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Structure of tetrakis(pentafluorophenoxido)-bis(tetrahydrofuran)titanium(IV)

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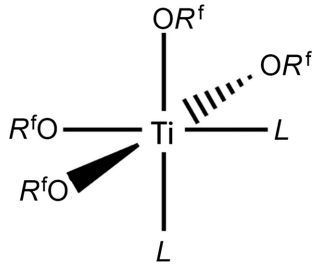
Titanium(IV) chloride was reacted with a slight excess of barium pentafluorophenoxide in tetrahydrofuran (THF) solution. After filtration and solvent evaporation, the resulting orange crystalline material was obtained. The product was recrystallized by preparing a concentrated solution in THF at room temperature, followed by cooling to 253 K. The supernatant solution was decanted using a pipet, and the crystals were dried by allowing the solvent to evaporate in the atmosphere of a glovebox. It was possible to obtain good-quality X-ray data at 100 K on a crystal, namely, tetrakis(pentafluorophenoxido-κO)bis(tetrahydrofuran-κO)titanium(IV), $[Ti(C_6F_5O)_4(C_4H_8O)_2]$, having monoclinic ($P2_1/n$) symmetry. This compound adopts a solid-state structure in which the titanium(IV) ions have a distorted octahedral coordination environment with two coordinated THF molecules occupying *cis* positions.

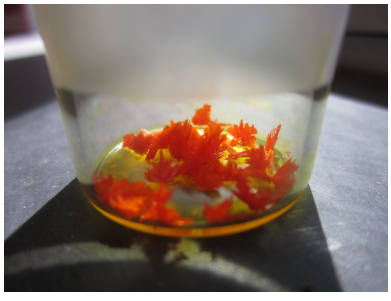
1. Chemical context

Early transition-metal alkoxides have been of interest for applications ranging from organic synthesis and catalysis to the preparation of metal oxide materials *via* the sol-gel process (Bradley, 1959; Bradley *et al.*, 1978; Bradley *et al.* 2001). Earlier work by the author of this article assumed the use of fluorinated alkoxides would provide enhanced Lewis acidity, while maintaining steric and stereochemical control over Ziegler–Natta polymerization-type processes. These publications described the partial substitution of alkyl alkoxides by fluoroalkoxides in alcoholysis-type reactions (Campbell *et al.*, 1994; Fisher *et al.*, 1993).



In addition, the structure of an acetonitrile adduct of tetrakisfluoroalkoxide titanium(IV), $Ti[OCH(CF_3)_2]_4(N{\equiv}CCH_3)_2$, was described, in which the coordinated solvent molecules act as Lewis bases in *cis* positions by way of nitrogen lone pairs. The coordination geometry of the titanium(IV) ion was best described as being a distorted octahedral structure. It was tempting to assume that this structure was typical for the disolvates of the tetrakisfluoralkoxide titanium(IV) complexes.

However, it was not possible to obtain suitable quality X-ray data for the analogous tetrahydrofuran (THF) adduct



due to the significantly low melting point. However, the data that were obtained seemed to suggest that the THF adduct was an ionization isomer in the solid state comprised of a $Ti(OPr^f)_2$-THF_4^{2+} cation and a $Ti(OPr^f)_6^{2-}$ anion (OPr^f is hexafluoroisopropoxide). Ionization isomers of metal complexes are known (Barbier *et al.*, 1972; Tebbe & Muetterties, 1967; Kamata *et al.*, 2012; Giesbrecht *et al.*, 2004; Xie *et al.*, 1996; Niemeyer, 2001), and it was assumed that the enhanced electron-withdrawing ability of the fluoroalkoxides as compared with the electron-donor properties of alkyl alkoxides would have a preference for such an ionization isomer in a polar solvent such as THF. Malinowski & Koteras (2026) recently described the crystal structure of $[Ti\{OC(CF_3)_3\}_2(N{\equiv}CCH_3)_4][Al\{OC(CF_3)_3\}_4]$, with the perfluoroalkoxide ligands coordinated to the titanium(III) cation exhibiting a significant amount of disorder.

Some recent efforts to obtain X-ray-quality crystals of the $Ti[OCH(CF_3)_2]_4THF_2$ complex, which was prepared by way of a metathesis reaction between titanium(IV) chloride and sodium hexafluoroisopropoxide in THF as a solvent, have been published (Van Der Sluys, 2024), but were again not entirely successful. However, it was possible to obtain the structure of a slightly higher melting minor product, in which only three chlorides had been substituted by fluoroalkoxides, producing $TiCl(OPr^f)_3THF_2$. In the present article, the X-ray crystal structure of the related pentafluorophenoxide complex, $Ti(OC_6F_5)_4THF_2$ (complex **1**), is reported.

2. Structural commentary

The molecular structure of **1** shown in Fig. 1 emphasizes the nearly octahedral coordination geometry of the Ti atom, with the THF ligands adopting a *cis* configuration. Guzei & Winter (1997) have presented arguments concerning the factors that affect the formation of *cis versus trans* isomers in $TiCl_4L_2$ complexes containing pyrazole ligands. Their arguments suggest that π-donor ligands greatly influence the stability of the *cis versus trans* isomers. Alkoxide ligands are generally considered better π-donor ligands than chloride ligands, but presumably the fluorophenoxide ligands somewhat attenuate these properties due to the electron-withdrawing nature of the F atoms and the potential delocalization of the oxygen lone pairs into the benzene π-ring system. Fractional coordinates and other crystallographic data can be found in the supporting information.

The coordination geometry of **1** is best described as distorted octahedral. The fluorophenoxide Ti—O bond lengths [average 1.8691 (19) Å] are comparable to those found in other fluorophenoxide compounds whose structures have been published previously (Campbell *et al.*, 1994; Fisher *et al.*, 1993). The Ti—O bond lengths for the coordinated THF ligands [average 2.1195 (18) Å] are significantly longer than the phenoxide bond lengths, comparable to those previously observed (Van Der Sluys, 2024), and consistent with the weaker polar coordinate bonds associated with the neutral ether ligands as compared with the phenoxide ligands.

3. Supramolecular features

Two of the fluorophenoxides in **1** have significantly more obtuse Ti—O—C bond angles and shorter Ti—O bond lengths than the other two fluorophenoxides. Specifically, the bond lengths and angles for the fluorophenoxides that are *trans* to the THF ligands are Ti1—O2 and Ti1—O3, which are 1.8777 (18) and 1.8370 (18) Å, respectively, while the Ti1—O2—C7 and Ti1—O3—C13 angles are 131.35 (17) and 158.45 (17)°, respectively. Alternatively, the fluorophenoxide ligands that are *trans* to each other, Ti1—O1 and Ti1—O4, have bond lengths of 1.8548 (19) and 1.9068 (19) Å, respec-

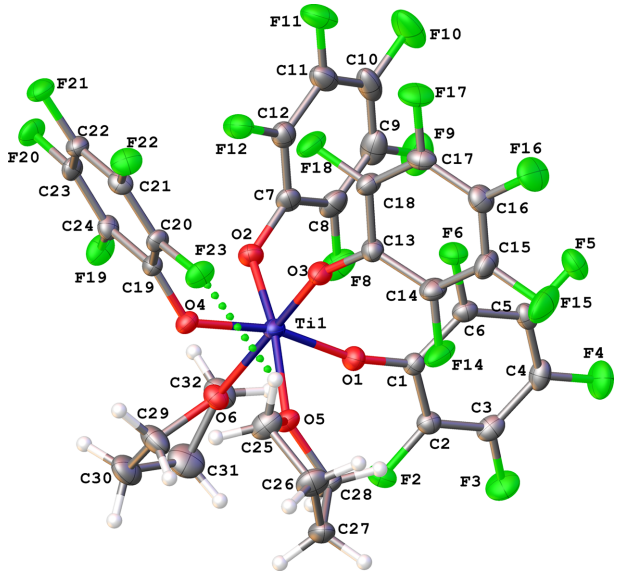


Figure 1
The molecular structure of **1**, showing the atom-numbering scheme used. Displacement ellipsoids are drawn at the 50% probability level.

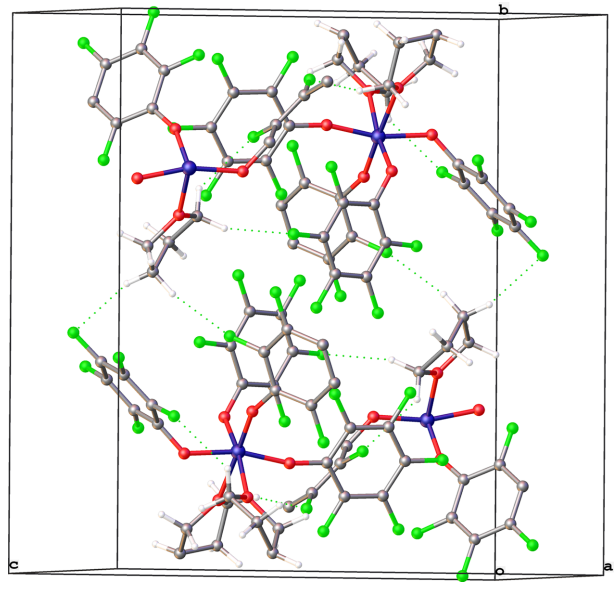


Figure 2
Packing diagram for the unit cell of **1**.

tively, and Ti1—O1—C1 and Ti1—O4—C1 angles of 166.99 (17) and 129.21 (16)°, respectively. These bond angles do not seem to correlate well with anticipated *trans*-influence effects associated with phenoxide ligands being *trans* to a phenoxide *versus* a THF ligand. The larger Ti—O—C bond angles and shorter Ti—O bond lengths could be interpreted as resulting from more significant π bonding interactions of the oxygen lone-pair interactions with the empty t_{2g} (d_{xy}, d_{xz} and d_{yz}) set of *d* orbitals of the titanium(IV) ion in an octahedral ligand field, which has a $3d^0$ electronic configuration. These variations do not seem to correlate with significant changes in the C—O bond lengths, which might be anticipated from changes in the bonding delocalization interactions of the benzene and the oxygen lone pairs. These variations in bond angles and lengths may simply be a result of crystal packing forces that influence the orientations of the benzene rings, as shown in the unit-cell packing diagram in Fig. 2.

4. Synthesis and crystallization

The reaction of pentafluorophenol with various alkoxides of titanium(IV) resulted in incomplete substitution of the alkyl alkoxide ligands (Campbell *et al.*, 1994). Mazdiyasni *et al.* (1971) described the synthesis of a series of hexafluoroisopropoxide Group IV element compounds by way of a metathesis approach, in which the metal chlorides were reacted with four equivalents of the sodium fluoroalkoxides, with the corresponding liquid fluoroalcohols as the solvent. The desired compounds were obtained by fractional distillation and could be recrystallized from various organic solvents, including diethyl ether and THF. It was hoped that a similar metathesis approach could be used to prepare the corresponding titanium(IV) pentafluorophenoxide compounds, but since pentafluorophenol is a solid at room temperature, THF was used as the solvent. A potential complicating factor in the reaction with greater than four equivalents of alkoxide is the potential formation of anionic species, such as $[Ti(OR)_5]^-$ (Boyle *et al.*, 1999; Chandler *et al.*, 1993) and $[Ti(OR)_6]^{2-}$ (Day *et al.*, 1995), which have been shown to be useful in controlling sol-gel production of titanium oxide solid-state materials.

Reaction of titanium(IV) chloride with greater than two equivalents of barium pentafluorophenoxide, which was prepared *in situ* from barium metal and pentafluorophenol, resulted in the rapid formation of an orange solution and a white precipitate. The solution was stirred at room temperature for 12 h, after which the solution was filtered, and the volume of the solution was reduced *in vacuo*. Cooling the solution to 253 K resulted in the formation of orange crystals, which were characterized by SEM-XPS and IR spectroscopy (see supporting information). The crystalline product has been formulated as $Ti(OC_6F_5)_4THF_2$. It was somewhat disappointing that this reaction did not appear to produce a double alkoxide complex containing barium and titanium(IV) ions similar to the $BaTi(OC_6H_5)_6{\cdot}2DMF$ compound (Day *et al.*, 1995), which was used to prepare barium titanate by way of the sol-gel process.

Liquid $TiCl_4$ and solid $TiCl_4THF_2$ were purchased from Aldrich and used as received. All synthetic procedures were carried out using standard Schlenk techniques or in a purified nitrogen atmosphere using a Braun UNIlab glovebox. Solvents were purified by distillation from a sodium benzophenone ketal solution and stored in glass containers with solvent seal fittings. IR spectra were recorded as KBr pellets, by grinding small portions of the sample with dried potassium bromide using an agate mortar and pestle in the glovebox. Fourier transform IR (FT–IR) spectra (Fig. S1 in the supporting information) were recorded on a ThermoScientific Nicolet iS10 FT–IR spectrometer. Residual gaseous carbon dioxide asymmetric vibrations were sometimes observed in the 2400 cm^{-1} region, due to incomplete background subtraction, and calibration was checked regularly using a film of polystyrene. Scanning electron micrograph (SEM) images and X-ray photoelectron spectroscopy (XPS) for compositional analysis (Fig. S2) were obtained by the Materials Characterization Lab of the Materials Research Institute at the PSU University Park campus.

5. Refinement

Crystal data collection and structure refinement details are summarized in Table 1. The positions of the H atoms were initially determined by geometry and were refined using a riding model. Non-H atoms were refined with anisotropic displacement parameters. H-atom displacement parameters

Table 1
Experimental details.

Crystal data	
Chemical formula	$[Ti(C_6F_5O)_4(C_4H_8O)_2]$
M_r	924.35
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	100
a, *b*, *c* (Å)	10.7678 (3), 18.6224 (5), 17.1245 (5)
β (°)	90.204 (2)
V (Å^3)	3433.82 (17)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.40
Crystal size (mm)	0.14 × 0.14 × 0.09
Data collection	
Diffractometer	Bruker APEX CCD
Absorption correction	Multi-scan (*SADABS2016*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.623, 0.695
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	41654, 6043, 4550
R_{int}	0.068
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.039, 0.097, 1.00
No. of reflections	6043
No. of parameters	532
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.34, −0.46

Computer programs: *APEX3* (Bruker, 2007), *SAINT* (Bruker, 2007), *SHELXT* (Sheldrick, 2015), *SHELXL2025* (Sheldrick, 2025) and *OLEX2* (Dolomanov *et al.*, 2009).

were set at 1.2 times the isotropic equivalent displacement parameters of the bonded atoms.

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Conflict of interest

The author declares no competing financial interest.

Funding information

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References

Barbier, J. P., Kappenstein, C. & Hugel, R. (1972). *J. Chem. Educ.* **49**, 204–205.
Boyle, T. J., Alam, T. M., Tafoya, C. J., Mechenbier, E. R. & Ziller, J. W. (1999). *Inorg. Chem.* **38**, 2422–2428.
Bradley, D. C. (1959). *Metal Alkoxides*, ch. 2, in *Metal–Organic Compounds*. Washington: ACS.
Bradley, D. C., Mehrotra, R. C. & Gaur, D. P. (1978). In *Metal Alkoxides*. New York: Academic Press.
Bradley, D. C., Mehrotra, R. C., Rothwell, I. P. & Singh, A. (2001). In *Alkoxo and Aryloxo Derivatives of Metals*. San Diego: Academic Press.
Bruker (2007). *APEX3* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Campbell, C., Bott, S., Larsen, R. & Van Der Sluys, W. G. (1994). *Inorg. Chem.* **33**, 4950–4958.
Chandler, C. D., Roger, C. & Hampden-Smith, M. (1993). *Chem. Rev.* **93**, 1205–1241.
Day, V. W., Eberspacher, T. A., Klemperer, W. G. & Liang, S. (1995). *Chem. Mater.* **7**, 1607–1608.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Fisher, J., Van DerSluys, W. G., Huffman, J. C. & Sears, J. (1993). *Synth. React. Inorg. Met.-Org. Chem.* **23**, 479–491.
Giesbrecht, G. R., Gordon, J. C., Clark, D. L. & Scott, B. L. (2004). *Inorg. Chem.* **43**, 1065–1070.
Guzei, I. A. & Winter, C. H. (1997). *Inorg. Chem.* **36**, 4415–4420.
Kamata, K., Suzuki, A., Nakai, Y. & Nakazawa, H. (2012). *Organometallics* **31**, 3825–3828.
Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.
Malinowski, P. J. & Koteras, K. (2026). *Acta Cryst.* E**82**, 86–90.
Mazdiyasni, K. S., Schaper, & B. J., Brown, L. M. (1971). *Inorg. Chem.* **10**, 889–892.
Niemeyer, M. (2001). *Acta Cryst.* E**57**, m363–m364.
Sheldrick, G. M. (2015). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2025). *SHELXL2025*. University of Göttingen, Germany.
Tebbe, F. N. & Muetterties, E. L. (1967). *Inorg. Chem.* **6**, 129–132.
Van Der Sluys, W. G. (2024). *Acta Cryst.* C**80**, 562–566.
Xie, Z., Chiu, K., Wu, B. & Mak, T. C. W. (1996). *Inorg. Chem.* **35**, 5957–5958.

supporting information

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Structure of tetrakis(pentafluorophenoxido)bis(tetrahydrofuran)titanium(IV)

William G. Van Der Sluys

Computing details

Tetrakis(pentafluorophenoxido-κO)bis(tetrahydrofuran-κO)titanium(IV), [Ti(C_6F_5O)$_4$(C_4H_8O)$_2$]

Crystal data

[Ti(C_6F_5O)$_4$(C_4H_8O)$_2$]
M_r = 924.35
Monoclinic, $P2_1/n$
a = 10.7678 (3) Å
b = 18.6224 (5) Å
c = 17.1245 (5) Å
β = 90.204 (2)°
V = 3433.82 (17) Å^3
Z = 4
$F(000)$ = 1832
D_x = 1.788 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8410 reflections
θ = 2.4–30.4°
μ = 0.40 mm^{-1}
T = 100 K
Block, orange
0.14 × 0.14 × 0.09 mm

Data collection

Bruker APEX CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS2016; Krause *et al.*, 2015)
T_{min} = 0.623, T_{max} = 0.695
41654 measured reflections
6043 independent reflections
4550 reflections with $I > 2\sigma(I)$
R_{int} = 0.068
θ_{max} = 25.0°, θ_{min} = 2.2°
h = −12→12
k = −22→22
l = −19→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.097
S = 1.00
6043 reflections
532 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0415P)^2 + 2.4623P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 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}
Ti1	0.54379 (4)	0.21700 (2)	0.65158 (3)	0.01836 (13)
F2	0.48061 (15)	0.07750 (8)	0.46061 (9)	0.0275 (4)
F3	0.46785 (16)	0.08295 (9)	0.30352 (10)	0.0361 (4)
F4	0.52382 (17)	0.20695 (10)	0.22618 (9)	0.0392 (4)
F5	0.58924 (15)	0.32564 (9)	0.30822 (10)	0.0330 (4)
F6	0.60174 (15)	0.32125 (8)	0.46622 (9)	0.0285 (4)
F8	0.30266 (16)	0.27450 (9)	0.50221 (10)	0.0389 (5)
F9	0.27079 (18)	0.39576 (11)	0.41814 (11)	0.0532 (6)
F10	0.33334 (18)	0.52580 (10)	0.48005 (12)	0.0534 (6)
F11	0.42690 (17)	0.53281 (9)	0.62739 (12)	0.0439 (5)
F12	0.45684 (16)	0.41232 (8)	0.71255 (10)	0.0311 (4)
F14	0.82314 (16)	0.23242 (8)	0.53812 (11)	0.0375 (4)
F15	1.02058 (17)	0.30959 (10)	0.48959 (12)	0.0504 (5)
F16	1.06352 (16)	0.44323 (9)	0.54877 (11)	0.0417 (5)
F17	0.90700 (15)	0.49807 (8)	0.65763 (10)	0.0350 (4)
F18	0.71103 (16)	0.42083 (8)	0.70748 (10)	0.0344 (4)
F19	0.31651 (14)	0.25946 (9)	0.80634 (10)	0.0299 (4)
F20	0.29102 (14)	0.36793 (8)	0.91024 (9)	0.0286 (4)
F21	0.49437 (15)	0.42573 (8)	0.98074 (9)	0.0289 (4)
F22	0.72545 (14)	0.37964 (8)	0.93880 (9)	0.0283 (4)
F23	0.75251 (14)	0.27640 (8)	0.83031 (9)	0.0265 (4)
O1	0.54289 (18)	0.19743 (9)	0.54538 (11)	0.0239 (4)
O2	0.40712 (17)	0.27960 (9)	0.64940 (11)	0.0240 (4)
O3	0.66287 (17)	0.28759 (9)	0.64923 (11)	0.0254 (4)
O4	0.54803 (16)	0.21227 (9)	0.76279 (10)	0.0210 (4)
O5	0.67766 (17)	0.13425 (9)	0.66137 (10)	0.0217 (4)
O6	0.41500 (17)	0.13131 (9)	0.66251 (11)	0.0232 (4)
C1	0.5398 (2)	0.19959 (13)	0.46761 (15)	0.0179 (6)
C2	0.5075 (2)	0.13973 (14)	0.42396 (16)	0.0209 (6)
C3	0.5019 (2)	0.14218 (15)	0.34369 (17)	0.0241 (6)
C4	0.5293 (3)	0.20430 (15)	0.30475 (16)	0.0244 (6)
C5	0.5616 (2)	0.26442 (14)	0.34650 (16)	0.0216 (6)
C6	0.5680 (2)	0.26185 (13)	0.42646 (16)	0.0202 (6)
C7	0.3861 (2)	0.33975 (14)	0.60855 (16)	0.0233 (6)
C8	0.3355 (3)	0.33817 (16)	0.53372 (18)	0.0293 (7)
C9	0.3184 (3)	0.39969 (18)	0.49046 (18)	0.0361 (8)
C10	0.3496 (3)	0.46504 (17)	0.52192 (19)	0.0359 (8)
C11	0.3969 (3)	0.46866 (15)	0.59653 (19)	0.0315 (7)
C12	0.4132 (3)	0.40705 (15)	0.63897 (17)	0.0256 (6)
C13	0.7608 (2)	0.32487 (13)	0.62373 (15)	0.0203 (6)
C14	0.8424 (3)	0.29829 (14)	0.56797 (17)	0.0257 (6)
C15	0.9432 (3)	0.33737 (16)	0.54330 (17)	0.0299 (7)
C16	0.9649 (3)	0.40483 (15)	0.57279 (17)	0.0270 (7)
C17	0.8863 (3)	0.43218 (14)	0.62814 (17)	0.0243 (6)
C18	0.7862 (2)	0.39280 (14)	0.65310 (16)	0.0218 (6)

C19	0.5350 (2)	0.26492 (13)	0.81489 (15)	0.0174 (6)
C20	0.6369 (2)	0.29737 (13)	0.85021 (16)	0.0193 (6)
C21	0.6242 (2)	0.35047 (13)	0.90531 (16)	0.0205 (6)
C22	0.5080 (3)	0.37395 (13)	0.92656 (15)	0.0207 (6)
C23	0.4055 (2)	0.34380 (14)	0.89140 (16)	0.0204 (6)
C24	0.4187 (2)	0.28991 (14)	0.83767 (15)	0.0195 (6)
C25	0.7764 (3)	0.13369 (16)	0.72070 (17)	0.0303 (7)
H25A	0.746264	0.112362	0.770084	0.036*
H25B	0.806424	0.182994	0.731279	0.036*
C26	0.8780 (3)	0.08829 (16)	0.68563 (19)	0.0332 (7)
H26A	0.927828	0.064229	0.726705	0.040*
H26B	0.933751	0.117468	0.652470	0.040*
C27	0.8055 (3)	0.03401 (14)	0.63716 (17)	0.0293 (7)
H27A	0.858044	0.012813	0.595813	0.035*
H27B	0.772060	−0.004972	0.670294	0.035*
C28	0.7021 (3)	0.07884 (14)	0.60249 (16)	0.0247 (6)
H28A	0.728349	0.100807	0.552551	0.030*
H28B	0.627176	0.049252	0.593037	0.030*
C29	0.4092 (3)	0.07952 (15)	0.72628 (18)	0.0347 (8)
H29A	0.406771	0.104471	0.777298	0.042*
H29B	0.482501	0.047409	0.725375	0.042*
C30	0.2905 (3)	0.03692 (16)	0.7130 (2)	0.0380 (8)
H30A	0.304888	−0.015034	0.721297	0.046*
H30B	0.223958	0.053268	0.748501	0.046*
C31	0.2572 (3)	0.05210 (18)	0.6292 (2)	0.0456 (9)
H31A	0.301009	0.018998	0.593386	0.055*
H31B	0.166589	0.047790	0.620419	0.055*
C32	0.3000 (3)	0.12791 (16)	0.61809 (19)	0.0322 (7)
H32A	0.314747	0.138376	0.562205	0.039*
H32B	0.238228	0.162378	0.638617	0.039*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ti1	0.0195 (3)	0.0161 (2)	0.0194 (3)	−0.00047 (19)	0.0011 (2)	−0.0020 (2)
F2	0.0306 (9)	0.0192 (8)	0.0327 (10)	−0.0024 (7)	−0.0023 (7)	0.0027 (7)
F3	0.0415 (11)	0.0354 (9)	0.0313 (10)	−0.0037 (8)	−0.0082 (8)	−0.0142 (8)
F4	0.0424 (11)	0.0569 (12)	0.0184 (10)	−0.0050 (9)	−0.0027 (8)	0.0001 (8)
F5	0.0330 (10)	0.0343 (9)	0.0316 (10)	−0.0014 (8)	0.0022 (8)	0.0128 (8)
F6	0.0367 (10)	0.0187 (8)	0.0303 (10)	−0.0020 (7)	0.0008 (7)	−0.0030 (7)
F8	0.0360 (10)	0.0458 (11)	0.0348 (11)	0.0117 (8)	−0.0100 (8)	−0.0138 (9)
F9	0.0499 (13)	0.0814 (15)	0.0280 (11)	0.0230 (11)	−0.0068 (9)	0.0092 (10)
F10	0.0467 (12)	0.0537 (12)	0.0598 (14)	0.0116 (10)	0.0023 (10)	0.0352 (10)
F11	0.0465 (12)	0.0229 (9)	0.0623 (13)	0.0021 (8)	0.0018 (10)	0.0067 (8)
F12	0.0384 (10)	0.0241 (8)	0.0307 (10)	0.0034 (7)	−0.0037 (8)	−0.0005 (7)
F14	0.0363 (10)	0.0299 (9)	0.0465 (12)	−0.0084 (8)	0.0153 (8)	−0.0211 (8)
F15	0.0387 (11)	0.0573 (12)	0.0554 (13)	−0.0122 (9)	0.0263 (10)	−0.0242 (10)
F16	0.0271 (10)	0.0412 (10)	0.0568 (13)	−0.0143 (8)	0.0083 (9)	0.0010 (9)

F17	0.0348 (10)	0.0201 (8)	0.0502 (12)	−0.0078 (7)	−0.0045 (8)	−0.0067 (8)
F18	0.0341 (10)	0.0291 (9)	0.0399 (11)	−0.0026 (7)	0.0113 (8)	−0.0162 (8)
F19	0.0159 (8)	0.0402 (9)	0.0338 (10)	−0.0069 (7)	0.0026 (7)	−0.0108 (8)
F20	0.0178 (8)	0.0334 (9)	0.0348 (10)	0.0041 (7)	0.0089 (7)	−0.0058 (7)
F21	0.0349 (10)	0.0222 (8)	0.0296 (10)	−0.0008 (7)	0.0060 (7)	−0.0105 (7)
F22	0.0232 (9)	0.0294 (8)	0.0322 (10)	−0.0030 (7)	−0.0082 (7)	−0.0069 (7)
F23	0.0149 (8)	0.0322 (8)	0.0322 (10)	0.0025 (7)	−0.0008 (7)	−0.0070 (7)
O1	0.0301 (11)	0.0221 (9)	0.0194 (11)	0.0002 (8)	0.0005 (8)	−0.0005 (8)
O2	0.0245 (11)	0.0215 (9)	0.0260 (11)	0.0037 (8)	0.0010 (8)	0.0003 (8)
O3	0.0251 (11)	0.0225 (10)	0.0287 (12)	−0.0041 (8)	0.0059 (9)	−0.0035 (8)
O4	0.0208 (10)	0.0203 (9)	0.0219 (11)	0.0003 (8)	0.0022 (8)	−0.0045 (8)
O5	0.0220 (10)	0.0222 (9)	0.0210 (11)	0.0030 (8)	−0.0011 (8)	−0.0050 (8)
O6	0.0241 (10)	0.0219 (9)	0.0236 (11)	−0.0040 (8)	−0.0036 (8)	0.0027 (8)
C1	0.0176 (14)	0.0216 (13)	0.0145 (14)	0.0029 (11)	−0.0013 (11)	−0.0001 (11)
C2	0.0179 (14)	0.0209 (13)	0.0240 (16)	−0.0005 (11)	−0.0008 (11)	−0.0010 (12)
C3	0.0162 (14)	0.0291 (15)	0.0271 (17)	0.0000 (12)	−0.0039 (12)	−0.0091 (13)
C4	0.0176 (14)	0.0400 (17)	0.0157 (15)	0.0009 (12)	−0.0016 (11)	−0.0015 (13)
C5	0.0157 (14)	0.0265 (14)	0.0225 (16)	−0.0015 (11)	0.0013 (11)	0.0067 (12)
C6	0.0162 (14)	0.0207 (13)	0.0235 (16)	0.0024 (11)	−0.0013 (11)	−0.0050 (11)
C7	0.0193 (14)	0.0252 (14)	0.0253 (16)	0.0067 (12)	0.0022 (12)	0.0021 (12)
C8	0.0220 (15)	0.0346 (16)	0.0314 (18)	0.0092 (13)	0.0027 (13)	−0.0060 (14)
C9	0.0294 (17)	0.054 (2)	0.0251 (18)	0.0159 (15)	−0.0012 (14)	0.0071 (15)
C10	0.0275 (17)	0.0403 (18)	0.040 (2)	0.0107 (14)	0.0079 (15)	0.0216 (16)
C11	0.0272 (17)	0.0250 (15)	0.042 (2)	0.0025 (13)	0.0059 (14)	0.0064 (14)
C12	0.0218 (15)	0.0297 (15)	0.0253 (16)	0.0031 (12)	0.0023 (12)	0.0030 (13)
C13	0.0205 (14)	0.0216 (13)	0.0187 (15)	−0.0029 (11)	0.0007 (11)	−0.0008 (11)
C14	0.0284 (16)	0.0200 (14)	0.0287 (17)	−0.0033 (12)	−0.0006 (13)	−0.0064 (12)
C15	0.0260 (16)	0.0349 (16)	0.0288 (18)	−0.0008 (13)	0.0075 (13)	−0.0072 (13)
C16	0.0194 (15)	0.0304 (15)	0.0313 (18)	−0.0059 (12)	0.0016 (13)	0.0017 (13)
C17	0.0269 (16)	0.0168 (13)	0.0293 (17)	−0.0014 (12)	−0.0086 (13)	−0.0009 (12)
C18	0.0202 (14)	0.0221 (14)	0.0232 (16)	0.0029 (11)	0.0013 (12)	−0.0047 (12)
C19	0.0200 (14)	0.0166 (12)	0.0156 (14)	−0.0003 (11)	0.0019 (11)	0.0009 (11)
C20	0.0128 (13)	0.0220 (13)	0.0231 (15)	0.0032 (11)	0.0039 (11)	0.0018 (11)
C21	0.0181 (14)	0.0208 (13)	0.0226 (15)	−0.0049 (11)	−0.0040 (11)	0.0003 (11)
C22	0.0250 (15)	0.0178 (13)	0.0192 (15)	0.0005 (11)	0.0039 (12)	−0.0012 (11)
C23	0.0151 (14)	0.0241 (14)	0.0219 (15)	0.0024 (11)	0.0068 (11)	0.0031 (11)
C24	0.0174 (14)	0.0243 (13)	0.0170 (14)	−0.0045 (11)	0.0008 (11)	0.0016 (11)
C25	0.0263 (16)	0.0374 (16)	0.0273 (17)	0.0060 (13)	−0.0067 (13)	−0.0071 (13)
C26	0.0270 (17)	0.0330 (16)	0.0396 (19)	0.0090 (13)	−0.0019 (14)	−0.0047 (14)
C27	0.0400 (18)	0.0218 (14)	0.0261 (17)	0.0073 (13)	0.0064 (14)	0.0023 (12)
C28	0.0321 (17)	0.0191 (13)	0.0227 (16)	0.0017 (12)	0.0054 (12)	−0.0063 (12)
C29	0.046 (2)	0.0271 (15)	0.0309 (18)	−0.0110 (14)	−0.0019 (15)	0.0081 (13)
C30	0.0323 (18)	0.0322 (16)	0.049 (2)	−0.0087 (14)	0.0087 (16)	0.0071 (15)
C31	0.037 (2)	0.0425 (19)	0.058 (2)	−0.0156 (16)	−0.0047 (17)	−0.0011 (17)
C32	0.0236 (16)	0.0362 (17)	0.0369 (19)	−0.0074 (13)	−0.0096 (14)	0.0041 (14)

Geometric parameters (Å, º)

Ti1—O1	1.8548 (19)	C7—C8	1.391 (4)
Ti1—O2	1.8777 (18)	C7—C12	1.388 (4)
Ti1—O3	1.8370 (18)	C8—C9	1.376 (4)
Ti1—O4	1.9068 (19)	C9—C10	1.372 (5)
Ti1—O5	2.1163 (18)	C10—C11	1.375 (4)
Ti1—O6	2.1227 (18)	C11—C12	1.369 (4)
F2—C2	1.350 (3)	C13—C14	1.391 (4)
F3—C3	1.350 (3)	C13—C18	1.388 (4)
F4—C4	1.347 (3)	C14—C15	1.375 (4)
F5—C5	1.349 (3)	C15—C16	1.374 (4)
F6—C6	1.348 (3)	C16—C17	1.371 (4)
F8—C8	1.349 (3)	C17—C18	1.374 (4)
F9—C9	1.341 (3)	C19—C20	1.390 (4)
F10—C10	1.351 (3)	C19—C24	1.392 (4)
F11—C11	1.345 (3)	C20—C21	1.374 (4)
F12—C12	1.347 (3)	C21—C22	1.376 (4)
F14—C14	1.345 (3)	C22—C23	1.375 (4)
F15—C15	1.347 (3)	C23—C24	1.369 (4)
F16—C16	1.346 (3)	C25—H25A	0.9900
F17—C17	1.345 (3)	C25—H25B	0.9900
F18—C18	1.341 (3)	C25—C26	1.509 (4)
F19—C24	1.348 (3)	C26—H26A	0.9900
F20—C23	1.352 (3)	C26—H26B	0.9900
F21—C22	1.347 (3)	C26—C27	1.522 (4)
F22—C21	1.344 (3)	C27—H27A	0.9900
F23—C20	1.350 (3)	C27—H27B	0.9900
O1—C1	1.333 (3)	C27—C28	1.511 (4)
O2—C7	1.340 (3)	C28—H28A	0.9900
O3—C13	1.337 (3)	C28—H28B	0.9900
O4—C19	1.333 (3)	C29—H29A	0.9900
O5—C25	1.468 (3)	C29—H29B	0.9900
O5—C28	1.467 (3)	C29—C30	1.521 (4)
O6—C29	1.458 (3)	C30—H30A	0.9900
O6—C32	1.452 (3)	C30—H30B	0.9900
C1—C2	1.386 (4)	C30—C31	1.505 (5)
C1—C6	1.391 (4)	C31—H31A	0.9900
C2—C3	1.376 (4)	C31—H31B	0.9900
C3—C4	1.368 (4)	C31—C32	1.497 (4)
C4—C5	1.373 (4)	C32—H32A	0.9900
C5—C6	1.371 (4)	C32—H32B	0.9900
O1—Ti1—O2	95.80 (8)	F17—C17—C16	119.8 (2)
O1—Ti1—O4	165.98 (8)	F17—C17—C18	119.9 (3)
O1—Ti1—O5	86.32 (8)	C18—C17—C16	120.3 (2)
O1—Ti1—O6	86.42 (8)	F18—C18—C13	119.2 (2)
O2—Ti1—O4	93.70 (8)	F18—C18—C17	119.0 (2)

O2—Ti1—O5	170.82 (8)	C17—C18—C13	121.8 (2)
O2—Ti1—O6	87.49 (8)	O4—C19—C20	121.7 (2)
O3—Ti1—O1	96.91 (8)	O4—C19—C24	122.0 (2)
O3—Ti1—O2	95.87 (8)	C20—C19—C24	116.2 (2)
O3—Ti1—O4	92.33 (8)	F23—C20—C19	119.5 (2)
O3—Ti1—O5	92.73 (8)	F23—C20—C21	118.4 (2)
O3—Ti1—O6	174.99 (8)	C21—C20—C19	122.1 (2)
O4—Ti1—O5	82.73 (7)	F22—C21—C20	120.1 (2)
O4—Ti1—O6	83.72 (7)	F22—C21—C22	119.7 (2)
O5—Ti1—O6	83.72 (7)	C20—C21—C22	120.2 (2)
C1—O1—Ti1	166.88 (17)	F21—C22—C21	120.7 (2)
C7—O2—Ti1	131.35 (17)	F21—C22—C23	120.3 (2)
C13—O3—Ti1	158.45 (17)	C23—C22—C21	118.9 (2)
C19—O4—Ti1	129.21 (16)	F20—C23—C22	119.4 (2)
C25—O5—Ti1	123.46 (15)	F20—C23—C24	120.1 (2)
C25—O5—C28	109.84 (19)	C24—C23—C22	120.5 (2)
C28—O5—Ti1	125.56 (15)	F19—C24—C19	118.8 (2)
C29—O6—Ti1	126.34 (16)	F19—C24—C23	119.3 (2)
C32—O6—Ti1	122.87 (15)	C23—C24—C19	122.0 (2)
C32—O6—C29	109.0 (2)	O5—C25—H25A	110.8
O1—C1—C2	121.3 (2)	O5—C25—H25B	110.8
O1—C1—C6	121.8 (2)	O5—C25—C26	104.7 (2)
C2—C1—C6	116.9 (2)	H25A—C25—H25B	108.9
F2—C2—C1	119.6 (2)	C26—C25—H25A	110.8
F2—C2—C3	119.0 (2)	C26—C25—H25B	110.8
C3—C2—C1	121.5 (2)	C25—C26—H26A	111.3
F3—C3—C2	119.5 (2)	C25—C26—H26B	111.3
F3—C3—C4	120.1 (3)	C25—C26—C27	102.6 (2)
C4—C3—C2	120.4 (2)	H26A—C26—H26B	109.2
F4—C4—C3	120.6 (2)	C27—C26—H26A	111.3
F4—C4—C5	120.0 (2)	C27—C26—H26B	111.3
C3—C4—C5	119.4 (3)	C26—C27—H27A	111.2
F5—C5—C4	119.5 (2)	C26—C27—H27B	111.2
F5—C5—C6	120.3 (2)	H27A—C27—H27B	109.1
C4—C5—C6	120.2 (2)	C28—C27—C26	102.9 (2)
F6—C6—C1	119.1 (2)	C28—C27—H27A	111.2
F6—C6—C5	119.2 (2)	C28—C27—H27B	111.2
C5—C6—C1	121.6 (2)	O5—C28—C27	104.6 (2)
O2—C7—C8	121.9 (2)	O5—C28—H28A	110.8
O2—C7—C12	121.6 (3)	O5—C28—H28B	110.8
C12—C7—C8	116.5 (3)	C27—C28—H28A	110.8
F8—C8—C7	119.2 (3)	C27—C28—H28B	110.8
F8—C8—C9	118.8 (3)	H28A—C28—H28B	108.9
C9—C8—C7	122.0 (3)	O6—C29—H29A	110.6
F9—C9—C8	120.1 (3)	O6—C29—H29B	110.6
F9—C9—C10	120.2 (3)	O6—C29—C30	105.7 (2)
C10—C9—C8	119.6 (3)	H29A—C29—H29B	108.7
F10—C10—C9	120.2 (3)	C30—C29—H29A	110.6

F10—C10—C11	119.9 (3)	C30—C29—H29B	110.6
C9—C10—C11	119.8 (3)	C29—C30—H30A	111.0
F11—C11—C10	119.7 (3)	C29—C30—H30B	111.0
F11—C11—C12	120.4 (3)	H30A—C30—H30B	109.0
C12—C11—C10	119.9 (3)	C31—C30—C29	104.0 (2)
F12—C12—C7	119.3 (2)	C31—C30—H30A	111.0
F12—C12—C11	118.6 (3)	C31—C30—H30B	111.0
C11—C12—C7	122.1 (3)	C30—C31—H31A	111.2
O3—C13—C14	122.7 (2)	C30—C31—H31B	111.2
O3—C13—C18	120.6 (2)	H31A—C31—H31B	109.1
C14—C13—C18	116.7 (2)	C32—C31—C30	103.0 (3)
F14—C14—C13	119.3 (2)	C32—C31—H31A	111.2
F14—C14—C15	119.1 (3)	C32—C31—H31B	111.2
C15—C14—C13	121.6 (2)	O6—C32—C31	103.7 (2)
F15—C15—C14	119.8 (3)	O6—C32—H32A	111.0
F15—C15—C16	119.8 (3)	O6—C32—H32B	111.0
C14—C15—C16	120.3 (3)	C31—C32—H32A	111.0
F16—C16—C15	120.5 (3)	C31—C32—H32B	111.0
F16—C16—C17	120.2 (3)	H32A—C32—H32B	109.0
C17—C16—C15	119.3 (3)		

Ti1—O1—C1—C2	−159.0 (7)	O4—C19—C20—C21	−178.4 (2)
Ti1—O1—C1—C6	20.6 (9)	O4—C19—C24—F19	0.5 (4)
Ti1—O2—C7—C8	86.4 (3)	O4—C19—C24—C23	179.7 (2)
Ti1—O2—C7—C12	−93.8 (3)	O5—Ti1—O1—C1	−141.9 (8)
Ti1—O3—C13—C14	−14.4 (7)	O5—Ti1—O3—C13	61.0 (5)
Ti1—O3—C13—C18	166.3 (4)	O5—C25—C26—C27	−32.4 (3)
Ti1—O4—C19—C20	−98.6 (3)	O6—Ti1—O1—C1	134.1 (8)
Ti1—O4—C19—C24	82.2 (3)	O6—Ti1—O2—C7	−142.4 (2)
Ti1—O5—C25—C26	−155.01 (18)	O6—C29—C30—C31	17.0 (3)
Ti1—O5—C28—C27	179.54 (16)	C1—C2—C3—F3	−178.8 (2)
Ti1—O6—C29—C30	171.78 (18)	C1—C2—C3—C4	0.4 (4)
Ti1—O6—C32—C31	166.3 (2)	C2—C1—C6—F6	−179.0 (2)
F2—C2—C3—F3	1.1 (4)	C2—C1—C6—C5	1.3 (4)
F2—C2—C3—C4	−179.6 (2)	C2—C3—C4—F4	−179.9 (2)
F3—C3—C4—F4	−0.7 (4)	C2—C3—C4—C5	−0.4 (4)
F3—C3—C4—C5	178.9 (2)	C3—C4—C5—F5	179.7 (2)
F4—C4—C5—F5	−0.8 (4)	C3—C4—C5—C6	0.9 (4)
F4—C4—C5—C6	−179.6 (2)	C4—C5—C6—F6	179.0 (2)
F5—C5—C6—F6	0.2 (4)	C4—C5—C6—C1	−1.3 (4)
F5—C5—C6—C1	179.9 (2)	C6—C1—C2—F2	179.2 (2)
F8—C8—C9—F9	−0.6 (4)	C6—C1—C2—C3	−0.9 (4)
F8—C8—C9—C10	179.1 (3)	C7—C8—C9—F9	179.2 (3)
F9—C9—C10—F10	−0.4 (5)	C7—C8—C9—C10	−1.2 (5)
F9—C9—C10—C11	179.2 (3)	C8—C7—C12—F12	176.9 (2)
F10—C10—C11—F11	−0.1 (4)	C8—C7—C12—C11	−3.0 (4)
F10—C10—C11—C12	179.9 (3)	C8—C9—C10—F10	180.0 (3)
F11—C11—C12—F12	1.6 (4)	C8—C9—C10—C11	−0.5 (5)

F11—C11—C12—C7	−178.5 (3)	C9—C10—C11—F11	−179.7 (3)
F14—C14—C15—F15	0.4 (4)	C9—C10—C11—C12	0.4 (5)
F14—C14—C15—C16	179.9 (3)	C10—C11—C12—F12	−178.4 (3)
F15—C15—C16—F16	−0.4 (4)	C10—C11—C12—C7	1.5 (4)
F15—C15—C16—C17	−179.2 (3)	C12—C7—C8—F8	−177.4 (2)
F16—C16—C17—F17	1.0 (4)	C12—C7—C8—C9	2.8 (4)
F16—C16—C17—C18	−179.5 (3)	C13—C14—C15—F15	179.5 (3)
F17—C17—C18—F18	−0.7 (4)	C13—C14—C15—C16	−0.9 (5)
F17—C17—C18—C13	179.4 (2)	C14—C13—C18—F18	−179.5 (2)
F20—C23—C24—F19	−2.6 (4)	C14—C13—C18—C17	0.4 (4)
F20—C23—C24—C19	178.1 (2)	C14—C15—C16—F16	180.0 (3)
F21—C22—C23—F20	1.7 (4)	C14—C15—C16—C17	1.2 (5)
F21—C22—C23—C24	−178.4 (2)	C15—C16—C17—F17	179.8 (3)
F22—C21—C22—F21	−0.2 (4)	C15—C16—C17—C18	−0.7 (4)
F22—C21—C22—C23	179.6 (2)	C16—C17—C18—F18	179.8 (2)
F23—C20—C21—F22	−0.9 (4)	C16—C17—C18—C13	−0.1 (4)
F23—C20—C21—C22	179.2 (2)	C18—C13—C14—F14	179.3 (2)
O1—Ti1—O2—C7	−56.3 (2)	C18—C13—C14—C15	0.1 (4)
O1—Ti1—O3—C13	−25.6 (5)	C19—C20—C21—F22	179.0 (2)
O1—C1—C2—F2	−1.2 (4)	C19—C20—C21—C22	−0.9 (4)
O1—C1—C2—C3	178.7 (2)	C20—C19—C24—F19	−178.8 (2)
O1—C1—C6—F6	1.3 (4)	C20—C19—C24—C23	0.5 (4)
O1—C1—C6—C5	−178.3 (2)	C20—C21—C22—F21	179.7 (2)
O2—Ti1—O1—C1	47.0 (8)	C20—C21—C22—C23	−0.5 (4)
O2—Ti1—O3—C13	−122.2 (5)	C21—C22—C23—F20	−178.1 (2)
O2—C7—C8—F8	2.3 (4)	C21—C22—C23—C24	1.8 (4)
O2—C7—C8—C9	−177.4 (3)	C22—C23—C24—F19	177.5 (2)
O2—C7—C12—F12	−2.9 (4)	C22—C23—C24—C19	−1.8 (4)
O2—C7—C12—C11	177.2 (3)	C24—C19—C20—F23	−179.3 (2)
O3—Ti1—O1—C1	−49.6 (8)	C24—C19—C20—C21	0.8 (4)
O3—Ti1—O2—C7	41.3 (2)	C25—O5—C28—C27	11.5 (3)
O3—C13—C14—F14	−0.1 (4)	C25—C26—C27—C28	39.3 (3)
O3—C13—C14—C15	−179.3 (3)	C26—C27—C28—O5	−31.4 (3)
O3—C13—C18—F18	−0.1 (4)	C28—O5—C25—C26	13.4 (3)
O3—C13—C18—C17	179.8 (3)	C29—O6—C32—C31	−28.2 (3)
O4—Ti1—O1—C1	179.5 (7)	C29—C30—C31—C32	−33.7 (3)
O4—Ti1—O2—C7	134.1 (2)	C30—C31—C32—O6	38.1 (3)
O4—Ti1—O3—C13	143.8 (5)	C32—O6—C29—C30	7.0 (3)
O4—C19—C20—F23	1.5 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C25—H25*A*···F9^{i}	0.99	2.55	3.426 (4)	147
C25—H25*B*···F23	0.99	2.50	3.264 (3)	134
C27—H27*A*···F21^{ii}	0.99	2.62	3.580 (3)	162
C27—H27*B*···F18^{ii}	0.99	2.51	3.399 (3)	149
C28—H28*A*···F20^{iii}	0.99	2.60	3.572 (3)	168

C29—H29*B*···F3^{iv}	0.99	2.53	3.342 (4)	139
C29—H29*B*···F17^{ii}	0.99	2.50	3.184 (4)	126
C32—H32*A*···F22^{v}	0.99	2.34	3.174 (3)	141

Symmetry codes: (i) *x*+1/2, −*y*+1/2, *z*+1/2; (ii) −*x*+3/2, *y*−1/2, −*z*+3/2; (iii) *x*+1/2, −*y*+1/2, *z*−1/2; (iv) −*x*+1, −*y*, −*z*+1; (v) *x*−1/2, −*y*+1/2, *z*−1/2.