Electronic Supplementary Material (ESI) for Chemical Communications

Reductive deoxygenation of CO_2 by a bimetallic titanium bis(pentalene) complex.

Alexander F. R. Kilpatrick[a] and F. Geoffrey N. Cloke*[a]

[a] Department of Chemistry, School of Life Sciences, University of Sussex, Brighton, BN1 9QJ, UK.

ELECTRONIC SUPPORTING INFORMATION

General methods, instrumentation, and starting materials:

The manipulation of air-sensitive compounds and their spectroscopic measurements were undertaken using standard Schlenk techniques under Ar (BOC pureshield) passed through a column containing BASF R3-11(G) catalyst and activated molecular sieves (4 Å), or in a MBraun glovebox under N_2 or Ar (O_2 and H_2O <1 ppm). All glassware was dried at 160 °C overnight prior to use. Celite was pre-dried in a 200 °C oven and then flame dried under dynamic vacuum ($<2 \times 10^{-2}$ mbar) prior to use. Solvents were purified by pre-drying over sodium wire and then distilled over K (methylcyclohexane and hexane), CaH_2 (pyridine) or Na-K alloy (pentane) under a N_2 atmosphere. Dried solvents were collected, degassed and stored over argon in potassium-mirrored ampoules, except pyridine, which was stored in an ampoule containing activated 4 Å molecular sieves. Deuterated solvents were degassed by three freeze−thaw cycles, dried by refluxing over K (C_6D_6 and methylcyclohexane-d_{14}) or CaH_2 (pyridine-d_5) for 3 days, vacuum distilled into ampoules and stored under N_2. The gases used were of very high purity - CO (99.999%) and CO_2 (99.99%) - supplied by Union Carbide and used in combination with a high-purity regulator. N_2O (puriss >99.998%) was supplied by Fluka and added via Toepler line. Isotopically enriched gases ^{13}CO (99.7%) and $^{13}CO_2$ (99%) were supplied by Euriso-top and Cambridge Isotopes respectively, and added via Toepler line. $(Pn^{\dagger})_2Ti_2$ was prepared according to published procedures.[1]

NMR spectra were recorded on a Varian VNMRS 400 (^1H 399.5 MHz; $^{13}C\{^1H\}$ 100.25 MHz; $^{29}Si\{^1H\}$ 79.4 MHz) spectrometer. The spectra were referenced internally to the residual protic solvent (^1H) or the signals of the solvent (^{13}C). $^{29}Si\{^1H\}$ NMR spectra were referenced externally relative to $SiMe_4$. All spectra were recorded at 303 K unless otherwise stated. Mass spectra were recorded at the University of Sussex using a VG Autospec Fisons instrument (electron ionisation at 70 eV).

Elemental Analyses for **2**, **2(py)$_2$** and **3** were carried out at the Elemental Analysis Service, London Metropolitan University.

Syntheses:

*Reaction of **1** with 1 eq. $^{13}CO_2$ at room temperature:*

An ampoule charged with **1** (25 mg, 0.027 mmol) and methylcyclohexane-d_{14} (0.5 mL) was cooled to -78 °C and the headspace evacuated. The solution was allowed to warm to room temperature and $^{13}CO_2$ gas (0.027 mmol) admitted, resulting in a colour change from deep red to brown. The ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra were recorded, showing a mixture of **2** and **3**:

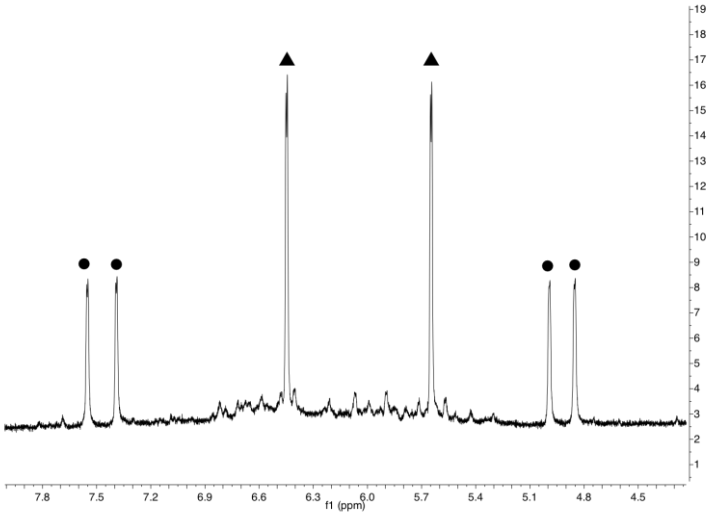

Figure S1. Aromatic region of ^{1}H NMR (methylcyclohexane-d_{14}) spectrum following reaction of **1** with 1 eq. $^{13}CO_2$ at 25 ˚C. ▲ labels Pn-*H* signals of **2**, ● labels Pn-*H* signals of **3**.

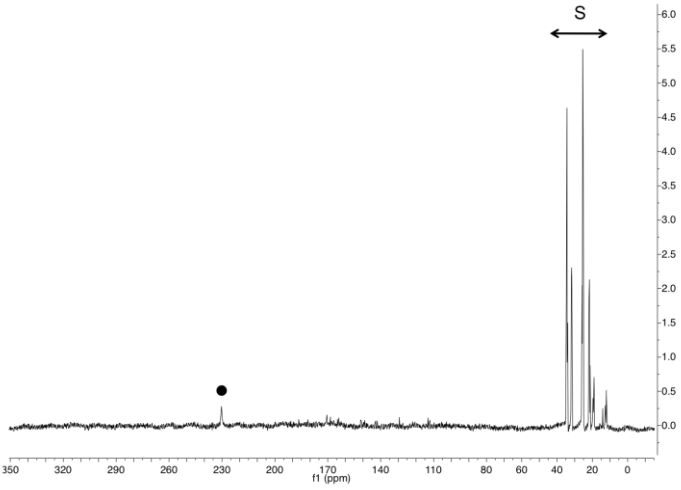

Figure S2. $^{13}C\{^{1}H\}$ NMR (methylcyclohexane-d_{14}) spectrum following reaction of **1** with 1 eq. $^{13}CO_2$ at 25 ˚C. ● labels the ^{13}CO signal of **3**. "S" denotes methylcyclohexane-d_{14} solvent signals.

Storage of this solution in a J. Young NMR tube overnight at room temperature afforded yellow crystals of **2** which were isolated by decantation, washed with pentane (0.5 mL) at -35 °C, and dried *in vacuo*. Total yield: 10 mg (77 % with respect to **1**, as per the stoichiometry in Scheme 1). Removal of the solvent from the mother liqour *in vacuo* resulted in a brown residue, which was extracted with TMS_2O (3 × 1 mL) at -35 °C, filtered, and stripped to dryness, affording **3** as a brown microcrystalline solid. Total yield: 12 mg (92 % with respect to **1**, as per the stoichiometry in Scheme 1).

Synthesis of $[(\eta^8\text{-}Pn^{\dagger})Ti(\mu\text{-}O)]_2$ ***(2):***

An ampoule charged with **1** (163.5 mg, 0.177 mmol) and toluene (3 mL) was cooled to -78 °C and the headspace evacuated. N_2O gas (0.37 mmol) was admitted and the reaction mixture was allowed to warm to room temperature, resulting in a colour change from deep red to yellow-brown. After stirring for 1 h a yellow precipitate formed which was taken back into solution by heating the mixture to 100 °C. The hot solution was filtered and the filtrate stripped to dryness, affording a yellow microcrystalline solid, which was treated with pentane (3 mL) and dried *in vacuo*. Total yield: 152 mg (90 % with respect to **1**).

^{1}H NMR (C_6D_6): δ_H 6.51 (4H, d, $^3J_{HH}$ = 3.3 Hz, Pn *H*), 5.76 (4H, d, $^3J_{HH}$ = 3.3 Hz, Pn *H*), 1.26 (12H, m, ^{i}Pr C*H*), 1.18 (36H, d, $^3J_{HH}$ = 7.1 Hz, ^{i}Pr CH_3), 1.12 (36H, d, $^3J_{HH}$ = 7.2 Hz, ^{i}Pr CH_3). ^{13}C{^{1}H} NMR (C_6D_6): δ_C 149.4 (Pn ring *C*), 129.9 (Pn ring *C*), 113.6 (Pn ring *C*), 112.6 (Pn ring *C*), 19.4 (^{i}Pr *C*H_3), 19.2 (^{i}Pr *C*H_3), 12.1 (^{i}Pr *C*H). ^{29}Si{^{1}H} NMR (C_6D_6): δ_{Si} -0.34.

EI-MS: *m/z* = 953-959 (principal peak 956, 100 %), $[M]^+$; 913 (25 %), $[M - {}^iPr_3]^+$.

Anal. found (calcd. for $C_{52}H_{92}O_2Si_4Ti_2$): C, 65.51 (65.24); H, 9.68 (9.69) %.

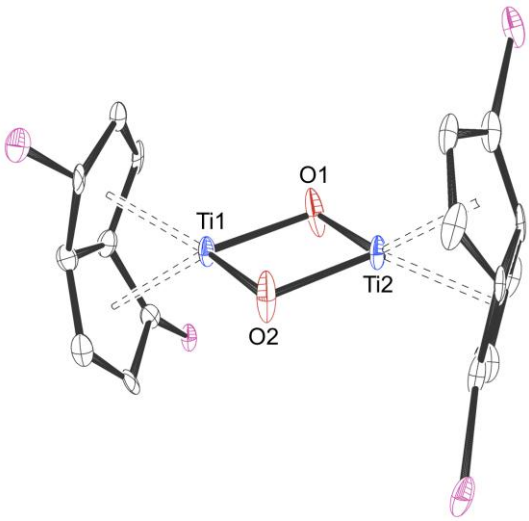

Figure S3. ORTEP view of unrefined (R_1 = 20.5%) molecular structure of **2**.

*Synthesis of [(η^5-Pn†)Ti(μ-O)(py)]$_2$ (**2(py)$_2$**):*

A frozen, degassed solution of **1** (52 mg, 0.056 mmol) in hexane (1.5 mL) was exposed to N_2O gas (0.11 mmol) and allowed warm to room temperature. After thawing and stirring for 1 h the reaction mixture appeared as a yellow-brown solution with yellow precipitate, characteristic of **2**. An excess of pyridine (0.4 mL) was added dropwise until the precipitate fully dissolved, giving a green solution, which was filtered and concentrated to ~1 mL. Storage of this solution at -35 °C afforded red crystals of **2(py)$_2$**, which were isolated by decantation. Total yield: 30 mg (48 % with respect to **1**). **2(py)$_2$** is prone to solvent loss and reforms **2** in the absence of excess pyridine, as confirmed by spectroscopic and analytical data.

^{1}H NMR (pyridine-d_5): δ_H 6.38 (2H, br d, $^3J_{HH}$ = 2.9 Hz, Pn *H*), 6.33 (2H, br d, $^3J_{HH}$ = 2.7 Hz, Pn *H*), 1.92-0.74 (72H, br m, ^{i}Pr CH_3). ^{13}C{^{1}H} NMR (pyridine-d_5): δ_C 140.7 (Pn ring *C*), 132.4 (Pn ring *C*), 111.8 (Pn ring *C*), 110.9 (Pn ring *C*), 20.05 (^{i}Pr *C*H$_3$), 13.05 (^{i}Pr *C*H). ^{29}Si{^{1}H} NMR (pyridine-d_5): resonances could not be identified.

EI-MS: *m/z* = 953-959 (principal peak 955, 100 %), [M - py]$^+$; 910-915 (principal peak 912, 25 %), [M - py - ^{i}Pr$_3$]$^+$.

Anal. found (calcd. for $C_{52}H_{92}O_2Si_4Ti_2$): C, 65.14 (65.24); H, 9.81 (9.69); N <0.1 (0.00) %.

*Synthesis of (μ:η^5,η^5-Pn†)$_2$[Ti(CO)]$_2$ (**3**):*

A freeze-thaw degassed solution of **1** (63 mg, 0.068 mmol) in pentane (5 mL), kept under static vacuum, was exposed to CO gas (1 atm) at -78 ºC before warming to room temperature. Shortly after gas addition the solution appeared orange-brown in colour. The reaction mixture was freeze-thaw degassed and exposed to an argon atmosphere, which resulted in a colour change to green-brown. Storage of this solution at -35 °C afforded brown crystals of **3** which were isolated by decantation and dried *in vacuo*. Total yield: 26 mg (39 % with respect to **1**).

^{1}H NMR (C_6D_6): δ_H 7.57 (2H, d, $^3J_{HH}$ = 3.1 Hz, Pn *H*), 7.49 (2H, d, $^3J_{HH}$ = 3.3 Hz, Pn *H*), 5.10 (2H, d, $^3J_{HH}$ = 3.3 Hz, Pn *H*), 4.70 (2H, d, $^3J_{HH}$ = 3.3 Hz, Pn *H*), 1.66 (6H, m, ^{i}Pr C*H*), 1.38 (6H, m, ^{i}Pr C*H*), 1.30 (18H, d, $^3J_{HH}$ = 7.4 Hz, ^{i}Pr CH_3), 1.17 (18H, d, $^3J_{HH}$ = 7.3 Hz, ^{i}Pr CH_3), 1.13 (18H, d, $^3J_{HH}$ = 7.4 Hz, ^{i}Pr CH_3), 0.91 (18H, d, $^3J_{HH}$ =

7.4 Hz, ^{i}Pr C*H*$_3$). ^{13}C{^{1}H} NMR (C_6D_6): δ_C 231.6 (CO), 122.8 (Pn ring *C*), 122.1 (Pn ring *C*), 121.9 (Pn ring *C*), 105.7 (Pn ring *C*), 103.0 (Pn ring *C*), 90.2 (Pn ring *C*), 85.0 (Pn ring *C*), 20.1 (^{i}Pr *C*H$_3$), 20.0 (^{i}Pr *C*H$_3$), 19.8 (^{i}Pr *C*H$_3$), 19.5 (^{i}Pr *C*H$_3$), 14.1 (^{i}Pr *C*H), 12.8 (^{i}Pr *C*H). ^{29}Si{^{1}H} NMR (C_6D_6): δ_{Si} 3.69, 2.85.

EI-MS: *m/z* = 915-926 (principal peak 923, 100 %), $[M - 2CO]^+$.

Anal. found (calcd. for $C_{54}H_{92}O_2Si_4Ti_2$): C, 65.99 (66.09); H, 9.49 (9.45) %.

IR ν(^{12}CO): (methylcyclohexane, 26 °C) 1991, 1910; (NaCl) 1987, 1910 cm^{-1}.

Alternatively, exposing a C_6D_6 solution of **1** to 2 eq. ^{13}CO via Toepler pump, yields the labeled product ^{13}C-**2**. NMR yield: quantitative with respect to **1**.

IR ν(^{13}CO): (methylcyclohexane, 26 °C) 1948, 1867; (NaCl) 1942, 1868 cm^{-1}.

X-Ray crystallography data:

X-Ray data collection, solution and refinement for ***2(py)$_2$****:*

Single crystal X-ray diffraction data for **2(py)$_2$** were collected at the University of Sussex on an Agilent Technologies Xcalibur Gemini Ultra diffractometer ($\lambda_{Cu\ K\alpha}$ = 1.54184 Å) equipped with a Eos CCD area detector. The data were collected at 173 K using an Oxford Cryosystems Cobra low temperature device. Data were processed using CrysAlisPro (version 1.171.36.32),[2] and unit cell parameters were refined against all data. Semi-empirical absorption corrections were carried out using the MULTI-SCAN program.[3] The structure was solved by Patterson methods (DIRDIF-2008[4]) and refined on F_o^2 by full-matrix least-squares refinements using SHELXL-2013.[5] All solutions and refinements were performed using the WinGX package and all software packages within.[6] All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were refined using a riding model. Atoms of the ^{i}Pr group C29, C30, C31 and ^{i}Pr CH$_3$ groups C45, C46 and C51, C52 were positionally disordered over two sites. The disorder was modelled adequately and refinement proceeded normally. Restrain instructions (DELU, SIMU) were applied to ^{i}Pr group C50>C52 to give the thermal parameters more chemically reasonable values. Each molecule of **2(py)$_2$** cocrystallized with two disordered pyridine solvate molecules. One of which was included in the model, with the N3 atom assigned to the largest Q-peak, the remaining Q-peaks assigned to C100>C104 and refined anisotropically. The more disordered molecule of pyridine could not be modelled properly; therefore, this disorder was treated by using the SQUEEZE[7] routine in PLATON.[8,9]

Table S.1. Crystal data and structure refinement for **2(py)$_2$.pyridine**

Identification code	**2(py)$_2$.pyridine**	
Empirical formula	C62 H102 N2 O2 Si4 Ti2. (C5 H5 N)	
Formula weight	1194.71	
Temperature	173(2) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 13.7134(6) Å	a= 85.689(3)°.
	b = 16.0497(6) Å	b= 86.517(3)°.
	c = 18.5403(6) Å	g = 66.630(4)°.
Volume	3733.1(3) Å^3	
Z	2	
Density (calculated)	1.063 Mg/m^3	
Absorption coefficient	2.727 mm^{-1}	
F(000)	1292	
Crystal size	0.400 x 0.400 x 0.200 mm^3	
Theta range for data collection	3.004 to 71.480°.	
Index ranges	-16<=h<=16, -13<=k<=19, -20<=l<=22	
Reflections collected	22701	
Independent reflections	13931 [R(int) = 0.0406]	
Completeness to theta = 67.684°	98.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.67895	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13931 / 72 / 769	
Goodness-of-fit on F^2	0.999	
Final R indices [I>2sigma(I)]	R1 = 0.0560, wR2 = 0.1561	
R indices (all data)	R1 = 0.0652, wR2 = 0.1622	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.611 and -0.436 e.Å^{-3}	

Table S.2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **2(py)$_2$.pyridine**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor. Ct(1) and Ct(2) are the η^5- centroids of the Pn(1) and Pn(2) rings respectively.

	x	y	z	U(eq)
C(1)	368(2)	238(2)	2380(1)	35(1)
C(2)	1295(2)	224(2)	1966(1)	36(1)
C(3)	2180(2)	-38(2)	2403(2)	36(1)
C(4)	1859(2)	-236(2)	3120(1)	34(1)
C(5)	740(2)	-55(2)	3111(1)	32(1)
C(6)	410(2)	-218(2)	3829(2)	36(1)
C(7)	1314(2)	-516(2)	4247(2)	38(1)
C(8)	2231(2)	-538(2)	3836(2)	36(1)
C(9)	-614(2)	4495(2)	2486(1)	33(1)
C(10)	111(2)	4052(2)	3051(1)	34(1)
C(11)	1172(2)	3861(2)	2812(1)	34(1)
C(12)	1153(2)	4212(2)	2076(1)	32(1)
C(13)	46(2)	4604(2)	1878(1)	32(1)
C(14)	19(2)	4941(2)	1144(2)	37(1)
C(15)	1069(2)	4746(2)	915(2)	41(1)
C(16)	1808(2)	4281(2)	1464(2)	37(1)
C(17)	-2008(3)	632(3)	2624(2)	58(1)
C(18)	-3005(3)	554(4)	2364(3)	89(2)
C(19)	-2267(3)	1591(3)	2861(3)	81(1)
C(20)	-492(3)	-1091(2)	1935(2)	67(1)
C(21)	538(4)	-1551(3)	1481(3)	93(2)
C(22)	-419(5)	-1607(3)	2672(3)	96(2)
C(23)	-978(3)	697(3)	1032(2)	58(1)
C(24)	-1666(4)	409(3)	563(2)	81(1)
C(25)	-1376(4)	1733(3)	993(2)	83(1)
C(26)	4000(3)	-2408(2)	4033(2)	61(1)
C(27)	3386(5)	-2790(3)	4584(3)	99(2)
C(28)	3863(4)	-2625(3)	3275(3)	85(1)
C(29A)	3917(12)	-829(12)	5015(7)	65(3)
C(30A)	3305(15)	-62(8)	5309(8)	84(4)
C(31A)	4847(19)	-1575(13)	5355(12)	89(6)
C(29B)	3629(12)	-1081(9)	5139(7)	54(3)
C(30B)	3004(10)	-403(13)	5490(6)	77(4)

C(31B)	4727(18)	-1678(18)	5489(14)	108(8)
C(32)	4531(3)	-817(2)	3434(2)	60(1)
C(33)	5722(3)	-1356(3)	3566(3)	88(2)
C(34)	4283(3)	185(3)	3341(3)	72(1)
C(35)	-2780(2)	5011(2)	1798(2)	44(1)
C(36)	-2649(3)	4042(2)	1656(2)	60(1)
C(37)	-3965(3)	5646(2)	1791(2)	61(1)
C(38)	-2515(2)	4645(2)	3509(2)	49(1)
C(39)	-2338(3)	3641(2)	3544(2)	70(1)
C(40)	-3666(3)	5209(3)	3757(2)	73(1)
C(41)	-2356(2)	6334(2)	2721(2)	46(1)
C(42)	-1798(3)	6467(3)	3366(2)	66(1)
C(43)	-2057(3)	6787(2)	2037(2)	58(1)
C(44A)	3477(4)	5106(4)	1263(3)	84(2)
C(45A)	2840(40)	5920(40)	710(40)	130(17)
C(46A)	2670(50)	5783(19)	1980(40)	139(18)
C(44B)	3477(4)	5106(4)	1263(3)	84(2)
C(45B)	3265(19)	5493(15)	462(8)	90(5)
C(46B)	2969(14)	5750(12)	1791(12)	91(4)
C(47)	3811(2)	3494(2)	2340(2)	54(1)
C(48)	3913(3)	2508(3)	2471(3)	73(1)
C(49)	4858(3)	3557(3)	2514(3)	79(1)
C(50A)	3962(4)	3153(4)	709(3)	93(2)
C(51A)	3570(40)	3090(40)	210(30)	108(13)
C(52A)	5030(20)	3560(40)	430(20)	98(10)
C(50B)	3962(4)	3153(4)	709(3)	93(2)
C(51B)	3395(12)	3324(10)	-12(6)	95(3)
C(52B)	5159(6)	2927(15)	619(7)	121(5)
C(53)	1619(3)	1890(2)	4108(2)	47(1)
C(54)	1630(3)	2176(3)	4787(2)	62(1)
C(55)	808(4)	2235(3)	5277(2)	66(1)
C(56)	5(3)	2010(2)	5071(2)	59(1)
C(57)	41(3)	1737(2)	4381(2)	46(1)
C(58)	1733(3)	2103(2)	803(2)	53(1)
C(59)	1930(4)	1864(3)	94(2)	72(1)
C(60)	1179(4)	2305(3)	-406(2)	71(1)
C(61)	242(4)	2970(2)	-192(2)	62(1)
C(62)	86(3)	3185(2)	525(2)	49(1)
N(1)	831(2)	1665(1)	3898(1)	35(1)

N(2)	820(2)	2762(2)	1023(1)	38(1)
O(1)	1689(1)	1962(1)	2455(1)	33(1)
O(2)	-266(1)	2374(1)	2462(1)	34(1)
Si(1)	-820(1)	174(1)	1992(1)	42(1)
Si(2)	3628(1)	-1147(1)	4106(1)	43(1)
Si(3)	-2087(1)	5089(1)	2623(1)	37(1)
Si(4)	3253(1)	4024(1)	1428(1)	48(1)
Ti(1)	848(1)	1338(1)	2779(1)	30(1)
Ti(2)	570(1)	3018(1)	2164(1)	30(1)
Ct(1)	1289	26	2596	29(1)
Ct(2)	373	4245	2461	29(1)
C(104)	1587(7)	4467(5)	4601(4)	115(2)
C(105)	2551(7)	3933(5)	4609(4)	118(2)
C(103)	1220(8)	5302(7)	4315(6)	155(3)
C(101)	3086(9)	5010(6)	4057(6)	151(3)
C(100)	3231(9)	4212(6)	4361(5)	142(3)
N(3)	2012(12)	5634(6)	3972(6)	209(4)

Table S.3. Bond lengths [Å] and angles [°] for **2(py)$_2$.pyridine**.

C(1)-C(2)	1.438(4)
C(1)-C(5)	1.455(4)
C(1)-Si(1)	1.862(3)
C(1)-Ti(1)	2.297(3)
C(2)-C(3)	1.404(4)
C(2)-Ti(1)	2.295(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.428(4)
C(3)-Ti(1)	2.362(2)
C(3)-H(3)	0.9500
C(4)-C(8)	1.429(4)
C(4)-C(5)	1.446(3)
C(4)-Ti(1)	2.407(2)
C(5)-C(6)	1.418(4)
C(5)-Ti(1)	2.334(2)
C(6)-C(7)	1.400(4)
C(6)-H(6)	0.9500
C(7)-C(8)	1.419(4)
C(7)-H(7)	0.9500
C(8)-Si(2)	1.853(3)
C(9)-C(10)	1.430(4)
C(9)-C(13)	1.447(4)
C(9)-Si(3)	1.870(2)
C(9)-Ti(2)	2.377(2)
C(10)-C(11)	1.413(4)
C(10)-Ti(2)	2.304(2)
C(10)-H(10)	0.9500
C(11)-C(12)	1.435(4)
C(11)-Ti(2)	2.283(2)
C(11)-H(11)	0.9500
C(12)-C(16)	1.429(4)
C(12)-C(13)	1.452(3)
C(12)-Ti(2)	2.343(2)
C(13)-C(14)	1.424(4)
C(13)-Ti(2)	2.380(2)
C(14)-C(15)	1.393(4)
C(14)-H(14)	0.9500

C(15)-C(16)	1.426(4)
C(15)-H(15)	0.9500
C(16)-Si(4)	1.855(3)
C(17)-C(19)	1.528(5)
C(17)-C(18)	1.531(5)
C(17)-Si(1)	1.875(4)
C(17)-H(17)	1.0000
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-C(22)	1.530(6)
C(20)-C(21)	1.540(7)
C(20)-Si(1)	1.906(4)
C(20)-H(20)	1.0000
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-C(25)	1.529(5)
C(23)-C(24)	1.539(5)
C(23)-Si(1)	1.897(3)
C(23)-H(23)	1.0000
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-C(28)	1.512(6)
C(26)-C(27)	1.529(6)
C(26)-Si(2)	1.895(3)
C(26)-H(26)	1.0000
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800

C(27)-H(27C)	0.9800
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29A)-C(30A)	1.320(17)
C(29A)-C(31A)	1.49(2)
C(29A)-Si(2)	1.904(11)
C(29A)-H(29A)	1.0000
C(30A)-H(30A)	0.9800
C(30A)-H(30B)	0.9800
C(30A)-H(30C)	0.9800
C(31A)-H(31A)	0.9800
C(31A)-H(31B)	0.9800
C(31A)-H(31C)	0.9800
C(29B)-C(30B)	1.281(17)
C(29B)-C(31B)	1.58(2)
C(29B)-Si(2)	1.926(11)
C(29B)-H(29B)	1.0000
C(30B)-H(30D)	0.9800
C(30B)-H(30E)	0.9800
C(30B)-H(30F)	0.9800
C(31B)-H(31D)	0.9800
C(31B)-H(31E)	0.9800
C(31B)-H(31F)	0.9800
C(32)-C(34)	1.505(5)
C(32)-C(33)	1.541(5)
C(32)-Si(2)	1.898(4)
C(32)-H(32)	1.0000
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-C(36)	1.533(4)
C(35)-C(37)	1.538(4)
C(35)-Si(3)	1.887(3)
C(35)-H(35)	1.0000
C(36)-H(36A)	0.9800

C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
C(38)-C(39)	1.528(5)
C(38)-C(40)	1.538(4)
C(38)-Si(3)	1.894(3)
C(38)-H(38)	1.0000
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(41)-C(42)	1.530(5)
C(41)-C(43)	1.531(5)
C(41)-Si(3)	1.904(3)
C(41)-H(41)	1.0000
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(44A)-C(46A)	1.80(7)
C(44A)-C(45A)	1.59(3)
C(44A)-Si(4)	1.880(4)
C(44A)-H(44A)	1.0000
C(45A)-H(45A)	0.9800
C(45A)-H(45B)	0.9800
C(45A)-H(45C)	0.9800
C(46A)-H(46A)	0.9800
C(46A)-H(46B)	0.9800
C(46A)-H(46C)	0.9800
C(45B)-H(45D)	0.9800
C(45B)-H(45E)	0.9800
C(45B)-H(45F)	0.9800
C(46B)-H(46D)	0.9800

C(46B)-H(46E)	0.9800
C(46B)-H(46F)	0.9800
C(47)-C(49)	1.534(4)
C(47)-C(48)	1.534(5)
C(47)-Si(4)	1.897(3)
C(47)-H(47)	1.0000
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(49)-H(49A)	0.9800
C(49)-H(49B)	0.9800
C(49)-H(49C)	0.9800
C(50A)-C(51A)	1.13(5)
C(50A)-C(52A)	1.85(4)
C(50A)-Si(4)	1.928(5)
C(50A)-H(50A)	1.0000
C(51A)-H(51A)	0.9800
C(51A)-H(51B)	0.9800
C(51A)-H(51C)	0.9800
C(52A)-H(52A)	0.9800
C(52A)-H(52B)	0.9800
C(52A)-H(52C)	0.9800
C(51B)-H(51D)	0.9800
C(51B)-H(51E)	0.9800
C(51B)-H(51F)	0.9800
C(52B)-H(52D)	0.9800
C(52B)-H(52E)	0.9800
C(52B)-H(52F)	0.9800
C(53)-N(1)	1.354(4)
C(53)-C(54)	1.376(5)
C(53)-H(53)	0.9500
C(54)-C(55)	1.381(6)
C(54)-H(54)	0.9500
C(55)-C(56)	1.369(6)
C(55)-H(55)	0.9500
C(56)-C(57)	1.375(5)
C(56)-H(56)	0.9500
C(57)-N(1)	1.337(4)
C(57)-H(57)	0.9500

C(58)-N(2)	1.344(4)
C(58)-C(59)	1.377(5)
C(58)-H(58)	0.9500
C(59)-C(60)	1.365(6)
C(59)-H(59)	0.9500
C(60)-C(61)	1.364(6)
C(60)-H(60)	0.9500
C(61)-C(62)	1.381(5)
C(61)-H(61)	0.9500
C(62)-N(2)	1.344(4)
C(62)-H(62)	0.9500
N(1)-Ti(1)	2.174(2)
N(2)-Ti(2)	2.165(2)
O(1)-Ti(2)	1.8495(17)
O(1)-Ti(1)	1.8531(17)
O(2)-Ti(1)	1.8416(17)
O(2)-Ti(2)	1.8615(17)
Ti(1)-Ct(1)	1.9962(9)
Ti(2)-Ct(2)	1.9936(9)
Ti(1)-Ti(2)	2.7376(6)
C(104)-C(105)	1.259(10)
C(104)-C(103)	1.311(11)
C(104)-H(104)	0.9500
C(105)-C(100)	1.238(10)
C(105)-H(105)	0.9500
C(103)-N(3)	1.481(13)
C(103)-H(103)	0.9500
C(101)-C(100)	1.304(11)
C(101)-N(3)	1.425(13)
C(101)-H(101)	0.9500
C(100)-H(100)	0.9500

C(2)-C(1)-C(5)	104.3(2)
C(2)-C(1)-Si(1)	124.8(2)
C(5)-C(1)-Si(1)	126.59(19)
C(2)-C(1)-Ti(1)	71.67(14)
C(5)-C(1)-Ti(1)	73.05(14)
Si(1)-C(1)-Ti(1)	137.60(13)
C(3)-C(2)-C(1)	111.4(2)

C(3)-C(2)-Ti(1)	75.06(15)
C(1)-C(2)-Ti(1)	71.83(14)
C(3)-C(2)-H(2)	124.3
C(1)-C(2)-H(2)	124.3
Ti(1)-C(2)-H(2)	120.4
C(2)-C(3)-C(4)	107.8(2)
C(2)-C(3)-Ti(1)	69.88(14)
C(4)-C(3)-Ti(1)	74.31(14)
C(2)-C(3)-H(3)	126.1
C(4)-C(3)-H(3)	126.1
Ti(1)-C(3)-H(3)	121.4
C(8)-C(4)-C(3)	143.4(2)
C(8)-C(4)-C(5)	109.4(2)
C(3)-C(4)-C(5)	107.2(2)
C(8)-C(4)-Ti(1)	122.48(18)
C(3)-C(4)-Ti(1)	70.84(14)
C(5)-C(4)-Ti(1)	69.50(13)
C(6)-C(5)-C(4)	107.3(2)
C(6)-C(5)-C(1)	143.4(2)
C(4)-C(5)-C(1)	109.3(2)
C(6)-C(5)-Ti(1)	119.37(18)
C(4)-C(5)-Ti(1)	75.03(14)
C(1)-C(5)-Ti(1)	70.32(13)
C(7)-C(6)-C(5)	106.6(2)
C(7)-C(6)-H(6)	126.7
C(5)-C(6)-H(6)	126.7
C(6)-C(7)-C(8)	112.4(2)
C(6)-C(7)-H(7)	123.8
C(8)-C(7)-H(7)	123.8
C(7)-C(8)-C(4)	104.2(2)
C(7)-C(8)-Si(2)	126.1(2)
C(4)-C(8)-Si(2)	127.3(2)
C(10)-C(9)-C(13)	104.7(2)
C(10)-C(9)-Si(3)	124.77(19)
C(13)-C(9)-Si(3)	128.17(18)
C(10)-C(9)-Ti(2)	69.44(14)
C(13)-C(9)-Ti(2)	72.43(13)
Si(3)-C(9)-Ti(2)	135.44(13)
C(11)-C(10)-C(9)	111.4(2)

C(11)-C(10)-Ti(2)	71.26(14)
C(9)-C(10)-Ti(2)	75.02(14)
C(11)-C(10)-H(10)	124.3
C(9)-C(10)-H(10)	124.3
Ti(2)-C(10)-H(10)	120.9
C(10)-C(11)-C(12)	107.6(2)
C(10)-C(11)-Ti(2)	72.86(14)
C(12)-C(11)-Ti(2)	74.22(14)
C(10)-C(11)-H(11)	126.2
C(12)-C(11)-H(11)	126.2
Ti(2)-C(11)-H(11)	118.7
C(16)-C(12)-C(11)	143.8(2)
C(16)-C(12)-C(13)	109.5(2)
C(11)-C(12)-C(13)	106.6(2)
C(16)-C(12)-Ti(2)	118.60(18)
C(11)-C(12)-Ti(2)	69.68(13)
C(13)-C(12)-Ti(2)	73.51(13)
C(14)-C(13)-C(9)	143.3(2)
C(14)-C(13)-C(12)	107.1(2)
C(9)-C(13)-C(12)	109.6(2)
C(14)-C(13)-Ti(2)	120.29(18)
C(9)-C(13)-Ti(2)	72.16(13)
C(12)-C(13)-Ti(2)	70.69(13)
C(15)-C(14)-C(13)	106.6(2)
C(15)-C(14)-H(14)	126.7
C(13)-C(14)-H(14)	126.7
C(14)-C(15)-C(16)	112.8(2)
C(14)-C(15)-H(15)	123.6
C(16)-C(15)-H(15)	123.6
C(15)-C(16)-C(12)	104.0(2)
C(15)-C(16)-Si(4)	126.8(2)
C(12)-C(16)-Si(4)	128.4(2)
C(19)-C(17)-C(18)	110.5(4)
C(19)-C(17)-Si(1)	115.2(3)
C(18)-C(17)-Si(1)	113.9(3)
C(19)-C(17)-H(17)	105.4
C(18)-C(17)-H(17)	105.4
Si(1)-C(17)-H(17)	105.4
C(17)-C(18)-H(18A)	109.5

C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(17)-C(19)-H(19A)	109.5
C(17)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(17)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(22)-C(20)-C(21)	109.9(4)
C(22)-C(20)-Si(1)	114.0(3)
C(21)-C(20)-Si(1)	111.1(3)
C(22)-C(20)-H(20)	107.1
C(21)-C(20)-H(20)	107.1
Si(1)-C(20)-H(20)	107.1
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(25)-C(23)-C(24)	109.5(3)
C(25)-C(23)-Si(1)	113.4(3)
C(24)-C(23)-Si(1)	114.5(3)
C(25)-C(23)-H(23)	106.3
C(24)-C(23)-H(23)	106.3
Si(1)-C(23)-H(23)	106.3
C(23)-C(24)-H(24A)	109.5
C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(23)-C(24)-H(24C)	109.5

H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(23)-C(25)-H(25A)	109.5
C(23)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(23)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(28)-C(26)-C(27)	110.3(4)
C(28)-C(26)-Si(2)	111.6(3)
C(27)-C(26)-Si(2)	112.6(3)
C(28)-C(26)-H(26)	107.4
C(27)-C(26)-H(26)	107.4
Si(2)-C(26)-H(26)	107.4
C(26)-C(27)-H(27A)	109.5
C(26)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(26)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(26)-C(28)-H(28A)	109.5
C(26)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(26)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(30A)-C(29A)-C(31A)	126.1(12)
C(30A)-C(29A)-Si(2)	122.2(8)
C(31A)-C(29A)-Si(2)	111.6(10)
C(30A)-C(29A)-H(29A)	91.3
C(31A)-C(29A)-H(29A)	91.3
Si(2)-C(29A)-H(29A)	91.3
C(29A)-C(30A)-H(30A)	109.5
C(29A)-C(30A)-H(30B)	109.5
H(30A)-C(30A)-H(30B)	109.5
C(29A)-C(30A)-H(30C)	109.5
H(30A)-C(30A)-H(30C)	109.5
H(30B)-C(30A)-H(30C)	109.5
C(29A)-C(31A)-H(31A)	109.5

C(29A)-C(31A)-H(31B)	109.5
H(31A)-C(31A)-H(31B)	109.5
C(29A)-C(31A)-H(31C)	109.5
H(31A)-C(31A)-H(31C)	109.5
H(31B)-C(31A)-H(31C)	109.5
C(30B)-C(29B)-C(31B)	116.6(13)
C(30B)-C(29B)-Si(2)	124.2(8)
C(31B)-C(29B)-Si(2)	114.3(12)
C(30B)-C(29B)-H(29B)	97.4
C(31B)-C(29B)-H(29B)	97.4
Si(2)-C(29B)-H(29B)	97.4
C(29B)-C(30B)-H(30D)	109.5
C(29B)-C(30B)-H(30E)	109.5
H(30D)-C(30B)-H(30E)	109.5
C(29B)-C(30B)-H(30F)	109.5
H(30D)-C(30B)-H(30F)	109.5
H(30E)-C(30B)-H(30F)	109.5
C(29B)-C(31B)-H(31D)	109.5
C(29B)-C(31B)-H(31E)	109.5
H(31D)-C(31B)-H(31E)	109.5
C(29B)-C(31B)-H(31F)	109.5
H(31D)-C(31B)-H(31F)	109.5
H(31E)-C(31B)-H(31F)	109.5
C(34)-C(32)-C(33)	110.5(3)
C(34)-C(32)-Si(2)	115.3(3)
C(33)-C(32)-Si(2)	113.5(3)
C(34)-C(32)-H(32)	105.6
C(33)-C(32)-H(32)	105.6
Si(2)-C(32)-H(32)	105.6
C(32)-C(33)-H(33A)	109.5
C(32)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(32)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(32)-C(34)-H(34A)	109.5
C(32)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(32)-C(34)-H(34C)	109.5

H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(36)-C(35)-C(37)	109.6(3)
C(36)-C(35)-Si(3)	114.1(2)
C(37)-C(35)-Si(3)	113.7(2)
C(36)-C(35)-H(35)	106.2
C(37)-C(35)-H(35)	106.2
Si(3)-C(35)-H(35)	106.2
C(35)-C(36)-H(36A)	109.5
C(35)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(35)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(35)-C(37)-H(37A)	109.5
C(35)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
C(35)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
C(39)-C(38)-C(40)	109.0(3)
C(39)-C(38)-Si(3)	115.3(2)
C(40)-C(38)-Si(3)	114.1(2)
C(39)-C(38)-H(38)	105.9
C(40)-C(38)-H(38)	105.9
Si(3)-C(38)-H(38)	105.9
C(38)-C(39)-H(39A)	109.5
C(38)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(38)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(38)-C(40)-H(40A)	109.5
C(38)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(38)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(42)-C(41)-C(43)	109.4(3)

C(42)-C(41)-Si(3)	112.2(2)
C(43)-C(41)-Si(3)	113.1(2)
C(42)-C(41)-H(41)	107.3
C(43)-C(41)-H(41)	107.3
Si(3)-C(41)-H(41)	107.3
C(41)-C(42)-H(42A)	109.5
C(41)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(41)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(41)-C(43)-H(43A)	109.5
C(41)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
C(41)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
C(46A)-C(44A)-C(45A)	88(3)
C(46A)-C(44A)-Si(4)	102.1(15)
C(45A)-C(44A)-Si(4)	125.2(18)
C(46A)-C(44A)-H(44A)	112.6
C(45A)-C(44A)-H(44A)	112.6
Si(4)-C(44A)-H(44A)	112.6
C(44A)-C(45A)-H(45A)	109.5
C(44A)-C(45A)-H(45B)	109.5
H(45A)-C(45A)-H(45B)	109.5
C(44A)-C(45A)-H(45C)	109.5
H(45A)-C(45A)-H(45C)	109.5
H(45B)-C(45A)-H(45C)	109.5
C(44A)-C(46A)-H(46A)	109.5
C(44A)-C(46A)-H(46B)	109.5
H(46A)-C(46A)-H(46B)	109.5
C(44A)-C(46A)-H(46C)	109.5
H(46A)-C(46A)-H(46C)	109.5
H(46B)-C(46A)-H(46C)	109.5
H(45D)-C(45B)-H(45E)	109.5
H(45D)-C(45B)-H(45F)	109.5
H(45E)-C(45B)-H(45F)	109.5
H(46D)-C(46B)-H(46E)	109.5

H(46D)-C(46B)-H(46F)	109.5
H(46E)-C(46B)-H(46F)	109.5
C(49)-C(47)-C(48)	109.7(3)
C(49)-C(47)-Si(4)	115.6(3)
C(48)-C(47)-Si(4)	113.2(3)
C(49)-C(47)-H(47)	105.9
C(48)-C(47)-H(47)	105.9
Si(4)-C(47)-H(47)	105.9
C(47)-C(48)-H(48A)	109.5
C(47)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(47)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
C(47)-C(49)-H(49A)	109.5
C(47)-C(49)-H(49B)	109.5
H(49A)-C(49)-H(49B)	109.5
C(47)-C(49)-H(49C)	109.5
H(49A)-C(49)-H(49C)	109.5
H(49B)-C(49)-H(49C)	109.5
C(51A)-C(50A)-C(52A)	109(3)
C(51A)-C(50A)-Si(4)	123(2)
C(52A)-C(50A)-Si(4)	97.7(14)
C(51A)-C(50A)-H(50A)	108.5
C(52A)-C(50A)-H(50A)	108.5
Si(4)-C(50A)-H(50A)	108.5
C(50A)-C(51A)-H(51A)	109.5
C(50A)-C(51A)-H(51B)	109.5
H(51A)-C(51A)-H(51B)	109.5
C(50A)-C(51A)-H(51C)	109.5
H(51A)-C(51A)-H(51C)	109.5
H(51B)-C(51A)-H(51C)	109.5
C(50A)-C(52A)-H(52A)	109.5
C(50A)-C(52A)-H(52B)	109.5
H(52A)-C(52A)-H(52B)	109.5
C(50A)-C(52A)-H(52C)	109.5
H(52A)-C(52A)-H(52C)	109.5
H(52B)-C(52A)-H(52C)	109.5
H(51D)-C(51B)-H(51E)	109.5

H(51D)-C(51B)-H(51F)	109.5
H(51E)-C(51B)-H(51F)	109.5
H(52D)-C(52B)-H(52E)	109.5
H(52D)-C(52B)-H(52F)	109.5
H(52E)-C(52B)-H(52F)	109.5
N(1)-C(53)-C(54)	122.5(3)
N(1)-C(53)-H(53)	118.7
C(54)-C(53)-H(53)	118.7
C(53)-C(54)-C(55)	119.0(3)
C(53)-C(54)-H(54)	120.5
C(55)-C(54)-H(54)	120.5
C(56)-C(55)-C(54)	119.0(3)
C(56)-C(55)-H(55)	120.5
C(54)-C(55)-H(55)	120.5
C(55)-C(56)-C(57)	118.8(3)
C(55)-C(56)-H(56)	120.6
C(57)-C(56)-H(56)	120.6
N(1)-C(57)-C(56)	123.5(3)
N(1)-C(57)-H(57)	118.2
C(56)-C(57)-H(57)	118.2
N(2)-C(58)-C(59)	122.2(3)
N(2)-C(58)-H(58)	118.9
C(59)-C(58)-H(58)	118.9
C(60)-C(59)-C(58)	119.5(4)
C(60)-C(59)-H(59)	120.2
C(58)-C(59)-H(59)	120.2
C(61)-C(60)-C(59)	119.2(3)
C(61)-C(60)-H(60)	120.4
C(59)-C(60)-H(60)	120.4
C(60)-C(61)-C(62)	119.0(3)
C(60)-C(61)-H(61)	120.5
C(62)-C(61)-H(61)	120.5
N(2)-C(62)-C(61)	122.6(3)
N(2)-C(62)-H(62)	118.7
C(61)-C(62)-H(62)	118.7
C(57)-N(1)-C(53)	117.1(3)
C(57)-N(1)-Ti(1)	124.28(19)
C(53)-N(1)-Ti(1)	118.39(19)
C(62)-N(2)-C(58)	117.5(3)

C(62)-N(2)-Ti(2)	123.8(2)
C(58)-N(2)-Ti(2)	118.6(2)
Ti(2)-O(1)-Ti(1)	95.35(8)
Ti(1)-O(2)-Ti(2)	95.33(8)
C(1)-Si(1)-C(17)	110.66(14)
C(1)-Si(1)-C(23)	109.24(14)
C(17)-Si(1)-C(23)	116.50(18)
C(1)-Si(1)-C(20)	105.46(14)
C(17)-Si(1)-C(20)	107.08(19)
C(23)-Si(1)-C(20)	107.26(17)
C(8)-Si(2)-C(26)	108.03(14)
C(8)-Si(2)-C(32)	109.16(14)
C(26)-Si(2)-C(32)	106.48(17)
C(8)-Si(2)-C(29A)	114.2(4)
C(26)-Si(2)-C(29A)	114.3(6)
C(32)-Si(2)-C(29A)	104.3(7)
C(8)-Si(2)-C(29B)	106.7(4)
C(26)-Si(2)-C(29B)	100.8(5)
C(32)-Si(2)-C(29B)	124.5(6)
C(9)-Si(3)-C(35)	110.08(13)
C(9)-Si(3)-C(38)	109.25(12)
C(35)-Si(3)-C(38)	115.56(15)
C(9)-Si(3)-C(41)	105.97(12)
C(35)-Si(3)-C(41)	108.18(14)
C(38)-Si(3)-C(41)	107.35(14)
C(16)-Si(4)-C(44A)	109.98(18)
C(16)-Si(4)-C(47)	108.41(13)
C(44A)-Si(4)-C(47)	107.61(19)
C(16)-Si(4)-C(50A)	109.89(18)
C(44A)-Si(4)-C(50A)	112.9(3)
C(47)-Si(4)-C(50A)	108.0(2)
O(2)-Ti(1)-O(1)	84.85(7)
O(2)-Ti(1)-N(1)	98.65(8)
O(1)-Ti(1)-N(1)	93.42(8)
O(2)-Ti(1)-C(2)	111.13(9)
O(1)-Ti(1)-C(2)	102.40(9)
N(1)-Ti(1)-C(2)	147.20(9)
O(2)-Ti(1)-C(1)	100.60(9)
O(1)-Ti(1)-C(1)	137.84(9)

N(1)-Ti(1)-C(1)	126.23(9)
C(2)-Ti(1)-C(1)	36.50(9)
O(2)-Ti(1)-C(5)	125.09(8)
O(1)-Ti(1)-C(5)	147.98(8)
N(1)-Ti(1)-C(5)	92.77(8)
C(2)-Ti(1)-C(5)	59.16(9)
C(1)-Ti(1)-C(5)	36.62(9)
O(2)-Ti(1)-C(3)	143.57(9)
O(1)-Ti(1)-C(3)	90.53(8)
N(1)-Ti(1)-C(3)	117.71(9)
C(2)-Ti(1)-C(3)	35.06(9)
C(1)-Ti(1)-C(3)	60.51(9)
C(5)-Ti(1)-C(3)	59.02(9)
O(2)-Ti(1)-C(4)	159.90(8)
O(1)-Ti(1)-C(4)	113.27(8)
N(1)-Ti(1)-C(4)	89.21(8)
C(2)-Ti(1)-C(4)	58.19(9)
C(1)-Ti(1)-C(4)	60.34(9)
C(5)-Ti(1)-C(4)	35.47(8)
C(3)-Ti(1)-C(4)	34.84(9)
O(2)-Ti(1)-Ti(2)	42.61(5)
O(1)-Ti(1)-Ti(2)	42.27(5)
N(1)-Ti(1)-Ti(2)	96.95(6)
C(2)-Ti(1)-Ti(2)	114.12(7)
C(1)-Ti(1)-Ti(2)	129.94(7)
C(5)-Ti(1)-Ti(2)	165.43(7)
C(3)-Ti(1)-Ti(2)	124.20(7)
C(4)-Ti(1)-Ti(2)	154.88(6)
O(1)-Ti(2)-O(2)	84.40(7)
O(1)-Ti(2)-N(2)	94.75(8)
O(2)-Ti(2)-N(2)	101.22(8)
O(1)-Ti(2)-C(11)	90.90(8)
O(2)-Ti(2)-C(11)	129.95(9)
N(2)-Ti(2)-C(11)	128.83(9)
O(1)-Ti(2)-C(10)	110.13(9)
O(2)-Ti(2)-C(10)	100.44(9)
N(2)-Ti(2)-C(10)	148.34(9)
C(11)-Ti(2)-C(10)	35.87(9)
O(1)-Ti(2)-C(12)	108.42(8)

O(2)-Ti(2)-C(12)	158.45(9)
N(2)-Ti(2)-C(12)	95.03(9)
C(11)-Ti(2)-C(12)	36.10(9)
C(10)-Ti(2)-C(12)	59.27(9)
O(1)-Ti(2)-C(9)	145.65(9)
O(2)-Ti(2)-C(9)	99.32(8)
N(2)-Ti(2)-C(9)	117.56(9)
C(11)-Ti(2)-C(9)	60.48(9)
C(10)-Ti(2)-C(9)	35.53(9)
C(12)-Ti(2)-C(9)	60.25(8)
O(1)-Ti(2)-C(13)	144.22(8)
O(2)-Ti(2)-C(13)	129.28(8)
N(2)-Ti(2)-C(13)	90.19(9)
C(11)-Ti(2)-C(13)	59.48(9)
C(10)-Ti(2)-C(13)	58.17(9)
C(12)-Ti(2)-C(13)	35.80(8)
C(9)-Ti(2)-C(13)	35.41(8)
O(1)-Ti(2)-Ti(1)	42.37(5)
O(2)-Ti(2)-Ti(1)	42.05(5)
N(2)-Ti(2)-Ti(1)	102.01(6)
C(11)-Ti(2)-Ti(1)	115.41(7)
C(10)-Ti(2)-Ti(1)	109.54(7)
C(12)-Ti(2)-Ti(1)	146.72(6)
C(9)-Ti(2)-Ti(1)	130.78(6)
C(13)-Ti(2)-Ti(1)	166.06(7)
C(105)-C(104)-C(103)	125.4(9)
C(105)-C(104)-H(104)	117.3
C(103)-C(104)-H(104)	117.3
C(100)-C(105)-C(104)	118.9(8)
C(100)-C(105)-H(105)	120.6
C(104)-C(105)-H(105)	120.6
C(104)-C(103)-N(3)	116.8(9)
C(104)-C(103)-H(103)	121.6
N(3)-C(103)-H(103)	121.6
C(100)-C(101)-N(3)	116.6(10)
C(100)-C(101)-H(101)	121.7
N(3)-C(101)-H(101)	121.7
C(105)-C(100)-C(101)	128.1(11)
C(105)-C(100)-H(100)	115.9

C(101)-C(100)-H(100)	115.9
C(101)-N(3)-C(103)	113.8(9)

Symmetry transformations used to generate equivalent atoms:

Table S.4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **2(py)$_2$.pyridine**. The anisotropic displacement factor exponent takes the form: $-2p^2[\, h^2a^{*2}U^{11} + ... + 2\, h\, k\, a^*\, b^*\, U^{12}\,]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	35(1)	29(1)	44(1)	-4(1)	-5(1)	-14(1)
C(2)	40(1)	34(1)	38(1)	-7(1)	-2(1)	-17(1)
C(3)	31(1)	31(1)	44(1)	-7(1)	2(1)	-10(1)
C(4)	31(1)	26(1)	43(1)	-1(1)	-1(1)	-10(1)
C(5)	33(1)	24(1)	43(1)	0(1)	-4(1)	-15(1)
C(6)	33(1)	32(1)	46(1)	-2(1)	1(1)	-16(1)
C(7)	41(1)	35(1)	41(1)	3(1)	-4(1)	-17(1)
C(8)	32(1)	30(1)	45(1)	1(1)	-7(1)	-12(1)
C(9)	27(1)	25(1)	44(1)	-2(1)	-3(1)	-9(1)
C(10)	36(1)	30(1)	36(1)	-3(1)	-2(1)	-12(1)
C(11)	32(1)	30(1)	40(1)	-2(1)	-9(1)	-12(1)
C(12)	26(1)	28(1)	45(1)	3(1)	-9(1)	-14(1)
C(13)	26(1)	25(1)	45(1)	4(1)	-8(1)	-12(1)
C(14)	35(1)	30(1)	46(1)	7(1)	-11(1)	-12(1)
C(15)	43(1)	38(1)	42(1)	8(1)	-6(1)	-19(1)
C(16)	30(1)	38(1)	47(1)	6(1)	-6(1)	-17(1)
C(17)	40(2)	67(2)	76(2)	-2(2)	-9(2)	-31(2)
C(18)	52(2)	127(4)	109(4)	-15(3)	-9(2)	-56(3)
C(19)	49(2)	69(3)	129(4)	-28(3)	20(2)	-26(2)
C(20)	80(3)	50(2)	85(3)	-3(2)	-31(2)	-37(2)
C(21)	96(3)	52(2)	127(4)	-32(3)	-23(3)	-18(2)
C(22)	145(5)	54(2)	110(4)	16(2)	-40(3)	-61(3)
C(23)	65(2)	64(2)	54(2)	4(2)	-21(2)	-35(2)
C(24)	111(4)	83(3)	68(2)	1(2)	-37(2)	-55(3)
C(25)	123(4)	70(3)	75(3)	21(2)	-47(3)	-57(3)
C(26)	48(2)	36(2)	92(3)	4(2)	-15(2)	-9(1)
C(27)	108(4)	66(3)	128(5)	21(3)	-10(3)	-44(3)
C(28)	90(3)	45(2)	113(4)	-23(2)	-14(3)	-14(2)
C(29A)	68(6)	69(7)	56(5)	-1(5)	-20(4)	-23(5)
C(30A)	128(10)	66(6)	65(6)	-2(5)	-33(6)	-42(6)
C(31A)	122(15)	67(7)	73(10)	4(6)	-58(10)	-26(7)
C(29B)	58(6)	53(5)	50(5)	7(4)	-22(4)	-18(4)
C(30B)	92(7)	91(10)	51(5)	-9(5)	-16(5)	-36(6)

C(31B)	59(7)	161(19)	60(7)	25(8)	-29(5)	1(9)
C(32)	36(2)	48(2)	93(3)	0(2)	-4(2)	-15(1)
C(33)	36(2)	72(3)	148(5)	5(3)	-3(2)	-13(2)
C(34)	50(2)	55(2)	114(3)	6(2)	-7(2)	-25(2)
C(35)	32(1)	42(2)	61(2)	2(1)	-10(1)	-16(1)
C(36)	51(2)	47(2)	85(2)	-8(2)	-18(2)	-20(2)
C(37)	36(2)	53(2)	91(3)	-2(2)	-19(2)	-13(1)
C(38)	39(2)	42(2)	60(2)	0(1)	6(1)	-10(1)
C(39)	69(2)	45(2)	85(3)	6(2)	28(2)	-16(2)
C(40)	51(2)	63(2)	88(3)	-1(2)	24(2)	-9(2)
C(41)	35(1)	32(1)	66(2)	-5(1)	-3(1)	-8(1)
C(42)	67(2)	53(2)	80(2)	-12(2)	-14(2)	-24(2)
C(43)	61(2)	31(1)	80(2)	3(1)	-5(2)	-15(1)
C(44A)	74(3)	88(3)	111(4)	37(3)	-26(3)	-59(3)
C(45A)	100(20)	130(30)	160(30)	80(30)	-30(20)	-70(20)
C(46A)	160(30)	43(10)	240(40)	-12(15)	-40(30)	-61(15)
C(44B)	74(3)	88(3)	111(4)	37(3)	-26(3)	-59(3)
C(45B)	96(9)	94(9)	101(7)	48(6)	-17(6)	-66(7)
C(46B)	83(7)	65(7)	138(10)	24(6)	-22(6)	-46(5)
C(47)	33(1)	57(2)	78(2)	13(2)	-19(1)	-26(1)
C(48)	45(2)	58(2)	113(3)	24(2)	-22(2)	-20(2)
C(49)	49(2)	88(3)	109(3)	21(3)	-31(2)	-39(2)
C(50A)	51(2)	137(5)	83(3)	-28(3)	7(2)	-25(3)
C(51A)	79(18)	150(30)	90(20)	-90(20)	28(13)	-39(19)
C(52A)	36(10)	140(30)	94(17)	-21(18)	28(10)	-15(12)
C(50B)	51(2)	137(5)	83(3)	-28(3)	7(2)	-25(3)
C(51B)	86(5)	133(7)	64(5)	-15(5)	7(4)	-41(5)
C(52B)	54(3)	176(14)	121(7)	-47(9)	27(4)	-27(5)
C(53)	51(2)	49(2)	47(2)	4(1)	-13(1)	-27(1)
C(54)	79(2)	68(2)	56(2)	-2(2)	-17(2)	-43(2)
C(55)	100(3)	60(2)	46(2)	-10(2)	-7(2)	-39(2)
C(56)	77(2)	55(2)	52(2)	-14(2)	13(2)	-33(2)
C(57)	50(2)	41(2)	51(2)	-7(1)	4(1)	-22(1)
C(58)	60(2)	49(2)	43(2)	-3(1)	2(1)	-14(2)
C(59)	89(3)	66(2)	53(2)	-14(2)	13(2)	-21(2)
C(60)	128(4)	58(2)	40(2)	-5(2)	-1(2)	-50(2)
C(61)	102(3)	49(2)	49(2)	6(1)	-25(2)	-42(2)
C(62)	62(2)	41(2)	48(2)	3(1)	-18(1)	-24(1)
N(1)	41(1)	26(1)	39(1)	1(1)	-6(1)	-14(1)

N(2)	45(1)	33(1)	38(1)	2(1)	-4(1)	-19(1)
O(1)	26(1)	30(1)	43(1)	5(1)	-5(1)	-11(1)
O(2)	26(1)	31(1)	45(1)	0(1)	-4(1)	-11(1)
Si(1)	42(1)	40(1)	52(1)	-1(1)	-14(1)	-23(1)
Si(2)	35(1)	34(1)	54(1)	0(1)	-12(1)	-7(1)
Si(3)	26(1)	29(1)	52(1)	0(1)	-3(1)	-8(1)
Si(4)	32(1)	61(1)	58(1)	4(1)	-3(1)	-24(1)
Ti(1)	29(1)	26(1)	36(1)	0(1)	-4(1)	-12(1)
Ti(2)	28(1)	27(1)	35(1)	2(1)	-4(1)	-11(1)
C(104)	143(6)	108(5)	110(5)	-8(4)	-10(4)	-66(5)
C(105)	129(6)	106(5)	116(5)	22(4)	0(4)	-48(5)
C(103)	142(7)	119(7)	196(10)	-27(6)	-41(7)	-35(6)
C(101)	177(9)	107(6)	190(9)	-46(6)	30(7)	-76(6)
C(100)	178(9)	118(6)	133(6)	-5(5)	-22(6)	-60(6)
N(3)	295(14)	106(6)	226(10)	-21(6)	-2(10)	-79(7)

Table S.5. Torsion angles [º] for **2(py)$_2$.pyridine**.

C(5)-C(1)-C(2)-C(3)	-1.2(3)
Si(1)-C(1)-C(2)-C(3)	-159.02(19)
Ti(1)-C(1)-C(2)-C(3)	65.16(19)
C(5)-C(1)-C(2)-Ti(1)	-66.33(16)
Si(1)-C(1)-C(2)-Ti(1)	135.8(2)
C(1)-C(2)-C(3)-C(4)	2.0(3)
Ti(1)-C(2)-C(3)-C(4)	65.16(18)
C(1)-C(2)-C(3)-Ti(1)	-63.18(18)
C(2)-C(3)-C(4)-C(8)	178.7(3)
Ti(1)-C(3)-C(4)-C(8)	-119.1(4)
C(2)-C(3)-C(4)-C(5)	-2.0(3)
Ti(1)-C(3)-C(4)-C(5)	60.31(17)
C(2)-C(3)-C(4)-Ti(1)	-62.26(18)
C(8)-C(4)-C(5)-C(6)	1.8(3)
C(3)-C(4)-C(5)-C(6)	-177.8(2)
Ti(1)-C(4)-C(5)-C(6)	-116.64(19)
C(8)-C(4)-C(5)-C(1)	-179.1(2)
C(3)-C(4)-C(5)-C(1)	1.3(3)
Ti(1)-C(4)-C(5)-C(1)	62.44(16)
C(8)-C(4)-C(5)-Ti(1)	118.43(19)
C(3)-C(4)-C(5)-Ti(1)	-61.17(17)
C(2)-C(1)-C(5)-C(6)	178.4(3)
Si(1)-C(1)-C(5)-C(6)	-24.2(5)
Ti(1)-C(1)-C(5)-C(6)	113.1(4)
C(2)-C(1)-C(5)-C(4)	-0.1(3)
Si(1)-C(1)-C(5)-C(4)	157.23(19)
Ti(1)-C(1)-C(5)-C(4)	-65.44(17)
C(2)-C(1)-C(5)-Ti(1)	65.35(16)
Si(1)-C(1)-C(5)-Ti(1)	-137.3(2)
C(4)-C(5)-C(6)-C(7)	-1.8(3)
C(1)-C(5)-C(6)-C(7)	179.6(3)
Ti(1)-C(5)-C(6)-C(7)	-84.1(2)
C(5)-C(6)-C(7)-C(8)	1.3(3)
C(6)-C(7)-C(8)-C(4)	-0.2(3)
C(6)-C(7)-C(8)-Si(2)	-163.6(2)
C(3)-C(4)-C(8)-C(7)	178.4(3)
C(5)-C(4)-C(8)-C(7)	-1.0(3)

Ti(1)-C(4)-C(8)-C(7)	76.6(2)
C(3)-C(4)-C(8)-Si(2)	-18.4(5)
C(5)-C(4)-C(8)-Si(2)	162.19(19)
Ti(1)-C(4)-C(8)-Si(2)	-120.3(2)
C(13)-C(9)-C(10)-C(11)	-1.9(3)
Si(3)-C(9)-C(10)-C(11)	-165.75(18)
Ti(2)-C(9)-C(10)-C(11)	62.49(18)
C(13)-C(9)-C(10)-Ti(2)	-64.41(16)
Si(3)-C(9)-C(10)-Ti(2)	131.77(19)
C(9)-C(10)-C(11)-C(12)	1.9(3)
Ti(2)-C(10)-C(11)-C(12)	66.65(17)
C(9)-C(10)-C(11)-Ti(2)	-64.79(18)
C(10)-C(11)-C(12)-C(16)	-176.7(3)
Ti(2)-C(11)-C(12)-C(16)	-111.0(4)
C(10)-C(11)-C(12)-C(13)	-1.0(3)
Ti(2)-C(11)-C(12)-C(13)	64.75(17)
C(10)-C(11)-C(12)-Ti(2)	-65.74(17)
C(10)-C(9)-C(13)-C(14)	179.4(3)
Si(3)-C(9)-C(13)-C(14)	-17.5(5)
Ti(2)-C(9)-C(13)-C(14)	117.1(4)
C(10)-C(9)-C(13)-C(12)	1.3(3)
Si(3)-C(9)-C(13)-C(12)	164.33(19)
Ti(2)-C(9)-C(13)-C(12)	-61.09(17)
C(10)-C(9)-C(13)-Ti(2)	62.35(16)
Si(3)-C(9)-C(13)-Ti(2)	-134.6(2)
C(16)-C(12)-C(13)-C(14)	-1.7(3)
C(11)-C(12)-C(13)-C(14)	-179.0(2)
Ti(2)-C(12)-C(13)-C(14)	-116.83(19)
C(16)-C(12)-C(13)-C(9)	177.1(2)
C(11)-C(12)-C(13)-C(9)	-0.2(3)
Ti(2)-C(12)-C(13)-C(9)	62.00(17)
C(16)-C(12)-C(13)-Ti(2)	115.1(2)
C(11)-C(12)-C(13)-Ti(2)	-62.20(16)
C(9)-C(13)-C(14)-C(15)	-177.5(3)
C(12)-C(13)-C(14)-C(15)	0.6(3)
Ti(2)-C(13)-C(14)-C(15)	-76.6(2)
C(13)-C(14)-C(15)-C(16)	0.7(3)
C(14)-C(15)-C(16)-C(12)	-1.7(3)
C(14)-C(15)-C(16)-Si(4)	-171.7(2)

C(11)-C(12)-C(16)-C(15)	177.7(3)
C(13)-C(12)-C(16)-C(15)	2.0(3)
Ti(2)-C(12)-C(16)-C(15)	83.4(2)
C(11)-C(12)-C(16)-Si(4)	-12.5(5)
C(13)-C(12)-C(16)-Si(4)	171.8(2)
Ti(2)-C(12)-C(16)-Si(4)	-106.8(2)
N(1)-C(53)-C(54)-C(55)	0.2(5)
C(53)-C(54)-C(55)-C(56)	-0.3(6)
C(54)-C(55)-C(56)-C(57)	-0.3(6)
C(55)-C(56)-C(57)-N(1)	1.1(5)
N(2)-C(58)-C(59)-C(60)	-0.1(6)
C(58)-C(59)-C(60)-C(61)	-0.6(6)
C(59)-C(60)-C(61)-C(62)	0.8(6)
C(60)-C(61)-C(62)-N(2)	-0.3(5)
C(56)-C(57)-N(1)-C(53)	-1.2(4)
C(56)-C(57)-N(1)-Ti(1)	-175.0(3)
C(54)-C(53)-N(1)-C(57)	0.5(4)
C(54)-C(53)-N(1)-Ti(1)	174.7(3)
C(61)-C(62)-N(2)-C(58)	-0.4(4)
C(61)-C(62)-N(2)-Ti(2)	-176.0(2)
C(59)-C(58)-N(2)-C(62)	0.6(5)
C(59)-C(58)-N(2)-Ti(2)	176.4(3)
C(2)-C(1)-Si(1)-C(17)	-159.2(2)
C(5)-C(1)-Si(1)-C(17)	47.9(3)
Ti(1)-C(1)-Si(1)-C(17)	-58.1(2)
C(2)-C(1)-Si(1)-C(23)	-29.6(3)
C(5)-C(1)-Si(1)-C(23)	177.4(2)
Ti(1)-C(1)-Si(1)-C(23)	71.5(2)
C(2)-C(1)-Si(1)-C(20)	85.4(3)
C(5)-C(1)-Si(1)-C(20)	-67.6(3)
Ti(1)-C(1)-Si(1)-C(20)	-173.5(2)
C(19)-C(17)-Si(1)-C(1)	54.0(4)
C(18)-C(17)-Si(1)-C(1)	-176.7(3)
C(19)-C(17)-Si(1)-C(23)	-71.5(4)
C(18)-C(17)-Si(1)-C(23)	57.7(4)
C(19)-C(17)-Si(1)-C(20)	168.5(3)
C(18)-C(17)-Si(1)-C(20)	-62.3(4)
C(25)-C(23)-Si(1)-C(1)	-73.2(3)
C(24)-C(23)-Si(1)-C(1)	160.1(3)

C(25)-C(23)-Si(1)-C(17)	53.1(3)
C(24)-C(23)-Si(1)-C(17)	-73.6(4)
C(25)-C(23)-Si(1)-C(20)	173.0(3)
C(24)-C(23)-Si(1)-C(20)	46.3(4)
C(7)-C(8)-Si(2)-C(26)	72.9(3)
C(4)-C(8)-Si(2)-C(26)	-86.8(3)
C(7)-C(8)-Si(2)-C(32)	-171.7(2)
C(4)-C(8)-Si(2)-C(32)	28.6(3)
C(7)-C(8)-Si(2)-C(29A)	-55.4(8)
C(4)-C(8)-Si(2)-C(29A)	144.9(8)
C(7)-C(8)-Si(2)-C(29B)	-34.8(6)
C(4)-C(8)-Si(2)-C(29B)	165.5(6)
C(28)-C(26)-Si(2)-C(8)	57.9(3)
C(27)-C(26)-Si(2)-C(8)	-66.8(4)
C(28)-C(26)-Si(2)-C(32)	-59.2(3)
C(27)-C(26)-Si(2)-C(32)	176.1(3)
C(28)-C(26)-Si(2)-C(29A)	-173.8(7)
C(27)-C(26)-Si(2)-C(29A)	61.5(7)
C(28)-C(26)-Si(2)-C(29B)	169.7(6)
C(27)-C(26)-Si(2)-C(29B)	45.0(6)
C(34)-C(32)-Si(2)-C(8)	56.8(3)
C(33)-C(32)-Si(2)-C(8)	-174.4(3)
C(34)-C(32)-Si(2)-C(26)	173.2(3)
C(33)-C(32)-Si(2)-C(26)	-58.0(4)
C(34)-C(32)-Si(2)-C(29A)	-65.6(5)
C(33)-C(32)-Si(2)-C(29A)	63.2(5)
C(34)-C(32)-Si(2)-C(29B)	-70.6(5)
C(33)-C(32)-Si(2)-C(29B)	58.2(5)
C(10)-C(9)-Si(3)-C(35)	-149.5(2)
C(13)-C(9)-Si(3)-C(35)	50.6(3)
Ti(2)-C(9)-Si(3)-C(35)	-54.0(2)
C(10)-C(9)-Si(3)-C(38)	-21.6(3)
C(13)-C(9)-Si(3)-C(38)	178.5(2)
Ti(2)-C(9)-Si(3)-C(38)	73.9(2)
C(10)-C(9)-Si(3)-C(41)	93.8(2)
C(13)-C(9)-Si(3)-C(41)	-66.2(3)
Ti(2)-C(9)-Si(3)-C(41)	-170.70(18)
C(36)-C(35)-Si(3)-C(9)	65.6(3)
C(37)-C(35)-Si(3)-C(9)	-167.6(2)

C(36)-C(35)-Si(3)-C(38)	-58.7(3)
C(37)-C(35)-Si(3)-C(38)	68.1(3)
C(36)-C(35)-Si(3)-C(41)	-179.0(2)
C(37)-C(35)-Si(3)-C(41)	-52.2(3)
C(39)-C(38)-Si(3)-C(9)	-64.2(3)
C(40)-C(38)-Si(3)-C(9)	168.5(3)
C(39)-C(38)-Si(3)-C(35)	60.5(3)
C(40)-C(38)-Si(3)-C(35)	-66.8(3)
C(39)-C(38)-Si(3)-C(41)	-178.7(3)
C(40)-C(38)-Si(3)-C(41)	54.0(3)
C(15)-C(16)-Si(4)-C(44A)	57.3(3)
C(12)-C(16)-Si(4)-C(44A)	-110.3(3)
C(15)-C(16)-Si(4)-C(47)	174.7(3)
C(12)-C(16)-Si(4)-C(47)	7.1(3)
C(15)-C(16)-Si(4)-C(50A)	-67.5(3)
C(12)-C(16)-Si(4)-C(50A)	124.9(3)
C(46A)-C(44A)-Si(4)-C(16)	54.0(14)
C(45A)-C(44A)-Si(4)-C(16)	-42(4)
C(46A)-C(44A)-Si(4)-C(47)	-63.9(14)
C(45A)-C(44A)-Si(4)-C(47)	-160(4)
C(46A)-C(44A)-Si(4)-C(50A)	177.1(14)
C(45A)-C(44A)-Si(4)-C(50A)	81(4)
C(49)-C(47)-Si(4)-C(16)	-158.3(3)
C(48)-C(47)-Si(4)-C(16)	74.1(3)
C(49)-C(47)-Si(4)-C(44A)	-39.4(4)
C(48)-C(47)-Si(4)-C(44A)	-167.0(3)
C(49)-C(47)-Si(4)-C(50A)	82.7(4)
C(48)-C(47)-Si(4)-C(50A)	-44.9(3)
Ti(2)-O(2)-Ti(1)-O(1)	-1.81(8)
Ti(2)-O(2)-Ti(1)-N(1)	90.88(9)
Ti(2)-O(2)-Ti(1)-C(2)	-103.13(10)
Ti(2)-O(2)-Ti(1)-C(1)	-139.57(9)
Ti(2)-O(2)-Ti(1)-C(5)	-169.53(9)
Ti(2)-O(2)-Ti(1)-C(3)	-85.71(15)
Ti(2)-O(2)-Ti(1)-C(4)	-157.1(2)
Ti(2)-O(1)-Ti(1)-O(2)	1.82(8)
Ti(2)-O(1)-Ti(1)-N(1)	-96.57(9)
Ti(2)-O(1)-Ti(1)-C(2)	112.35(9)
Ti(2)-O(1)-Ti(1)-C(1)	101.95(13)

Ti(2)-O(1)-Ti(1)-C(5)	162.67(13)
Ti(2)-O(1)-Ti(1)-C(3)	145.62(9)
Ti(2)-O(1)-Ti(1)-C(4)	172.82(8)
Ti(1)-O(1)-Ti(2)-O(2)	-1.80(8)
Ti(1)-O(1)-Ti(2)-N(2)	-102.64(9)
Ti(1)-O(1)-Ti(2)-C(11)	128.27(9)
Ti(1)-O(1)-Ti(2)-C(10)	97.29(9)
Ti(1)-O(1)-Ti(2)-C(12)	160.44(8)
Ti(1)-O(1)-Ti(2)-C(9)	96.52(14)
Ti(1)-O(1)-Ti(2)-C(13)	160.40(12)
Ti(1)-O(2)-Ti(2)-O(1)	1.81(8)
Ti(1)-O(2)-Ti(2)-N(2)	95.56(9)
Ti(1)-O(2)-Ti(2)-C(11)	-84.66(12)
Ti(1)-O(2)-Ti(2)-C(10)	-107.67(9)
Ti(1)-O(2)-Ti(2)-C(12)	-126.2(2)
Ti(1)-O(2)-Ti(2)-C(9)	-143.74(9)
Ti(1)-O(2)-Ti(2)-C(13)	-164.84(9)
C(103)-C(104)-C(105)-C(100)	3.5(14)
C(105)-C(104)-C(103)-N(3)	0.5(14)
C(104)-C(105)-C(100)-C(101)	-2.4(16)
N(3)-C(101)-C(100)-C(105)	-2.6(16)
C(100)-C(101)-N(3)-C(103)	6.0(14)
C(104)-C(103)-N(3)-C(101)	-5.1(14)

Symmetry transformations used to generate equivalent atoms:

*X-Ray data collection, solution and refinement for **3**:*

Single crystal X-ray diffraction data for **3** were collected at the UK National Crystallography Service,[10] University of Southampton on a Rigaku FR-E+ Ultra High Flux diffractometer ($\lambda_{Mo\ K\alpha}$ = 0.71073 Å) equipped with VariMax VHF optics and a Saturn 724+ CCD area detector. The data were collected at 100 K using an Oxford Cryosystems Cobra low temperature device. Data were processed using CrystalClear-SM Expert 3.1 b18,[11] and unit cell parameters were refined against all data. Semi-empirical absorption corrections were carried out using the MULTI-SCAN program.[3] The structure was solved by direct methods (SHELXS-97[12]) and refined on F_o^2 by full-matrix least-squares refinements using SHELXL-2013.[5] All solutions and refinements were performed using the WinGX package and all software packages

within.[6] All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were refined using a riding model. Atoms of the ^{i}Pr CH_3 group C10 was positionally disordered over two sites. The disorder was modelled adequately and refinement proceeded normally. Restrain instructions (DELU, SIMU) were applied to this ^{i}Pr group C9>C11 to give the thermal parameters more chemically reasonable values.

Table S.6. Crystal data and structure refinement for **3**.

Identification code	**3**	
Empirical formula	C54 H92 O2 Si4 Ti2	
Formula weight	981.43	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 12.894(3) Å	a= 90°.
	b = 22.342(5) Å	b= 92.18(3)°.
	c = 19.113(4) Å	g = 90°.
Volume	5502.1(19) Å^3	
Z	4	
Density (calculated)	1.185 Mg/m^3	
Absorption coefficient	0.415 mm^{-1}	
F(000)	2128	
Crystal size	0.120 x 0.120 x 0.030 mm^3	
Theta range for data collection	3.159 to 27.483°.	
Index ranges	-16<=h<=16, -29<=k<=28, -24<=l<=20	
Reflections collected	72543	
Independent reflections	12581 [R(int) = 0.0621]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9877 and 0.9519	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12581 / 38 / 557	
Goodness-of-fit on F^2	1.067	
Final R indices [I>2sigma(I)]	R1 = 0.0766, wR2 = 0.2107	
R indices (all data)	R1 = 0.1018, wR2 = 0.2279	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.997 and -0.793 e.Å^{-3}	

Table S.7. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor. Ct(1), Ct(2) and Ct(3), Ct(4) are the η^5:η^5- centroids of the Pn(1) and Pn(2) rings respectively.

	x	y	z	U(eq)
C(1)	4359(3)	1509(2)	7610(2)	20(1)
C(2)	3665(3)	1560(2)	7006(2)	21(1)
C(3)	3923(3)	2038(2)	6575(2)	20(1)
C(4)	4758(3)	2361(2)	6923(2)	20(1)
C(5)	5035(3)	2030(2)	7552(2)	20(1)
C(6)	5848(3)	2356(2)	7917(2)	23(1)
C(7)	5989(3)	2896(2)	7553(2)	26(1)
C(8)	5372(3)	2920(2)	6909(2)	24(1)
C(9A)	2619(5)	1353(3)	8596(3)	63(1)
C(10A)	1735(9)	1223(9)	8195(6)	63(1)
C(9B)	2619(5)	1353(3)	8596(3)	63(1)
C(10B)	1786(15)	944(15)	8243(11)	63(1)
C(11)	2581(5)	2037(3)	8625(4)	73(2)
C(12)	4061(4)	262(2)	8327(2)	42(1)
C(13)	3689(7)	-84(3)	8960(3)	79(2)
C(14)	3507(6)	35(2)	7666(3)	67(2)
C(15)	4878(4)	1362(2)	9186(2)	33(1)
C(16)	4419(5)	1296(2)	9910(2)	47(1)
C(17)	5970(4)	1080(2)	9196(2)	40(1)
C(18)	3805(5)	3922(2)	6979(3)	53(1)
C(19)	3999(4)	3992(2)	7741(3)	46(1)
C(20)	2902(5)	3487(3)	6836(4)	64(2)
C(21)	4653(6)	3682(2)	5557(3)	69(2)
C(22)	3944(6)	4134(3)	5283(3)	71(2)
C(23)	5665(6)	3836(3)	5071(3)	64(2)
C(24)	6107(5)	4216(3)	6771(3)	55(1)
C(25)	5848(6)	4863(3)	6545(3)	66(2)
C(26)	7266(5)	3992(3)	6570(3)	73(2)
C(27)	5184(3)	1339(2)	5420(2)	22(1)
C(28)	5576(3)	757(2)	5612(2)	23(1)
C(29)	6561(3)	787(2)	5941(2)	25(1)
C(53)	6067(4)	742(2)	7300(2)	47(1)
C(30)	6894(3)	1400(2)	5919(2)	21(1)

C(31)	6046(3)	1743(2)	5610(2)	20(1)
C(32)	6394(3)	2350(2)	5559(2)	21(1)
C(33)	7445(3)	2364(2)	5781(2)	23(1)
C(34)	7791(3)	1794(2)	6043(2)	23(1)
C(35)	2869(3)	1036(2)	5060(2)	27(1)
C(36)	2092(3)	879(2)	4461(2)	34(1)
C(37)	3063(3)	474(2)	5507(2)	32(1)
C(38)	3852(3)	2232(2)	4570(2)	27(1)
C(39)	2762(4)	2390(2)	4281(3)	41(1)
C(40)	4664(4)	2519(2)	4100(2)	36(1)
C(41)	4592(3)	988(2)	3950(2)	33(1)
C(54)	7484(4)	1672(2)	7505(2)	45(1)
C(42)	3974(4)	1089(2)	3255(2)	42(1)
C(43)	5754(4)	1087(3)	3835(2)	47(1)
C(44)	9634(4)	996(2)	6717(3)	49(1)
C(45)	8884(4)	457(3)	6725(3)	54(1)
C(46)	10697(4)	732(3)	6515(4)	62(2)
C(47)	9580(4)	1388(2)	5178(3)	43(1)
C(48)	9033(4)	822(3)	4901(4)	58(2)
C(49)	9387(6)	1890(3)	4650(3)	64(2)
C(50)	9913(3)	2343(2)	6308(2)	34(1)
C(51)	9709(5)	2580(4)	7035(4)	85(3)
C(52)	11090(4)	2318(3)	6211(4)	58(2)
O(1)	6486(3)	408(2)	7663(2)	59(1)
O(2)	8011(3)	1429(2)	7904(2)	60(1)
Si(1)	4002(1)	1099(1)	8429(1)	25(1)
Si(2)	5077(1)	3675(1)	6514(1)	32(1)
Si(3)	4104(1)	1410(1)	4740(1)	21(1)
Si(4)	9219(1)	1619(1)	6098(1)	26(1)
Ti(1)	5308(1)	1336(1)	6611(1)	18(1)
Ti(2)	6529(1)	2153(1)	6780(1)	20(1)
Ct(1)	4348	1899	7133	24(1)
Ct(2)	5401	2512	7371	24(1)
Ct(3)	6052	1205	5701	25(1)
Ct(4)	6914	1930	5782	24(1)

Table S.8. Bond lengths [Å] and angles [°] for **3**.

C(1)-C(2)	1.436(5)
C(1)-C(5)	1.461(5)
C(1)-Si(1)	1.886(4)
C(1)-Ti(1)	2.338(4)
C(2)-C(3)	1.397(5)
C(2)-Ti(1)	2.330(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.439(5)
C(3)-Ti(1)	2.375(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.445(5)
C(4)-C(8)	1.479(5)
C(4)-Ti(2)	2.356(4)
C(4)-Ti(1)	2.477(4)
C(5)-C(6)	1.435(5)
C(5)-Ti(1)	2.410(4)
C(5)-Ti(2)	2.485(4)
Ti(1)-Ct(1)	2.0510(15)
Ti(1)-Ct(3)	2.0399(15)
C(6)-C(7)	1.409(5)
C(6)-Ti(2)	2.417(4)
C(6)-H(6)	0.9500
C(7)-C(8)	1.441(5)
C(7)-Ti(2)	2.344(4)
C(7)-H(7)	0.9500
C(8)-Si(2)	1.881(4)
C(8)-Ti(2)	2.291(4)
Ti(2)-Ct(2)	2.0397(16)
Ti(2)-Ct(4)	2.0505(16)
C(9A)-C(10A)	1.380(13)
C(9A)-C(11)	1.530(9)
C(9A)-Si(1)	1.910(6)
C(9A)-H(9A)	1.0000
C(10A)-H(10A)	0.9800
C(10A)-H(10B)	0.9800
C(10A)-H(10C)	0.9800
C(10B)-H(10D)	0.9800

C(10B)-H(10E)	0.9800
C(10B)-H(10F)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-C(14)	1.515(7)
C(12)-C(13)	1.528(7)
C(12)-Si(1)	1.883(5)
C(12)-H(12)	1.0000
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-C(16)	1.532(6)
C(15)-C(17)	1.543(7)
C(15)-Si(1)	1.894(4)
C(15)-H(15)	1.0000
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-C(19)	1.475(8)
C(18)-C(20)	1.533(9)
C(18)-Si(2)	1.974(6)
C(18)-H(18)	1.0000
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-C(22)	1.448(8)
C(21)-C(23)	1.667(10)
C(21)-Si(2)	1.890(6)
C(21)-H(21)	1.0000

C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-C(25)	1.542(8)
C(24)-C(26)	1.634(9)
C(24)-Si(2)	1.847(6)
C(24)-H(24)	1.0000
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-C(28)	1.438(5)
C(27)-C(31)	1.467(5)
C(27)-Si(3)	1.876(4)
C(27)-Ti(1)	2.275(4)
C(28)-C(29)	1.397(5)
C(28)-Ti(1)	2.342(4)
C(28)-H(28)	0.9500
C(29)-C(30)	1.436(5)
C(29)-Ti(1)	2.431(4)
C(29)-H(29)	0.9500
C(53)-O(1)	1.141(6)
C(53)-Ti(1)	2.087(5)
C(30)-C(31)	1.443(5)
C(30)-C(34)	1.465(5)
C(30)-Ti(2)	2.413(4)
C(30)-Ti(1)	2.482(4)
C(31)-C(32)	1.433(5)
C(31)-Ti(1)	2.352(3)
C(31)-Ti(2)	2.476(4)
C(32)-C(33)	1.405(5)
C(32)-Ti(2)	2.376(3)
C(32)-H(32)	0.9500
C(33)-C(34)	1.432(5)

C(33)-Ti(2)	2.331(4)
C(33)-H(33)	0.9500
C(34)-Si(4)	1.881(4)
C(34)-Ti(2)	2.334(4)
C(35)-C(36)	1.532(5)
C(35)-C(37)	1.535(6)
C(35)-Si(3)	1.919(4)
C(35)-H(35)	1.0000
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
C(38)-C(39)	1.530(6)
C(38)-C(40)	1.544(6)
C(38)-Si(3)	1.891(4)
C(38)-H(38)	1.0000
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(41)-C(43)	1.538(7)
C(41)-C(42)	1.539(6)
C(41)-Si(3)	1.907(4)
C(41)-H(41)	1.0000
C(54)-O(2)	1.140(6)
C(54)-Ti(2)	2.111(5)
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(44)-C(45)	1.544(8)
C(44)-C(46)	1.553(8)
C(44)-Si(4)	1.891(5)

C(44)-H(44)	1.0000
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(46)-H(46A)	0.9800
C(46)-H(46B)	0.9800
C(46)-H(46C)	0.9800
C(47)-C(49)	1.523(8)
C(47)-C(48)	1.532(7)
C(47)-Si(4)	1.907(5)
C(47)-H(47)	1.0000
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(49)-H(49A)	0.9800
C(49)-H(49B)	0.9800
C(49)-H(49C)	0.9800
C(50)-C(51)	1.519(7)
C(50)-C(52)	1.538(6)
C(50)-Si(4)	1.886(5)
C(50)-H(50)	1.0000
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800
C(52)-H(52A)	0.9800
C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800
Ti(1)-Ti(2)	2.4250(10)

C(2)-C(1)-C(5)	103.4(3)
C(2)-C(1)-Si(1)	122.7(3)
C(5)-C(1)-Si(1)	127.9(3)
C(2)-C(1)-Ti(1)	71.75(19)
C(5)-C(1)-Ti(1)	74.8(2)
Si(1)-C(1)-Ti(1)	138.55(19)
C(3)-C(2)-C(1)	112.3(3)
C(3)-C(2)-Ti(1)	74.5(2)
C(1)-C(2)-Ti(1)	72.4(2)
C(3)-C(2)-H(2)	123.9

C(1)-C(2)-H(2)	123.9
Ti(1)-C(2)-H(2)	120.7
C(2)-C(3)-C(4)	107.6(3)
C(2)-C(3)-Ti(1)	71.0(2)
C(4)-C(3)-Ti(1)	76.7(2)
C(2)-C(3)-H(3)	126.2
C(4)-C(3)-H(3)	126.2
Ti(1)-C(3)-H(3)	118.1
C(3)-C(4)-C(5)	106.5(3)
C(3)-C(4)-C(8)	143.8(3)
C(5)-C(4)-C(8)	109.5(3)
C(3)-C(4)-Ti(2)	124.0(2)
C(5)-C(4)-Ti(2)	77.6(2)
C(8)-C(4)-Ti(2)	69.07(19)
C(3)-C(4)-Ti(1)	68.91(19)
C(5)-C(4)-Ti(1)	70.3(2)
C(8)-C(4)-Ti(1)	128.2(2)
Ti(2)-C(4)-Ti(1)	60.17(8)
C(6)-C(5)-C(4)	107.3(3)
C(6)-C(5)-C(1)	142.6(3)
C(4)-C(5)-C(1)	109.9(3)
C(6)-C(5)-Ti(1)	124.4(2)
C(4)-C(5)-Ti(1)	75.4(2)
C(1)-C(5)-Ti(1)	69.41(19)
C(6)-C(5)-Ti(2)	70.4(2)
C(4)-C(5)-Ti(2)	67.79(19)
C(1)-C(5)-Ti(2)	127.7(2)
Ti(1)-C(5)-Ti(2)	59.36(8)
C(7)-C(6)-C(5)	107.5(3)
C(7)-C(6)-Ti(2)	70.0(2)
C(5)-C(6)-Ti(2)	75.6(2)
C(7)-C(6)-H(6)	126.2
C(5)-C(6)-H(6)	126.2
Ti(2)-C(6)-H(6)	120.0
C(6)-C(7)-C(8)	112.1(3)
C(6)-C(7)-Ti(2)	75.7(2)
C(8)-C(7)-Ti(2)	69.9(2)
C(6)-C(7)-H(7)	123.9
C(8)-C(7)-H(7)	123.9

Ti(2)-C(7)-H(7)	122.0
C(7)-C(8)-C(4)	103.3(3)
C(7)-C(8)-Si(2)	118.2(3)
C(4)-C(8)-Si(2)	131.7(3)
C(7)-C(8)-Ti(2)	73.9(2)
C(4)-C(8)-Ti(2)	73.8(2)
Si(2)-C(8)-Ti(2)	138.6(2)
C(10A)-C(9A)-C(11)	101.8(10)
C(10A)-C(9A)-Si(1)	126.9(7)
C(11)-C(9A)-Si(1)	109.5(4)
C(10A)-C(9A)-H(9A)	105.7
C(11)-C(9A)-H(9A)	105.7
Si(1)-C(9A)-H(9A)	105.7
C(9A)-C(10A)-H(10A)	109.5
C(9A)-C(10A)-H(10B)	109.5
H(10A)-C(10A)-H(10B)	109.5
C(9A)-C(10A)-H(10C)	109.5
H(10A)-C(10A)-H(10C)	109.5
H(10B)-C(10A)-H(10C)	109.5
H(10D)-C(10B)-H(10E)	109.5
H(10D)-C(10B)-H(10F)	109.5
H(10E)-C(10B)-H(10F)	109.5
C(9A)-C(11)-H(11A)	109.5
C(9A)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(9A)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(14)-C(12)-C(13)	109.8(4)
C(14)-C(12)-Si(1)	113.5(4)
C(13)-C(12)-Si(1)	114.0(4)
C(14)-C(12)-H(12)	106.3
C(13)-C(12)-H(12)	106.3
Si(1)-C(12)-H(12)	106.3
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5

H(13B)-C(13)-H(13C)	109.5
C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(16)-C(15)-C(17)	109.4(4)
C(16)-C(15)-Si(1)	114.8(3)
C(17)-C(15)-Si(1)	113.6(3)
C(16)-C(15)-H(15)	106.1
C(17)-C(15)-H(15)	106.1
Si(1)-C(15)-H(15)	106.1
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(15)-C(17)-H(17A)	109.5
C(15)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(15)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(19)-C(18)-C(20)	110.0(5)
C(19)-C(18)-Si(2)	111.2(4)
C(20)-C(18)-Si(2)	112.4(4)
C(19)-C(18)-H(18)	107.7
C(20)-C(18)-H(18)	107.7
Si(2)-C(18)-H(18)	107.7
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(18)-C(20)-H(20A)	109.5
C(18)-C(20)-H(20B)	109.5

H(20A)-C(20)-H(20B)	109.5
C(18)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(22)-C(21)-C(23)	98.6(6)
C(22)-C(21)-Si(2)	120.7(4)
C(23)-C(21)-Si(2)	109.7(4)
C(22)-C(21)-H(21)	109.0
C(23)-C(21)-H(21)	109.0
Si(2)-C(21)-H(21)	109.0
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(21)-C(23)-H(23A)	109.5
C(21)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(21)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(25)-C(24)-C(26)	114.3(5)
C(25)-C(24)-Si(2)	113.1(4)
C(26)-C(24)-Si(2)	113.1(4)
C(25)-C(24)-H(24)	105.1
C(26)-C(24)-H(24)	105.1
Si(2)-C(24)-H(24)	105.1
C(24)-C(25)-H(25A)	109.5
C(24)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(24)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(24)-C(26)-H(26A)	109.5
C(24)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(24)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5

H(26B)-C(26)-H(26C)	109.5
C(28)-C(27)-C(31)	103.7(3)
C(28)-C(27)-Si(3)	119.9(3)
C(31)-C(27)-Si(3)	130.9(3)
C(28)-C(27)-Ti(1)	74.4(2)
C(31)-C(27)-Ti(1)	74.4(2)
Si(3)-C(27)-Ti(1)	135.72(19)
C(29)-C(28)-C(27)	112.1(3)
C(29)-C(28)-Ti(1)	76.5(2)
C(27)-C(28)-Ti(1)	69.3(2)
C(29)-C(28)-H(28)	124.0
C(27)-C(28)-H(28)	124.0
Ti(1)-C(28)-H(28)	121.7
C(28)-C(29)-C(30)	107.5(3)
C(28)-C(29)-Ti(1)	69.5(2)
C(30)-C(29)-Ti(1)	75.0(2)
C(28)-C(29)-H(29)	126.2
C(30)-C(29)-H(29)	126.2
Ti(1)-C(29)-H(29)	121.0
O(1)-C(53)-Ti(1)	178.2(5)
C(29)-C(30)-C(31)	107.2(3)
C(29)-C(30)-C(34)	143.4(3)
C(31)-C(30)-C(34)	109.2(3)
C(29)-C(30)-Ti(2)	125.3(2)
C(31)-C(30)-Ti(2)	75.2(2)
C(34)-C(30)-Ti(2)	69.1(2)
C(29)-C(30)-Ti(1)	71.1(2)
C(31)-C(30)-Ti(1)	67.79(19)
C(34)-C(30)-Ti(1)	127.6(2)
Ti(2)-C(30)-Ti(1)	59.38(8)
C(32)-C(31)-C(30)	107.2(3)
C(32)-C(31)-C(27)	143.3(3)
C(30)-C(31)-C(27)	109.3(3)
C(32)-C(31)-Ti(1)	123.9(2)
C(30)-C(31)-Ti(1)	77.6(2)
C(27)-C(31)-Ti(1)	68.66(19)
C(32)-C(31)-Ti(2)	69.0(2)
C(30)-C(31)-Ti(2)	70.5(2)
C(27)-C(31)-Ti(2)	127.8(2)

Ti(1)-C(31)-Ti(2)	60.23(8)
C(33)-C(32)-C(31)	107.5(3)
C(33)-C(32)-Ti(2)	70.9(2)
C(31)-C(32)-Ti(2)	76.7(2)
C(33)-C(32)-H(32)	126.3
C(31)-C(32)-H(32)	126.3
Ti(2)-C(32)-H(32)	118.1
C(32)-C(33)-C(34)	111.8(3)
C(32)-C(33)-Ti(2)	74.4(2)
C(34)-C(33)-Ti(2)	72.3(2)
C(32)-C(33)-H(33)	124.1
C(34)-C(33)-H(33)	124.1
Ti(2)-C(33)-H(33)	120.8
C(33)-C(34)-C(30)	104.1(3)
C(33)-C(34)-Si(4)	119.7(3)
C(30)-C(34)-Si(4)	130.4(3)
C(33)-C(34)-Ti(2)	72.0(2)
C(30)-C(34)-Ti(2)	75.0(2)
Si(4)-C(34)-Ti(2)	137.86(19)
C(36)-C(35)-C(37)	108.4(3)
C(36)-C(35)-Si(3)	112.9(3)
C(37)-C(35)-Si(3)	114.4(3)
C(36)-C(35)-H(35)	106.9
C(37)-C(35)-H(35)	106.9
Si(3)-C(35)-H(35)	106.9
C(35)-C(36)-H(36A)	109.5
C(35)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(35)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(35)-C(37)-H(37A)	109.5
C(35)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
C(35)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
C(39)-C(38)-C(40)	109.2(3)
C(39)-C(38)-Si(3)	115.7(3)

C(40)-C(38)-Si(3)	112.7(3)
C(39)-C(38)-H(38)	106.1
C(40)-C(38)-H(38)	106.1
Si(3)-C(38)-H(38)	106.1
C(38)-C(39)-H(39A)	109.5
C(38)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(38)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(38)-C(40)-H(40A)	109.5
C(38)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(38)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(43)-C(41)-C(42)	109.3(4)
C(43)-C(41)-Si(3)	113.2(3)
C(42)-C(41)-Si(3)	115.8(3)
C(43)-C(41)-H(41)	105.9
C(42)-C(41)-H(41)	105.9
Si(3)-C(41)-H(41)	105.9
O(2)-C(54)-Ti(2)	177.9(5)
C(41)-C(42)-H(42A)	109.5
C(41)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(41)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(41)-C(43)-H(43A)	109.5
C(41)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
C(41)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
C(45)-C(44)-C(46)	105.4(5)
C(45)-C(44)-Si(4)	114.7(3)
C(46)-C(44)-Si(4)	110.8(4)
C(45)-C(44)-H(44)	108.6

C(46)-C(44)-H(44)	108.6
Si(4)-C(44)-H(44)	108.6
C(44)-C(45)-H(45A)	109.5
C(44)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(44)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
C(44)-C(46)-H(46A)	109.5
C(44)-C(46)-H(46B)	109.5
H(46A)-C(46)-H(46B)	109.5
C(44)-C(46)-H(46C)	109.5
H(46A)-C(46)-H(46C)	109.5
H(46B)-C(46)-H(46C)	109.5
C(49)-C(47)-C(48)	108.5(5)
C(49)-C(47)-Si(4)	111.8(3)
C(48)-C(47)-Si(4)	114.6(4)
C(49)-C(47)-H(47)	107.2
C(48)-C(47)-H(47)	107.2
Si(4)-C(47)-H(47)	107.2
C(47)-C(48)-H(48A)	109.5
C(47)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(47)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
C(47)-C(49)-H(49A)	109.5
C(47)-C(49)-H(49B)	109.5
H(49A)-C(49)-H(49B)	109.5
C(47)-C(49)-H(49C)	109.5
H(49A)-C(49)-H(49C)	109.5
H(49B)-C(49)-H(49C)	109.5
C(51)-C(50)-C(52)	109.2(4)
C(51)-C(50)-Si(4)	113.4(4)
C(52)-C(50)-Si(4)	113.9(3)
C(51)-C(50)-H(50)	106.6
C(52)-C(50)-H(50)	106.6
Si(4)-C(50)-H(50)	106.6
C(50)-C(51)-H(51A)	109.5

C(50)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(50)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(50)-C(52)-H(52A)	109.5
C(50)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
C(50)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
C(12)-Si(1)-C(1)	112.59(19)
C(12)-Si(1)-C(15)	111.2(2)
C(1)-Si(1)-C(15)	109.05(17)
C(12)-Si(1)-C(9A)	110.7(3)
C(1)-Si(1)-C(9A)	104.7(2)
C(15)-Si(1)-C(9A)	108.3(3)
C(24)-Si(2)-C(8)	110.4(2)
C(24)-Si(2)-C(21)	115.5(3)
C(8)-Si(2)-C(21)	116.2(2)
C(24)-Si(2)-C(18)	107.5(3)
C(8)-Si(2)-C(18)	103.2(2)
C(21)-Si(2)-C(18)	102.6(3)
C(27)-Si(3)-C(38)	108.65(17)
C(27)-Si(3)-C(41)	104.39(18)
C(38)-Si(3)-C(41)	113.88(18)
C(27)-Si(3)-C(35)	110.18(17)
C(38)-Si(3)-C(35)	109.75(18)
C(41)-Si(3)-C(35)	109.84(19)
C(34)-Si(4)-C(50)	106.74(18)
C(34)-Si(4)-C(44)	116.2(2)
C(50)-Si(4)-C(44)	112.2(2)
C(34)-Si(4)-C(47)	106.2(2)
C(50)-Si(4)-C(47)	107.3(2)
C(44)-Si(4)-C(47)	107.7(3)
C(53)-Ti(1)-C(27)	130.30(16)
C(53)-Ti(1)-C(2)	109.98(16)
C(27)-Ti(1)-C(2)	107.09(13)
C(53)-Ti(1)-C(1)	80.62(15)

C(27)-Ti(1)-C(1)	142.85(13)
C(2)-Ti(1)-C(1)	35.84(12)
C(53)-Ti(1)-C(28)	94.75(17)
C(27)-Ti(1)-C(28)	36.26(13)
C(2)-Ti(1)-C(28)	123.18(13)
C(1)-Ti(1)-C(28)	148.71(13)
C(53)-Ti(1)-C(31)	124.38(16)
C(27)-Ti(1)-C(31)	36.91(13)
C(2)-Ti(1)-C(31)	125.60(13)
C(1)-Ti(1)-C(31)	147.22(13)
C(28)-Ti(1)-C(31)	58.25(13)
C(53)-Ti(1)-C(3)	140.49(15)
C(27)-Ti(1)-C(3)	86.87(13)
C(2)-Ti(1)-C(3)	34.52(12)
C(1)-Ti(1)-C(3)	59.87(12)
C(28)-Ti(1)-C(3)	118.41(13)
C(31)-Ti(1)-C(3)	92.80(12)
C(53)-Ti(1)-C(5)	90.88(17)
C(27)-Ti(1)-C(5)	137.57(13)
C(2)-Ti(1)-C(5)	57.31(12)
C(1)-Ti(1)-C(5)	35.79(12)
C(28)-Ti(1)-C(5)	173.50(13)
C(31)-Ti(1)-C(5)	115.71(13)
C(3)-Ti(1)-C(5)	57.74(12)
C(53)-Ti(1)-Ti(2)	96.19(18)
C(27)-Ti(1)-Ti(2)	98.74(10)
C(2)-Ti(1)-Ti(2)	112.88(10)
C(1)-Ti(1)-Ti(2)	97.11(9)
C(28)-Ti(1)-Ti(2)	114.17(10)
C(31)-Ti(1)-Ti(2)	62.41(9)
C(3)-Ti(1)-Ti(2)	89.44(9)
C(5)-Ti(1)-Ti(2)	61.86(9)
C(53)-Ti(1)-C(29)	72.94(15)
C(27)-Ti(1)-C(29)	59.86(13)
C(2)-Ti(1)-C(29)	155.47(13)
C(1)-Ti(1)-C(29)	153.13(13)
C(28)-Ti(1)-C(29)	33.97(13)
C(31)-Ti(1)-C(29)	57.92(12)
C(3)-Ti(1)-C(29)	146.30(12)

C(5)-Ti(1)-C(29)	146.69(13)
Ti(2)-Ti(1)-C(29)	90.50(10)
C(53)-Ti(1)-C(4)	124.53(17)
C(27)-Ti(1)-C(4)	103.22(12)
C(2)-Ti(1)-C(4)	56.75(12)
C(1)-Ti(1)-C(4)	59.14(12)
C(28)-Ti(1)-C(4)	139.45(12)
C(31)-Ti(1)-C(4)	88.12(12)
C(3)-Ti(1)-C(4)	34.41(12)
C(5)-Ti(1)-C(4)	34.36(11)
Ti(2)-Ti(1)-C(4)	57.43(9)
C(29)-Ti(1)-C(4)	142.66(13)
C(53)-Ti(1)-C(30)	89.83(16)
C(27)-Ti(1)-C(30)	59.66(12)
C(2)-Ti(1)-C(30)	159.76(13)
C(1)-Ti(1)-C(30)	153.23(13)
C(28)-Ti(1)-C(30)	56.46(13)
C(31)-Ti(1)-C(30)	34.60(11)
C(3)-Ti(1)-C(30)	125.49(12)
C(5)-Ti(1)-C(30)	120.45(12)
Ti(2)-Ti(1)-C(30)	58.89(9)
C(29)-Ti(1)-C(30)	33.98(12)
C(4)-Ti(1)-C(30)	108.91(12)
C(54)-Ti(2)-C(8)	132.54(17)
C(54)-Ti(2)-C(33)	109.81(17)
C(8)-Ti(2)-C(33)	106.82(14)
C(54)-Ti(2)-C(34)	79.53(16)
C(8)-Ti(2)-C(34)	142.50(13)
C(33)-Ti(2)-C(34)	35.75(13)
C(54)-Ti(2)-C(7)	97.28(17)
C(8)-Ti(2)-C(7)	36.21(14)
C(33)-Ti(2)-C(7)	123.04(14)
C(34)-Ti(2)-C(7)	148.61(14)
C(54)-Ti(2)-C(4)	124.59(17)
C(8)-Ti(2)-C(4)	37.09(13)
C(33)-Ti(2)-C(4)	125.36(13)
C(34)-Ti(2)-C(4)	146.99(13)
C(7)-Ti(2)-C(4)	58.35(13)
C(54)-Ti(2)-C(32)	139.27(16)

C(8)-Ti(2)-C(32)	86.75(13)
C(33)-Ti(2)-C(32)	34.72(12)
C(34)-Ti(2)-C(32)	59.82(12)
C(7)-Ti(2)-C(32)	118.41(13)
C(4)-Ti(2)-C(32)	92.43(13)
C(54)-Ti(2)-C(30)	88.19(16)
C(8)-Ti(2)-C(30)	137.68(13)
C(33)-Ti(2)-C(30)	57.55(13)
C(34)-Ti(2)-C(30)	35.92(13)
C(7)-Ti(2)-C(30)	173.52(13)
C(4)-Ti(2)-C(30)	115.58(13)
C(32)-Ti(2)-C(30)	57.81(12)
C(54)-Ti(2)-C(6)	74.25(16)
C(8)-Ti(2)-C(6)	60.22(13)
C(33)-Ti(2)-C(6)	155.73(14)
C(34)-Ti(2)-C(6)	153.15(13)
C(7)-Ti(2)-C(6)	34.38(13)
C(4)-Ti(2)-C(6)	58.11(12)
C(32)-Ti(2)-C(6)	146.44(13)
C(30)-Ti(2)-C(6)	146.18(13)
C(54)-Ti(2)-Ti(1)	93.66(16)
C(8)-Ti(2)-Ti(1)	98.93(10)
C(33)-Ti(2)-Ti(1)	112.88(10)
C(34)-Ti(2)-Ti(1)	97.16(10)
C(7)-Ti(2)-Ti(1)	114.23(10)
C(4)-Ti(2)-Ti(1)	62.40(9)
C(32)-Ti(2)-Ti(1)	89.13(10)
C(30)-Ti(2)-Ti(1)	61.73(9)
C(6)-Ti(2)-Ti(1)	90.26(9)
C(54)-Ti(2)-C(31)	121.63(16)
C(8)-Ti(2)-C(31)	103.39(13)
C(33)-Ti(2)-C(31)	56.77(13)
C(34)-Ti(2)-C(31)	58.97(12)
C(7)-Ti(2)-C(31)	139.56(13)
C(4)-Ti(2)-C(31)	88.08(12)
C(32)-Ti(2)-C(31)	34.28(12)
C(30)-Ti(2)-C(31)	34.30(11)
C(6)-Ti(2)-C(31)	142.58(12)
Ti(1)-Ti(2)-C(31)	57.36(8)

C(54)-Ti(2)-C(5)	89.99(17)
C(8)-Ti(2)-C(5)	59.81(13)
C(33)-Ti(2)-C(5)	159.52(13)
C(34)-Ti(2)-C(5)	153.32(13)
C(7)-Ti(2)-C(5)	56.61(12)
C(4)-Ti(2)-C(5)	34.60(12)
C(32)-Ti(2)-C(5)	125.06(12)
C(30)-Ti(2)-C(5)	120.21(12)
C(6)-Ti(2)-C(5)	33.99(12)
Ti(1)-Ti(2)-C(5)	58.78(8)
C(31)-Ti(2)-C(5)	108.75(12)
Ct(1)-Ti(1)-Ct(3)	144.62(8)
Ct(2)-Ti(2)-Ct(4)	144.43(8)

Symmetry transformations used to generate equivalent atoms:

Table S.9. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **3**. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	19(2)	18(2)	23(2)	0(1)	3(1)	0(1)
C(2)	16(2)	23(2)	23(2)	-4(1)	2(1)	0(1)
C(3)	17(2)	22(2)	21(2)	-2(1)	1(1)	4(1)
C(4)	19(2)	18(2)	24(2)	1(1)	3(1)	2(1)
C(5)	19(2)	20(2)	22(2)	0(1)	2(1)	0(1)
C(6)	22(2)	25(2)	23(2)	1(1)	2(1)	-3(1)
C(7)	30(2)	20(2)	27(2)	-4(1)	4(2)	-4(2)
C(8)	23(2)	19(2)	30(2)	0(1)	5(1)	3(1)
C(9A)	46(2)	83(4)	61(3)	10(3)	19(2)	1(3)
C(10A)	46(2)	83(4)	61(3)	10(3)	19(2)	1(3)
C(9B)	46(2)	83(4)	61(3)	10(3)	19(2)	1(3)
C(10B)	46(2)	83(4)	61(3)	10(3)	19(2)	1(3)
C(11)	60(4)	91(5)	69(4)	-17(4)	16(3)	40(4)
C(12)	60(3)	28(2)	38(2)	2(2)	0(2)	-11(2)
C(13)	149(7)	45(3)	42(3)	15(2)	-15(4)	-48(4)
C(14)	135(6)	30(3)	33(3)	-3(2)	-5(3)	-27(3)
C(15)	45(2)	27(2)	26(2)	0(2)	4(2)	-7(2)
C(16)	66(3)	51(3)	22(2)	-3(2)	5(2)	-6(3)
C(17)	42(3)	44(3)	32(2)	3(2)	-3(2)	-6(2)
C(18)	65(4)	35(3)	58(3)	7(2)	7(3)	8(2)
C(19)	55(3)	44(3)	41(3)	3(2)	12(2)	10(2)
C(20)	51(3)	57(4)	87(5)	5(3)	11(3)	6(3)
C(21)	97(5)	34(3)	73(4)	-19(3)	-49(4)	28(3)
C(22)	125(6)	46(3)	42(3)	18(2)	-21(3)	-5(4)
C(23)	92(5)	53(4)	49(3)	1(3)	14(3)	-4(3)
C(24)	69(4)	44(3)	53(3)	4(2)	2(3)	-9(3)
C(25)	93(5)	39(3)	65(4)	0(3)	-1(3)	-12(3)
C(26)	74(4)	91(5)	56(3)	-11(3)	22(3)	-55(4)
C(27)	23(2)	21(2)	22(2)	0(1)	3(1)	2(1)
C(28)	26(2)	20(2)	24(2)	-2(1)	5(1)	3(1)
C(29)	24(2)	24(2)	26(2)	4(1)	5(1)	8(2)
C(53)	57(3)	50(3)	35(2)	15(2)	14(2)	30(2)
C(30)	17(2)	23(2)	23(2)	1(1)	4(1)	6(1)

C(31)	18(2)	22(2)	19(2)	3(1)	3(1)	3(1)
C(32)	22(2)	21(2)	21(2)	5(1)	4(1)	4(1)
C(33)	20(2)	26(2)	24(2)	3(1)	7(1)	0(1)
C(34)	18(2)	28(2)	23(2)	3(1)	3(1)	2(1)
C(35)	23(2)	28(2)	31(2)	-7(2)	1(2)	-1(2)
C(36)	27(2)	35(2)	38(2)	-8(2)	-1(2)	-4(2)
C(37)	30(2)	29(2)	37(2)	-6(2)	11(2)	-7(2)
C(38)	31(2)	29(2)	22(2)	4(2)	-4(2)	1(2)
C(39)	39(2)	35(2)	49(3)	0(2)	-10(2)	8(2)
C(40)	39(2)	35(2)	33(2)	10(2)	-3(2)	-2(2)
C(41)	40(2)	33(2)	25(2)	-1(2)	4(2)	6(2)
C(54)	49(3)	52(3)	32(2)	1(2)	-3(2)	18(2)
C(42)	55(3)	46(3)	25(2)	-7(2)	1(2)	-2(2)
C(43)	45(3)	66(4)	31(2)	-1(2)	12(2)	17(2)
C(44)	30(2)	49(3)	66(3)	26(3)	-10(2)	-1(2)
C(45)	46(3)	59(4)	57(3)	12(3)	-3(2)	5(3)
C(46)	27(2)	44(3)	114(5)	19(3)	-14(3)	6(2)
C(47)	30(2)	41(3)	59(3)	-20(2)	17(2)	-2(2)
C(48)	40(3)	53(3)	82(4)	-27(3)	10(3)	-3(2)
C(49)	87(5)	74(4)	32(3)	-5(3)	23(3)	-10(4)
C(50)	21(2)	36(2)	45(2)	-8(2)	2(2)	-1(2)
C(51)	47(3)	134(7)	76(4)	-63(5)	10(3)	-28(4)
C(52)	26(2)	49(3)	98(5)	-24(3)	8(3)	-5(2)
O(1)	64(2)	66(3)	46(2)	15(2)	5(2)	23(2)
O(2)	63(3)	70(3)	45(2)	5(2)	-4(2)	19(2)
Si(1)	29(1)	26(1)	21(1)	1(1)	5(1)	-5(1)
Si(2)	52(1)	16(1)	27(1)	1(1)	4(1)	-1(1)
Si(3)	21(1)	22(1)	21(1)	-2(1)	0(1)	2(1)
Si(4)	16(1)	27(1)	37(1)	7(1)	3(1)	2(1)
Ti(1)	18(1)	18(1)	20(1)	2(1)	3(1)	3(1)
Ti(2)	17(1)	22(1)	22(1)	2(1)	2(1)	1(1)

Table S.10. Torsion angles [º] for **3**.

C(5)-C(1)-C(2)-C(3)	4.4(4)
Si(1)-C(1)-C(2)-C(3)	159.0(3)
Ti(1)-C(1)-C(2)-C(3)	-64.4(3)
C(5)-C(1)-C(2)-Ti(1)	68.7(2)
Si(1)-C(1)-C(2)-Ti(1)	-136.6(3)
C(1)-C(2)-C(3)-C(4)	-5.5(4)
Ti(1)-C(2)-C(3)-C(4)	-68.6(2)
C(1)-C(2)-C(3)-Ti(1)	63.1(3)
C(2)-C(3)-C(4)-C(5)	4.2(4)
Ti(1)-C(3)-C(4)-C(5)	-60.6(2)
C(2)-C(3)-C(4)-C(8)	-168.8(5)
Ti(1)-C(3)-C(4)-C(8)	126.5(5)
C(2)-C(3)-C(4)-Ti(2)	90.2(3)
Ti(1)-C(3)-C(4)-Ti(2)	25.4(2)
C(2)-C(3)-C(4)-Ti(1)	64.7(2)
C(3)-C(4)-C(5)-C(6)	-178.3(3)
C(8)-C(4)-C(5)-C(6)	-2.7(4)
Ti(2)-C(4)-C(5)-C(6)	59.6(3)
Ti(1)-C(4)-C(5)-C(6)	122.0(3)
C(3)-C(4)-C(5)-C(1)	-1.5(4)
C(8)-C(4)-C(5)-C(1)	174.1(3)
Ti(2)-C(4)-C(5)-C(1)	-123.7(3)
Ti(1)-C(4)-C(5)-C(1)	-61.2(2)
C(3)-C(4)-C(5)-Ti(1)	59.7(2)
C(8)-C(4)-C(5)-Ti(1)	-124.7(3)
Ti(2)-C(4)-C(5)-Ti(1)	-62.47(7)
C(3)-C(4)-C(5)-Ti(2)	122.1(3)
C(8)-C(4)-C(5)-Ti(2)	-62.3(2)
Ti(1)-C(4)-C(5)-Ti(2)	62.47(7)
C(2)-C(1)-C(5)-C(6)	173.3(5)
Si(1)-C(1)-C(5)-C(6)	20.4(7)
Ti(1)-C(1)-C(5)-C(6)	-120.2(5)
C(2)-C(1)-C(5)-C(4)	-1.6(4)
Si(1)-C(1)-C(5)-C(4)	-154.5(3)
Ti(1)-C(1)-C(5)-C(4)	64.9(3)
C(2)-C(1)-C(5)-Ti(1)	-66.5(2)
Si(1)-C(1)-C(5)-Ti(1)	140.6(3)

C(2)-C(1)-C(5)-Ti(2)	-78.4(3)
Si(1)-C(1)-C(5)-Ti(2)	128.7(3)
Ti(1)-C(1)-C(5)-Ti(2)	-11.9(2)
C(4)-C(5)-C(6)-C(7)	5.2(4)
C(1)-C(5)-C(6)-C(7)	-169.7(5)
Ti(1)-C(5)-C(6)-C(7)	89.0(4)
Ti(2)-C(5)-C(6)-C(7)	63.1(3)
C(4)-C(5)-C(6)-Ti(2)	-57.9(2)
C(1)-C(5)-C(6)-Ti(2)	127.1(5)
Ti(1)-C(5)-C(6)-Ti(2)	25.9(2)
C(5)-C(6)-C(7)-C(8)	-6.0(4)
Ti(2)-C(6)-C(7)-C(8)	60.9(3)
C(5)-C(6)-C(7)-Ti(2)	-66.9(3)
C(6)-C(7)-C(8)-C(4)	4.2(4)
Ti(2)-C(7)-C(8)-C(4)	68.5(2)
C(6)-C(7)-C(8)-Si(2)	158.7(3)
Ti(2)-C(7)-C(8)-Si(2)	-137.0(3)
C(6)-C(7)-C(8)-Ti(2)	-64.3(3)
C(3)-C(4)-C(8)-C(7)	172.0(5)
C(5)-C(4)-C(8)-C(7)	-0.8(4)
Ti(2)-C(4)-C(8)-C(7)	-68.6(2)
Ti(1)-C(4)-C(8)-C(7)	-80.6(4)
C(3)-C(4)-C(8)-Si(2)	22.6(7)
C(5)-C(4)-C(8)-Si(2)	-150.3(3)
Ti(2)-C(4)-C(8)-Si(2)	142.0(3)
Ti(1)-C(4)-C(8)-Si(2)	129.9(3)
C(3)-C(4)-C(8)-Ti(2)	-119.4(5)
C(5)-C(4)-C(8)-Ti(2)	67.8(3)
Ti(1)-C(4)-C(8)-Ti(2)	-12.0(2)
C(31)-C(27)-C(28)-C(29)	4.2(4)
Si(3)-C(27)-C(28)-C(29)	160.8(3)
Ti(1)-C(27)-C(28)-C(29)	-65.0(3)
C(31)-C(27)-C(28)-Ti(1)	69.2(2)
Si(3)-C(27)-C(28)-Ti(1)	-134.2(3)
C(27)-C(28)-C(29)-C(30)	-5.2(4)
Ti(1)-C(28)-C(29)-C(30)	-65.9(3)
C(27)-C(28)-C(29)-Ti(1)	60.7(3)
C(28)-C(29)-C(30)-C(31)	3.9(4)
Ti(1)-C(29)-C(30)-C(31)	-58.4(2)

C(28)-C(29)-C(30)-C(34)	-169.4(5)
Ti(1)-C(29)-C(30)-C(34)	128.2(5)
C(28)-C(29)-C(30)-Ti(2)	87.7(3)
Ti(1)-C(29)-C(30)-Ti(2)	25.4(2)
C(28)-C(29)-C(30)-Ti(1)	62.3(2)
C(29)-C(30)-C(31)-C(32)	-177.5(3)
C(34)-C(30)-C(31)-C(32)	-1.7(4)
Ti(2)-C(30)-C(31)-C(32)	59.5(2)
Ti(1)-C(30)-C(31)-C(32)	122.0(3)
C(29)-C(30)-C(31)-C(27)	-1.4(4)
C(34)-C(30)-C(31)-C(27)	174.4(3)
Ti(2)-C(30)-C(31)-C(27)	-124.4(3)
Ti(1)-C(30)-C(31)-C(27)	-61.9(2)
C(29)-C(30)-C(31)-Ti(1)	60.5(2)
C(34)-C(30)-C(31)-Ti(1)	-123.7(3)
Ti(2)-C(30)-C(31)-Ti(1)	-62.52(7)
C(29)-C(30)-C(31)-Ti(2)	123.0(3)
C(34)-C(30)-C(31)-Ti(2)	-61.2(2)
Ti(1)-C(30)-C(31)-Ti(2)	62.52(7)
C(28)-C(27)-C(31)-C(32)	172.2(5)
Si(3)-C(27)-C(31)-C(32)	19.3(7)
Ti(1)-C(27)-C(31)-C(32)	-118.6(5)
C(28)-C(27)-C(31)-C(30)	-1.6(4)
Si(3)-C(27)-C(31)-C(30)	-154.5(3)
Ti(1)-C(27)-C(31)-C(30)	67.6(2)
C(28)-C(27)-C(31)-Ti(1)	-69.2(2)
Si(3)-C(27)-C(31)-Ti(1)	137.9(3)
C(28)-C(27)-C(31)-Ti(2)	-81.4(3)
Si(3)-C(27)-C(31)-Ti(2)	125.7(3)
Ti(1)-C(27)-C(31)-Ti(2)	-12.2(2)
C(30)-C(31)-C(32)-C(33)	4.3(4)
C(27)-C(31)-C(32)-C(33)	-169.5(5)
Ti(1)-C(31)-C(32)-C(33)	90.7(3)
Ti(2)-C(31)-C(32)-C(33)	64.7(2)
C(30)-C(31)-C(32)-Ti(2)	-60.4(2)
C(27)-C(31)-C(32)-Ti(2)	125.8(5)
Ti(1)-C(31)-C(32)-Ti(2)	26.0(2)
C(31)-C(32)-C(33)-C(34)	-5.5(4)
Ti(2)-C(32)-C(33)-C(34)	63.1(3)

C(31)-C(32)-C(33)-Ti(2)	-68.6(2)
C(32)-C(33)-C(34)-C(30)	4.3(4)
Ti(2)-C(33)-C(34)-C(30)	68.7(2)
C(32)-C(33)-C(34)-Si(4)	160.2(3)
Ti(2)-C(33)-C(34)-Si(4)	-135.4(3)
C(32)-C(33)-C(34)-Ti(2)	-64.4(3)
C(29)-C(30)-C(34)-C(33)	171.8(5)
C(31)-C(30)-C(34)-C(33)	-1.5(4)
Ti(2)-C(30)-C(34)-C(33)	-66.6(2)
Ti(1)-C(30)-C(34)-C(33)	-77.8(3)
C(29)-C(30)-C(34)-Si(4)	19.6(7)
C(31)-C(30)-C(34)-Si(4)	-153.7(3)
Ti(2)-C(30)-C(34)-Si(4)	141.2(3)
Ti(1)-C(30)-C(34)-Si(4)	130.0(3)
C(29)-C(30)-C(34)-Ti(2)	-121.6(5)
C(31)-C(30)-C(34)-Ti(2)	65.1(2)
Ti(1)-C(30)-C(34)-Ti(2)	-11.2(2)
C(14)-C(12)-Si(1)-C(1)	-48.4(5)
C(13)-C(12)-Si(1)-C(1)	-175.1(4)
C(14)-C(12)-Si(1)-C(15)	-171.2(4)
C(13)-C(12)-Si(1)-C(15)	62.1(5)
C(14)-C(12)-Si(1)-C(9A)	68.4(5)
C(13)-C(12)-Si(1)-C(9A)	-58.3(5)
C(2)-C(1)-Si(1)-C(12)	76.1(4)
C(5)-C(1)-Si(1)-C(12)	-135.6(3)
Ti(1)-C(1)-Si(1)-C(12)	-23.4(4)
C(2)-C(1)-Si(1)-C(15)	-159.9(3)
C(5)-C(1)-Si(1)-C(15)	-11.7(4)
Ti(1)-C(1)-Si(1)-C(15)	100.5(3)
C(2)-C(1)-Si(1)-C(9A)	-44.2(4)
C(5)-C(1)-Si(1)-C(9A)	104.0(4)
Ti(1)-C(1)-Si(1)-C(9A)	-143.8(3)
C(16)-C(15)-Si(1)-C(12)	-80.7(4)
C(17)-C(15)-Si(1)-C(12)	46.3(4)
C(16)-C(15)-Si(1)-C(1)	154.5(3)
C(17)-C(15)-Si(1)-C(1)	-78.5(3)
C(16)-C(15)-Si(1)-C(9A)	41.1(4)
C(17)-C(15)-Si(1)-C(9A)	168.2(3)
C(25)-C(24)-Si(2)-C(8)	-172.6(4)

C(26)-C(24)-Si(2)-C(8)	55.4(5)
C(25)-C(24)-Si(2)-C(21)	53.1(5)
C(26)-C(24)-Si(2)-C(21)	-78.9(5)
C(25)-C(24)-Si(2)-C(18)	-60.8(5)
C(26)-C(24)-Si(2)-C(18)	167.3(4)
C(7)-C(8)-Si(2)-C(24)	27.3(4)
C(4)-C(8)-Si(2)-C(24)	173.1(4)
Ti(2)-C(8)-Si(2)-C(24)	-70.4(4)
C(7)-C(8)-Si(2)-C(21)	161.2(4)
C(4)-C(8)-Si(2)-C(21)	-52.9(5)
Ti(2)-C(8)-Si(2)-C(21)	63.6(4)
C(7)-C(8)-Si(2)-C(18)	-87.3(3)
C(4)-C(8)-Si(2)-C(18)	58.6(4)
Ti(2)-C(8)-Si(2)-C(18)	175.1(3)
C(22)-C(21)-Si(2)-C(24)	-79.4(7)
C(23)-C(21)-Si(2)-C(24)	34.1(4)
C(22)-C(21)-Si(2)-C(8)	149.0(6)
C(23)-C(21)-Si(2)-C(8)	-97.5(4)
C(22)-C(21)-Si(2)-C(18)	37.2(7)
C(23)-C(21)-Si(2)-C(18)	150.7(4)
C(28)-C(27)-Si(3)-C(38)	-175.9(3)
C(31)-C(27)-Si(3)-C(38)	-26.6(4)
Ti(1)-C(27)-Si(3)-C(38)	85.7(3)
C(28)-C(27)-Si(3)-C(41)	-54.1(3)
C(31)-C(27)-Si(3)-C(41)	95.3(4)
Ti(1)-C(27)-Si(3)-C(41)	-152.4(3)
C(28)-C(27)-Si(3)-C(35)	63.8(3)
C(31)-C(27)-Si(3)-C(35)	-146.8(3)
Ti(1)-C(27)-Si(3)-C(35)	-34.5(3)
C(39)-C(38)-Si(3)-C(27)	-155.6(3)
C(40)-C(38)-Si(3)-C(27)	77.6(3)
C(39)-C(38)-Si(3)-C(41)	88.5(4)
C(40)-C(38)-Si(3)-C(41)	-38.3(3)
C(39)-C(38)-Si(3)-C(35)	-35.1(4)
C(40)-C(38)-Si(3)-C(35)	-161.9(3)
C(33)-C(34)-Si(4)-C(50)	33.7(4)
C(30)-C(34)-Si(4)-C(50)	-177.7(3)
Ti(2)-C(34)-Si(4)-C(50)	-62.1(3)
C(33)-C(34)-Si(4)-C(44)	159.7(3)

C(30)-C(34)-Si(4)-C(44)	-51.7(4)
Ti(2)-C(34)-Si(4)-C(44)	63.9(4)
C(33)-C(34)-Si(4)-C(47)	-80.6(3)
C(30)-C(34)-Si(4)-C(47)	68.1(4)
Ti(2)-C(34)-Si(4)-C(47)	-176.3(3)
C(51)-C(50)-Si(4)-C(34)	67.3(5)
C(52)-C(50)-Si(4)-C(34)	-167.0(4)
C(51)-C(50)-Si(4)-C(44)	-61.1(5)
C(52)-C(50)-Si(4)-C(44)	64.7(5)
C(51)-C(50)-Si(4)-C(47)	-179.2(4)
C(52)-C(50)-Si(4)-C(47)	-53.5(5)
C(45)-C(44)-Si(4)-C(34)	39.1(5)
C(46)-C(44)-Si(4)-C(34)	158.3(4)
C(45)-C(44)-Si(4)-C(50)	162.3(4)
C(46)-C(44)-Si(4)-C(50)	-78.5(5)
C(45)-C(44)-Si(4)-C(47)	-79.8(5)
C(46)-C(44)-Si(4)-C(47)	39.4(5)

Symmetry transformations used to generate equivalent atoms:

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