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{6,6′-Dimethyl-2,2′-bis[(2-oxidobenzylidene)amino]-1,1′-biphenyl-κ^4O,N,N',O'}bis(propan-2-olato-κO)titanium(IV) *n*-hexane hemisolvate

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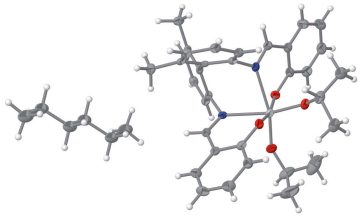
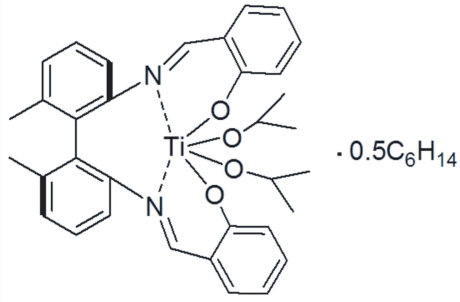
Structural data: full structural data are available from iucrdata.iucr.org

The mononuclear Ti^{IV} title complex, $[Ti(C_{28}H_{22}N_2O_2)(C_3H_7O)_2]\cdot 0.5C_6H_{14}$, crystallizes as an *n*-hexane hemisolvate. The Ti^{IV} atom is coordinated by a dianionic tetradentate biphenyl Schiff base ligand and two O atoms of two propan-2-olate anions in a distorted TiN_2O_4 octahedral coordination geometry, in which the two N atoms are in a *cis* configuration. In the crystal, complex molecules are stacked parallel to [100], leaving space for channels parallel to [001] where the solvent molecules are located.

3D view



Chemical scheme



Structure description

The structure determination of the title compound was undertaken as part of a project on the synthesis of new titanium catalysts (Zi, 2011). For similar structures of titanium complexes with biaryl Schiff base ligands, see: Chen *et al.* (2013). The structure of the title Ti^{IV} complex consists of molecules with the metal atom in an N_2O_4 coordination environment defined by one tetradentate dianionic 6,6′-dimethyl-2,2′-bis[(2-oxidobenzylidene)amino]-1,1′-biphenyl ligand and two propanolate anionic ligands (Fig. 1). The bond lengths involving the N-atom donors are elongated [Ti—N = 2.229 (3)–2.306 (3) Å], whereas the O-atom donors have normal Ti—O bond lengths [1.782 (2)–1.974 (2) Å]. The biphenyl group is twisted, with a dihedral angle between the benzene rings of 69.9 (4)°. The solvent molecule sits about a centre of inversion in channels propagating parallel to [001]. In the crystal packing (Fig. 2), a weak intermolecular C—H···O interaction is found between an aryl H atom and one of the phenolate O atoms of the Schiff base ligand (Table 1).

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10···O2^{i}	0.95	2.47	3.312 (4)	147

Symmetry code: (i) $-x, -y, -z$.

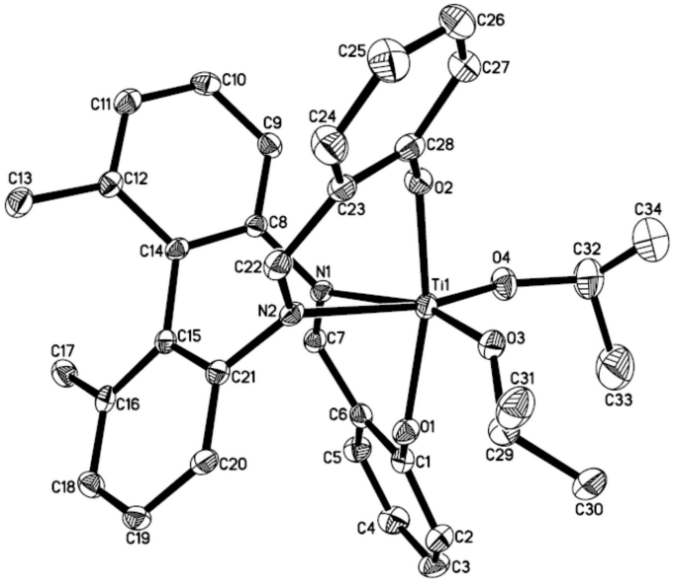


Figure 1
The asymmetric unit of the title compound, showing 50% probability displacement ellipsoids (the H atoms and *n*-hexane solvent molecule have been omitted for clarity).

Synthesis and crystallization

An *n*-hexane solution (10 ml) of the Schiff base ligand 2,2′-bis[(2-hydroxybenzylidene)amino]-6,6′-dimethyl-1,1′-biphenyl (0.42 g, 1.0 mmol) was added slowly to an *n*-hexane solution (10 ml) of titanium isopropoxide (0.28 g, 1.0 mmol) with stirring at room temperature. After the resulting yellow solution had been stirred at room temperature for 1 d, the solution was filtered. The filtrate was concentrated to about 2 ml under vacuum. Yellow crystals of the title compound were isolated when this solution was kept at room temperature for 3 d (yield: 0.43 g, 68%).

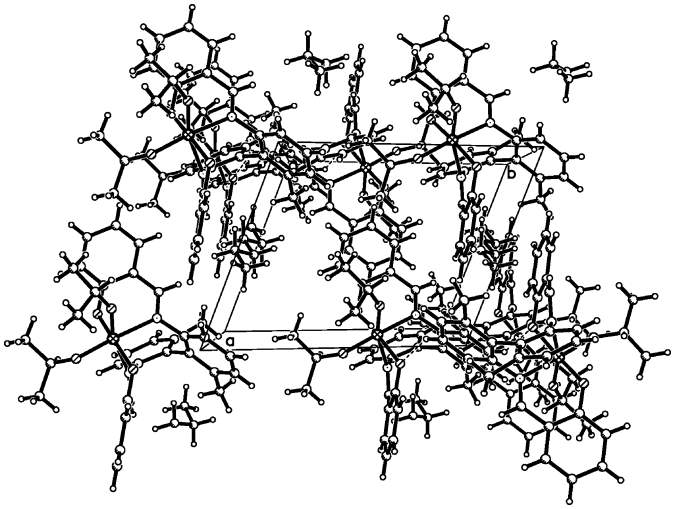


Figure 2
The crystal packing of the title compound, viewed along [001].

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Ti(C_{28}H_{22}N_2O_2)(C_3H_7O)_2]\cdot 0.5C_6H_{14}$
M_r	627.63
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	110
a, b, c (Å)	9.4212 (17), 12.062 (2), 16.116 (3)
α, β, γ (°)	107.369 (3), 95.857 (3), 107.938 (4)
V (Å^3)	1624.5 (5)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.31
Crystal size (mm)	0.12 × 0.11 × 0.10
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.61, 0.75
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8216, 5869, 4345
R_{int}	0.032
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.064, 0.176, 1.05
No. of reflections	5869
No. of parameters	404
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.76, −0.60

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS97* and *SHELXTL* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

We thank Professor Guofu Zi for providing the Schiff-base ligand and helpful discussion.

References

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full crystallographic data

IUCrData (2016). **1**, x161482 [doi:10.1107/S2414314616014826]

{6,6′-Dimethyl-2,2′-bis[(2-oxidobenzylidene)amino]-1,1′-biphenyl-κ^4O,N,N',O'}bis(propan-2-olato-κO)titanium(IV) *n*-hexane hemisolvate

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Crystal data

$[Ti(C_{28}H_{22}N_2O_2)(C_3H_7O)_2]\cdot 0.5C_6H_{14}$
M_r = 627.63
Triclinic, $P\overline{1}$
a = 9.4212 (17) Å
b = 12.062 (2) Å
c = 16.116 (3) Å
α = 107.369 (3)°
β = 95.857 (3)°
γ = 107.938 (4)°
V = 1624.5 (5) Å^3
Z = 2
$F(000)$ = 666
D_x = 1.283 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2116 reflections
θ = 2.7–24.7°
μ = 0.31 mm^{-1}
T = 110 K
Block, yellow
0.12 × 0.11 × 0.10 mm

Data collection

Bruker APEX-II CCD diffractometer
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.61, T_{max} = 0.75
8216 measured reflections
5869 independent reflections
4345 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 25.3°, θ_{min} = 1.9°
h = −11→9
k = −8→14
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.176
S = 1.05
5869 reflections
404 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0919P)^2 + 1.0825P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 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}
C1	0.3053 (4)	0.4834 (3)	0.3414 (2)	0.0219 (8)
C2	0.4005 (4)	0.6037 (3)	0.3970 (2)	0.0253 (8)
H2	0.3617	0.6695	0.4085	0.030*
C3	0.5501 (4)	0.6277 (3)	0.4353 (2)	0.0296 (9)
H3	0.6131	0.7102	0.4715	0.036*
C4	0.6096 (4)	0.5340 (4)	0.4217 (2)	0.0299 (9)
H4	0.7125	0.5518	0.4483	0.036*
C5	0.5183 (4)	0.4150 (3)	0.3695 (2)	0.0257 (8)
H5	0.5575	0.3497	0.3617	0.031*
C6	0.3677 (4)	0.3883 (3)	0.3274 (2)	0.0202 (7)
C7	0.2727 (4)	0.2605 (3)	0.2786 (2)	0.0189 (7)
H7	0.3094	0.1982	0.2858	0.023*
C8	0.0519 (4)	0.0938 (3)	0.1981 (2)	0.0163 (7)
C9	0.0534 (4)	0.0112 (3)	0.1183 (2)	0.0199 (7)
H9	0.1177	0.0382	0.0811	0.024*
C10	−0.0413 (4)	−0.1124 (3)	0.0933 (2)	0.0219 (8)
H10	−0.0412	−0.1712	0.0389	0.026*
C11	−0.1351 (4)	−0.1497 (3)	0.1475 (2)	0.0219 (8)
H11	−0.1998	−0.2344	0.1291	0.026*
C12	−0.1382 (4)	−0.0675 (3)	0.2282 (2)	0.0183 (7)
C13	−0.2465 (4)	−0.1129 (3)	0.2835 (2)	0.0253 (8)
H13A	−0.1987	−0.1472	0.3216	0.038*
H13B	−0.3406	−0.1777	0.2442	0.038*
H13C	−0.2708	−0.0434	0.3207	0.038*
C14	−0.0408 (4)	0.0573 (3)	0.2549 (2)	0.0165 (7)
C15	−0.0408 (4)	0.1526 (3)	0.3394 (2)	0.0162 (7)
C16	0.0160 (4)	0.1510 (3)	0.4232 (2)	0.0184 (7)
C17	0.0993 (4)	0.0656 (3)	0.4303 (2)	0.0246 (8)
H17A	0.1406	0.0835	0.4932	0.037*
H17B	0.1832	0.0782	0.3988	0.037*
H17C	0.0287	−0.0208	0.4038	0.037*
C18	0.0018 (4)	0.2358 (3)	0.4990 (2)	0.0217 (8)
H18	0.0383	0.2345	0.5557	0.026*
C19	−0.0644 (4)	0.3224 (3)	0.4941 (2)	0.0212 (8)
H19	−0.0775	0.3768	0.5467	0.025*
C20	−0.1115 (4)	0.3287 (3)	0.4116 (2)	0.0200 (7)
H20	−0.1525	0.3901	0.4074	0.024*
C21	−0.0982 (4)	0.2444 (3)	0.3353 (2)	0.0174 (7)
C22	−0.2790 (4)	0.2087 (3)	0.2125 (2)	0.0210 (8)
H22	−0.3500	0.1815	0.2465	0.025*
C23	−0.3400 (4)	0.1951 (3)	0.1223 (2)	0.0208 (8)
C24	−0.4958 (4)	0.1660 (4)	0.0952 (3)	0.0319 (9)
H24	−0.5588	0.1614	0.1374	0.038*
C25	−0.5610 (5)	0.1439 (4)	0.0089 (3)	0.0369 (10)
H25	−0.6673	0.1263	−0.0083	0.044*

C26	−0.4679 (5)	0.1477 (4)	−0.0526 (3)	0.0326 (9)
H26	−0.5117	0.1320	−0.1126	0.039*
C27	−0.3143 (4)	0.1738 (3)	−0.0284 (2)	0.0280 (9)
H27	−0.2537	0.1744	−0.0721	0.034*
C28	−0.2454 (4)	0.1995 (3)	0.0594 (2)	0.0220 (8)
C29	−0.0782 (5)	0.5564 (3)	0.2484 (2)	0.0291 (9)
H29	−0.0670	0.5455	0.3076	0.035*
C30	0.0412 (5)	0.6796 (3)	0.2564 (3)	0.0334 (9)
H30A	0.1429	0.6816	0.2791	0.050*
H30B	0.0204	0.7481	0.2976	0.050*
H30C	0.0373	0.6883	0.1978	0.050*
C31	−0.2383 (5)	0.5478 (4)	0.2201 (3)	0.0362 (10)
H31A	−0.2537	0.5508	0.1599	0.054*
H31B	−0.2569	0.6175	0.2613	0.054*
H31C	−0.3096	0.4693	0.2205	0.054*
C32	0.2837 (6)	0.4602 (4)	0.0844 (3)	0.0493 (13)
H32	0.3418	0.4129	0.0500	0.059*
C33	0.3973 (6)	0.5811 (5)	0.1525 (4)	0.0682 (17)
H33A	0.3418	0.6305	0.1847	0.102*
H33B	0.4628	0.6282	0.1219	0.102*
H33C	0.4605	0.5622	0.1946	0.102*
C34	0.1792 (7)	0.4810 (5)	0.0215 (3)	0.0691 (17)
H34A	0.1097	0.4008	−0.0213	0.104*
H34B	0.2384	0.5302	−0.0103	0.104*
H34C	0.1199	0.5261	0.0541	0.104*
C35	0.3909 (5)	−0.0331 (4)	0.2955 (3)	0.0445 (11)
H35A	0.4148	−0.1086	0.2723	0.067*
H35B	0.4179	0.0179	0.2583	0.067*
H35C	0.2814	−0.0560	0.2949	0.067*
C36	0.4824 (5)	0.0410 (4)	0.3913 (3)	0.0394 (11)
H36A	0.5924	0.0720	0.3905	0.047*
H36B	0.4524	0.1141	0.4157	0.047*
C37	0.4578 (5)	−0.0358 (4)	0.4523 (3)	0.0397 (11)
H37A	0.3472	−0.0694	0.4510	0.048*
H37B	0.4908	−0.1074	0.4287	0.048*
N1	0.1428 (3)	0.2243 (2)	0.22620 (17)	0.0166 (6)
N2	−0.1374 (3)	0.2544 (2)	0.25002 (18)	0.0172 (6)
O1	0.1623 (3)	0.4616 (2)	0.30682 (15)	0.0215 (5)
O2	−0.0966 (3)	0.2237 (2)	0.08126 (15)	0.0212 (5)
O3	−0.0504 (3)	0.4588 (2)	0.18582 (15)	0.0232 (6)
O4	0.1998 (3)	0.3891 (2)	0.13028 (16)	0.0277 (6)
Ti1	0.04656 (7)	0.35195 (6)	0.18542 (4)	0.0188 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.024 (2)	0.0194 (17)	0.0212 (18)	0.0046 (15)	0.0052 (15)	0.0088 (14)
C2	0.025 (2)	0.0199 (18)	0.029 (2)	0.0073 (16)	0.0034 (16)	0.0078 (15)

C3	0.026 (2)	0.0225 (19)	0.028 (2)	−0.0001 (16)	0.0013 (16)	0.0015 (16)
C4	0.018 (2)	0.032 (2)	0.030 (2)	0.0019 (16)	0.0012 (16)	0.0062 (17)
C5	0.021 (2)	0.0253 (19)	0.028 (2)	0.0059 (16)	0.0049 (15)	0.0072 (16)
C6	0.0204 (19)	0.0216 (18)	0.0189 (17)	0.0056 (15)	0.0058 (14)	0.0089 (14)
C7	0.0216 (19)	0.0169 (17)	0.0211 (17)	0.0087 (15)	0.0080 (15)	0.0076 (14)
C8	0.0187 (18)	0.0139 (16)	0.0168 (16)	0.0069 (14)	0.0029 (13)	0.0052 (13)
C9	0.0234 (19)	0.0213 (18)	0.0178 (17)	0.0101 (15)	0.0068 (14)	0.0078 (14)
C10	0.025 (2)	0.0216 (18)	0.0184 (17)	0.0123 (15)	0.0036 (14)	0.0020 (14)
C11	0.0219 (19)	0.0171 (17)	0.0249 (18)	0.0067 (15)	0.0011 (15)	0.0061 (15)
C12	0.0173 (18)	0.0164 (17)	0.0225 (17)	0.0070 (14)	0.0024 (14)	0.0082 (14)
C13	0.024 (2)	0.0203 (18)	0.030 (2)	0.0046 (15)	0.0089 (16)	0.0079 (16)
C14	0.0178 (18)	0.0127 (16)	0.0179 (16)	0.0055 (13)	0.0002 (13)	0.0048 (13)
C15	0.0132 (17)	0.0158 (16)	0.0177 (16)	0.0017 (13)	0.0062 (13)	0.0060 (14)
C16	0.0161 (18)	0.0156 (16)	0.0242 (18)	0.0028 (14)	0.0066 (14)	0.0100 (14)
C17	0.029 (2)	0.0267 (19)	0.0207 (18)	0.0112 (16)	0.0050 (15)	0.0109 (16)
C18	0.0207 (19)	0.0244 (18)	0.0174 (17)	0.0051 (15)	0.0029 (14)	0.0072 (15)
C19	0.0232 (19)	0.0193 (18)	0.0185 (17)	0.0066 (15)	0.0076 (14)	0.0031 (14)
C20	0.0204 (19)	0.0141 (16)	0.0226 (18)	0.0049 (14)	0.0056 (14)	0.0037 (14)
C21	0.0154 (17)	0.0162 (16)	0.0186 (17)	0.0028 (14)	0.0043 (13)	0.0059 (14)
C22	0.022 (2)	0.0178 (17)	0.0242 (18)	0.0075 (15)	0.0066 (15)	0.0081 (15)
C23	0.0226 (19)	0.0171 (17)	0.0203 (17)	0.0057 (15)	0.0009 (14)	0.0058 (14)
C24	0.024 (2)	0.040 (2)	0.031 (2)	0.0074 (18)	0.0060 (17)	0.0157 (18)
C25	0.021 (2)	0.050 (3)	0.038 (2)	0.0085 (19)	−0.0020 (17)	0.020 (2)
C26	0.033 (2)	0.035 (2)	0.026 (2)	0.0096 (19)	−0.0039 (17)	0.0128 (17)
C27	0.032 (2)	0.028 (2)	0.0236 (19)	0.0093 (17)	0.0056 (16)	0.0090 (16)
C28	0.022 (2)	0.0173 (17)	0.0241 (18)	0.0067 (15)	0.0006 (15)	0.0052 (14)
C29	0.042 (2)	0.0237 (19)	0.0243 (19)	0.0147 (18)	0.0089 (17)	0.0083 (16)
C30	0.044 (3)	0.0202 (19)	0.033 (2)	0.0109 (18)	0.0041 (18)	0.0062 (17)
C31	0.039 (3)	0.028 (2)	0.049 (3)	0.0171 (19)	0.019 (2)	0.0149 (19)
C32	0.057 (3)	0.044 (3)	0.048 (3)	0.006 (2)	0.023 (2)	0.026 (2)
C33	0.055 (3)	0.059 (3)	0.068 (4)	−0.017 (3)	0.007 (3)	0.031 (3)
C34	0.116 (5)	0.049 (3)	0.041 (3)	0.022 (3)	0.013 (3)	0.023 (3)
C35	0.042 (3)	0.028 (2)	0.064 (3)	0.012 (2)	0.024 (2)	0.012 (2)
C36	0.032 (2)	0.024 (2)	0.066 (3)	0.0114 (18)	0.021 (2)	0.015 (2)
C37	0.033 (2)	0.022 (2)	0.064 (3)	0.0103 (18)	0.019 (2)	0.011 (2)
N1	0.0165 (15)	0.0142 (14)	0.0175 (14)	0.0035 (12)	0.0057 (12)	0.0044 (11)
N2	0.0193 (16)	0.0117 (13)	0.0190 (14)	0.0050 (12)	0.0012 (12)	0.0044 (11)
O1	0.0213 (14)	0.0180 (12)	0.0241 (13)	0.0071 (10)	0.0012 (10)	0.0070 (10)
O2	0.0195 (13)	0.0228 (13)	0.0201 (12)	0.0063 (10)	0.0041 (10)	0.0070 (10)
O3	0.0282 (14)	0.0188 (12)	0.0235 (13)	0.0088 (11)	0.0037 (10)	0.0088 (10)
O4	0.0242 (14)	0.0307 (14)	0.0298 (14)	0.0057 (11)	0.0081 (11)	0.0162 (12)
Ti1	0.0194 (4)	0.0163 (3)	0.0200 (3)	0.0039 (3)	0.0028 (3)	0.0083 (3)

Geometric parameters (Å, º)

C1—O1	1.318 (4)	C23—C28	1.418 (5)
C1—C2	1.404 (5)	C24—C25	1.372 (5)
C1—C6	1.414 (5)	C24—H24	0.9500

C2—C3	1.383 (5)	C25—C26	1.392 (6)
C2—H2	0.9500	C25—H25	0.9500
C3—C4	1.381 (6)	C26—C27	1.370 (5)
C3—H3	0.9500	C26—H26	0.9500
C4—C5	1.371 (5)	C27—C28	1.396 (5)
C4—H4	0.9500	C27—H27	0.9500
C5—C6	1.403 (5)	C28—O2	1.327 (4)
C5—H5	0.9500	C29—O3	1.417 (4)
C6—C7	1.442 (5)	C29—C31	1.493 (6)
C7—N1	1.281 (4)	C29—C30	1.522 (5)
C7—H7	0.9500	C29—H29	1.0000
C8—C9	1.376 (4)	C30—H30A	0.9800
C8—C14	1.400 (5)	C30—H30B	0.9800
C8—N1	1.443 (4)	C30—H30C	0.9800
C9—C10	1.389 (5)	C31—H31A	0.9800
C9—H9	0.9500	C31—H31B	0.9800
C10—C11	1.375 (5)	C31—H31C	0.9800
C10—H10	0.9500	C32—O4	1.410 (5)
C11—C12	1.389 (5)	C32—C34	1.469 (7)
C11—H11	0.9500	C32—C33	1.523 (7)
C12—C14	1.406 (4)	C32—H32	1.0000
C12—C13	1.507 (5)	C33—H33A	0.9800
C13—H13A	0.9800	C33—H33B	0.9800
C13—H13B	0.9800	C33—H33C	0.9800
C13—H13C	0.9800	C34—H34A	0.9800
C14—C15	1.497 (4)	C34—H34B	0.9800
C15—C21	1.389 (5)	C34—H34C	0.9800
C15—C16	1.408 (5)	C35—C36	1.534 (6)
C16—C18	1.389 (5)	C35—H35A	0.9800
C16—C17	1.497 (5)	C35—H35B	0.9800
C17—H17A	0.9800	C35—H35C	0.9800
C17—H17B	0.9800	C36—C37	1.530 (6)
C17—H17C	0.9800	C36—H36A	0.9900
C18—C19	1.388 (5)	C36—H36B	0.9900
C18—H18	0.9500	C37—C37^{i}	1.508 (9)
C19—C20	1.391 (5)	C37—H37A	0.9900
C19—H19	0.9500	C37—H37B	0.9900
C20—C21	1.387 (5)	N1—Ti1	2.229 (3)
C20—H20	0.9500	N2—Ti1	2.306 (3)
C21—N2	1.436 (4)	O1—Ti1	1.974 (2)
C22—N2	1.277 (4)	O2—Ti1	1.932 (2)
C22—C23	1.450 (5)	O3—Ti1	1.793 (2)
C22—H22	0.9500	O4—Ti1	1.782 (2)
C23—C24	1.389 (5)		

O1—C1—C2	120.1 (3)	C26—C27—H27	119.5
O1—C1—C6	122.4 (3)	C28—C27—H27	119.5
C2—C1—C6	117.4 (3)	O2—C28—C27	119.9 (3)

C3—C2—C1	120.8 (3)	O2—C28—C23	122.1 (3)
C3—C2—H2	119.6	C27—C28—C23	117.9 (3)
C1—C2—H2	119.6	O3—C29—C31	108.9 (3)
C4—C3—C2	121.3 (3)	O3—C29—C30	108.7 (3)
C4—C3—H3	119.4	C31—C29—C30	113.5 (3)
C2—C3—H3	119.4	O3—C29—H29	108.5
C5—C4—C3	119.2 (4)	C31—C29—H29	108.5
C5—C4—H4	120.4	C30—C29—H29	108.5
C3—C4—H4	120.4	C29—C30—H30A	109.5
C4—C5—C6	120.9 (4)	C29—C30—H30B	109.5
C4—C5—H5	119.6	H30A—C30—H30B	109.5
C6—C5—H5	119.6	C29—C30—H30C	109.5
C5—C6—C1	120.3 (3)	H30A—C30—H30C	109.5
C5—C6—C7	118.8 (3)	H30B—C30—H30C	109.5
C1—C6—C7	120.5 (3)	C29—C31—H31A	109.5
N1—C7—C6	125.3 (3)	C29—C31—H31B	109.5
N1—C7—H7	117.4	H31A—C31—H31B	109.5
C6—C7—H7	117.4	C29—C31—H31C	109.5
C9—C8—C14	122.3 (3)	H31A—C31—H31C	109.5
C9—C8—N1	121.3 (3)	H31B—C31—H31C	109.5
C14—C8—N1	116.4 (3)	O4—C32—C34	110.0 (4)
C8—C9—C10	118.5 (3)	O4—C32—C33	108.5 (4)
C8—C9—H9	120.7	C34—C32—C33	112.6 (5)
C10—C9—H9	120.7	O4—C32—H32	108.5
C11—C10—C9	120.0 (3)	C34—C32—H32	108.5
C11—C10—H10	120.0	C33—C32—H32	108.5
C9—C10—H10	120.0	C32—C33—H33A	109.5
C10—C11—C12	122.1 (3)	C32—C33—H33B	109.5
C10—C11—H11	118.9	H33A—C33—H33B	109.5
C12—C11—H11	118.9	C32—C33—H33C	109.5
C11—C12—C14	118.3 (3)	H33A—C33—H33C	109.5
C11—C12—C13	119.8 (3)	H33B—C33—H33C	109.5
C14—C12—C13	121.8 (3)	C32—C34—H34A	109.5
C12—C13—H13A	109.5	C32—C34—H34B	109.5
C12—C13—H13B	109.5	H34A—C34—H34B	109.5
H13A—C13—H13B	109.5	C32—C34—H34C	109.5
C12—C13—H13C	109.5	H34A—C34—H34C	109.5
H13A—C13—H13C	109.5	H34B—C34—H34C	109.5
H13B—C13—H13C	109.5	C36—C35—H35A	109.5
C8—C14—C12	118.6 (3)	C36—C35—H35B	109.5
C8—C14—C15	119.6 (3)	H35A—C35—H35B	109.5
C12—C14—C15	121.7 (3)	C36—C35—H35C	109.5
C21—C15—C16	119.2 (3)	H35A—C35—H35C	109.5
C21—C15—C14	119.4 (3)	H35B—C35—H35C	109.5
C16—C15—C14	121.4 (3)	C37—C36—C35	112.9 (3)
C18—C16—C15	118.6 (3)	C37—C36—H36A	109.0
C18—C16—C17	120.8 (3)	C35—C36—H36A	109.0
C15—C16—C17	120.5 (3)	C37—C36—H36B	109.0

C16—C17—H17A	109.5	C35—C36—H36B	109.0
C16—C17—H17B	109.5	H36A—C36—H36B	107.8
H17A—C17—H17B	109.5	C37^{i}—C37—C36	114.1 (4)
C16—C17—H17C	109.5	C37^{i}—C37—H37A	108.7
H17A—C17—H17C	109.5	C36—C37—H37A	108.7
H17B—C17—H17C	109.5	C37^{i}—C37—H37B	108.7
C19—C18—C16	121.8 (3)	C36—C37—H37B	108.7
C19—C18—H18	119.1	H37A—C37—H37B	107.6
C16—C18—H18	119.1	C7—N1—C8	116.4 (3)
C18—C19—C20	119.3 (3)	C7—N1—Ti1	123.9 (2)
C18—C19—H19	120.3	C8—N1—Ti1	119.5 (2)
C20—C19—H19	120.3	C22—N2—C21	116.9 (3)
C21—C20—C19	119.4 (3)	C22—N2—Ti1	121.7 (2)
C21—C20—H20	120.3	C21—N2—Ti1	121.4 (2)
C19—C20—H20	120.3	C1—O1—Ti1	127.0 (2)
C20—C21—C15	121.4 (3)	C28—O2—Ti1	127.1 (2)
C20—C21—N2	120.1 (3)	C29—O3—Ti1	138.5 (2)
C15—C21—N2	118.4 (3)	C32—O4—Ti1	151.0 (3)
N2—C22—C23	125.3 (3)	O4—Ti1—O3	107.05 (12)
N2—C22—H22	117.4	O4—Ti1—O2	95.59 (11)
C23—C22—H22	117.4	O3—Ti1—O2	92.98 (11)
C24—C23—C28	119.7 (3)	O4—Ti1—O1	96.70 (11)
C24—C23—C22	119.2 (3)	O3—Ti1—O1	88.61 (10)
C28—C23—C22	120.8 (3)	O2—Ti1—O1	166.56 (10)
C25—C24—C23	121.6 (4)	O4—Ti1—N1	88.78 (11)
C25—C24—H24	119.2	O3—Ti1—N1	161.50 (11)
C23—C24—H24	119.2	O2—Ti1—N1	94.97 (10)
C24—C25—C26	118.5 (4)	O1—Ti1—N1	79.89 (10)
C24—C25—H25	120.7	O4—Ti1—N2	164.22 (11)
C26—C25—H25	120.7	O3—Ti1—N2	88.20 (11)
C27—C26—C25	121.3 (4)	O2—Ti1—N2	79.22 (10)
C27—C26—H26	119.3	O1—Ti1—N2	87.50 (10)
C25—C26—H26	119.3	N1—Ti1—N2	76.95 (10)
C26—C27—C28	121.0 (4)		

O1—C1—C2—C3	178.7 (3)	N2—C22—C23—C24	−168.0 (3)
C6—C1—C2—C3	0.9 (5)	N2—C22—C23—C28	18.0 (5)
C1—C2—C3—C4	−1.5 (6)	C28—C23—C24—C25	−1.4 (6)
C2—C3—C4—C5	−0.1 (6)	C22—C23—C24—C25	−175.5 (4)
C3—C4—C5—C6	2.2 (6)	C23—C24—C25—C26	1.7 (6)
C4—C5—C6—C1	−2.7 (5)	C24—C25—C26—C27	−0.4 (6)
C4—C5—C6—C7	−175.5 (3)	C25—C26—C27—C28	−1.1 (6)
O1—C1—C6—C5	−176.6 (3)	C26—C27—C28—O2	179.5 (3)
C2—C1—C6—C5	1.1 (5)	C26—C27—C28—C23	1.4 (5)
O1—C1—C6—C7	−4.0 (5)	C24—C23—C28—O2	−178.2 (3)
C2—C1—C6—C7	173.7 (3)	C22—C23—C28—O2	−4.2 (5)
C5—C6—C7—N1	−168.7 (3)	C24—C23—C28—C27	−0.1 (5)
C1—C6—C7—N1	18.6 (5)	C22—C23—C28—C27	173.9 (3)

C14—C8—C9—C10	0.3 (5)	C35—C36—C37—C37^{i}	−178.1 (4)
N1—C8—C9—C10	−177.4 (3)	C6—C7—N1—C8	−167.6 (3)
C8—C9—C10—C11	0.7 (5)	C6—C7—N1—Ti1	8.0 (5)
C9—C10—C11—C12	−0.6 (5)	C9—C8—N1—C7	−96.2 (4)
C10—C11—C12—C14	−0.6 (5)	C14—C8—N1—C7	85.9 (4)
C10—C11—C12—C13	178.2 (3)	C9—C8—N1—Ti1	88.1 (3)
C9—C8—C14—C12	−1.5 (5)	C14—C8—N1—Ti1	−89.8 (3)
N1—C8—C14—C12	176.4 (3)	C23—C22—N2—C21	−171.7 (3)
C9—C8—C14—C15	−178.0 (3)	C23—C22—N2—Ti1	9.6 (5)
N1—C8—C14—C15	−0.1 (4)	C20—C21—N2—C22	−81.2 (4)
C11—C12—C14—C8	1.6 (5)	C15—C21—N2—C22	101.6 (4)
C13—C12—C14—C8	−177.2 (3)	C20—C21—N2—Ti1	97.6 (3)
C11—C12—C14—C15	178.0 (3)	C15—C21—N2—Ti1	−79.7 (3)
C13—C12—C14—C15	−0.8 (5)	C2—C1—O1—Ti1	140.6 (3)
C8—C14—C15—C21	66.3 (4)	C6—C1—O1—Ti1	−41.7 (4)
C12—C14—C15—C21	−110.0 (4)	C27—C28—O2—Ti1	137.2 (3)
C8—C14—C15—C16	−113.8 (4)	C23—C28—O2—Ti1	−44.8 (4)
C12—C14—C15—C16	69.9 (4)	C31—C29—O3—Ti1	−140.4 (3)
C21—C15—C16—C18	5.0 (5)	C30—C29—O3—Ti1	95.4 (4)
C14—C15—C16—C18	−175.0 (3)	C34—C32—O4—Ti1	−40.5 (7)
C21—C15—C16—C17	−170.9 (3)	C33—C32—O4—Ti1	83.1 (7)
C14—C15—C16—C17	9.2 (5)	C32—O4—Ti1—O3	−2.0 (6)
C15—C16—C18—C19	−1.0 (5)	C32—O4—Ti1—O2	92.8 (6)
C17—C16—C18—C19	174.9 (3)	C32—O4—Ti1—O1	−92.6 (6)
C16—C18—C19—C20	−3.1 (5)	C32—O4—Ti1—N1	−172.3 (6)
C18—C19—C20—C21	3.1 (5)	C32—O4—Ti1—N2	162.6 (5)
C19—C20—C21—C15	1.0 (5)	C29—O3—Ti1—O4	−115.0 (3)
C19—C20—C21—N2	−176.2 (3)	C29—O3—Ti1—O2	148.3 (3)
C16—C15—C21—C20	−5.0 (5)	C29—O3—Ti1—O1	−18.4 (3)
C14—C15—C21—C20	174.9 (3)	C29—O3—Ti1—N1	32.9 (6)
C16—C15—C21—N2	172.2 (3)	C29—O3—Ti1—N2	69.2 (3)
C14—C15—C21—N2	−7.9 (4)		

Symmetry code: (i) −*x*+1, −*y*, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10···O2^{ii}	0.95	2.47	3.312 (4)	147

Symmetry code: (ii) −*x*, −*y*, −*z*.