)	Ni1^{xxiii}—Ti2—Ti2^{xx}	55.72 (2)
Ti1^{ii}—Ni1—Ti2^{xii}	70.38 (3)	Ni1^{vi}—Ti2—Ti2^{xx}	112.73 (2)
Ti2^{xi}—Ni1—Ti2^{xii}	68.57 (5)	Ni1—Ti2—Ti2^{xx}	149.262 (5)
Ti1^{vi}—Ni1—Ti2^{xiii}	70.38 (3)	Ti1^{ii}—Ti2—Ti2^{xx}	100.245 (14)
Ti1^{v}—Ni1—Ti2^{xiii}	125.12 (2)	Ti1^{v}—Ti2—Ti2^{xx}	149.135 (4)
Ti1^{ii}—Ni1—Ti2^{xiii}	125.12 (2)	Ti2^{xviii}—Ti2—Ti2^{xx}	60.0
Ti2^{xi}—Ni1—Ti2^{xiii}	68.57 (5)	Ti2^{xix}—Ti2—Ti2^{xx}	90.001 (1)
Ti2^{xii}—Ni1—Ti2^{xiii}	68.57 (5)	C1^{xvi}—Ti2—Ti2^{xxi}	104.34 (3)
Ti1^{vi}—Ni1—Ni1^{v}	55.837 (19)	C1^{xvii}—Ti2—Ti2^{xxi}	45.58 (2)
Ti1^{v}—Ni1—Ni1^{v}	104.31 (2)	Ni1^{xxii}—Ti2—Ti2^{xxi}	55.72 (2)
Ti1^{ii}—Ni1—Ni1^{v}	55.837 (19)	Ni1^{xxiii}—Ti2—Ti2^{xxi}	115.62 (3)
Ti2^{xi}—Ni1—Ni1^{v}	174.69 (3)	Ni1^{vi}—Ti2—Ti2^{xxi}	112.73 (2)
Ti2^{xii}—Ni1—Ni1^{v}	115.62 (3)	Ni1—Ti2—Ti2^{xxi}	149.262 (5)
Ti2^{xiii}—Ni1—Ni1^{v}	115.62 (3)	Ti1^{ii}—Ti2—Ti2^{xxi}	149.135 (3)
Ti1^{vi}—Ni1—Ni1^{vi}	104.31 (2)	Ti1^{v}—Ti2—Ti2^{xxi}	100.245 (14)
Ti1^{v}—Ni1—Ni1^{vi}	55.837 (19)	Ti2^{xviii}—Ti2—Ti2^{xxi}	90.0
Ti1^{ii}—Ni1—Ni1^{vi}	55.837 (19)	Ti2^{xix}—Ti2—Ti2^{xxi}	60.0
Ti2^{xi}—Ni1—Ni1^{vi}	115.62 (3)	Ti2^{xx}—Ti2—Ti2^{xxi}	60.0
Ti2^{xii}—Ni1—Ni1^{vi}	115.62 (3)	Ti2^{xxiv}—C1—Ti2^{xxv}	91.17 (4)
Ti2^{xiii}—Ni1—Ni1^{vi}	174.69 (3)	Ti2^{xxiv}—C1—Ti2^{xxvi}	88.83 (4)
Ni1^{v}—Ni1—Ni1^{vi}	60.0	Ti2^{xxv}—C1—Ti2^{xxvi}	180.0
Ti1^{vi}—Ni1—Ni1^{ii}	55.837 (19)	Ti2^{xxiv}—C1—Ti2^{xxvii}	91.17 (4)
Ti1^{v}—Ni1—Ni1^{ii}	55.837 (19)	Ti2^{xxv}—C1—Ti2^{xxvii}	88.83 (4)
Ti1^{ii}—Ni1—Ni1^{ii}	104.31 (2)	Ti2^{xxvi}—C1—Ti2^{xxvii}	91.17 (4)
Ti2^{xi}—Ni1—Ni1^{ii}	115.62 (3)	Ti2^{xxiv}—C1—Ti2^{xxviii}	88.83 (4)
Ti2^{xii}—Ni1—Ni1^{ii}	174.69 (3)	Ti2^{xxv}—C1—Ti2^{xxviii}	91.17 (4)
Ti2^{xiii}—Ni1—Ni1^{ii}	115.62 (3)	Ti2^{xxvi}—C1—Ti2^{xxviii}	88.83 (4)
Ni1^{v}—Ni1—Ni1^{ii}	60.0	Ti2^{xxvii}—C1—Ti2^{xxviii}	180.0
Ni1^{vi}—Ni1—Ni1^{ii}	60.0	Ti2^{xxiv}—C1—Ti2^{xxix}	180.0
Ti1^{vi}—Ni1—Ti2^{xiv}	65.185 (5)	Ti2^{xxv}—C1—Ti2^{xxix}	88.83 (4)
Ti1^{v}—Ni1—Ti2^{xiv}	166.08 (5)	Ti2^{xxvi}—C1—Ti2^{xxix}	91.17 (4)
Ti1^{ii}—Ni1—Ti2^{xiv}	65.185 (5)	Ti2^{xxvii}—C1—Ti2^{xxix}	88.83 (4)
Ti2^{xi}—Ni1—Ti2^{xiv}	123.55 (5)	Ti2^{xxviii}—C1—Ti2^{xxix}	91.17 (4)
Ti2^{xii}—Ni1—Ti2^{xiv}	65.437 (12)		

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