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$Ti_4Fe_2C_{0.82}O_{0.18}$

Huizi Liu,[a] Changzeng Fan,[a,b]* Bin Wen[a] and Lifeng Zhang[a,c]

[a]State Key Laboratory of Metastable Materials Science and Technology, Yanshan University, Qinhuangdao 066004, People's Republic of China, [b]Hebei Key Lab for Optimizing Metal Product Technology and Performance, Yanshan University, Qinhuangdao 066004, People's Republic of China, and [c]School of Mechanical and Materials Engineering, North China University of Technology, Beijing 100144, People's Republic of China. *Correspondence e-mail: chzfan@ysu.edu.cn

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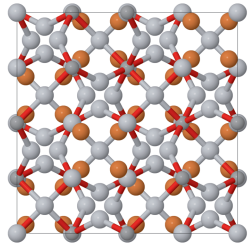
The phase with composition $Ti_4Fe_2C_{0.82}O_{0.18}$, tetratitanium diiron carbide oxide, was unexpectedly synthesized by high-pressure sintering (HPS) of a stoichiometric mixture with nominal composition Ti_2Fe. The $Ti_4Fe_2C_{0.82}O_{0.18}$ phase crystallizes in the $Fd\bar{3}m$ space group and can be considered as the Ti_2Fe structure filled with C and O atoms co-occupying the same octahedral void [occupancy ratio 0.82 (7):0.18 (7)]. The $Ti_4Fe_2C_{0.82}O_{0.18}$ phase is isotypic with Ti_4Ni_2C and $Ti_4Fe_2O_{0.407}$, and is the first example where C and O atoms co-occupy the same site in filled Ti_2Fe structures.

3D view



Structure description

Intermetallic phases usually are classified by structural or chemical similarities. For example, Duwez & Taylor (1950) investigated the crystal structure of Ti_2Fe on the basis of X-ray powder data. They determined that the Ti_2Fe phase crystallizes in a face centered cubic (f.c.c.) unit cell, with cell parameter a = 11.305 Å and with 96 atoms per unit cell. The related crystal structure of cubic $Ti_4Fe_2O_{0.407}$ was refined on the basis of neutron powder diffraction, affording the cell parameter a = 11.3326 (5) Å in space group $Fd\bar{3}m$ with Ti on position 48 f and on 16 d, Fe on 32 e and O (with a site occupation factor of 0.407) on 16 c (Rupp & Fischer, 1988). Liu *et al.* (2024) reported the isotypic crystal structure of Ti_4Ni_2C [a = 11.3235 (8) Å] by using single-crystal X-ray diffraction (SXRD) measurements. The latter phase can be considered as a partially filled Ti_2Ni structure with the C atom occupying an octahedral void. Holleck & Thummler (1967) studied a series of carbides, nitrides and oxides in ternary systems including Nb_4Ni_2C (a = 11.64 Å) and Ta_4Ni_2C (a =11.61 Å) phases. Although the title $Ti_4Fe_2C_{0.82}O_{0.18}$ phase is isotypic with Ti_4Ni_2C and $Ti_4Fe_2O_{0.407}$, no detailed study has been performed so far with respect to a phase where C and O atoms co-occupy the same site. The carbon present in the crystal structure of $Ti_4Fe_2C_{0.82}O_{0.18}$ most likely originated from the graphite crucible used during

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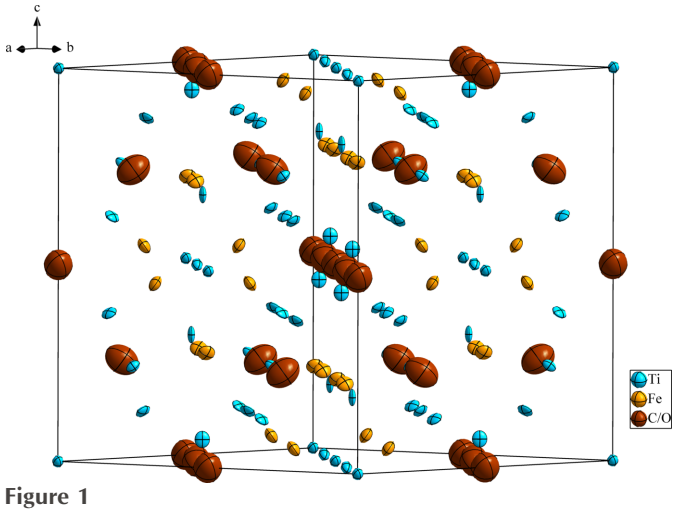

Figure 1
The crystal structure of $Ti_4Fe_2C_{0.82}O_{0.18}$, with displacement ellipsoids drawn at the 99.9% probability level.

high pressure sintering (HPS), whereas oxygen may be incorporated due to surface oxidation during sample storage and subsequent HPS.

$Ti_4Fe_2C_{0.82}O_{0.18}$ crystallizes isotypically with $Ti_4Fe_2O_{0.407}$ and Ti_4Ni_2C in a partially filled Ti_2Fe structure in space group type $Fd\bar{3}m$. Fig. 1 shows the distribution of the atoms in the the unit cell of $Ti_4Fe_2C_{0.82}O_{0.18}$. The environments of the Ti1 and (C1/O1) sites are shown in Figs. 2 and 3, respectively. The Ti1 atom is situated at a position with site symmetry $.\bar{3}m$ (multiplicity 16, Wyckoff letter *c*). It is surrounded by six Ti2 atoms (2.*mm*, 48 *f*) and six Fe1 atoms (.3*m*, 32 *e*), defining the center of an icosahedron. The (C1/O1) atoms co-occupy a position with site symmetry $.\bar{3}m$ (16 *d*) and center an octahedron defined by six Ti2 atoms. The shortest Ti1 to Ti2 separation is 2.9084 (10) Å and the shortest Ti1 to Fe1 separation is 2.4650 (4) Å; the (C1/O1)—Ti2 bond length is 2.1273 (5) Å.

Synthesis and crystallization

Pure titanium powder (indicated purity 99.5%, 0.6312 g) and iron powder (indicated purity 99.9%, 0.3693 g) were evenly mixed according to the stoichiometric ratio of 2:1 and thoroughly ground in an agate mortar. The mixed powder was put 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. Details 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 1473 K for 20 minutes, cooled to 1173 K, held at the temperature for 1 h, and then the furnace power was turned off to rapidly cool to room temperature. Different phases were isolated from two samples from the same batch. $Ti_4Fe_2C_{0.82}O_{0.18}$ originated from sample 1, together with TiFe. The refined chemical formula of $Ti_4Fe_2C_{0.82}O_{0.18}$ from sample 1 is in accordance with the complementary EDX results (see Table S1 of the electronic supporting information, ESI). Another phase with very similar refined composition, $Ti_4Fe_2C_{0.87}O_{0.13}$, was isolated from sample 2, and its composition is also in accordance with the complementary EDX results (see Table S2 of the ESI). Different options for refinements for the two phases $Ti_4Fe_2C_{1-\delta}O_\delta$ ($\delta = 0.18$; $\delta = 0.13$) are listed in Table S3 of the ESI. The crystal structures of $Ti_4Fe_2C_{0.82}O_{0.18}$ and $Ti_4Fe_2C_{0.87}O_{0.13}$ are very similar, just different in atomic proportions at the 16 *d* site, so the $Ti_4Fe_2C_{0.82}O_{0.18}$ phase was selected for the current report. Structural data for $Ti_4Fe_2C_{0.87}O_{0.13}$ can be found in Table S4 of the ESI.

Refinement

Crystal data, data collection and structure refinement details of $Ti_4Fe_2C_{0.82}O_{0.18}$ are summarized in Table 1. The labeling scheme and atomic coordinates of $Ti_4Fe_2C_{0.82}O_{0.18}$ were adapted from Ti_4Ni_2C for better comparison (Liu *et al.*, 2024). The 16 *d* site is co-occupied by C and O atoms, with site occupancies refined to 0.82 (7) for C1 and 0.18 (7) for O1, assuming full occupancy. Both atoms were refined with the same displacement parameters. The maximum and minimum residual electron densities in the final difference map are located 1.16 Å from site Fe1 and 1.67 Å from Fe1, respectively.

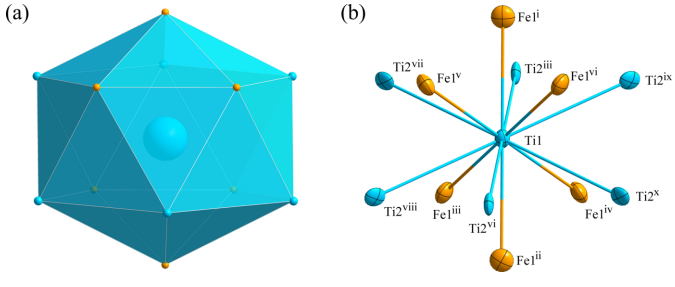

Figure 2
(*a*) The icosahedron formed around the Ti1 atom at the 16 *c* site; (*b*) the environment of the Ti1 atom with displacement ellipsoids drawn at the 99.9% probability level. [Symmetry codes: (i) $-x, y-\frac{1}{4}, z-\frac{1}{4}$; (ii) $x, -y+\frac{1}{4}, -z+\frac{1}{4}$; (iii) $-x+\frac{1}{4}, -y+\frac{1}{4}, z$; (iv) $-x+\frac{1}{4}, y, -z+\frac{1}{4}$; (v) $x-\frac{1}{4}, -y, z-\frac{1}{4}$; (vi) $x-\frac{1}{4}, y-\frac{1}{4}, -z$; (vii) $y-\frac{1}{4}, -z, x-\frac{1}{4}$; (viii) $z, -x+\frac{1}{4}, -y+\frac{1}{4}$; (ix) $-z, x-\frac{1}{4}, y-\frac{1}{4}$; (*x*) $-y+\frac{1}{4}, z, -x+\frac{1}{4}$.]

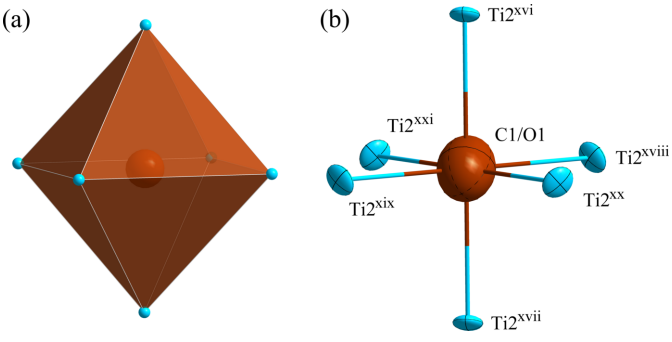

Figure 3
(*a*) The octahedron formed around the (C1/O1) atoms at the 16 *d* site; (*b*) the environment of the (C1/O1) atoms with displacement ellipsoids drawn at the 99.9% probability level. [Symmetry codes: (xvi) $-z+\frac{1}{2}, -x+1, -y+\frac{1}{2}$; (xvii) $z+\frac{1}{2}, x, y+\frac{1}{2}$; (xviii) $x, y+\frac{1}{2}, z+\frac{1}{2}$; (xix) $-x+1, -y+\frac{1}{2}, -z+\frac{1}{2}$; (xx) $-y+\frac{1}{2}, -z+\frac{1}{2}, -x+1$; (xxi) $y+\frac{1}{2}, z+\frac{1}{2}, x$.]

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Table 1
Experimental details.

Crystal data	
Chemical formula	$Ti_4Fe_2C_{0.82}O_{0.18}$
M_r	316.02
Crystal system, space group	Cubic, $Fd\bar{3}m$
Temperature (K)	296
a (Å)	11.323 (4)
V (Å^3)	1451.6 (3)
Z	16
Radiation type	Mo $K\alpha$
μ (mm^{-1})	15.91
Crystal size (mm)	0.10 × 0.06 × 0.06
Data collection	
Diffractometer	Bruker D8 Venture Photon 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.429, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5363, 102, 82
R_{int}	0.155
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.643
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.022, 0.040, 1.14
No. of reflections	102
No. of parameters	13
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.58, −0.83

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

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full crystallographic data

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$Ti_4Fe_2C_{0.82}O_{0.18}$

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Tetratitanium diiron carbide oxide

Crystal data

$Ti_4Fe_2C_{0.82}O_{0.18}$
M_r = 316.02
Cubic, $Fd\overline{3}m$
a = 11.323 (4) Å
V = 1451.6 (3) Å^3
Z = 16
$F(000)$ = 2342
D_x = 5.784 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1378 reflections
θ = 3.1–26.7°
μ = 15.91 mm^{-1}
T = 296 K
Lump, gray
0.10 × 0.06 × 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} = 0.429, T_{max} = 0.746
5363 measured reflections
102 independent reflections
82 reflections with $I > 2\sigma(I)$
R_{int} = 0.155
θ_{max} = 27.2°, θ_{min} = 3.1°
h = −14→14
k = −13→14
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.040
S = 1.14
102 reflections
13 parameters
0 restraints
$w = 1/[\sigma^2(F_o^2) + (0.0069P)^2 + 29.2966P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.83 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)
Ti1	0.000000	0.000000	0.000000	0.0018 (5)	
Fe1	0.21037 (6)	0.21037 (6)	0.21037 (6)	0.0028 (4)	
Ti2	0.43636 (12)	0.125000	0.125000	0.0021 (4)	

C1	0.500000	0.500000	0.500000	0.012 (4)	0.82 (7)
O1	0.500000	0.500000	0.500000	0.012 (4)	0.18 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ti1	0.0018 (5)	0.0018 (5)	0.0018 (5)	0.0004 (6)	0.0004 (6)	0.0004 (6)
Fe1	0.0028 (4)	0.0028 (4)	0.0028 (4)	−0.0007 (3)	−0.0007 (3)	−0.0007 (3)
Ti2	0.0033 (8)	0.0016 (5)	0.0016 (5)	0.000	0.000	−0.0010 (5)
C1	0.012 (4)	0.012 (4)	0.012 (4)	0.002 (4)	0.002 (4)	0.002 (4)
O1	0.012 (4)	0.012 (4)	0.012 (4)	0.002 (4)	0.002 (4)	0.002 (4)

Geometric parameters (Å, º)

Ti1—Fe1^{i}	2.4650 (4)	Fe1—Ti2^{xiii}	2.6501 (10)
Ti1—Fe1^{ii}	2.4650 (4)	Fe1—Fe1^{iii}	2.734 (2)
Ti1—Fe1^{iii}	2.4650 (4)	Fe1—Fe1^{ii}	2.734 (2)
Ti1—Fe1^{iv}	2.4650 (4)	Fe1—Fe1^{iv}	2.734 (2)
Ti1—Fe1^{v}	2.4650 (4)	Fe1—Ti2	2.9011 (12)
Ti1—Fe1^{vi}	2.4650 (4)	Fe1—Ti2^{xiv}	2.9011 (12)
Ti1—Ti2^{vii}	2.9084 (10)	Fe1—Ti2^{xv}	2.9011 (12)
Ti1—Ti2^{iii}	2.9084 (10)	Ti2—C1^{xvi}	2.1273 (5)
Ti1—Ti2^{vi}	2.9084 (10)	Ti2—C1^{xvii}	2.1273 (5)
Ti1—Ti2^{viii}	2.9084 (10)	Ti2—Ti2^{xviii}	2.9963 (6)
Ti1—Ti2^{ix}	2.9084 (10)	Ti2—Ti2^{xix}	2.9963 (6)
Ti1—Ti2^{x}	2.9084 (10)	Ti2—Ti2^{xi}	2.9963 (6)
Fe1—Ti2^{xi}	2.6501 (10)	Ti2—Ti2^{xii}	2.9963 (6)
Fe1—Ti2^{xii}	2.6501 (10)		

Fe1^{i}—Ti1—Fe1^{ii}	180.0	Ti2^{xi}—Fe1—Ti2^{xiv}	65.152 (14)
Fe1^{i}—Ti1—Fe1^{iii}	112.64 (4)	Ti2^{xii}—Fe1—Ti2^{xiv}	124.00 (6)
Fe1^{ii}—Ti1—Fe1^{iii}	67.36 (4)	Ti2^{xiii}—Fe1—Ti2^{xiv}	65.152 (14)
Fe1^{i}—Ti1—Fe1^{iv}	112.64 (4)	Fe1^{iii}—Fe1—Ti2^{xiv}	112.83 (2)
Fe1^{ii}—Ti1—Fe1^{iv}	67.36 (4)	Fe1^{ii}—Fe1—Ti2^{xiv}	112.83 (2)
Fe1^{iii}—Ti1—Fe1^{iv}	67.36 (4)	Fe1^{iv}—Fe1—Ti2^{xiv}	61.89 (3)
Fe1^{i}—Ti1—Fe1^{v}	67.36 (4)	Ti2—Fe1—Ti2^{xiv}	118.474 (12)
Fe1^{ii}—Ti1—Fe1^{v}	112.64 (4)	Ti1^{ii}—Fe1—Ti2^{xv}	65.047 (6)
Fe1^{iii}—Ti1—Fe1^{v}	112.64 (4)	Ti1^{iii}—Fe1—Ti2^{xv}	166.80 (5)
Fe1^{iv}—Ti1—Fe1^{v}	180.0	Ti1^{iv}—Fe1—Ti2^{xv}	65.047 (6)
Fe1^{i}—Ti1—Fe1^{vi}	67.36 (4)	Ti2^{xi}—Fe1—Ti2^{xv}	124.00 (6)
Fe1^{ii}—Ti1—Fe1^{vi}	112.64 (4)	Ti2^{xii}—Fe1—Ti2^{xv}	65.152 (14)
Fe1^{iii}—Ti1—Fe1^{vi}	180.0	Ti2^{xiii}—Fe1—Ti2^{xv}	65.152 (14)
Fe1^{iv}—Ti1—Fe1^{vi}	112.64 (4)	Fe1^{iii}—Fe1—Ti2^{xv}	61.89 (3)
Fe1^{v}—Ti1—Fe1^{vi}	67.36 (4)	Fe1^{ii}—Fe1—Ti2^{xv}	112.83 (2)
Fe1^{i}—Ti1—Ti2^{vii}	64.739 (17)	Fe1^{iv}—Fe1—Ti2^{xv}	112.83 (2)
Fe1^{ii}—Ti1—Ti2^{vii}	115.261 (17)	Ti2—Fe1—Ti2^{xv}	118.474 (12)
Fe1^{iii}—Ti1—Ti2^{vii}	58.40 (3)	Ti2^{xiv}—Fe1—Ti2^{xv}	118.474 (12)
Fe1^{iv}—Ti1—Ti2^{vii}	115.261 (17)	C1^{xvi}—Ti2—C1^{xvii}	140.40 (7)

Fe1^{v}—Ti1—Ti2^{vii}	64.739 (17)	C1^{xvi}—Ti2—Fe1^{xx}	88.009 (14)
Fe1^{vi}—Ti1—Ti2^{vii}	121.60 (3)	C1^{xvii}—Ti2—Fe1^{xx}	88.009 (14)
Fe1^{i}—Ti1—Ti2^{iii}	58.40 (3)	C1^{xvi}—Ti2—Fe1^{xxi}	88.009 (14)
Fe1^{ii}—Ti1—Ti2^{iii}	121.60 (3)	C1^{xvii}—Ti2—Fe1^{xxi}	88.009 (14)
Fe1^{iii}—Ti1—Ti2^{iii}	64.739 (17)	Fe1^{xx}—Ti2—Fe1^{xxi}	168.22 (7)
Fe1^{iv}—Ti1—Ti2^{iii}	64.739 (17)	C1^{xvi}—Ti2—Fe1^{ii}	137.91 (5)
Fe1^{v}—Ti1—Ti2^{iii}	115.261 (17)	C1^{xvii}—Ti2—Fe1^{ii}	81.68 (3)
Fe1^{vi}—Ti1—Ti2^{iii}	115.261 (17)	Fe1^{xx}—Ti2—Fe1^{ii}	95.19 (3)
Ti2^{vii}—Ti1—Ti2^{iii}	62.010 (9)	Fe1^{xxi}—Ti2—Fe1^{ii}	95.19 (3)
Fe1^{i}—Ti1—Ti2^{vi}	121.60 (3)	C1^{xvi}—Ti2—Fe1	81.69 (3)
Fe1^{ii}—Ti1—Ti2^{vi}	58.40 (3)	C1^{xvii}—Ti2—Fe1	137.91 (5)
Fe1^{iii}—Ti1—Ti2^{vi}	115.261 (17)	Fe1^{xx}—Ti2—Fe1	95.19 (3)
Fe1^{iv}—Ti1—Ti2^{vi}	115.261 (17)	Fe1^{xxi}—Ti2—Fe1	95.19 (3)
Fe1^{v}—Ti1—Ti2^{vi}	64.739 (17)	Fe1^{ii}—Ti2—Fe1	56.23 (6)
Fe1^{vi}—Ti1—Ti2^{vi}	64.739 (17)	C1^{xvi}—Ti2—Ti1^{iv}	104.226 (19)
Ti2^{vii}—Ti1—Ti2^{vi}	117.990 (9)	C1^{xvii}—Ti2—Ti1^{iv}	104.226 (19)
Ti2^{iii}—Ti1—Ti2^{vi}	180.0	Fe1^{xx}—Ti2—Ti1^{iv}	52.40 (2)
Fe1^{i}—Ti1—Ti2^{viii}	115.261 (17)	Fe1^{xxi}—Ti2—Ti1^{iv}	139.38 (5)
Fe1^{ii}—Ti1—Ti2^{viii}	64.739 (17)	Fe1^{ii}—Ti2—Ti1^{iv}	50.21 (2)
Fe1^{iii}—Ti1—Ti2^{viii}	64.739 (17)	Fe1—Ti2—Ti1^{iv}	50.21 (2)
Fe1^{iv}—Ti1—Ti2^{viii}	121.60 (3)	C1^{xvi}—Ti2—Ti1^{iii}	104.226 (19)
Fe1^{v}—Ti1—Ti2^{viii}	58.40 (3)	C1^{xvii}—Ti2—Ti1^{iii}	104.226 (19)
Fe1^{vi}—Ti1—Ti2^{viii}	115.261 (17)	Fe1^{xx}—Ti2—Ti1^{iii}	139.38 (5)
Ti2^{vii}—Ti1—Ti2^{viii}	62.010 (9)	Fe1^{xxi}—Ti2—Ti1^{iii}	52.40 (2)
Ti2^{iii}—Ti1—Ti2^{viii}	117.990 (9)	Fe1^{ii}—Ti2—Ti1^{iii}	50.21 (2)
Ti2^{vi}—Ti1—Ti2^{viii}	62.010 (9)	Fe1—Ti2—Ti1^{iii}	50.21 (2)
Fe1^{i}—Ti1—Ti2^{ix}	64.739 (17)	Ti1^{iv}—Ti2—Ti1^{iii}	86.98 (4)
Fe1^{ii}—Ti1—Ti2^{ix}	115.261 (17)	C1^{xvi}—Ti2—Ti2^{xviii}	149.47 (3)
Fe1^{iii}—Ti1—Ti2^{ix}	115.261 (17)	C1^{xvii}—Ti2—Ti2^{xviii}	45.23 (2)
Fe1^{iv}—Ti1—Ti2^{ix}	58.40 (3)	Fe1^{xx}—Ti2—Ti2^{xviii}	121.68 (3)
Fe1^{v}—Ti1—Ti2^{ix}	121.60 (3)	Fe1^{xxi}—Ti2—Ti2^{xviii}	61.47 (2)
Fe1^{vi}—Ti1—Ti2^{ix}	64.739 (17)	Fe1^{ii}—Ti2—Ti2^{xviii}	53.38 (3)
Ti2^{vii}—Ti1—Ti2^{ix}	117.990 (9)	Fe1—Ti2—Ti2^{xviii}	100.81 (3)
Ti2^{iii}—Ti1—Ti2^{ix}	62.010 (9)	Ti1^{iv}—Ti2—Ti2^{xviii}	100.29 (4)
Ti2^{vi}—Ti1—Ti2^{ix}	117.990 (9)	Ti1^{iii}—Ti2—Ti2^{xviii}	58.995 (4)
Ti2^{viii}—Ti1—Ti2^{ix}	180.0	C1^{xvi}—Ti2—Ti2^{xix}	149.47 (3)
Fe1^{i}—Ti1—Ti2^{x}	115.261 (17)	C1^{xvii}—Ti2—Ti2^{xix}	45.23 (2)
Fe1^{ii}—Ti1—Ti2^{x}	64.739 (17)	Fe1^{xx}—Ti2—Ti2^{xix}	61.47 (2)
Fe1^{iii}—Ti1—Ti2^{x}	121.60 (3)	Fe1^{xxi}—Ti2—Ti2^{xix}	121.68 (3)
Fe1^{iv}—Ti1—Ti2^{x}	64.739 (17)	Fe1^{ii}—Ti2—Ti2^{xix}	53.38 (3)
Fe1^{v}—Ti1—Ti2^{x}	115.261 (17)	Fe1—Ti2—Ti2^{xix}	100.81 (3)
Fe1^{vi}—Ti1—Ti2^{x}	58.40 (3)	Ti1^{iv}—Ti2—Ti2^{xix}	58.995 (4)
Ti2^{vii}—Ti1—Ti2^{x}	180.0	Ti1^{iii}—Ti2—Ti2^{xix}	100.29 (4)
Ti2^{iii}—Ti1—Ti2^{x}	117.990 (9)	Ti2^{xviii}—Ti2—Ti2^{xix}	60.54 (6)
Ti2^{vi}—Ti1—Ti2^{x}	62.010 (9)	C1^{xvi}—Ti2—Ti2^{xi}	45.23 (2)
Ti2^{viii}—Ti1—Ti2^{x}	117.990 (9)	C1^{xvii}—Ti2—Ti2^{xi}	149.47 (3)
Ti2^{ix}—Ti1—Ti2^{x}	62.010 (9)	Fe1^{xx}—Ti2—Ti2^{xi}	121.68 (3)
Ti1^{ii}—Fe1—Ti1^{iii}	108.58 (3)	Fe1^{xxi}—Ti2—Ti2^{xi}	61.47 (2)

Ti1^{ii}—Fe1—Ti1^{iv}	108.58 (3)	Fe1^{ii}—Ti2—Ti2^{xi}	100.81 (3)
Ti1^{iii}—Fe1—Ti1^{iv}	108.58 (3)	Fe1—Ti2—Ti2^{xi}	53.38 (3)
Ti1^{ii}—Fe1—Ti2^{xi}	124.77 (2)	Ti1^{iv}—Ti2—Ti2^{xi}	100.29 (4)
Ti1^{iii}—Fe1—Ti2^{xi}	69.20 (3)	Ti1^{iii}—Ti2—Ti2^{xi}	58.995 (4)
Ti1^{iv}—Fe1—Ti2^{xi}	124.77 (2)	Ti2^{xviii}—Ti2—Ti2^{xi}	112.60 (3)
Ti1^{ii}—Fe1—Ti2^{xii}	124.77 (2)	Ti2^{xix}—Ti2—Ti2^{xi}	153.19 (5)
Ti1^{iii}—Fe1—Ti2^{xii}	124.77 (2)	C1^{xvi}—Ti2—Ti2^{xii}	45.23 (2)
Ti1^{iv}—Fe1—Ti2^{xii}	69.20 (3)	C1^{xvii}—Ti2—Ti2^{xii}	149.47 (3)
Ti2^{xi}—Fe1—Ti2^{xii}	69.49 (5)	Fe1^{xx}—Ti2—Ti2^{xii}	61.47 (2)
Ti1^{ii}—Fe1—Ti2^{xiii}	69.20 (3)	Fe1^{xxi}—Ti2—Ti2^{xii}	121.68 (3)
Ti1^{iii}—Fe1—Ti2^{xiii}	124.77 (2)	Fe1^{ii}—Ti2—Ti2^{xii}	100.81 (3)
Ti1^{iv}—Fe1—Ti2^{xiii}	124.77 (2)	Fe1—Ti2—Ti2^{xii}	53.38 (3)
Ti2^{xi}—Fe1—Ti2^{xiii}	69.49 (5)	Ti1^{iv}—Ti2—Ti2^{xii}	58.995 (4)
Ti2^{xii}—Fe1—Ti2^{xiii}	69.49 (5)	Ti1^{iii}—Ti2—Ti2^{xii}	100.29 (4)
Ti1^{ii}—Fe1—Fe1^{iii}	56.32 (2)	Ti2^{xviii}—Ti2—Ti2^{xii}	153.19 (5)
Ti1^{iii}—Fe1—Fe1^{iii}	104.92 (3)	Ti2^{xix}—Ti2—Ti2^{xii}	112.60 (3)
Ti1^{iv}—Fe1—Fe1^{iii}	56.32 (2)	Ti2^{xi}—Ti2—Ti2^{xii}	60.54 (6)
Ti2^{xi}—Fe1—Fe1^{iii}	174.11 (3)	Ti2^{xxii}—C1—Ti2^{xxiii}	180.0
Ti2^{xii}—Fe1—Fe1^{iii}	115.14 (3)	Ti2^{xxii}—C1—Ti2^{xxiv}	89.54 (5)
Ti2^{xiii}—Fe1—Fe1^{iii}	115.14 (3)	Ti2^{xxiii}—C1—Ti2^{xxiv}	90.46 (5)
Ti1^{ii}—Fe1—Fe1^{ii}	104.92 (3)	Ti2^{xxii}—C1—Ti2^{xxv}	90.46 (5)
Ti1^{iii}—Fe1—Fe1^{ii}	56.32 (2)	Ti2^{xxiii}—C1—Ti2^{xxv}	89.54 (5)
Ti1^{iv}—Fe1—Fe1^{ii}	56.32 (2)	Ti2^{xxiv}—C1—Ti2^{xxv}	180.0
Ti2^{xi}—Fe1—Fe1^{ii}	115.14 (3)	Ti2^{xxii}—C1—Ti2^{xxvi}	90.46 (5)
Ti2^{xii}—Fe1—Fe1^{ii}	115.14 (3)	Ti2^{xxiii}—C1—Ti2^{xxvi}	89.54 (5)
Ti2^{xiii}—Fe1—Fe1^{ii}	174.11 (3)	Ti2^{xxiv}—C1—Ti2^{xxvi}	89.54 (5)
Fe1^{iii}—Fe1—Fe1^{ii}	60.0	Ti2^{xxv}—C1—Ti2^{xxvi}	90.46 (5)
Ti1^{ii}—Fe1—Fe1^{iv}	56.32 (2)	Ti2^{xxii}—C1—Ti2^{xxvii}	89.54 (5)
Ti1^{iii}—Fe1—Fe1^{iv}	56.32 (2)	Ti2^{xxiii}—C1—Ti2^{xxvii}	90.46 (5)
Ti1^{iv}—Fe1—Fe1^{iv}	104.92 (3)	Ti2^{xxiv}—C1—Ti2^{xxvii}	90.46 (5)
Ti2^{xi}—Fe1—Fe1^{iv}	115.14 (3)	Ti2^{xxv}—C1—Ti2^{xxvii}	89.54 (5)
Ti2^{xii}—Fe1—Fe1^{iv}	174.11 (3)	Ti2^{xxvi}—C1—Ti2^{xxvii}	180.0
Ti2^{xiii}—Fe1—Fe1^{iv}	115.14 (3)	Ti2^{xxii}—O1—Ti2^{xxiii}	180.0
Fe1^{iii}—Fe1—Fe1^{iv}	60.0	Ti2^{xxii}—O1—Ti2^{xxiv}	89.54 (5)
Fe1^{ii}—Fe1—Fe1^{iv}	60.0	Ti2^{xxiii}—O1—Ti2^{xxiv}	90.46 (5)
Ti1^{ii}—Fe1—Ti2	166.80 (5)	Ti2^{xxii}—O1—Ti2^{xxv}	90.46 (5)
Ti1^{iii}—Fe1—Ti2	65.047 (6)	Ti2^{xxiii}—O1—Ti2^{xxv}	89.54 (5)
Ti1^{iv}—Fe1—Ti2	65.047 (6)	Ti2^{xxiv}—O1—Ti2^{xxv}	180.0
Ti2^{xi}—Fe1—Ti2	65.152 (14)	Ti2^{xxii}—O1—Ti2^{xxvi}	90.46 (5)
Ti2^{xii}—Fe1—Ti2	65.152 (14)	Ti2^{xxiii}—O1—Ti2^{xxvi}	89.54 (5)
Ti2^{xiii}—Fe1—Ti2	124.00 (6)	Ti2^{xxiv}—O1—Ti2^{xxvi}	89.54 (5)
Fe1^{iii}—Fe1—Ti2	112.83 (2)	Ti2^{xxv}—O1—Ti2^{xxvi}	90.46 (5)
Fe1^{ii}—Fe1—Ti2	61.89 (3)	Ti2^{xxii}—O1—Ti2^{xxvii}	89.54 (5)
Fe1^{iv}—Fe1—Ti2	112.83 (2)	Ti2^{xxiii}—O1—Ti2^{xxvii}	90.46 (5)
Ti1^{ii}—Fe1—Ti2^{xiv}	65.047 (6)	Ti2^{xxiv}—O1—Ti2^{xxvii}	90.46 (5)

Ti1^{iii}—Fe1—Ti2^{xiv}	65.047 (6)	Ti2^{xxv}—O1—Ti2^{xxvii}	89.54 (5)
Ti1^{iv}—Fe1—Ti2^{xiv}	166.80 (5)	Ti2^{xxvi}—O1—Ti2^{xxvii}	180.0

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