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{*N*,*N*-Bis[bis(2,2,2-trifluoroethoxy)-phosphanyl]methylamine-κ^2P,P'}bis(η^5-cyclopentadienyl)titanium(II)

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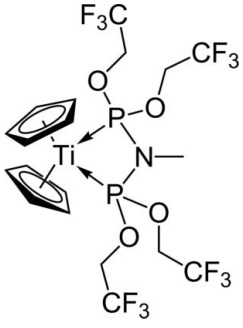
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.003 Å; R factor = 0.031; wR factor = 0.079; data-to-parameter ratio = 17.9.

The title compound, $[Ti(C_5H_5)_2(C_9H_{11}F_{12}NO_4P_2)]$, is a four-membered titanacycle obtained from the reaction of $Cp_2Ti(\eta^2$-$Me_3SiC_2SiMe_3)$ and $CH_3N[P(OCH_2CF_3)_2]_2$ {*N*,*N*-bis[bis(trifluoroethoxy)phosphanyl]methylamine, tfepma}. The Ti^{II} atom is coordinated by two cyclopentadienyl (Cp) ligands and the chelating tfepma ligand in a strongly distorted tetrahedral geometry. The molecule is located on a mirror plane.

Related literature

For other titanocene complexes with four-membered metallacycles [TiPNP], see: Haehnel *et al.* (2012). For selected examples of four-membered metallacycles with a chelating tfepma ligand, see: *M* = Rh, Esswein *et al.* (2005, 2007); *M* = Ir, Heyduk & Nocera (1999, 2000); Gray *et al.* (2004); Veige *et al.* (2005); Esswein *et al.* (2008). The starting alkyne complex $Cp_2Ti(\eta^2$-$Me_3SiC_2SiMe_3)$ is described by Burlakov *et al.* (1988).



Experimental

Crystal data

$[Ti(C_5H_5)_2(C_9H_{11}F_{12}NO_4P_2)]$
M_r = 665.21
Orthorhombic, *Pnma*
a = 14.6494 (2) Å
b = 20.0535 (3) Å
c = 8.7694 (1) Å
V = 2576.20 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.57 mm^{-1}
T = 150 K
0.42 × 0.41 × 0.16 mm

Data collection

Bruker Kappa APEXII DUO diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.90, T_{max} = 1.00
60903 measured reflections
3420 independent reflections
2988 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.079
S = 1.06
3420 reflections
191 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Data collection: *APEX2* (Bruker, 2011); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT6910).

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supplementary materials

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{*N*,*N*-Bis[bis(2,2,2-trifluoroethoxy)phosphanyl]methylamine-κ^2P,P'}bis(η^5-cyclopentadienyl)titanium(II)

Martin Haehnel, Sven Hansen, Anke Spannenberg and Torsten Beweries

Comment

The reaction of tfepma with the titanocene precursor $Cp_2Ti(\eta^2\text{-}Me_3SiC_2SiMe_3)$ was investigated to synthesize a new 4-membered hetero-metallacycle. In this reaction, the spectator ligand $Me_3SiC_2SiMe_3$ is replaced by the chelating tfepma ligand, which is binding over both phosphorus atoms to result in the four membered metallacycle.

In the title compound the titanium center is coordinated by two Cp units and the chelating tfepma ligand (Fig. 1). The molecule is located on a mirror plane which passes through H5A, C5, N1, Ti1, C7, H7, C11 and H11. The geometry at the titanium center is found to be strongly distorted tetrahedral. The largest deviation from the ideal tetrahedral angle is observed for P1—Ti1—$P1^i$ [63.94 (2)°, symmetry code to generate equivalent atoms: (i) x, $-y + 1/2$, z]. The four membered metallacycle Ti1,P1,N1,$P1^i$ is planar with a mean deviation from the best plane of 0.015 Å. The following bond lengths and angles of the cyclic unit were observed: Ti1—P1 = 2.4266 (4) Å, P1—N1 = 1.696 (1) Å, P1—N1—$P1^i$ = 98.51 (8)°.

Experimental

To a stirred solution of $Cp_2Ti(\eta^2\text{-}Me_3SiC_2SiMe_3)$ (150 mg, 0.430 mmol) in 5 ml of toluene was added a solution of tfepma (210 mg, 0.430 mmol) in 5 ml of toluene at room temperature. The colour of the reaction mixture instantly changed from brown to dark green. After additional stirring for 1 h, all volatiles were removed in vacuum and the resulting green precipitate was dissolved in 7 ml of toluene and stored at -30°C for several weeks. The resulting dark green single crystals were filtered, washed with cold *n*-hexane and dried in vacuum. Yield: 96% (274 mg, 0.412 mmol).

Refinement

H5A and H5B were found from the difference Fourier map and refined freely. All other H atoms were placed in idealized positions with d(C—H) = 0.95 Å (CH), 0.99 Å (CH_2) and refined using a riding model with U_{iso}(H) fixed at 1.2 U_{eq}(C).

Computing details

Data collection: *APEX2* (Bruker, 2011); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

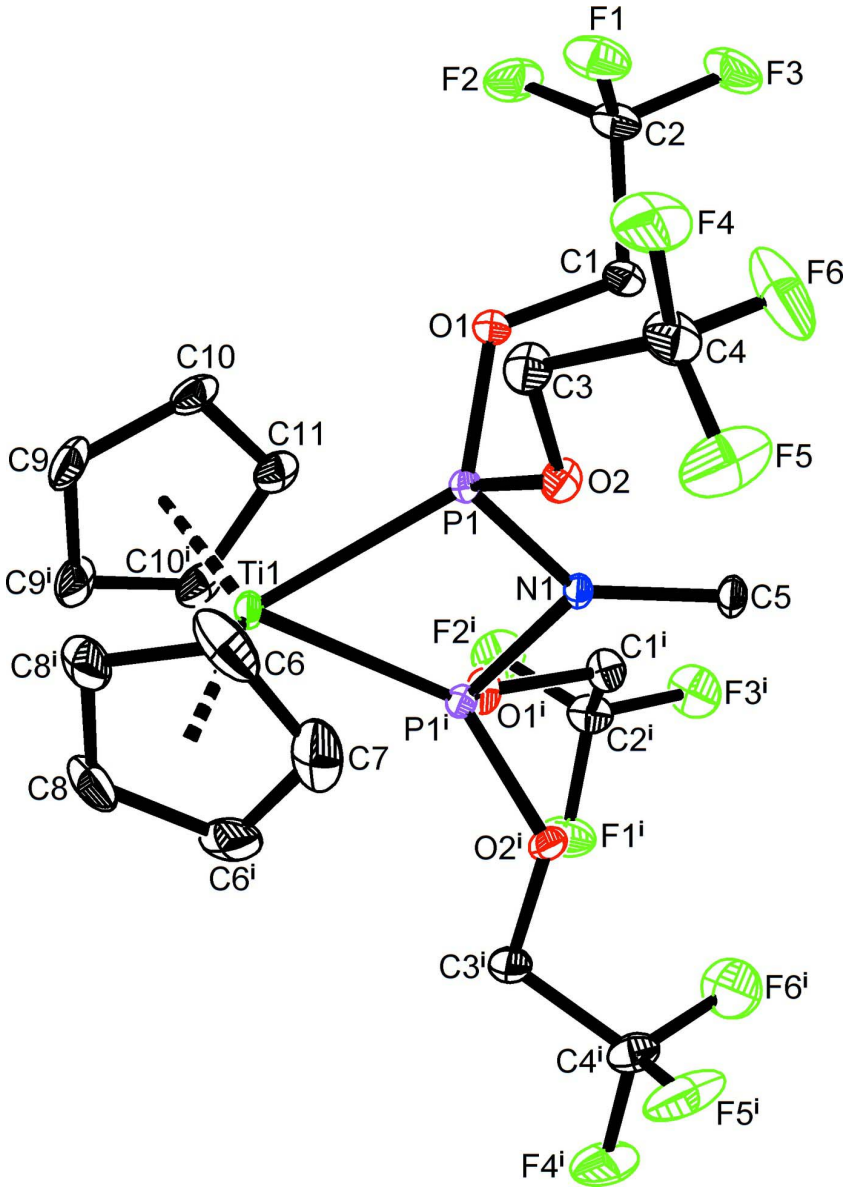

Figure 1

The molecular structure of the title compound in the crystal (symmetry code to generate equivalent atoms: (i) *x*, -*y* + 1/2, *z*). Hydrogen atoms are omitted for clarity. Displacement ellipsoids are drawn at the 30% probability level.

{*N*,*N*-Bis[bis(2,2,2-trifluoroethoxy)phosphanyl]methylamine-κ^2P,P'}bis(η^5-cyclopentadienyl)titanium(II)

Crystal data

$[Ti(C_5H_5)_2(C_9H_{11}F_{12}NO_4P_2)]$
M_r = 665.21
Orthorhombic, *Pnma*
a = 14.6494 (2) Å
b = 20.0535 (3) Å
c = 8.7694 (1) Å
V = 2576.20 (6) Å^3
Z = 4
F(000) = 1336
D_x = 1.715 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 9979 reflections
θ = 2.5–28.6°
μ = 0.57 mm^{-1}
T = 150 K
Prism, dark green
0.42 × 0.41 × 0.16 mm

Data collection

Bruker Kappa APEXII DUO diffractometer
Radiation source: fine-focus sealed tube
Curved graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
ω and phi scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.90, T_{max} = 1.00
60903 measured reflections
3420 independent reflections
2988 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 28.7°, θ_{min} = 2.5°
h = −19→19
k = −27→24
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.079
S = 1.06
3420 reflections
191 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0339P)^2 + 1.9223P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	y	z	U_{iso}*/U_{eq}
C1	0.92098 (11)	0.13133 (8)	0.72113 (17)	0.0261 (3)
H1A	0.9235	0.1703	0.6520	0.031*
H1B	0.8574	0.1259	0.7574	0.031*
C2	0.95209 (12)	0.06964 (8)	0.63952 (18)	0.0296 (3)
C3	0.88445 (11)	0.07502 (8)	1.1082 (2)	0.0310 (4)
H3A	0.9098	0.0719	1.2126	0.037*
H3B	0.9278	0.0537	1.0367	0.037*
C4	0.79412 (13)	0.04136 (9)	1.1005 (2)	0.0379 (4)
C5	0.79887 (14)	0.2500	0.8632 (3)	0.0228 (4)
H5A	0.8034 (17)	0.2500	0.752 (3)	0.023 (6)*
H5B	0.7653 (14)	0.2887 (10)	0.897 (2)	0.033 (5)*
C6	1.01942 (18)	0.19336 (12)	1.3387 (2)	0.0528 (6)
H6	0.9998	0.1483	1.3320	0.063*
C7	0.9650 (2)	0.2500	1.3137 (3)	0.0561 (9)
H7	0.9025	0.2500	1.2850	0.067*
C8	1.10686 (16)	0.28522 (10)	1.3748 (2)	0.0437 (5)

H8	1.1578	0.3131	1.3959	0.052*
C9	1.22452 (11)	0.21453 (9)	1.0707 (3)	0.0404 (5)
H9	1.2574	0.1868	1.1392	0.049*
C10	1.16817 (10)	0.19273 (8)	0.9531 (2)	0.0336 (4)
H10	1.1565	0.1476	0.9265	0.040*
C11	1.13093 (15)	0.2500	0.8793 (3)	0.0292 (5)
H11	1.0891	0.2500	0.7964	0.035*
F1	0.94470 (9)	0.01516 (5)	0.72635 (13)	0.0447 (3)
F2	1.03855 (8)	0.07332 (6)	0.59488 (13)	0.0441 (3)
F3	0.90112 (9)	0.05987 (6)	0.51500 (12)	0.0455 (3)
F4	0.80238 (10)	−0.02315 (5)	1.13574 (17)	0.0569 (4)
F5	0.73432 (10)	0.06669 (6)	1.1954 (2)	0.0734 (5)
F6	0.75798 (12)	0.04567 (8)	0.96213 (19)	0.0813 (5)
N1	0.89119 (11)	0.2500	0.93043 (19)	0.0167 (3)
O1	0.98087 (7)	0.14063 (5)	0.84642 (12)	0.0253 (2)
O2	0.87059 (7)	0.14299 (5)	1.06745 (13)	0.0239 (2)
P1	0.95613 (2)	0.185927 (17)	0.99495 (4)	0.01645 (9)
Ti1	1.07370 (2)	0.2500	1.12354 (4)	0.01905 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0296 (7)	0.0269 (7)	0.0217 (7)	0.0021 (6)	−0.0017 (6)	−0.0068 (6)
C2	0.0402 (9)	0.0244 (7)	0.0242 (7)	−0.0003 (6)	0.0027 (6)	−0.0049 (6)
C3	0.0308 (8)	0.0214 (7)	0.0409 (9)	−0.0025 (6)	−0.0028 (7)	0.0091 (7)
C4	0.0424 (10)	0.0239 (8)	0.0473 (10)	−0.0106 (7)	0.0011 (8)	0.0034 (7)
C5	0.0146 (9)	0.0275 (11)	0.0263 (10)	0.000	−0.0043 (8)	0.000
C6	0.0838 (16)	0.0552 (13)	0.0192 (8)	−0.0323 (12)	−0.0119 (9)	0.0102 (8)
C7	0.0390 (15)	0.113 (3)	0.0162 (11)	0.000	0.0021 (10)	0.000
C8	0.0644 (13)	0.0359 (10)	0.0308 (9)	−0.0074 (9)	−0.0247 (9)	−0.0022 (7)
C9	0.0156 (7)	0.0351 (9)	0.0707 (13)	0.0046 (6)	−0.0038 (8)	0.0044 (9)
C10	0.0183 (7)	0.0251 (8)	0.0573 (11)	0.0015 (6)	0.0114 (7)	−0.0044 (7)
C11	0.0196 (9)	0.0327 (11)	0.0354 (12)	0.000	0.0116 (9)	0.000
F1	0.0710 (8)	0.0228 (5)	0.0403 (6)	−0.0047 (5)	0.0008 (6)	0.0001 (4)
F2	0.0448 (6)	0.0437 (6)	0.0437 (6)	0.0072 (5)	0.0161 (5)	−0.0106 (5)
F3	0.0649 (8)	0.0431 (6)	0.0285 (5)	−0.0021 (6)	−0.0079 (5)	−0.0152 (5)
F4	0.0704 (8)	0.0208 (5)	0.0794 (9)	−0.0123 (5)	0.0114 (7)	0.0060 (6)
F5	0.0586 (8)	0.0395 (7)	0.1222 (13)	−0.0053 (6)	0.0509 (9)	0.0120 (8)
F6	0.0961 (12)	0.0685 (10)	0.0791 (10)	−0.0436 (9)	−0.0491 (9)	0.0132 (8)
N1	0.0136 (7)	0.0184 (7)	0.0180 (7)	0.000	−0.0020 (6)	0.000
O1	0.0226 (5)	0.0269 (5)	0.0263 (5)	0.0036 (4)	−0.0020 (4)	−0.0097 (4)
O2	0.0197 (5)	0.0187 (5)	0.0335 (6)	−0.0029 (4)	0.0012 (4)	0.0048 (4)
P1	0.01472 (15)	0.01642 (16)	0.01822 (16)	−0.00044 (12)	−0.00029 (12)	−0.00094 (12)
Ti1	0.01473 (16)	0.01974 (17)	0.02269 (18)	0.000	−0.00488 (13)	0.000

Geometric parameters (Å, º)

C1—O1	1.4183 (18)	C8—C8^{i}	1.413 (4)
C1—C2	1.500 (2)	C8—Ti1	2.3644 (18)
C1—H1A	0.9900	C8—H8	0.9500

C1—H1B	0.9900	C9—C10	1.392 (3)
C2—F2	1.328 (2)	C9—C9^{i}	1.422 (4)
C2—F1	1.3360 (19)	C9—Ti1	2.3670 (17)
C2—F3	1.3374 (19)	C9—H9	0.9500
C3—O2	1.4235 (18)	C10—C11	1.427 (2)
C3—C4	1.487 (2)	C10—Ti1	2.3387 (17)
C3—H3A	0.9900	C10—H10	0.9500
C3—H3B	0.9900	C11—C10^{i}	1.427 (2)
C4—F5	1.311 (2)	C11—Ti1	2.300 (2)
C4—F6	1.327 (2)	C11—H11	0.9500
C4—F4	1.336 (2)	N1—P1^{i}	1.6959 (11)
C5—N1	1.475 (2)	N1—P1	1.6959 (11)
C5—H5A	0.98 (3)	O1—P1	1.6287 (11)
C5—H5B	0.97 (2)	O2—P1	1.6481 (10)
C6—C8^{i}	1.388 (3)	P1—Ti1	2.4266 (4)
C6—C7	1.405 (3)	P1—P1^{i}	2.5697 (7)
C6—Ti1	2.3412 (19)	Ti1—C10^{i}	2.3387 (17)
C6—H6	0.9500	Ti1—C6^{i}	2.3412 (19)
C7—C6^{i}	1.405 (3)	Ti1—C8^{i}	2.3644 (18)
C7—Ti1	2.305 (3)	Ti1—C9^{i}	2.3670 (17)
C7—H7	0.9500	Ti1—P1^{i}	2.4266 (4)
C8—C6^{i}	1.388 (3)		

O1—C1—C2	106.86 (13)	O2—P1—Ti1	129.57 (4)
O1—C1—H1A	110.3	N1—P1—Ti1	98.74 (4)
C2—C1—H1A	110.3	O1—P1—P1^{i}	123.89 (4)
O1—C1—H1B	110.3	O2—P1—P1^{i}	121.50 (4)
C2—C1—H1B	110.3	Ti1—P1—P1^{i}	58.029 (9)
H1A—C1—H1B	108.6	C11—Ti1—C7	157.70 (10)
F2—C2—F1	106.91 (14)	C11—Ti1—C10	35.81 (6)
F2—C2—F3	107.46 (13)	C7—Ti1—C10	150.58 (4)
F1—C2—F3	107.48 (14)	C11—Ti1—C10^{i}	35.81 (6)
F2—C2—C1	112.62 (14)	C7—Ti1—C10^{i}	150.58 (4)
F1—C2—C1	112.20 (13)	C10—Ti1—C10^{i}	58.82 (8)
F3—C2—C1	109.92 (14)	C11—Ti1—C6^{i}	150.94 (6)
O2—C3—C4	107.24 (14)	C7—Ti1—C6^{i}	35.18 (8)
O2—C3—H3A	110.3	C10—Ti1—C6^{i}	162.62 (7)
C4—C3—H3A	110.3	C10^{i}—Ti1—C6^{i}	118.54 (8)
O2—C3—H3B	110.3	C11—Ti1—C6	150.94 (6)
C4—C3—H3B	110.3	C7—Ti1—C6	35.18 (8)
H3A—C3—H3B	108.5	C10—Ti1—C6	118.54 (8)
F5—C4—F6	106.78 (19)	C10^{i}—Ti1—C6	162.61 (7)
F5—C4—F4	106.79 (15)	C6^{i}—Ti1—C6	58.05 (12)
F6—C4—F4	108.12 (16)	C11—Ti1—C8^{i}	142.46 (8)
F5—C4—C3	112.95 (16)	C7—Ti1—C8^{i}	57.85 (9)
F6—C4—C3	111.54 (16)	C10—Ti1—C8^{i}	109.11 (7)
F4—C4—C3	110.41 (16)	C10^{i}—Ti1—C8^{i}	128.38 (8)
N1—C5—H5A	109.7 (15)	C6^{i}—Ti1—C8^{i}	57.57 (7)
N1—C5—H5B	110.2 (12)	C6—Ti1—C8^{i}	34.30 (8)

H5A—C5—H5B	109.9 (14)	C11—Ti1—C8	142.46 (8)
C8^{i}—C6—C7	108.0 (2)	C7—Ti1—C8	57.85 (9)
C8^{i}—C6—Ti1	73.76 (12)	C10—Ti1—C8	128.38 (8)
C7—C6—Ti1	71.01 (13)	C10^{i}—Ti1—C8	109.11 (7)
C8^{i}—C6—H6	126.0	C6^{i}—Ti1—C8	34.30 (8)
C7—C6—H6	126.0	C6—Ti1—C8	57.57 (7)
Ti1—C6—H6	121.0	C8^{i}—Ti1—C8	34.76 (9)
C6^{i}—C7—C6	107.9 (3)	C11—Ti1—C9	58.49 (8)
C6^{i}—C7—Ti1	73.80 (14)	C7—Ti1—C9	141.84 (8)
C6—C7—Ti1	73.80 (14)	C10—Ti1—C9	34.39 (7)
C6^{i}—C7—H7	126.0	C10^{i}—Ti1—C9	57.99 (6)
C6—C7—H7	126.0	C6^{i}—Ti1—C9	128.36 (8)
Ti1—C7—H7	118.3	C6—Ti1—C9	109.21 (9)
C6^{i}—C8—C8^{i}	108.03 (13)	C8^{i}—Ti1—C9	84.32 (8)
C6^{i}—C8—Ti1	71.93 (10)	C8—Ti1—C9	94.62 (8)
C8^{i}—C8—Ti1	72.62 (5)	C11—Ti1—C9^{i}	58.49 (8)
C6^{i}—C8—H8	126.0	C7—Ti1—C9^{i}	141.84 (8)
C8^{i}—C8—H8	126.0	C10—Ti1—C9^{i}	57.99 (6)
Ti1—C8—H8	121.2	C10^{i}—Ti1—C9^{i}	34.39 (7)
C10—C9—C9^{i}	108.31 (10)	C6^{i}—Ti1—C9^{i}	109.21 (9)
C10—C9—Ti1	71.69 (9)	C6—Ti1—C9^{i}	128.36 (8)
C9^{i}—C9—Ti1	72.51 (4)	C8^{i}—Ti1—C9^{i}	94.62 (8)
C10—C9—H9	125.8	C8—Ti1—C9^{i}	84.32 (8)
C9^{i}—C9—H9	125.8	C9—Ti1—C9^{i}	34.97 (9)
Ti1—C9—H9	121.7	C11—Ti1—P1^{i}	79.98 (5)
C9—C10—C11	108.07 (16)	C7—Ti1—P1^{i}	81.14 (6)
C9—C10—Ti1	73.91 (10)	C10—Ti1—P1^{i}	112.52 (5)
C11—C10—Ti1	70.63 (11)	C10^{i}—Ti1—P1^{i}	82.12 (4)
C9—C10—H10	126.0	C6^{i}—Ti1—P1^{i}	82.91 (5)
C11—C10—H10	126.0	C6—Ti1—P1^{i}	112.97 (7)
Ti1—C10—H10	121.2	C8^{i}—Ti1—P1^{i}	137.48 (6)
C10—C11—C10^{i}	107.2 (2)	C8—Ti1—P1^{i}	114.88 (5)
C10—C11—Ti1	73.56 (12)	C9—Ti1—P1^{i}	136.94 (6)
C10^{i}—C11—Ti1	73.56 (12)	C9^{i}—Ti1—P1^{i}	114.36 (5)
C10—C11—H11	126.4	C11—Ti1—P1	79.98 (5)
C10^{i}—C11—H11	126.4	C7—Ti1—P1	81.14 (6)
Ti1—C11—H11	118.5	C10—Ti1—P1	82.12 (4)
C5—N1—P1^{i}	130.36 (4)	C10^{i}—Ti1—P1	112.52 (5)
C5—N1—P1	130.36 (4)	C6^{i}—Ti1—P1	112.97 (7)
P1^{i}—N1—P1	98.51 (8)	C6—Ti1—P1	82.91 (5)
C1—O1—P1	123.73 (9)	C8^{i}—Ti1—P1	114.88 (5)
C3—O2—P1	119.25 (10)	C8—Ti1—P1	137.48 (6)
O1—P1—O2	100.73 (6)	C9—Ti1—P1	114.35 (5)
O1—P1—N1	106.29 (7)	C9^{i}—Ti1—P1	136.94 (6)
O2—P1—N1	95.62 (6)	P1^{i}—Ti1—P1	63.942 (18)
O1—P1—Ti1	120.60 (4)		

Symmetry code: (i) x, $-y+1/2$, z.