Bis(pentalene)di-titanium: a bent double-sandwich complex with a very short Ti–Ti bond.

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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 predried in a 200 °C oven and then flame-dried under dynamic vacuum (<2 × 10^{-2} mbar) prior to use. Solvents were purified by pre-drying over sodium wire and then distilled over K (toluene, hexane and THF), or Na-K alloy (pentane) under a N_2 atmosphere. Dried solvents were collected, degassed and stored over argon in potassium-mirrored ampoules, except THF, which was stored in ampoules containing activated 4 Å molecular sieves. Deuterated benzene and toluene were degassed by three freeze−thaw cycles, dried by refluxing over K for 3 days, vacuum distilled into ampoules and stored under N_2. The starting materials $TiCl_3(THF)_3$ and K_2Pn[†] were prepared according to published procedures.[1,2]

NMR spectra were recorded on a Varian VNMRS 400 (^{1}H 399.5 MHz; ^{13}C{^{1}H} 100.25 MHz; ^{29}Si{^{1}H} 79.4 MHz) spectrometer. The spectra were referenced internally to the residual protic solvent (^{1}H) or the signals of the solvent (^{13}C). ^{29}Si{^{1}H} 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 **1** were carried out at the Mikroanalytisches Labor Pascher, Remagen and for **2** at the Elemental Analysis Service, London Metropolitan University.

Magnetism data of crystalline powdered samples (20-30 mg) were recorded at the University of Erlangen with a SQUID magnetometer (Quantum Design) at 10 kOe. Values of the magnetic susceptibility were corrected for the underlying diamagnetic increment (χ_{dia} = -7.33 × 10^{-4} cm^3 mol^{-1} for **1**) using Pascal's constants,[3] and the effect of the blank sample holders (gelatin capsule/straw).

EPR spectra were obtained at the EPSRC National UK EPR Facility and Service, the University of Manchester. X- and Q-band continuous wave EPR spectra measurements were performed using a Bruker E580 ELEXSYS spectrometer and simulated with the XSophe (Bruker Biospin GmbH) suite.

Single crystal X-ray diffraction data for **2** were collected at the UK National Crystallography Service,[4] 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 cryostream device. Data were processed using CrystalClear-SM Expert 3.1 b18,[5] and unit cell parameters were refined against all data. An empirical absorption correction was carried out using the MULTI-SCAN program. The structures were solved by direct methods using SHELXL-97 and refined on F_o^2 by full-matrix least-squares refinements using SHELXL-97.[6] All solutions and refinements were performed using the WinGX package and all software packages within.[7] All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were refined using a riding model.

Theoretical calculations were carried out using the Amsterdam Density Functional package (version ADF2010.02).[8-11] The Slater-type orbital (STO) basis sets were of triple-ζ quality augmented with a one polarization function (ADF basis TZP). Core electrons were frozen (C 1s; Ti 2p) in our model of the electronic configuration for each atom. The local density approximation (LDA) by Vosko, Wilk and Nusair (VWN)[12] was used together with the exchange correlation corrections of Becke and Perdew (BP86).[13,14] Tight optimization conditions were used. Frequency calculations were used to confirm minima.

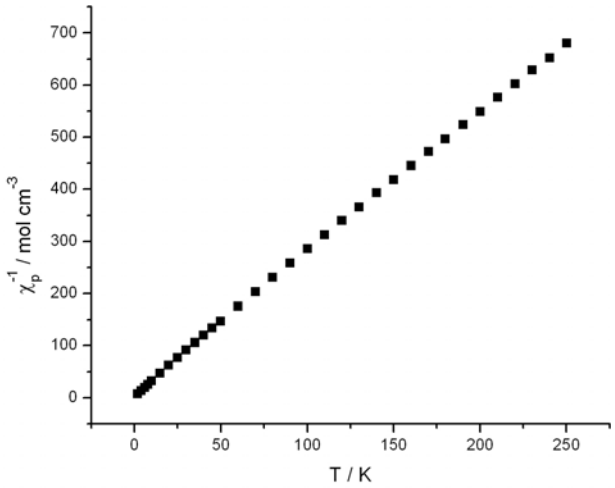

Figure S.1. Temperature dependence of the reciprocal magnetic susceptibility of **1**, determined by SQUID magnetometry.

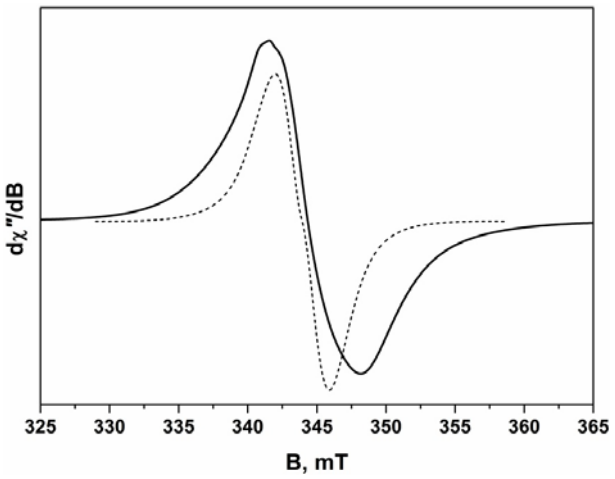

Figure S.2. X-band EPR spectra of polycrystalline **1** at 293 K (solid line) and 10 K (dashed line).

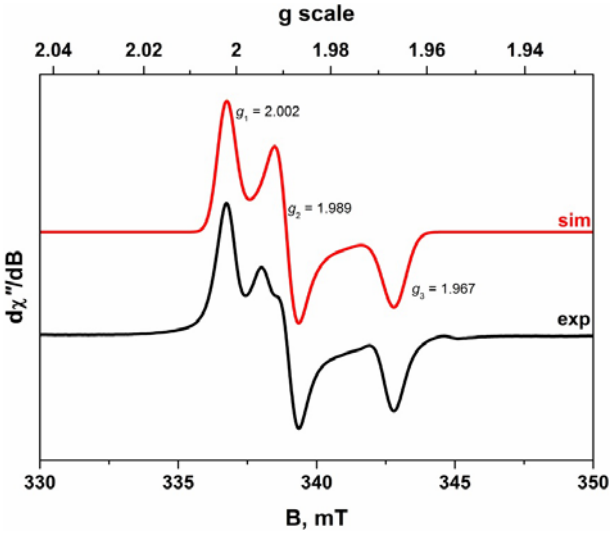

Figure S.3. X-band EPR spectrum of **1** in toluene solution at 150 K (black) and corresponding simulation (red).

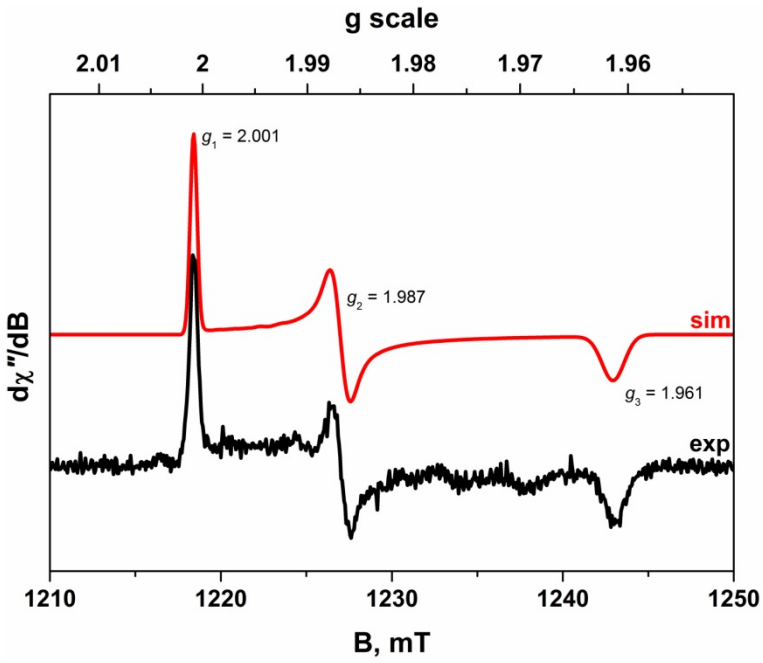

Figure S.3. Q-band EPR spectrum of **1** in toluene solution at 150 K (black) and corresponding simulation (red).

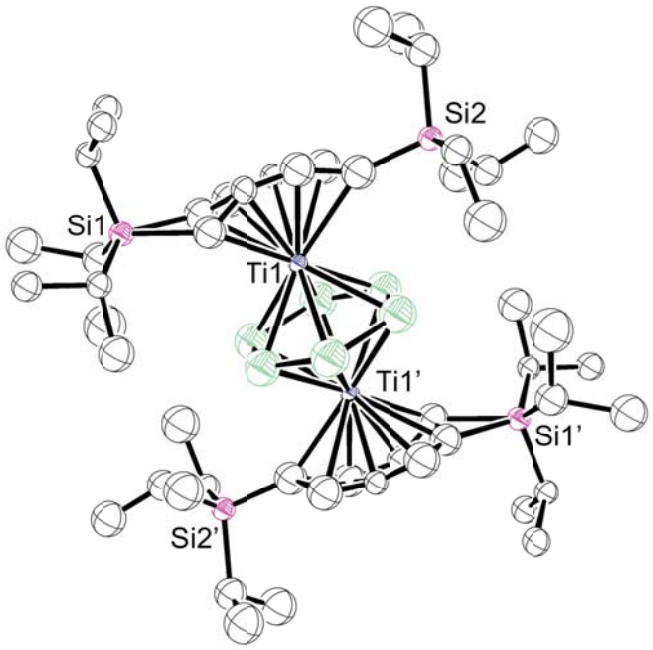

Figure S.4. ORTEP view of unrefined (R_1 = 25.4%) molecular structure of **1**. Cl atoms shown in green.

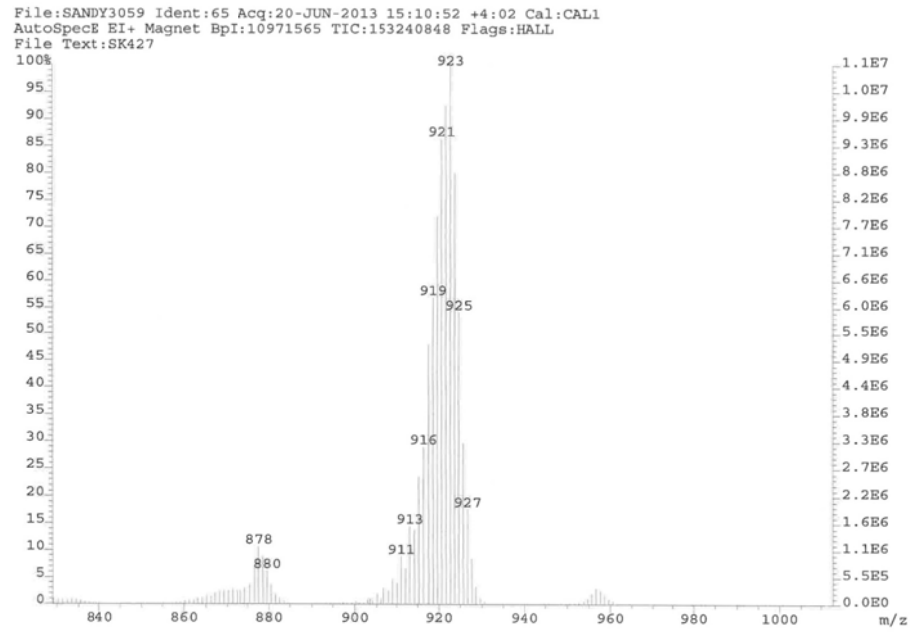

Figure S.5. Mass spectrum (EI) of **2**.

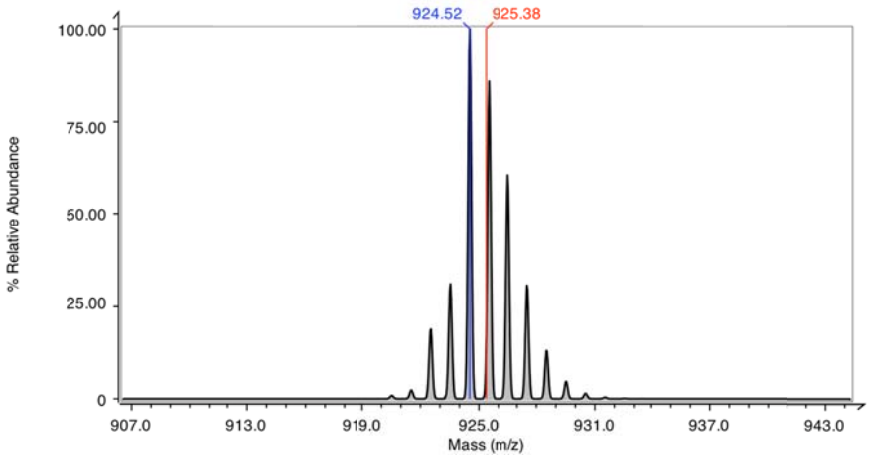

Figure S.6. Simulated mass spectrum for the proposed formulation of **2**, $C_{52}H_{92}Si_4Ti_2$.

Table S.1. Crystal data and structure refinement for **2**.

Identification code	**2**
Empirical formula	C52 H92 Si4 Ti2
Formula weight	925.42
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 13.055(7) A alpha = 95.75(6) deg. b = 13.064(5) A beta = 103.67(7) deg. c = 19.698(10) A gamma = 119.44(3) deg.
Volume	2749(2) A^3
Z, Calculated density	2, 1.118 Mg/m^3
Absorption coefficient	0.409 mm^-1
F(000)	1008
Crystal size	0.05 x 0.04 x 0.01 mm
Theta range for data collection	2.97 to 24.71 deg.
Limiting indices	-15<=h<=15, -15<=k<=15, -21<=l<=23
Reflections collected / unique	28563 / 9280 [R(int) = 0.1059]

Completeness to theta = 24.71	98.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9959 and 0.9799
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9280 / 0 / 524
Goodness-of-fit on F^2	1.079
Final R indices [I>2sigma(I)]	R1 = 0.0927, wR2 = 0.1865
R indices (all data)	R1 = 0.1117, wR2 = 0.2008
Largest diff. peak and hole	0.487 and -0.746 e.A^-3

Table S.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **2**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	4683(7)	813(6)	2559(4)	32(2)
C(2)	3911(6)	275(6)	1792(4)	29(2)
C(3)	3144(7)	741(6)	1579(4)	33(2)
C(4)	3340(7)	1581(6)	2201(4)	34(2)
C(5)	4288(7)	1636(7)	2801(4)	34(2)
C(6)	4389(7)	2370(7)	3445(4)	35(2)
C(7)	3496(7)	2695(7)	3244(4)	35(2)
C(8)	2874(7)	2293(7)	2481(4)	32(2)
C(9)	6756(7)	920(7)	3877(4)	37(2)
C(10)	6966(7)	144(8)	4370(5)	48(2)
C(11)	6818(7)	2004(7)	4333(4)	41(2)
C(12)	5669(7)	-840(7)	2346(4)	38(2)
C(13)	5995(9)	-1727(9)	2610(5)	53(2)
C(14)	6664(8)	59(7)	2059(5)	47(2)
C(15)	3959(7)	-1257(7)	3273(4)	41(2)
C(16)	2793(7)	-2092(7)	2603(5)	48(2)
C(17)	3620(8)	-719(8)	3846(5)	52(2)
C(18)	-10(8)	968(7)	1911(5)	47(2)
C(19)	-46(8)	689(9)	2648(5)	60(3)
C(20)	-273(9)	-149(8)	1377(7)	81(4)

C(21)	1580(8)	2616(8)	1073(5)	50(2)
C(22)	2864(8)	3696(9)	1119(5)	59(3)
C(23)	513(9)	2686(10)	617(5)	65(3)
C(24)	1640(7)	3728(7)	2627(5)	41(2)
C(25)	2788(8)	5011(7)	2735(5)	53(2)
C(26)	447(8)	3754(9)	2435(5)	59(3)
C(27)	6913(6)	3749(7)	1647(4)	34(2)
C(28)	7522(7)	3310(7)	2131(5)	39(2)
C(29)	7514(6)	3609(6)	2839(4)	32(2)
C(30)	7021(7)	4384(7)	2851(4)	36(2)
C(31)	6610(6)	4451(6)	2122(4)	29(2)
C(32)	6185(7)	5284(6)	2130(4)	35(2)
C(33)	6381(7)	5749(6)	2851(4)	34(2)
C(34)	6874(6)	5209(6)	3339(4)	32(2)
C(35)	5290(7)	3352(7)	159(5)	43(2)
C(36)	5013(8)	3113(8)	-666(4)	48(2)
C(37)	4269(7)	2280(8)	350(5)	49(2)
C(38)	7430(7)	2733(7)	371(4)	37(2)
C(39)	6464(8)	1376(7)	232(5)	50(2)
C(40)	7856(8)	2980(7)	-292(4)	45(2)
C(41)	8116(8)	5381(7)	702(5)	44(2)
C(42)	9456(8)	5773(9)	1177(5)	60(2)
C(43)	7841(8)	6373(8)	915(5)	51(2)
C(44)	8242(7)	5382(7)	4939(4)	37(2)
C(45)	7156(8)	4729(8)	5230(5)	48(2)
C(46)	9487(8)	6167(8)	5577(4)	50(2)
C(47)	9522(8)	7325(8)	4171(5)	47(2)
C(48)	10058(8)	6644(8)	3866(5)	55(2)
C(49)	9487(8)	8204(8)	3730(5)	59(3)
C(50)	7340(7)	7191(7)	4576(4)	39(2)
C(51)	5951(8)	6466(8)	4554(5)	50(2)
C(52)	8224(8)	8153(8)	5316(5)	53(2)
Si(1)	5300(2)	-38(2)	3037(1)	33(1)
Si(2)	1519(2)	2413(2)	2010(1)	36(1)
Si(3)	6925(2)	3794(2)	707(1)	34(1)
Si(4)	7951(2)	6235(2)	4269(1)	35(1)
Ti(1)	5362(1)	2350(1)	2002(1)	34(1)
Ti(2)	4926(1)	3677(1)	2635(1)	34(1)

Table S.3. Bond lengths [A] and angles [deg] for **2**.

C(1)-C(2)	1.471(10)
C(1)-C(5)	1.486(10)
C(1)-Si(1)	1.871(7)
C(1)-Ti(1)	2.274(7)
C(2)-C(3)	1.414(10)
C(2)-Ti(1)	2.337(7)

C(2)-H(003)	0.9500
C(3)-C(4)	1.442(10)
C(3)-Ti(1)	2.454(7)
C(3)-H(005)	0.9500
C(4)-C(5)	1.463(10)
C(4)-C(8)	1.467(10)
C(4)-Ti(2)	2.375(7)
C(4)-Ti(1)	2.468(7)
C(5)-C(6)	1.449(10)
C(5)-Ti(1)	2.316(7)
C(5)-Ti(2)	2.456(8)
C(6)-C(7)	1.414(10)
C(6)-Ti(2)	2.419(7)
C(6)-H(025)	0.9500
C(7)-C(8)	1.429(10)
C(7)-Ti(2)	2.363(7)
C(7)-H(013)	0.9500
C(8)-Si(2)	1.881(8)
C(8)-Ti(2)	2.298(7)
C(9)-C(10)	1.547(10)
C(9)-C(11)	1.556(10)
C(9)-Si(1)	1.918(8)
C(9)-H(049)	1.0000
C(10)-H(03J)	0.9800
C(10)-H(03K)	0.9800
C(10)-H(03L)	0.9800
C(11)-H(04M)	0.9800
C(11)-H(04N)	0.9800
C(11)-H(04O)	0.9800
C(12)-C(13)	1.515(11)
C(12)-C(14)	1.538(11)
C(12)-Si(1)	1.925(8)
C(12)-H(037)	1.0000
C(13)-H(05A)	0.9800
C(13)-H(05B)	0.9800
C(13)-H(05C)	0.9800
C(14)-H(03M)	0.9800
C(14)-H(03N)	0.9800
C(14)-H(03O)	0.9800
C(15)-C(17)	1.532(11)
C(15)-C(16)	1.543(11)
C(15)-Si(1)	1.900(8)
C(15)-H(009)	1.0000
C(16)-H(02J)	0.9800
C(16)-H(02K)	0.9800
C(16)-H(02L)	0.9800
C(17)-H(02M)	0.9800
C(17)-H(02N)	0.9800
C(17)-H(02O)	0.9800
C(18)-C(19)	1.539(12)

C(18)-C(20)	1.544(12)
C(18)-Si(2)	1.903(8)
C(18)-H(052)	1.0000
C(19)-H(04$)	0.9800
C(19)-H(04V)	0.9800
C(19)-H(04W)	0.9800
C(20)-H(04S)	0.9800
C(20)-H(04T)	0.9800
C(20)-H(04U)	0.9800
C(21)-C(23)	1.518(11)
C(21)-C(22)	1.545(11)
C(21)-Si(2)	1.906(9)
C(21)-H(012)	1.0000
C(22)-H(02P)	0.9800
C(22)-H(02Q)	0.9800
C(22)-H(02R)	0.9800
C(23)-H(03D)	0.9800
C(23)-H(03E)	0.9800
C(23)-H(03F)	0.9800
C(24)-C(26)	1.533(10)
C(24)-C(25)	1.552(11)
C(24)-Si(2)	1.917(8)
C(24)-H(001)	1.0000
C(25)-H(02D)	0.9800
C(25)-H(02E)	0.9800
C(25)-H(02F)	0.9800
C(26)-H(03G)	0.9800
C(26)-H(03H)	0.9800
C(26)-H(03I)	0.9800
C(27)-C(28)	1.439(11)
C(27)-C(31)	1.494(10)
C(27)-Si(3)	1.862(8)
C(27)-Ti(1)	2.284(7)
C(28)-C(29)	1.412(11)
C(28)-Ti(1)	2.389(7)
C(28)-H(014)	0.9500
C(29)-C(30)	1.444(10)
C(29)-Ti(1)	2.458(8)
C(29)-H(031)	0.9500
C(30)-C(31)	1.437(10)
C(30)-C(34)	1.485(10)
C(30)-Ti(2)	2.325(7)
C(30)-Ti(1)	2.508(8)
C(31)-C(32)	1.444(9)
C(31)-Ti(1)	2.353(7)
C(31)-Ti(2)	2.439(7)
C(32)-C(33)	1.397(11)
C(32)-Ti(2)	2.428(8)
C(32)-H(030)	0.9500
C(33)-C(34)	1.458(10)

C(33)-Ti(2)	2.335(7)
C(33)-H(006)	0.9500
C(34)-Si(4)	1.889(8)
C(34)-Ti(2)	2.274(8)
C(35)-C(36)	1.542(11)
C(35)-C(37)	1.544(11)
C(35)-Si(3)	1.905(8)
C(35)-H(017)	1.0000
C(36)-H(03A)	0.9800
C(36)-H(03B)	0.9800
C(36)-H(03C)	0.9800
C(37)-H(02G)	0.9800
C(37)-H(02H)	0.9800
C(37)-H(02I)	0.9800
C(38)-C(39)	1.534(11)
C(38)-C(40)	1.539(10)
C(38)-Si(3)	1.928(7)
C(38)-H(010)	1.0000
C(39)-H(02S)	0.9800
C(39)-H(02T)	0.9800
C(39)-H(02U)	0.9800
C(40)-H(02A)	0.9800
C(40)-H(02B)	0.9800
C(40)-H(02C)	0.9800
C(41)-C(43)	1.551(11)
C(41)-C(42)	1.564(11)
C(41)-Si(3)	1.887(8)
C(41)-H(040)	1.0000
C(42)-H(04D)	0.9800
C(42)-H(04E)	0.9800
C(42)-H(04F)	0.9800
C(43)-H(04J)	0.9800
C(43)-H(04K)	0.9800
C(43)-H(04L)	0.9800
C(44)-C(45)	1.537(10)
C(44)-C(46)	1.553(11)
C(44)-Si(4)	1.897(8)
C(44)-H(038)	1.0000
C(45)-H(04G)	0.9800
C(45)-H(04H)	0.9800
C(45)-H(04I)	0.9800
C(46)-H(04A)	0.9800
C(46)-H(04B)	0.9800
C(46)-H(04C)	0.9800
C(47)-C(49)	1.519(11)
C(47)-C(48)	1.531(11)
C(47)-Si(4)	1.908(8)
C(47)-H(039)	1.0000
C(48)-H(04P)	0.9800
C(48)-H(04Q)	0.9800

C(48)-H(04R)	0.9800
C(49)-H(05D)	0.9800
C(49)-H(05E)	0.9800
C(49)-H(05F)	0.9800
C(50)-C(52)	1.564(11)
C(50)-C(51)	1.567(11)
C(50)-Si(4)	1.902(8)
C(50)-H(002)	1.0000
C(51)-H(01D)	0.9800
C(51)-H(01E)	0.9800
C(51)-H(01F)	0.9800
C(52)-H(01A)	0.9800
C(52)-H(01B)	0.9800
C(52)-H(01C)	0.9800
Ti(1)-Ti(2)	2.399(2)

C(2)-C(1)-C(5)	102.5(6)
C(2)-C(1)-Si(1)	118.5(5)
C(5)-C(1)-Si(1)	133.0(6)
C(2)-C(1)-Ti(1)	73.7(4)
C(5)-C(1)-Ti(1)	72.6(4)
Si(1)-C(1)-Ti(1)	138.0(4)
C(3)-C(2)-C(1)	112.0(6)
C(3)-C(2)-Ti(1)	77.4(4)
C(1)-C(2)-Ti(1)	69.1(4)
C(3)-C(2)-H(003)	124.0
C(1)-C(2)-H(003)	124.0
Ti(1)-C(2)-H(003)	120.9
C(2)-C(3)-C(4)	108.5(7)
C(2)-C(3)-Ti(1)	68.4(4)
C(4)-C(3)-Ti(1)	73.5(4)
C(2)-C(3)-H(005)	125.7
C(4)-C(3)-H(005)	125.7
Ti(1)-C(3)-H(005)	124.0
C(3)-C(4)-C(5)	106.5(6)
C(3)-C(4)-C(8)	144.5(7)
C(5)-C(4)-C(8)	108.6(7)
C(3)-C(4)-Ti(2)	126.6(5)
C(5)-C(4)-Ti(2)	75.4(4)
C(8)-C(4)-Ti(2)	68.9(4)
C(3)-C(4)-Ti(1)	72.4(4)
C(5)-C(4)-Ti(1)	66.6(4)
C(8)-C(4)-Ti(1)	127.7(5)
Ti(2)-C(4)-Ti(1)	59.36(17)
C(6)-C(5)-C(4)	106.8(6)
C(6)-C(5)-C(1)	142.1(7)
C(4)-C(5)-C(1)	110.5(6)
C(6)-C(5)-Ti(1)	126.1(5)
C(4)-C(5)-Ti(1)	78.0(4)
C(1)-C(5)-Ti(1)	69.6(4)

C(6)-C(5)-Ti(2)	71.3(4)
C(4)-C(5)-Ti(2)	69.4(4)
C(1)-C(5)-Ti(2)	128.9(5)
Ti(1)-C(5)-Ti(2)	60.29(18)
C(7)-C(6)-C(5)	107.6(7)
C(7)-C(6)-Ti(2)	70.6(4)
C(5)-C(6)-Ti(2)	74.1(4)
C(7)-C(6)-H(025)	126.2
C(5)-C(6)-H(025)	126.2
Ti(2)-C(6)-H(025)	120.8
C(6)-C(7)-C(8)	111.5(7)
C(6)-C(7)-Ti(2)	75.0(4)
C(8)-C(7)-Ti(2)	69.7(4)
C(6)-C(7)-H(013)	124.2
C(8)-C(7)-H(013)	124.2
Ti(2)-C(7)-H(013)	122.6
C(7)-C(8)-C(4)	105.2(6)
C(7)-C(8)-Si(2)	124.5(5)
C(4)-C(8)-Si(2)	129.1(6)
C(7)-C(8)-Ti(2)	74.6(4)
C(4)-C(8)-Ti(2)	74.6(4)
Si(2)-C(8)-Ti(2)	125.2(4)
C(10)-C(9)-C(11)	109.7(6)
C(10)-C(9)-Si(1)	112.6(5)
C(11)-C(9)-Si(1)	114.9(5)
C(10)-C(9)-H(049)	106.3
C(11)-C(9)-H(049)	106.3
Si(1)-C(9)-H(049)	106.3
C(9)-C(10)-H(03J)	109.5
C(9)-C(10)-H(03K)	109.5
H(03J)-C(10)-H(03K)	109.5
C(9)-C(10)-H(03L)	109.5
H(03J)-C(10)-H(03L)	109.5
H(03K)-C(10)-H(03L)	109.5
C(9)-C(11)-H(04M)	109.5
C(9)-C(11)-H(04N)	109.5
H(04M)-C(11)-H(04N)	109.5
C(9)-C(11)-H(04O)	109.5
H(04M)-C(11)-H(04O)	109.5
H(04N)-C(11)-H(04O)	109.5
C(13)-C(12)-C(14)	111.1(7)
C(13)-C(12)-Si(1)	113.8(6)
C(14)-C(12)-Si(1)	112.6(5)
C(13)-C(12)-H(037)	106.2
C(14)-C(12)-H(037)	106.2
Si(1)-C(12)-H(037)	106.2
C(12)-C(13)-H(05A)	109.5
C(12)-C(13)-H(05B)	109.5
H(05A)-C(13)-H(05B)	109.5
C(12)-C(13)-H(05C)	109.5

H(05A)-C(13)-H(05C)	109.5
H(05B)-C(13)-H(05C)	109.5
C(12)-C(14)-H(03M)	109.5
C(12)-C(14)-H(03N)	109.5
H(03M)-C(14)-H(03N)	109.5
C(12)-C(14)-H(03O)	109.5
H(03M)-C(14)-H(03O)	109.5
H(03N)-C(14)-H(03O)	109.5
C(17)-C(15)-C(16)	110.1(7)
C(17)-C(15)-Si(1)	112.3(5)
C(16)-C(15)-Si(1)	112.4(6)
C(17)-C(15)-H(009)	107.3
C(16)-C(15)-H(009)	107.3
Si(1)-C(15)-H(009)	107.3
C(15)-C(16)-H(02J)	109.5
C(15)-C(16)-H(02K)	109.5
H(02J)-C(16)-H(02K)	109.5
C(15)-C(16)-H(02L)	109.5
H(02J)-C(16)-H(02L)	109.5
H(02K)-C(16)-H(02L)	109.5
C(15)-C(17)-H(02M)	109.5
C(15)-C(17)-H(02N)	109.5
H(02M)-C(17)-H(02N)	109.5
C(15)-C(17)-H(02O)	109.5
H(02M)-C(17)-H(02O)	109.5
H(02N)-C(17)-H(02O)	109.5
C(19)-C(18)-C(20)	109.6(8)
C(19)-C(18)-Si(2)	110.9(6)
C(20)-C(18)-Si(2)	113.2(6)
C(19)-C(18)-H(052)	107.6
C(20)-C(18)-H(052)	107.6
Si(2)-C(18)-H(052)	107.6
C(18)-C(19)-H(04$)	109.5
C(18)-C(19)-H(04V)	109.5
H(04$)-C(19)-H(04V)	109.5
C(18)-C(19)-H(04W)	109.5
H(04$)-C(19)-H(04W)	109.5
H(04V)-C(19)-H(04W)	109.5
C(18)-C(20)-H(04S)	109.5
C(18)-C(20)-H(04T)	109.5
H(04S)-C(20)-H(04T)	109.5
C(18)-C(20)-H(04U)	109.5
H(04S)-C(20)-H(04U)	109.5
H(04T)-C(20)-H(04U)	109.5
C(23)-C(21)-C(22)	112.2(8)
C(23)-C(21)-Si(2)	114.5(6)
C(22)-C(21)-Si(2)	111.0(7)
C(23)-C(21)-H(012)	106.2
C(22)-C(21)-H(012)	106.2
Si(2)-C(21)-H(012)	106.2

C(21)-C(22)-H(02P)	109.5
C(21)-C(22)-H(02Q)	109.5
H(02P)-C(22)-H(02Q)	109.5
C(21)-C(22)-H(02R)	109.5
H(02P)-C(22)-H(02R)	109.5
H(02Q)-C(22)-H(02R)	109.5
C(21)-C(23)-H(03D)	109.5
C(21)-C(23)-H(03E)	109.5
H(03D)-C(23)-H(03E)	109.5
C(21)-C(23)-H(03F)	109.5
H(03D)-C(23)-H(03F)	109.5
H(03E)-C(23)-H(03F)	109.5
C(26)-C(24)-C(25)	110.3(7)
C(26)-C(24)-Si(2)	113.9(6)
C(25)-C(24)-Si(2)	115.9(6)
C(26)-C(24)-H(001)	105.2
C(25)-C(24)-H(001)	105.2
Si(2)-C(24)-H(001)	105.2
C(24)-C(25)-H(02D)	109.5
C(24)-C(25)-H(02E)	109.5
H(02D)-C(25)-H(02E)	109.5
C(24)-C(25)-H(02F)	109.5
H(02D)-C(25)-H(02F)	109.5
H(02E)-C(25)-H(02F)	109.5
C(24)-C(26)-H(03G)	109.5
C(24)-C(26)-H(03H)	109.5
H(03G)-C(26)-H(03H)	109.5
C(24)-C(26)-H(03I)	109.5
H(03G)-C(26)-H(03I)	109.5
H(03H)-C(26)-H(03I)	109.5
C(28)-C(27)-C(31)	104.5(6)
C(28)-C(27)-Si(3)	126.0(6)
C(31)-C(27)-Si(3)	127.5(5)
C(28)-C(27)-Ti(1)	76.1(4)
C(31)-C(27)-Ti(1)	73.7(4)
Si(3)-C(27)-Ti(1)	127.6(4)
C(29)-C(28)-C(27)	110.9(7)
C(29)-C(28)-Ti(1)	75.7(4)
C(27)-C(28)-Ti(1)	68.1(4)
C(29)-C(28)-H(014)	124.5
C(27)-C(28)-H(014)	124.5
Ti(1)-C(28)-H(014)	123.1
C(28)-C(29)-C(30)	108.1(7)
C(28)-C(29)-Ti(1)	70.4(4)
C(30)-C(29)-Ti(1)	75.0(4)
C(28)-C(29)-H(031)	125.9
C(30)-C(29)-H(031)	125.9
Ti(1)-C(29)-H(031)	120.4
C(31)-C(30)-C(29)	107.5(6)
C(31)-C(30)-C(34)	108.8(6)

C(29)-C(30)-C(34)	143.5(7)
C(31)-C(30)-Ti(2)	76.8(4)
C(29)-C(30)-Ti(2)	124.1(5)
C(34)-C(30)-Ti(2)	69.3(4)
C(31)-C(30)-Ti(1)	67.0(4)
C(29)-C(30)-Ti(1)	71.2(4)
C(34)-C(30)-Ti(1)	128.3(5)
Ti(2)-C(30)-Ti(1)	59.40(19)
C(30)-C(31)-C(32)	108.2(6)
C(30)-C(31)-C(27)	108.6(6)
C(32)-C(31)-C(27)	142.7(7)
C(30)-C(31)-Ti(1)	78.8(5)
C(32)-C(31)-Ti(1)	125.1(5)
C(27)-C(31)-Ti(1)	68.7(4)
C(30)-C(31)-Ti(2)	68.1(4)
C(32)-C(31)-Ti(2)	72.3(4)
C(27)-C(31)-Ti(2)	128.4(5)
Ti(1)-C(31)-Ti(2)	60.06(17)
C(33)-C(32)-C(31)	107.4(7)
C(33)-C(32)-Ti(2)	69.3(4)
C(31)-C(32)-Ti(2)	73.2(4)
C(33)-C(32)-H(030)	126.3
C(31)-C(32)-H(030)	126.3
Ti(2)-C(32)-H(030)	122.8
C(32)-C(33)-C(34)	112.0(7)
C(32)-C(33)-Ti(2)	76.6(4)
C(34)-C(33)-Ti(2)	69.3(4)
C(32)-C(33)-H(006)	124.0
C(34)-C(33)-H(006)	124.0
Ti(2)-C(33)-H(006)	121.5
C(33)-C(34)-C(30)	103.5(6)
C(33)-C(34)-Si(4)	115.6(5)
C(30)-C(34)-Si(4)	128.7(5)
C(33)-C(34)-Ti(2)	73.8(4)
C(30)-C(34)-Ti(2)	73.0(4)
Si(4)-C(34)-Ti(2)	147.6(4)
C(36)-C(35)-C(37)	110.7(7)
C(36)-C(35)-Si(3)	114.9(5)
C(37)-C(35)-Si(3)	112.4(6)
C(36)-C(35)-H(017)	106.0
C(37)-C(35)-H(017)	106.0
Si(3)-C(35)-H(017)	106.0
C(35)-C(36)-H(03A)	109.5
C(35)-C(36)-H(03B)	109.5
H(03A)-C(36)-H(03B)	109.5
C(35)-C(36)-H(03C)	109.5
H(03A)-C(36)-H(03C)	109.5
H(03B)-C(36)-H(03C)	109.5
C(35)-C(37)-H(02G)	109.5
C(35)-C(37)-H(02H)	109.5

H(02G)-C(37)-H(02H)	109.5
C(35)-C(37)-H(02I)	109.5
H(02G)-C(37)-H(02I)	109.5
H(02H)-C(37)-H(02I)	109.5
C(39)-C(38)-C(40)	110.1(7)
C(39)-C(38)-Si(3)	114.2(5)
C(40)-C(38)-Si(3)	113.7(5)
C(39)-C(38)-H(010)	106.1
C(40)-C(38)-H(010)	106.1
Si(3)-C(38)-H(010)	106.1
C(38)-C(39)-H(02S)	109.5
C(38)-C(39)-H(02T)	109.5
H(02S)-C(39)-H(02T)	109.5
C(38)-C(39)-H(02U)	109.5
H(02S)-C(39)-H(02U)	109.5
H(02T)-C(39)-H(02U)	109.5
C(38)-C(40)-H(02A)	109.5
C(38)-C(40)-H(02B)	109.5
H(02A)-C(40)-H(02B)	109.5
C(38)-C(40)-H(02C)	109.5
H(02A)-C(40)-H(02C)	109.5
H(02B)-C(40)-H(02C)	109.5
C(43)-C(41)-C(42)	110.1(7)
C(43)-C(41)-Si(3)	115.4(6)
C(42)-C(41)-Si(3)	111.2(6)
C(43)-C(41)-H(040)	106.5
C(42)-C(41)-H(040)	106.5
Si(3)-C(41)-H(040)	106.5
C(41)-C(42)-H(04D)	109.5
C(41)-C(42)-H(04E)	109.5
H(04D)-C(42)-H(04E)	109.5
C(41)-C(42)-H(04F)	109.5
H(04D)-C(42)-H(04F)	109.5
H(04E)-C(42)-H(04F)	109.5
C(41)-C(43)-H(04J)	109.5
C(41)-C(43)-H(04K)	109.5
H(04J)-C(43)-H(04K)	109.5
C(41)-C(43)-H(04L)	109.5
H(04J)-C(43)-H(04L)	109.5
H(04K)-C(43)-H(04L)	109.5
C(45)-C(44)-C(46)	109.9(7)
C(45)-C(44)-Si(4)	112.6(6)
C(46)-C(44)-Si(4)	114.4(5)
C(45)-C(44)-H(038)	106.5
C(46)-C(44)-H(038)	106.5
Si(4)-C(44)-H(038)	106.5
C(44)-C(45)-H(04G)	109.5
C(44)-C(45)-H(04H)	109.5
H(04G)-C(45)-H(04H)	109.5
C(44)-C(45)-H(04I)	109.5

H(04G)-C(45)-H(04I)	109.5
H(04H)-C(45)-H(04I)	109.5
C(44)-C(46)-H(04A)	109.5
C(44)-C(46)-H(04B)	109.5
H(04A)-C(46)-H(04B)	109.5
C(44)-C(46)-H(04C)	109.5
H(04A)-C(46)-H(04C)	109.5
H(04B)-C(46)-H(04C)	109.5
C(49)-C(47)-C(48)	110.5(7)
C(49)-C(47)-Si(4)	113.4(6)
C(48)-C(47)-Si(4)	111.7(6)
C(49)-C(47)-H(039)	106.9
C(48)-C(47)-H(039)	106.9
Si(4)-C(47)-H(039)	106.9
C(47)-C(48)-H(04P)	109.5
C(47)-C(48)-H(04Q)	109.5
H(04P)-C(48)-H(04Q)	109.5
C(47)-C(48)-H(04R)	109.5
H(04P)-C(48)-H(04R)	109.5
H(04Q)-C(48)-H(04R)	109.5
C(47)-C(49)-H(05D)	109.5
C(47)-C(49)-H(05E)	109.5
H(05D)-C(49)-H(05E)	109.5
C(47)-C(49)-H(05F)	109.5
H(05D)-C(49)-H(05F)	109.5
H(05E)-C(49)-H(05F)	109.5
C(52)-C(50)-C(51)	111.7(7)
C(52)-C(50)-Si(4)	113.1(5)
C(51)-C(50)-Si(4)	115.7(5)
C(52)-C(50)-H(002)	105.0
C(51)-C(50)-H(002)	105.0
Si(4)-C(50)-H(002)	105.0
C(50)-C(51)-H(01D)	109.5
C(50)-C(51)-H(01E)	109.5
H(01D)-C(51)-H(01E)	109.5
C(50)-C(51)-H(01F)	109.5
H(01D)-C(51)-H(01F)	109.5
H(01E)-C(51)-H(01F)	109.5
C(50)-C(52)-H(01A)	109.5
C(50)-C(52)-H(01B)	109.5
H(01A)-C(52)-H(01B)	109.5
C(50)-C(52)-H(01C)	109.5
H(01A)-C(52)-H(01C)	109.5
H(01B)-C(52)-H(01C)	109.5
C(1)-Si(1)-C(15)	105.9(4)
C(1)-Si(1)-C(9)	115.9(3)
C(15)-Si(1)-C(9)	111.0(4)
C(1)-Si(1)-C(12)	107.0(3)
C(15)-Si(1)-C(12)	107.8(4)
C(9)-Si(1)-C(12)	108.9(3)

C(8)-Si(2)-C(18)	110.3(4)
C(8)-Si(2)-C(21)	108.5(3)
C(18)-Si(2)-C(21)	108.9(4)
C(8)-Si(2)-C(24)	106.6(4)
C(18)-Si(2)-C(24)	107.9(4)
C(21)-Si(2)-C(24)	114.7(4)
C(27)-Si(3)-C(41)	109.4(4)
C(27)-Si(3)-C(35)	105.8(3)
C(41)-Si(3)-C(35)	110.8(4)
C(27)-Si(3)-C(38)	109.3(3)
C(41)-Si(3)-C(38)	107.1(4)
C(35)-Si(3)-C(38)	114.3(4)
C(34)-Si(4)-C(44)	113.1(3)
C(34)-Si(4)-C(50)	108.7(3)
C(44)-Si(4)-C(50)	114.1(4)
C(34)-Si(4)-C(47)	106.8(4)
C(44)-Si(4)-C(47)	106.7(4)
C(50)-Si(4)-C(47)	107.0(4)
C(1)-Ti(1)-C(27)	148.9(3)
C(1)-Ti(1)-C(5)	37.8(3)
C(27)-Ti(1)-C(5)	155.0(3)
C(1)-Ti(1)-C(2)	37.2(3)
C(27)-Ti(1)-C(2)	144.2(3)
C(5)-Ti(1)-C(2)	59.4(3)
C(1)-Ti(1)-C(31)	147.6(3)
C(27)-Ti(1)-C(31)	37.5(2)
C(5)-Ti(1)-C(31)	120.6(3)
C(2)-Ti(1)-C(31)	172.7(2)
C(1)-Ti(1)-C(28)	113.6(3)
C(27)-Ti(1)-C(28)	35.8(3)
C(5)-Ti(1)-C(28)	132.0(3)
C(2)-Ti(1)-C(28)	127.6(3)
C(31)-Ti(1)-C(28)	58.5(3)
C(1)-Ti(1)-Ti(2)	100.00(19)
C(27)-Ti(1)-Ti(2)	99.1(2)
C(5)-Ti(1)-Ti(2)	62.76(19)
C(2)-Ti(1)-Ti(2)	114.99(18)
C(31)-Ti(1)-Ti(2)	61.75(18)
C(28)-Ti(1)-Ti(2)	112.2(2)
C(1)-Ti(1)-C(3)	60.6(3)
C(27)-Ti(1)-C(3)	143.4(3)
C(5)-Ti(1)-C(3)	58.3(3)
C(2)-Ti(1)-C(3)	34.2(2)
C(31)-Ti(1)-C(3)	138.7(2)
C(28)-Ti(1)-C(3)	157.7(3)
Ti(2)-Ti(1)-C(3)	90.10(19)
C(1)-Ti(1)-C(29)	97.5(3)
C(27)-Ti(1)-C(29)	59.2(3)
C(5)-Ti(1)-C(29)	100.8(3)
C(2)-Ti(1)-C(29)	129.5(3)

C(31)-Ti(1)-C(29)	57.7(2)
C(28)-Ti(1)-C(29)	33.8(3)
Ti(2)-Ti(1)-C(29)	87.36(19)
C(3)-Ti(1)-C(29)	157.1(2)
C(1)-Ti(1)-C(4)	61.3(2)
C(27)-Ti(1)-C(4)	149.4(2)
C(5)-Ti(1)-C(4)	35.4(3)
C(2)-Ti(1)-C(4)	57.6(2)
C(31)-Ti(1)-C(4)	117.6(2)
C(28)-Ti(1)-C(4)	165.5(3)
Ti(2)-Ti(1)-C(4)	58.38(18)
C(3)-Ti(1)-C(4)	34.1(2)
C(29)-Ti(1)-C(4)	131.7(3)
C(1)-Ti(1)-C(30)	113.7(3)
C(27)-Ti(1)-C(30)	59.3(3)
C(5)-Ti(1)-C(30)	95.7(3)
C(2)-Ti(1)-C(30)	150.7(3)
C(31)-Ti(1)-C(30)	34.2(2)
C(28)-Ti(1)-C(30)	56.3(3)
Ti(2)-Ti(1)-C(30)	56.51(17)
C(3)-Ti(1)-C(30)	145.8(2)
C(29)-Ti(1)-C(30)	33.8(2)
C(4)-Ti(1)-C(30)	111.9(2)
C(34)-Ti(2)-C(8)	151.3(3)
C(34)-Ti(2)-C(30)	37.7(2)
C(8)-Ti(2)-C(30)	156.7(3)
C(34)-Ti(2)-C(33)	36.9(3)
C(8)-Ti(2)-C(33)	143.2(3)
C(30)-Ti(2)-C(33)	59.5(3)
C(34)-Ti(2)-C(7)	116.3(3)
C(8)-Ti(2)-C(7)	35.7(3)
C(30)-Ti(2)-C(7)	134.5(3)
C(33)-Ti(2)-C(7)	128.7(3)
C(34)-Ti(2)-C(4)	151.1(3)
C(8)-Ti(2)-C(4)	36.5(2)
C(30)-Ti(2)-C(4)	122.6(3)
C(33)-Ti(2)-C(4)	169.9(3)
C(7)-Ti(2)-C(4)	58.1(3)
C(34)-Ti(2)-Ti(1)	101.52(19)
C(8)-Ti(2)-Ti(1)	98.5(2)
C(30)-Ti(2)-Ti(1)	64.1(2)
C(33)-Ti(2)-Ti(1)	115.0(2)
C(7)-Ti(2)-Ti(1)	113.14(19)
C(4)-Ti(2)-Ti(1)	62.26(19)
C(34)-Ti(2)-C(6)	100.2(3)
C(8)-Ti(2)-C(6)	59.7(3)
C(30)-Ti(2)-C(6)	102.7(3)
C(33)-Ti(2)-C(6)	131.7(3)
C(7)-Ti(2)-C(6)	34.4(2)
C(4)-Ti(2)-C(6)	58.4(3)

Ti(1)-Ti(2)-C(6)	89.04(19)
C(34)-Ti(2)-C(32)	60.4(3)
C(8)-Ti(2)-C(32)	140.4(3)
C(30)-Ti(2)-C(32)	58.8(3)
C(33)-Ti(2)-C(32)	34.1(3)
C(7)-Ti(2)-C(32)	156.9(3)
C(4)-Ti(2)-C(32)	136.8(3)
Ti(1)-Ti(2)-C(32)	89.44(19)
C(6)-Ti(2)-C(32)	159.7(3)
C(34)-Ti(2)-C(31)	60.4(3)
C(8)-Ti(2)-C(31)	148.1(3)
C(30)-Ti(2)-C(31)	35.0(2)
C(33)-Ti(2)-C(31)	57.3(3)
C(7)-Ti(2)-C(31)	167.2(2)
C(4)-Ti(2)-C(31)	117.9(2)
Ti(1)-Ti(2)-C(31)	58.19(17)
C(6)-Ti(2)-C(31)	132.9(2)
C(32)-Ti(2)-C(31)	34.5(2)
C(34)-Ti(2)-C(5)	116.2(3)
C(8)-Ti(2)-C(5)	59.9(3)
C(30)-Ti(2)-C(5)	96.9(2)
C(33)-Ti(2)-C(5)	152.8(3)
C(7)-Ti(2)-C(5)	57.2(2)
C(4)-Ti(2)-C(5)	35.2(2)
Ti(1)-Ti(2)-C(5)	56.96(17)
C(6)-Ti(2)-C(5)	34.6(2)
C(32)-Ti(2)-C(5)	145.8(2)
C(31)-Ti(2)-C(5)	111.9(2)

Symmetry transformations used to generate equivalent atoms:

Table S.4. Anisotropic displacement parameters (A^2 x 10^3) for **2**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	32(4)	28(4)	42(5)	11(3)	11(3)	21(3)
C(2)	28(4)	17(3)	44(5)	13(3)	17(3)	11(3)
C(3)	33(4)	28(4)	38(5)	16(3)	18(4)	11(3)
C(4)	34(4)	21(4)	51(5)	16(4)	18(4)	15(3)

C(5)	31(4)	41(4)	28(4)	9(4)	17(3)	15(4)
C(6)	36(4)	35(4)	41(5)	21(4)	20(4)	18(4)
C(7)	39(4)	48(5)	39(5)	20(4)	23(4)	32(4)
C(8)	34(4)	35(4)	34(4)	16(3)	14(3)	21(4)
C(9)	33(4)	36(4)	43(5)	9(4)	12(4)	19(4)
C(10)	35(4)	46(5)	58(6)	8(4)	1(4)	26(4)
C(11)	38(4)	31(4)	48(5)	11(4)	16(4)	15(4)
C(12)	33(4)	35(4)	40(5)	1(4)	4(3)	19(4)
C(13)	71(6)	66(6)	46(6)	13(5)	22(5)	52(5)
C(14)	49(5)	46(5)	61(6)	22(4)	34(5)	28(5)
C(15)	33(4)	39(5)	50(5)	24(4)	15(4)	16(4)
C(16)	35(5)	28(4)	52(6)	4(4)	6(4)	1(4)
C(17)	39(5)	43(5)	63(6)	12(5)	25(4)	9(4)
C(18)	36(4)	42(5)	64(6)	13(4)	17(4)	22(4)
C(19)	36(5)	72(7)	66(7)	36(6)	18(5)	21(5)
C(20)	47(6)	35(5)	147(11)	12(6)	33(7)	13(5)
C(21)	45(5)	63(6)	55(6)	22(5)	16(4)	38(5)
C(22)	53(6)	62(6)	61(6)	23(5)	31(5)	24(5)
C(23)	56(6)	106(8)	73(7)	56(7)	37(5)	58(6)
C(24)	36(4)	41(5)	46(5)	10(4)	6(4)	23(4)
C(25)	52(5)	42(5)	72(7)	11(5)	26(5)	30(4)
C(26)	46(5)	65(6)	74(7)	9(5)	15(5)	38(5)
C(27)	25(4)	32(4)	45(5)	8(4)	14(4)	16(3)
C(28)	27(4)	34(4)	57(6)	12(4)	15(4)	16(4)
C(29)	24(4)	32(4)	39(5)	13(3)	11(3)	14(3)
C(30)	28(4)	36(4)	52(5)	14(4)	15(4)	21(4)
C(31)	24(4)	28(4)	35(5)	5(3)	7(3)	16(3)
C(32)	28(4)	27(4)	49(5)	12(4)	14(4)	13(3)
C(33)	30(4)	26(4)	44(5)	13(3)	15(4)	13(3)
C(34)	20(3)	30(4)	45(5)	7(3)	10(3)	14(3)
C(35)	45(5)	45(5)	49(5)	12(4)	20(4)	30(4)
C(36)	51(5)	60(6)	46(5)	18(4)	12(4)	39(5)
C(37)	33(4)	55(6)	63(6)	23(5)	18(4)	24(4)
C(38)	36(4)	36(4)	42(5)	9(4)	14(4)	20(4)
C(39)	55(6)	40(5)	60(6)	18(4)	29(5)	24(4)
C(40)	46(5)	43(5)	43(5)	7(4)	20(4)	20(4)
C(41)	49(5)	40(5)	49(5)	15(4)	22(4)	23(4)
C(42)	41(5)	54(6)	70(7)	19(5)	19(5)	15(5)
C(43)	56(5)	43(5)	54(6)	14(4)	23(5)	25(5)
C(44)	37(4)	28(4)	43(5)	9(4)	12(4)	15(4)
C(45)	52(5)	55(5)	48(6)	17(4)	24(4)	31(5)
C(46)	50(5)	57(6)	41(5)	13(4)	8(4)	32(5)
C(47)	45(5)	41(5)	46(5)	13(4)	21(4)	14(4)
C(48)	32(5)	53(6)	75(7)	19(5)	24(5)	16(4)
C(49)	47(5)	35(5)	77(7)	24(5)	26(5)	4(4)
C(50)	31(4)	32(4)	45(5)	4(4)	10(4)	13(4)
C(51)	54(5)	55(6)	54(6)	11(5)	24(5)	37(5)
C(52)	50(5)	47(5)	54(6)	4(4)	12(5)	25(5)
Si(1)	31(1)	27(1)	44(1)	10(1)	13(1)	16(1)
Si(2)	29(1)	38(1)	46(1)	16(1)	14(1)	21(1)

Si(3)	32(1)	32(1)	38(1)	10(1)	14(1)	17(1)
Si(4)	32(1)	32(1)	39(1)	9(1)	12(1)	16(1)
Ti(1)	28(1)	32(1)	42(1)	10(1)	13(1)	17(1)
Ti(2)	30(1)	32(1)	45(1)	13(1)	16(1)	18(1)

Table S.5. Torsion angles [deg] for **2**.

C(5)-C(1)-C(2)-C(3)	1.4(8)
Si(1)-C(1)-C(2)-C(3)	157.7(5)
Ti(1)-C(1)-C(2)-C(3)	-66.1(5)
C(5)-C(1)-C(2)-Ti(1)	67.5(4)
Si(1)-C(1)-C(2)-Ti(1)	-136.2(5)
C(1)-C(2)-C(3)-C(4)	-1.9(8)
Ti(1)-C(2)-C(3)-C(4)	-62.9(5)
C(1)-C(2)-C(3)-Ti(1)	61.0(5)
C(2)-C(3)-C(4)-C(5)	1.6(8)
Ti(1)-C(3)-C(4)-C(5)	-58.1(5)
C(2)-C(3)-C(4)-C(8)	-169.0(9)
Ti(1)-C(3)-C(4)-C(8)	131.3(11)
C(2)-C(3)-C(4)-Ti(2)	85.5(7)
Ti(1)-C(3)-C(4)-Ti(2)	25.8(5)
C(2)-C(3)-C(4)-Ti(1)	59.7(5)
C(3)-C(4)-C(5)-C(6)	-173.7(6)
C(8)-C(4)-C(5)-C(6)	0.5(8)
Ti(2)-C(4)-C(5)-C(6)	61.9(5)
Ti(1)-C(4)-C(5)-C(6)	124.4(5)
C(3)-C(4)-C(5)-C(1)	-0.7(8)
C(8)-C(4)-C(5)-C(1)	173.5(6)
Ti(2)-C(4)-C(5)-C(1)	-125.2(5)
Ti(1)-C(4)-C(5)-C(1)	-62.6(5)
C(3)-C(4)-C(5)-Ti(1)	61.9(5)
C(8)-C(4)-C(5)-Ti(1)	-123.8(5)
Ti(2)-C(4)-C(5)-Ti(1)	-62.53(16)
C(3)-C(4)-C(5)-Ti(2)	124.4(5)
C(8)-C(4)-C(5)-Ti(2)	-61.3(5)
Ti(1)-C(4)-C(5)-Ti(2)	62.53(16)
C(2)-C(1)-C(5)-C(6)	168.7(9)
Si(1)-C(1)-C(5)-C(6)	17.5(14)
Ti(1)-C(1)-C(5)-C(6)	-123.0(10)
C(2)-C(1)-C(5)-C(4)	-0.4(8)
Si(1)-C(1)-C(5)-C(4)	-151.5(6)
Ti(1)-C(1)-C(5)-C(4)	67.9(5)
C(2)-C(1)-C(5)-Ti(1)	-68.3(4)
Si(1)-C(1)-C(5)-Ti(1)	140.6(7)
C(2)-C(1)-C(5)-Ti(2)	-79.9(7)

Si(1)-C(1)-C(5)-Ti(2)	129.0(6)
Ti(1)-C(1)-C(5)-Ti(2)	-11.6(5)
C(4)-C(5)-C(6)-C(7)	2.5(8)
C(1)-C(5)-C(6)-C(7)	-166.7(9)
Ti(1)-C(5)-C(6)-C(7)	89.8(7)
Ti(2)-C(5)-C(6)-C(7)	63.1(5)
C(4)-C(5)-C(6)-Ti(2)	-60.6(5)
C(1)-C(5)-C(6)-Ti(2)	130.1(10)
Ti(1)-C(5)-C(6)-Ti(2)	26.6(5)
C(5)-C(6)-C(7)-C(8)	-4.9(8)
Ti(2)-C(6)-C(7)-C(8)	60.5(5)
C(5)-C(6)-C(7)-Ti(2)	-65.4(5)
C(6)-C(7)-C(8)-C(4)	5.1(8)
Ti(2)-C(7)-C(8)-C(4)	68.9(5)
C(6)-C(7)-C(8)-Si(2)	173.8(5)
Ti(2)-C(7)-C(8)-Si(2)	-122.5(6)
C(6)-C(7)-C(8)-Ti(2)	-63.7(5)
C(3)-C(4)-C(8)-C(7)	167.1(10)
C(5)-C(4)-C(8)-C(7)	-3.4(8)
Ti(2)-C(4)-C(8)-C(7)	-68.9(5)
Ti(1)-C(4)-C(8)-C(7)	-77.7(8)
C(3)-C(4)-C(8)-Si(2)	-0.8(14)
C(5)-C(4)-C(8)-Si(2)	-171.3(5)
Ti(2)-C(4)-C(8)-Si(2)	123.2(6)
Ti(1)-C(4)-C(8)-Si(2)	114.4(6)
C(3)-C(4)-C(8)-Ti(2)	-124.0(11)
C(5)-C(4)-C(8)-Ti(2)	65.5(5)
Ti(1)-C(4)-C(8)-Ti(2)	-8.8(5)
C(31)-C(27)-C(28)-C(29)	4.7(8)
Si(3)-C(27)-C(28)-C(29)	169.3(5)
Ti(1)-C(27)-C(28)-C(29)	-64.1(5)
C(31)-C(27)-C(28)-Ti(1)	68.8(4)
Si(3)-C(27)-C(28)-Ti(1)	-126.6(6)
C(27)-C(28)-C(29)-C(30)	-6.6(9)
Ti(1)-C(28)-C(29)-C(30)	-66.1(5)
C(27)-C(28)-C(29)-Ti(1)	59.4(5)
C(28)-C(29)-C(30)-C(31)	5.8(8)
Ti(1)-C(29)-C(30)-C(31)	-57.3(5)
C(28)-C(29)-C(30)-C(34)	-167.1(10)
Ti(1)-C(29)-C(30)-C(34)	129.8(11)
C(28)-C(29)-C(30)-Ti(2)	91.5(7)
Ti(1)-C(29)-C(30)-Ti(2)	28.4(5)
C(28)-C(29)-C(30)-Ti(1)	63.1(5)
C(29)-C(30)-C(31)-C(32)	-176.5(6)
C(34)-C(30)-C(31)-C(32)	-1.0(8)
Ti(2)-C(30)-C(31)-C(32)	61.5(5)
Ti(1)-C(30)-C(31)-C(32)	123.5(5)
C(29)-C(30)-C(31)-C(27)	-2.9(8)
C(34)-C(30)-C(31)-C(27)	172.7(6)
Ti(2)-C(30)-C(31)-C(27)	-124.9(5)

Ti(1)-C(30)-C(31)-C(27)	-62.8(5)
C(29)-C(30)-C(31)-Ti(1)	60.0(5)
C(34)-C(30)-C(31)-Ti(1)	-124.5(5)
Ti(2)-C(30)-C(31)-Ti(1)	-62.05(15)
C(29)-C(30)-C(31)-Ti(2)	122.0(6)
C(34)-C(30)-C(31)-Ti(2)	-62.5(5)
Ti(1)-C(30)-C(31)-Ti(2)	62.05(15)
C(28)-C(27)-C(31)-C(30)	-1.0(8)
Si(3)-C(27)-C(31)-C(30)	-165.3(6)
Ti(1)-C(27)-C(31)-C(30)	69.5(5)
C(28)-C(27)-C(31)-C(32)	169.0(9)
Si(3)-C(27)-C(31)-C(32)	4.7(14)
Ti(1)-C(27)-C(31)-C(32)	-120.5(10)
C(28)-C(27)-C(31)-Ti(1)	-70.5(5)
Si(3)-C(27)-C(31)-Ti(1)	125.2(6)
C(28)-C(27)-C(31)-Ti(2)	-77.5(7)
Si(3)-C(27)-C(31)-Ti(2)	118.2(6)
Ti(1)-C(27)-C(31)-Ti(2)	-7.0(5)
C(30)-C(31)-C(32)-C(33)	2.4(8)
C(27)-C(31)-C(32)-C(33)	-167.7(9)
Ti(1)-C(31)-C(32)-C(33)	91.3(7)
Ti(2)-C(31)-C(32)-C(33)	61.3(5)
C(30)-C(31)-C(32)-Ti(2)	-58.9(5)
C(27)-C(31)-C(32)-Ti(2)	131.1(10)
Ti(1)-C(31)-C(32)-Ti(2)	30.1(5)
C(31)-C(32)-C(33)-C(34)	-3.0(8)
Ti(2)-C(32)-C(33)-C(34)	60.8(5)
C(31)-C(32)-C(33)-Ti(2)	-63.8(5)
C(32)-C(33)-C(34)-C(30)	2.3(8)
Ti(2)-C(33)-C(34)-C(30)	67.5(5)
C(32)-C(33)-C(34)-Si(4)	148.2(5)
Ti(2)-C(33)-C(34)-Si(4)	-146.6(5)
C(32)-C(33)-C(34)-Ti(2)	-65.2(5)
C(31)-C(30)-C(34)-C(33)	-0.7(8)
C(29)-C(30)-C(34)-C(33)	172.1(10)
Ti(2)-C(30)-C(34)-C(33)	-68.1(5)
Ti(1)-C(30)-C(34)-C(33)	-75.8(7)
C(31)-C(30)-C(34)-Si(4)	-140.3(6)
C(29)-C(30)-C(34)-Si(4)	32.5(15)
Ti(2)-C(30)-C(34)-Si(4)	152.4(6)
Ti(1)-C(30)-C(34)-Si(4)	144.6(5)
C(31)-C(30)-C(34)-Ti(2)	67.3(5)
C(29)-C(30)-C(34)-Ti(2)	-119.8(11)
Ti(1)-C(30)-C(34)-Ti(2)	-7.7(5)
C(2)-C(1)-Si(1)-C(15)	-79.5(6)
C(5)-C(1)-Si(1)-C(15)	68.1(8)
Ti(1)-C(1)-Si(1)-C(15)	-176.8(5)
C(2)-C(1)-Si(1)-C(9)	157.0(5)
C(5)-C(1)-Si(1)-C(9)	-55.5(8)
Ti(1)-C(1)-Si(1)-C(9)	59.7(7)

C(2)-C(1)-Si(1)-C(12)	35.3(6)
C(5)-C(1)-Si(1)-C(12)	-177.1(7)
Ti(1)-C(1)-Si(1)-C(12)	-62.0(6)
C(17)-C(15)-Si(1)-C(1)	-68.1(7)
C(16)-C(15)-Si(1)-C(1)	56.6(7)
C(17)-C(15)-Si(1)-C(9)	58.5(7)
C(16)-C(15)-Si(1)-C(9)	-176.8(6)
C(17)-C(15)-Si(1)-C(12)	177.7(6)
C(16)-C(15)-Si(1)-C(12)	-57.6(7)
C(10)-C(9)-Si(1)-C(1)	161.9(5)
C(11)-C(9)-Si(1)-C(1)	35.2(7)
C(10)-C(9)-Si(1)-C(15)	41.0(7)
C(11)-C(9)-Si(1)-C(15)	-85.6(6)
C(10)-C(9)-Si(1)-C(12)	-77.5(6)
C(11)-C(9)-Si(1)-C(12)	155.9(5)
C(13)-C(12)-Si(1)-C(1)	-171.2(6)
C(14)-C(12)-Si(1)-C(1)	61.2(7)
C(13)-C(12)-Si(1)-C(15)	-57.7(7)
C(14)-C(12)-Si(1)-C(15)	174.7(6)
C(13)-C(12)-Si(1)-C(9)	62.8(7)
C(14)-C(12)-Si(1)-C(9)	-64.7(7)
C(7)-C(8)-Si(2)-C(18)	-91.8(7)
C(4)-C(8)-Si(2)-C(18)	74.1(7)
Ti(2)-C(8)-Si(2)-C(18)	173.0(4)
C(7)-C(8)-Si(2)-C(21)	149.1(6)
C(4)-C(8)-Si(2)-C(21)	-45.1(7)
Ti(2)-C(8)-Si(2)-C(21)	53.8(6)
C(7)-C(8)-Si(2)-C(24)	25.1(7)
C(4)-C(8)-Si(2)-C(24)	-169.1(6)
Ti(2)-C(8)-Si(2)-C(24)	-70.2(5)
C(19)-C(18)-Si(2)-C(8)	55.2(7)
C(20)-C(18)-Si(2)-C(8)	-68.5(8)
C(19)-C(18)-Si(2)-C(21)	174.0(6)
C(20)-C(18)-Si(2)-C(21)	50.4(8)
C(19)-C(18)-Si(2)-C(24)	-60.9(7)
C(20)-C(18)-Si(2)-C(24)	175.5(7)
C(23)-C(21)-Si(2)-C(8)	178.1(7)
C(22)-C(21)-Si(2)-C(8)	-53.6(7)
C(23)-C(21)-Si(2)-C(18)	58.1(8)
C(22)-C(21)-Si(2)-C(18)	-173.6(6)
C(23)-C(21)-Si(2)-C(24)	-62.9(8)
C(22)-C(21)-Si(2)-C(24)	65.4(7)
C(26)-C(24)-Si(2)-C(8)	-164.8(6)
C(25)-C(24)-Si(2)-C(8)	65.6(7)
C(26)-C(24)-Si(2)-C(18)	-46.4(7)
C(25)-C(24)-Si(2)-C(18)	-176.0(6)
C(26)-C(24)-Si(2)-C(21)	75.1(7)
C(25)-C(24)-Si(2)-C(21)	-54.5(7)
C(28)-C(27)-Si(3)-C(41)	-99.7(7)
C(31)-C(27)-Si(3)-C(41)	61.4(7)

Ti(1)-C(27)-Si(3)-C(41)	159.7(4)
C(28)-C(27)-Si(3)-C(35)	140.8(6)
C(31)-C(27)-Si(3)-C(35)	-58.1(7)
Ti(1)-C(27)-Si(3)-C(35)	40.2(5)
C(28)-C(27)-Si(3)-C(38)	17.3(8)
C(31)-C(27)-Si(3)-C(38)	178.4(6)
Ti(1)-C(27)-Si(3)-C(38)	-83.3(5)
C(43)-C(41)-Si(3)-C(27)	-65.0(7)
C(42)-C(41)-Si(3)-C(27)	61.3(7)
C(43)-C(41)-Si(3)-C(35)	51.4(7)
C(42)-C(41)-Si(3)-C(35)	177.7(6)
C(43)-C(41)-Si(3)-C(38)	176.7(6)
C(42)-C(41)-Si(3)-C(38)	-57.0(7)
C(36)-C(35)-Si(3)-C(27)	-170.0(6)
C(37)-C(35)-Si(3)-C(27)	-42.2(7)
C(36)-C(35)-Si(3)-C(41)	71.5(7)
C(37)-C(35)-Si(3)-C(41)	-160.7(6)
C(36)-C(35)-Si(3)-C(38)	-49.7(7)
C(37)-C(35)-Si(3)-C(38)	78.1(7)
C(39)-C(38)-Si(3)-C(27)	70.2(7)
C(40)-C(38)-Si(3)-C(27)	-162.4(5)
C(39)-C(38)-Si(3)-C(41)	-171.4(6)
C(40)-C(38)-Si(3)-C(41)	-44.0(7)
C(39)-C(38)-Si(3)-C(35)	-48.2(7)
C(40)-C(38)-Si(3)-C(35)	79.2(6)
C(33)-C(34)-Si(4)-C(44)	166.1(5)
C(30)-C(34)-Si(4)-C(44)	-58.3(8)
Ti(2)-C(34)-Si(4)-C(44)	65.9(8)
C(33)-C(34)-Si(4)-C(50)	38.3(6)
C(30)-C(34)-Si(4)-C(50)	174.0(7)
Ti(2)-C(34)-Si(4)-C(50)	-61.8(8)
C(33)-C(34)-Si(4)-C(47)	-76.9(6)
C(30)-C(34)-Si(4)-C(47)	58.8(8)
Ti(2)-C(34)-Si(4)-C(47)	-177.1(6)
C(45)-C(44)-Si(4)-C(34)	-78.4(6)
C(46)-C(44)-Si(4)-C(34)	155.2(5)
C(45)-C(44)-Si(4)-C(50)	46.5(7)
C(46)-C(44)-Si(4)-C(50)	-79.9(6)
C(45)-C(44)-Si(4)-C(47)	164.5(6)
C(46)-C(44)-Si(4)-C(47)	38.1(7)
C(52)-C(50)-Si(4)-C(34)	-175.3(6)
C(51)-C(50)-Si(4)-C(34)	54.1(7)
C(52)-C(50)-Si(4)-C(44)	57.5(7)
C(51)-C(50)-Si(4)-C(44)	-73.2(7)
C(52)-C(50)-Si(4)-C(47)	-60.2(7)
C(51)-C(50)-Si(4)-C(47)	169.1(6)
C(49)-C(47)-Si(4)-C(34)	66.7(7)
C(48)-C(47)-Si(4)-C(34)	-59.0(7)
C(49)-C(47)-Si(4)-C(44)	-172.1(6)
C(48)-C(47)-Si(4)-C(44)	62.2(7)

C(49)-C(47)-Si(4)-C(50)	-49.7(7)
C(48)-C(47)-Si(4)-C(50)	-175.4(6)
C(2)-C(1)-Ti(1)-C(27)	-114.3(6)
C(5)-C(1)-Ti(1)-C(27)	136.5(5)
Si(1)-C(1)-Ti(1)-C(27)	0.5(10)
C(2)-C(1)-Ti(1)-C(5)	109.2(6)
Si(1)-C(1)-Ti(1)-C(5)	-136.0(8)
C(5)-C(1)-Ti(1)-C(2)	-109.2(6)
Si(1)-C(1)-Ti(1)-C(2)	114.8(7)
C(2)-C(1)-Ti(1)-C(31)	170.2(4)
C(5)-C(1)-Ti(1)-C(31)	61.1(6)
Si(1)-C(1)-Ti(1)-C(31)	-75.0(7)
C(2)-C(1)-Ti(1)-C(28)	-121.8(4)
C(5)-C(1)-Ti(1)-C(28)	129.0(4)
Si(1)-C(1)-Ti(1)-C(28)	-7.0(7)
C(2)-C(1)-Ti(1)-Ti(2)	118.5(4)
C(5)-C(1)-Ti(1)-Ti(2)	9.3(4)
Si(1)-C(1)-Ti(1)-Ti(2)	-126.7(5)
C(2)-C(1)-Ti(1)-C(3)	34.1(4)
C(5)-C(1)-Ti(1)-C(3)	-75.1(4)
Si(1)-C(1)-Ti(1)-C(3)	148.9(7)
C(2)-C(1)-Ti(1)-C(29)	-152.9(4)
C(5)-C(1)-Ti(1)-C(29)	98.0(4)
Si(1)-C(1)-Ti(1)-C(29)	-38.1(6)
C(2)-C(1)-Ti(1)-C(4)	73.2(4)
C(5)-C(1)-Ti(1)-C(4)	-35.9(4)
Si(1)-C(1)-Ti(1)-C(4)	-172.0(7)
C(2)-C(1)-Ti(1)-C(30)	176.2(4)
C(5)-C(1)-Ti(1)-C(30)	67.0(5)
Si(1)-C(1)-Ti(1)-C(30)	-69.0(6)
C(28)-C(27)-Ti(1)-C(1)	-11.8(8)
C(31)-C(27)-Ti(1)-C(1)	-121.8(6)
Si(3)-C(27)-Ti(1)-C(1)	113.2(6)
C(28)-C(27)-Ti(1)-C(5)	74.5(8)
C(31)-C(27)-Ti(1)-C(5)	-35.5(8)
Si(3)-C(27)-Ti(1)-C(5)	-160.5(5)
C(28)-C(27)-Ti(1)-C(2)	-82.0(6)
C(31)-C(27)-Ti(1)-C(2)	168.0(4)
Si(3)-C(27)-Ti(1)-C(2)	42.9(7)
C(28)-C(27)-Ti(1)-C(31)	109.9(6)
Si(3)-C(27)-Ti(1)-C(31)	-125.1(7)
C(31)-C(27)-Ti(1)-C(28)	-109.9(6)
Si(3)-C(27)-Ti(1)-C(28)	125.0(7)
C(28)-C(27)-Ti(1)-Ti(2)	115.5(4)
C(31)-C(27)-Ti(1)-Ti(2)	5.6(4)
Si(3)-C(27)-Ti(1)-Ti(2)	-119.5(4)
C(28)-C(27)-Ti(1)-C(3)	-141.8(5)
C(31)-C(27)-Ti(1)-C(3)	108.3(5)
Si(3)-C(27)-Ti(1)-C(3)	-16.8(7)
C(28)-C(27)-Ti(1)-C(29)	34.2(4)

C(31)-C(27)-Ti(1)-C(29)	-75.8(4)
Si(3)-C(27)-Ti(1)-C(29)	159.1(6)
C(28)-C(27)-Ti(1)-C(4)	155.1(5)
C(31)-C(27)-Ti(1)-C(4)	45.2(7)
Si(3)-C(27)-Ti(1)-C(4)	-79.9(7)
C(28)-C(27)-Ti(1)-C(30)	73.7(5)
C(31)-C(27)-Ti(1)-C(30)	-36.3(4)
Si(3)-C(27)-Ti(1)-C(30)	-161.3(6)
C(6)-C(5)-Ti(1)-C(1)	140.4(9)
C(4)-C(5)-Ti(1)-C(1)	-117.4(6)
Ti(2)-C(5)-Ti(1)-C(1)	169.6(5)
C(6)-C(5)-Ti(1)-C(27)	17.6(11)
C(4)-C(5)-Ti(1)-C(27)	119.8(6)
C(1)-C(5)-Ti(1)-C(27)	-122.8(6)
Ti(2)-C(5)-Ti(1)-C(27)	46.9(7)
C(6)-C(5)-Ti(1)-C(2)	-178.1(8)
C(4)-C(5)-Ti(1)-C(2)	-75.9(4)
C(1)-C(5)-Ti(1)-C(2)	41.5(4)
Ti(2)-C(5)-Ti(1)-C(2)	-148.9(3)
C(6)-C(5)-Ti(1)-C(31)	-6.7(8)
C(4)-C(5)-Ti(1)-C(31)	95.5(4)
C(1)-C(5)-Ti(1)-C(31)	-147.0(4)
Ti(2)-C(5)-Ti(1)-C(31)	22.6(3)
C(6)-C(5)-Ti(1)-C(28)	66.9(8)
C(4)-C(5)-Ti(1)-C(28)	169.1(4)
C(1)-C(5)-Ti(1)-C(28)	-73.5(5)
Ti(2)-C(5)-Ti(1)-C(28)	96.2(3)
C(6)-C(5)-Ti(1)-Ti(2)	-29.3(6)
C(4)-C(5)-Ti(1)-Ti(2)	72.9(4)
C(1)-C(5)-Ti(1)-Ti(2)	-169.6(5)
C(6)-C(5)-Ti(1)-C(3)	-137.9(8)
C(4)-C(5)-Ti(1)-C(3)	-35.7(4)
C(1)-C(5)-Ti(1)-C(3)	81.7(4)
Ti(2)-C(5)-Ti(1)-C(3)	-108.7(3)
C(6)-C(5)-Ti(1)-C(29)	52.1(7)
C(4)-C(5)-Ti(1)-C(29)	154.3(4)
C(1)-C(5)-Ti(1)-C(29)	-88.3(4)
Ti(2)-C(5)-Ti(1)-C(29)	81.3(2)
C(6)-C(5)-Ti(1)-C(4)	-102.2(8)
C(1)-C(5)-Ti(1)-C(4)	117.4(6)
Ti(2)-C(5)-Ti(1)-C(4)	-72.9(4)
C(6)-C(5)-Ti(1)-C(30)	18.3(7)
C(4)-C(5)-Ti(1)-C(30)	120.5(4)
C(1)-C(5)-Ti(1)-C(30)	-122.1(4)
Ti(2)-C(5)-Ti(1)-C(30)	47.6(2)
C(3)-C(2)-Ti(1)-C(1)	119.7(6)
C(3)-C(2)-Ti(1)-C(27)	-113.8(5)
C(1)-C(2)-Ti(1)-C(27)	126.5(5)
C(3)-C(2)-Ti(1)-C(5)	77.5(5)
C(1)-C(2)-Ti(1)-C(5)	-42.2(4)

C(3)-C(2)-Ti(1)-C(31)	-15(2)
C(1)-C(2)-Ti(1)-C(31)	-134.7(19)
C(3)-C(2)-Ti(1)-C(28)	-160.7(4)
C(1)-C(2)-Ti(1)-C(28)	79.6(5)
C(3)-C(2)-Ti(1)-Ti(2)	47.0(5)
C(1)-C(2)-Ti(1)-Ti(2)	-72.7(4)
C(1)-C(2)-Ti(1)-C(3)	-119.7(6)
C(3)-C(2)-Ti(1)-C(29)	155.6(4)
C(1)-C(2)-Ti(1)-C(29)	35.9(5)
C(3)-C(2)-Ti(1)-C(4)	35.8(4)
C(1)-C(2)-Ti(1)-C(4)	-83.9(4)
C(3)-C(2)-Ti(1)-C(30)	112.6(6)
C(1)-C(2)-Ti(1)-C(30)	-7.1(7)
C(30)-C(31)-Ti(1)-C(1)	9.8(7)
C(32)-C(31)-Ti(1)-C(1)	-94.8(8)
C(27)-C(31)-Ti(1)-C(1)	124.9(5)
Ti(2)-C(31)-Ti(1)-C(1)	-61.3(5)
C(30)-C(31)-Ti(1)-C(27)	-115.2(6)
C(32)-C(31)-Ti(1)-C(27)	140.3(9)
Ti(2)-C(31)-Ti(1)-C(27)	173.7(4)
C(30)-C(31)-Ti(1)-C(5)	48.3(5)
C(32)-C(31)-Ti(1)-C(5)	-56.2(7)
C(27)-C(31)-Ti(1)-C(5)	163.5(4)
Ti(2)-C(31)-Ti(1)-C(5)	-22.8(3)
C(30)-C(31)-Ti(1)-C(2)	136.5(19)
C(32)-C(31)-Ti(1)-C(2)	32(2)
C(27)-C(31)-Ti(1)-C(2)	-108(2)
Ti(2)-C(31)-Ti(1)-C(2)	65(2)
C(30)-C(31)-Ti(1)-C(28)	-75.1(4)
C(32)-C(31)-Ti(1)-C(28)	-179.6(8)
C(27)-C(31)-Ti(1)-C(28)	40.1(4)
Ti(2)-C(31)-Ti(1)-C(28)	-146.2(3)
C(30)-C(31)-Ti(1)-Ti(2)	71.1(4)
C(32)-C(31)-Ti(1)-Ti(2)	-33.4(6)
C(27)-C(31)-Ti(1)-Ti(2)	-173.7(4)
C(30)-C(31)-Ti(1)-C(3)	123.7(4)
C(32)-C(31)-Ti(1)-C(3)	19.2(9)
C(27)-C(31)-Ti(1)-C(3)	-121.1(5)
Ti(2)-C(31)-Ti(1)-C(3)	52.6(4)
C(30)-C(31)-Ti(1)-C(29)	-35.0(4)
C(32)-C(31)-Ti(1)-C(29)	-139.5(7)
C(27)-C(31)-Ti(1)-C(29)	80.2(4)
Ti(2)-C(31)-Ti(1)-C(29)	-106.1(3)
C(30)-C(31)-Ti(1)-C(4)	88.9(4)
C(32)-C(31)-Ti(1)-C(4)	-15.6(7)
C(27)-C(31)-Ti(1)-C(4)	-155.9(4)
Ti(2)-C(31)-Ti(1)-C(4)	17.8(3)
C(32)-C(31)-Ti(1)-C(30)	-104.5(8)
C(27)-C(31)-Ti(1)-C(30)	115.2(6)
Ti(2)-C(31)-Ti(1)-C(30)	-71.1(4)

C(29)-C(28)-Ti(1)-C(1)	-66.7(5)
C(27)-C(28)-Ti(1)-C(1)	173.4(4)
C(29)-C(28)-Ti(1)-C(27)	119.9(6)
C(29)-C(28)-Ti(1)-C(5)	-26.9(6)
C(27)-C(28)-Ti(1)-C(5)	-146.8(4)
C(29)-C(28)-Ti(1)-C(2)	-107.1(5)
C(27)-C(28)-Ti(1)-C(2)	133.0(4)
C(29)-C(28)-Ti(1)-C(31)	77.8(5)
C(27)-C(28)-Ti(1)-C(31)	-42.2(4)
C(29)-C(28)-Ti(1)-Ti(2)	45.8(5)
C(27)-C(28)-Ti(1)-Ti(2)	-74.1(5)
C(29)-C(28)-Ti(1)-C(3)	-136.4(7)
C(27)-C(28)-Ti(1)-C(3)	103.7(7)
C(27)-C(28)-Ti(1)-C(29)	-119.9(7)
C(29)-C(28)-Ti(1)-C(4)	-0.8(13)
C(27)-C(28)-Ti(1)-C(4)	-120.8(10)
C(29)-C(28)-Ti(1)-C(30)	37.0(4)
C(27)-C(28)-Ti(1)-C(30)	-83.0(5)
C(2)-C(3)-Ti(1)-C(1)	-37.0(4)
C(4)-C(3)-Ti(1)-C(1)	81.2(4)
C(2)-C(3)-Ti(1)-C(27)	116.0(5)
C(4)-C(3)-Ti(1)-C(27)	-125.8(5)
C(2)-C(3)-Ti(1)-C(5)	-81.1(5)
C(4)-C(3)-Ti(1)-C(5)	37.2(4)
C(4)-C(3)-Ti(1)-C(2)	118.3(6)
C(2)-C(3)-Ti(1)-C(31)	177.1(4)
C(4)-C(3)-Ti(1)-C(31)	-64.6(6)
C(2)-C(3)-Ti(1)-C(28)	43.5(9)
C(4)-C(3)-Ti(1)-C(28)	161.8(7)
C(2)-C(3)-Ti(1)-Ti(2)	-138.5(4)
C(4)-C(3)-Ti(1)-Ti(2)	-20.2(4)
C(2)-C(3)-Ti(1)-C(29)	-55.0(8)
C(4)-C(3)-Ti(1)-C(29)	63.2(8)
C(2)-C(3)-Ti(1)-C(4)	-118.3(6)
C(2)-C(3)-Ti(1)-C(30)	-126.6(5)
C(4)-C(3)-Ti(1)-C(30)	-8.3(7)
C(28)-C(29)-Ti(1)-C(1)	121.9(5)
C(30)-C(29)-Ti(1)-C(1)	-122.2(4)
C(28)-C(29)-Ti(1)-C(27)	-36.1(4)
C(30)-C(29)-Ti(1)-C(27)	79.8(5)
C(28)-C(29)-Ti(1)-C(5)	160.0(5)
C(30)-C(29)-Ti(1)-C(5)	-84.1(5)
C(28)-C(29)-Ti(1)-C(2)	101.0(5)
C(30)-C(29)-Ti(1)-C(2)	-143.1(4)
C(28)-C(29)-Ti(1)-C(31)	-80.4(5)
C(30)-C(29)-Ti(1)-C(31)	35.5(4)
C(30)-C(29)-Ti(1)-C(28)	115.9(7)
C(28)-C(29)-Ti(1)-Ti(2)	-138.4(4)
C(30)-C(29)-Ti(1)-Ti(2)	-22.5(4)
C(28)-C(29)-Ti(1)-C(3)	137.7(6)

C(30)-C(29)-Ti(1)-C(3)	-106.4(7)
C(28)-C(29)-Ti(1)-C(4)	179.7(4)
C(30)-C(29)-Ti(1)-C(4)	-64.4(5)
C(28)-C(29)-Ti(1)-C(30)	-115.9(7)
C(3)-C(4)-Ti(1)-C(1)	-79.2(4)
C(5)-C(4)-Ti(1)-C(1)	38.3(4)
C(8)-C(4)-Ti(1)-C(1)	134.3(8)
Ti(2)-C(4)-Ti(1)-C(1)	124.8(3)
C(3)-C(4)-Ti(1)-C(27)	108.5(6)
C(5)-C(4)-Ti(1)-C(27)	-134.0(6)
C(8)-C(4)-Ti(1)-C(27)	-38.0(10)
Ti(2)-C(4)-Ti(1)-C(27)	-47.6(6)
C(3)-C(4)-Ti(1)-C(5)	-117.5(6)
C(8)-C(4)-Ti(1)-C(5)	96.0(8)
Ti(2)-C(4)-Ti(1)-C(5)	86.5(4)
C(3)-C(4)-Ti(1)-C(2)	-35.9(4)
C(5)-C(4)-Ti(1)-C(2)	81.6(4)
C(8)-C(4)-Ti(1)-C(2)	177.6(8)
Ti(2)-C(4)-Ti(1)-C(2)	168.0(3)
C(3)-C(4)-Ti(1)-C(31)	137.7(4)
C(5)-C(4)-Ti(1)-C(31)	-104.9(4)
C(8)-C(4)-Ti(1)-C(31)	-8.9(7)
Ti(2)-C(4)-Ti(1)-C(31)	-18.4(3)
C(3)-C(4)-Ti(1)-C(28)	-151.7(9)
C(5)-C(4)-Ti(1)-C(28)	-34.2(12)
C(8)-C(4)-Ti(1)-C(28)	61.8(13)
Ti(2)-C(4)-Ti(1)-C(28)	52.2(10)
C(3)-C(4)-Ti(1)-Ti(2)	156.1(5)
C(5)-C(4)-Ti(1)-Ti(2)	-86.5(4)
C(8)-C(4)-Ti(1)-Ti(2)	9.6(6)
C(5)-C(4)-Ti(1)-C(3)	117.5(6)
C(8)-C(4)-Ti(1)-C(3)	-146.5(9)
Ti(2)-C(4)-Ti(1)-C(3)	-156.1(5)
C(3)-C(4)-Ti(1)-C(29)	-152.3(4)
C(5)-C(4)-Ti(1)-C(29)	-34.8(5)
C(8)-C(4)-Ti(1)-C(29)	61.2(8)
Ti(2)-C(4)-Ti(1)-C(29)	51.6(3)
C(3)-C(4)-Ti(1)-C(30)	175.0(4)
C(5)-C(4)-Ti(1)-C(30)	-67.6(4)
C(8)-C(4)-Ti(1)-C(30)	28.4(7)
Ti(2)-C(4)-Ti(1)-C(30)	18.9(3)
C(31)-C(30)-Ti(1)-C(1)	-174.3(4)
C(29)-C(30)-Ti(1)-C(1)	66.4(5)
C(34)-C(30)-Ti(1)-C(1)	-78.0(7)
Ti(2)-C(30)-Ti(1)-C(1)	-86.4(2)
C(31)-C(30)-Ti(1)-C(27)	39.9(4)
C(29)-C(30)-Ti(1)-C(27)	-79.4(5)
C(34)-C(30)-Ti(1)-C(27)	136.2(7)
Ti(2)-C(30)-Ti(1)-C(27)	127.8(3)
C(31)-C(30)-Ti(1)-C(5)	-139.8(4)

C(29)-C(30)-Ti(1)-C(5)	100.9(5)
C(34)-C(30)-Ti(1)-C(5)	-43.5(7)
Ti(2)-C(30)-Ti(1)-C(5)	-51.9(2)
C(31)-C(30)-Ti(1)-C(2)	-169.6(5)
C(29)-C(30)-Ti(1)-C(2)	71.1(6)
C(34)-C(30)-Ti(1)-C(2)	-73.3(8)
Ti(2)-C(30)-Ti(1)-C(2)	-81.7(5)
C(29)-C(30)-Ti(1)-C(31)	-119.3(6)
C(34)-C(30)-Ti(1)-C(31)	96.3(8)
Ti(2)-C(30)-Ti(1)-C(31)	87.9(4)
C(31)-C(30)-Ti(1)-C(28)	82.3(4)
C(29)-C(30)-Ti(1)-C(28)	-37.0(4)
C(34)-C(30)-Ti(1)-C(28)	178.6(8)
Ti(2)-C(30)-Ti(1)-C(28)	170.2(3)
C(31)-C(30)-Ti(1)-Ti(2)	-87.9(4)
C(29)-C(30)-Ti(1)-Ti(2)	152.8(5)
C(34)-C(30)-Ti(1)-Ti(2)	8.4(6)
C(31)-C(30)-Ti(1)-C(3)	-102.2(5)
C(29)-C(30)-Ti(1)-C(3)	138.5(5)
C(34)-C(30)-Ti(1)-C(3)	-5.9(9)
Ti(2)-C(30)-Ti(1)-C(3)	-14.3(5)
C(31)-C(30)-Ti(1)-C(29)	119.3(6)
C(34)-C(30)-Ti(1)-C(29)	-144.4(9)
Ti(2)-C(30)-Ti(1)-C(29)	-152.8(5)
C(31)-C(30)-Ti(1)-C(4)	-107.2(4)
C(29)-C(30)-Ti(1)-C(4)	133.5(4)
C(34)-C(30)-Ti(1)-C(4)	-10.9(7)
Ti(2)-C(30)-Ti(1)-C(4)	-19.3(3)
C(33)-C(34)-Ti(2)-C(8)	-110.0(6)
C(30)-C(34)-Ti(2)-C(8)	139.9(5)
Si(4)-C(34)-Ti(2)-C(8)	2.3(11)
C(33)-C(34)-Ti(2)-C(30)	110.1(6)
Si(4)-C(34)-Ti(2)-C(30)	-137.5(9)
C(30)-C(34)-Ti(2)-C(33)	-110.1(6)
Si(4)-C(34)-Ti(2)-C(33)	112.4(8)
C(33)-C(34)-Ti(2)-C(7)	-120.2(4)
C(30)-C(34)-Ti(2)-C(7)	129.7(4)
Si(4)-C(34)-Ti(2)-C(7)	-7.8(8)
C(33)-C(34)-Ti(2)-C(4)	168.6(5)
C(30)-C(34)-Ti(2)-C(4)	58.6(7)
Si(4)-C(34)-Ti(2)-C(4)	-79.0(9)
C(33)-C(34)-Ti(2)-Ti(1)	116.5(4)
C(30)-C(34)-Ti(2)-Ti(1)	6.5(4)
Si(4)-C(34)-Ti(2)-Ti(1)	-131.1(7)
C(33)-C(34)-Ti(2)-C(6)	-152.3(4)
C(30)-C(34)-Ti(2)-C(6)	97.6(4)
Si(4)-C(34)-Ti(2)-C(6)	-40.0(7)
C(33)-C(34)-Ti(2)-C(32)	33.9(4)
C(30)-C(34)-Ti(2)-C(32)	-76.2(4)
Si(4)-C(34)-Ti(2)-C(32)	146.3(8)

C(33)-C(34)-Ti(2)-C(31)	73.8(4)
C(30)-C(34)-Ti(2)-C(31)	-36.3(4)
Si(4)-C(34)-Ti(2)-C(31)	-173.8(8)
C(33)-C(34)-Ti(2)-C(5)	175.2(4)
C(30)-C(34)-Ti(2)-C(5)	65.1(5)
Si(4)-C(34)-Ti(2)-C(5)	-72.4(7)
C(7)-C(8)-Ti(2)-C(34)	-15.7(7)
C(4)-C(8)-Ti(2)-C(34)	-126.7(6)
Si(2)-C(8)-Ti(2)-C(34)	106.0(6)
C(7)-C(8)-Ti(2)-C(30)	78.7(8)
C(4)-C(8)-Ti(2)-C(30)	-32.3(9)
Si(2)-C(8)-Ti(2)-C(30)	-159.6(5)
C(7)-C(8)-Ti(2)-C(33)	-85.9(6)
C(4)-C(8)-Ti(2)-C(33)	163.1(5)
Si(2)-C(8)-Ti(2)-C(33)	35.8(8)
C(4)-C(8)-Ti(2)-C(7)	-111.0(6)
Si(2)-C(8)-Ti(2)-C(7)	121.7(7)
C(7)-C(8)-Ti(2)-C(4)	111.0(6)
Si(2)-C(8)-Ti(2)-C(4)	-127.3(7)
C(7)-C(8)-Ti(2)-Ti(1)	118.2(4)
C(4)-C(8)-Ti(2)-Ti(1)	7.2(4)
Si(2)-C(8)-Ti(2)-Ti(1)	-120.1(4)
C(7)-C(8)-Ti(2)-C(6)	34.4(4)
C(4)-C(8)-Ti(2)-C(6)	-76.6(5)
Si(2)-C(8)-Ti(2)-C(6)	156.1(6)
C(7)-C(8)-Ti(2)-C(32)	-142.2(5)
C(4)-C(8)-Ti(2)-C(32)	106.8(5)
Si(2)-C(8)-Ti(2)-C(32)	-20.6(7)
C(7)-C(8)-Ti(2)-C(31)	158.0(5)
C(4)-C(8)-Ti(2)-C(31)	47.0(7)
Si(2)-C(8)-Ti(2)-C(31)	-80.3(6)
C(7)-C(8)-Ti(2)-C(5)	74.6(4)
C(4)-C(8)-Ti(2)-C(5)	-36.4(4)
Si(2)-C(8)-Ti(2)-C(5)	-163.7(6)
C(31)-C(30)-Ti(2)-C(34)	-116.2(6)
C(29)-C(30)-Ti(2)-C(34)	141.4(9)
Ti(1)-C(30)-Ti(2)-C(34)	172.9(5)
C(31)-C(30)-Ti(2)-C(8)	115.3(7)
C(29)-C(30)-Ti(2)-C(8)	12.9(12)
C(34)-C(30)-Ti(2)-C(8)	-128.5(7)
Ti(1)-C(30)-Ti(2)-C(8)	44.4(7)
C(31)-C(30)-Ti(2)-C(33)	-75.4(5)
C(29)-C(30)-Ti(2)-C(33)	-177.8(8)
C(34)-C(30)-Ti(2)-C(33)	40.8(4)
Ti(1)-C(30)-Ti(2)-C(33)	-146.2(3)
C(31)-C(30)-Ti(2)-C(7)	168.6(4)
C(29)-C(30)-Ti(2)-C(7)	66.2(8)
C(34)-C(30)-Ti(2)-C(7)	-75.2(5)
Ti(1)-C(30)-Ti(2)-C(7)	97.8(3)
C(31)-C(30)-Ti(2)-C(4)	93.1(5)

C(29)-C(30)-Ti(2)-C(4)	-9.3(8)
C(34)-C(30)-Ti(2)-C(4)	-150.7(4)
Ti(1)-C(30)-Ti(2)-C(4)	22.2(3)
C(31)-C(30)-Ti(2)-Ti(1)	70.9(4)
C(29)-C(30)-Ti(2)-Ti(1)	-31.5(6)
C(34)-C(30)-Ti(2)-Ti(1)	-172.9(5)
C(31)-C(30)-Ti(2)-C(6)	153.5(4)
C(29)-C(30)-Ti(2)-C(6)	51.1(7)
C(34)-C(30)-Ti(2)-C(6)	-90.3(4)
Ti(1)-C(30)-Ti(2)-C(6)	82.6(2)
C(31)-C(30)-Ti(2)-C(32)	-35.5(4)
C(29)-C(30)-Ti(2)-C(32)	-137.9(8)
C(34)-C(30)-Ti(2)-C(32)	80.7(5)
Ti(1)-C(30)-Ti(2)-C(32)	-106.3(3)
C(29)-C(30)-Ti(2)-C(31)	-102.4(8)
C(34)-C(30)-Ti(2)-C(31)	116.2(6)
Ti(1)-C(30)-Ti(2)-C(31)	-70.9(4)
C(31)-C(30)-Ti(2)-C(5)	118.9(4)
C(29)-C(30)-Ti(2)-C(5)	16.5(7)
C(34)-C(30)-Ti(2)-C(5)	-124.9(4)
Ti(1)-C(30)-Ti(2)-C(5)	48.0(2)
C(32)-C(33)-Ti(2)-C(34)	120.1(6)
C(32)-C(33)-Ti(2)-C(8)	-108.7(5)
C(34)-C(33)-Ti(2)-C(8)	131.2(5)
C(32)-C(33)-Ti(2)-C(30)	78.3(5)
C(34)-C(33)-Ti(2)-C(30)	-41.8(4)
C(32)-C(33)-Ti(2)-C(7)	-156.8(4)
C(34)-C(33)-Ti(2)-C(7)	83.0(5)
C(32)-C(33)-Ti(2)-C(4)	-26.9(17)
C(34)-C(33)-Ti(2)-C(4)	-147.0(14)
C(32)-C(33)-Ti(2)-Ti(1)	44.9(5)
C(34)-C(33)-Ti(2)-Ti(1)	-75.3(4)
C(32)-C(33)-Ti(2)-C(6)	157.8(4)
C(34)-C(33)-Ti(2)-C(6)	37.7(6)
C(34)-C(33)-Ti(2)-C(32)	-120.1(6)
C(32)-C(33)-Ti(2)-C(31)	37.1(4)
C(34)-C(33)-Ti(2)-C(31)	-83.1(4)
C(32)-C(33)-Ti(2)-C(5)	110.7(6)
C(34)-C(33)-Ti(2)-C(5)	-9.4(8)
C(6)-C(7)-Ti(2)-C(34)	-68.1(5)
C(8)-C(7)-Ti(2)-C(34)	171.7(4)
C(6)-C(7)-Ti(2)-C(8)	120.3(7)
C(6)-C(7)-Ti(2)-C(30)	-26.8(6)
C(8)-C(7)-Ti(2)-C(30)	-147.1(4)
C(6)-C(7)-Ti(2)-C(33)	-109.7(5)
C(8)-C(7)-Ti(2)-C(33)	130.0(4)
C(6)-C(7)-Ti(2)-C(4)	79.4(5)
C(8)-C(7)-Ti(2)-C(4)	-40.9(4)
C(6)-C(7)-Ti(2)-Ti(1)	48.9(5)
C(8)-C(7)-Ti(2)-Ti(1)	-71.3(4)

C(8)-C(7)-Ti(2)-C(6)	-120.3(7)
C(6)-C(7)-Ti(2)-C(32)	-143.9(7)
C(8)-C(7)-Ti(2)-C(32)	95.9(8)
C(6)-C(7)-Ti(2)-C(31)	4.0(14)
C(8)-C(7)-Ti(2)-C(31)	-116.2(12)
C(6)-C(7)-Ti(2)-C(5)	37.5(4)
C(8)-C(7)-Ti(2)-C(5)	-82.8(5)
C(3)-C(4)-Ti(2)-C(34)	-89.6(8)
C(5)-C(4)-Ti(2)-C(34)	10.3(8)
C(8)-C(4)-Ti(2)-C(34)	127.2(6)
Ti(1)-C(4)-Ti(2)-C(34)	-60.9(6)
C(3)-C(4)-Ti(2)-C(8)	143.1(9)
C(5)-C(4)-Ti(2)-C(8)	-117.0(6)
Ti(1)-C(4)-Ti(2)-C(8)	171.9(5)
C(3)-C(4)-Ti(2)-C(30)	-51.4(7)
C(5)-C(4)-Ti(2)-C(30)	48.5(5)
C(8)-C(4)-Ti(2)-C(30)	165.5(4)
Ti(1)-C(4)-Ti(2)-C(30)	-22.6(3)
C(3)-C(4)-Ti(2)-C(33)	47.8(18)
C(5)-C(4)-Ti(2)-C(33)	147.7(14)
C(8)-C(4)-Ti(2)-C(33)	-95.3(15)
Ti(1)-C(4)-Ti(2)-C(33)	76.6(15)
C(3)-C(4)-Ti(2)-C(7)	-177.0(7)
C(5)-C(4)-Ti(2)-C(7)	-77.1(4)
C(8)-C(4)-Ti(2)-C(7)	39.9(4)
Ti(1)-C(4)-Ti(2)-C(7)	-148.2(3)
C(3)-C(4)-Ti(2)-Ti(1)	-28.8(6)
C(5)-C(4)-Ti(2)-Ti(1)	71.1(4)
C(8)-C(4)-Ti(2)-Ti(1)	-171.9(5)
C(3)-C(4)-Ti(2)-C(6)	-136.3(7)
C(5)-C(4)-Ti(2)-C(6)	-36.4(4)
C(8)-C(4)-Ti(2)-C(6)	80.5(5)
Ti(1)-C(4)-Ti(2)-C(6)	-107.6(3)
C(3)-C(4)-Ti(2)-C(32)	26.1(8)
C(5)-C(4)-Ti(2)-C(32)	126.0(4)
C(8)-C(4)-Ti(2)-C(32)	-117.0(5)
Ti(1)-C(4)-Ti(2)-C(32)	54.9(4)
C(3)-C(4)-Ti(2)-C(31)	-11.0(7)
C(5)-C(4)-Ti(2)-C(31)	88.9(4)
C(8)-C(4)-Ti(2)-C(31)	-154.1(4)
Ti(1)-C(4)-Ti(2)-C(31)	17.8(3)
C(3)-C(4)-Ti(2)-C(5)	-99.9(7)
C(8)-C(4)-Ti(2)-C(5)	117.0(6)
Ti(1)-C(4)-Ti(2)-C(5)	-71.1(4)
C(1)-Ti(1)-Ti(2)-C(34)	107.5(3)
C(27)-Ti(1)-Ti(2)-C(34)	-47.9(3)
C(5)-Ti(1)-Ti(2)-C(34)	113.9(3)
C(2)-Ti(1)-Ti(2)-C(34)	143.3(3)
C(31)-Ti(1)-Ti(2)-C(34)	-44.0(3)
C(28)-Ti(1)-Ti(2)-C(34)	-13.2(3)

C(3)-Ti(1)-Ti(2)-C(34)	167.6(3)
C(29)-Ti(1)-Ti(2)-C(34)	10.4(3)
C(4)-Ti(1)-Ti(2)-C(34)	154.5(3)
C(30)-Ti(1)-Ti(2)-C(34)	-4.4(3)
C(1)-Ti(1)-Ti(2)-C(8)	-51.9(3)
C(27)-Ti(1)-Ti(2)-C(8)	152.7(3)
C(5)-Ti(1)-Ti(2)-C(8)	-45.5(3)
C(2)-Ti(1)-Ti(2)-C(8)	-16.0(3)
C(31)-Ti(1)-Ti(2)-C(8)	156.6(3)
C(28)-Ti(1)-Ti(2)-C(8)	-172.6(3)
C(3)-Ti(1)-Ti(2)-C(8)	8.3(3)
C(29)-Ti(1)-Ti(2)-C(8)	-149.0(3)
C(4)-Ti(1)-Ti(2)-C(8)	-4.9(3)
C(30)-Ti(1)-Ti(2)-C(8)	-163.8(3)
C(1)-Ti(1)-Ti(2)-C(30)	111.9(3)
C(27)-Ti(1)-Ti(2)-C(30)	-43.5(3)
C(5)-Ti(1)-Ti(2)-C(30)	118.3(3)
C(2)-Ti(1)-Ti(2)-C(30)	147.7(3)
C(31)-Ti(1)-Ti(2)-C(30)	-39.6(3)
C(28)-Ti(1)-Ti(2)-C(30)	-8.8(3)
C(3)-Ti(1)-Ti(2)-C(30)	172.0(3)
C(29)-Ti(1)-Ti(2)-C(30)	14.8(3)
C(4)-Ti(1)-Ti(2)-C(30)	158.9(3)
C(1)-Ti(1)-Ti(2)-C(33)	143.8(3)
C(27)-Ti(1)-Ti(2)-C(33)	-11.6(3)
C(5)-Ti(1)-Ti(2)-C(33)	150.2(3)
C(2)-Ti(1)-Ti(2)-C(33)	179.6(3)
C(31)-Ti(1)-Ti(2)-C(33)	-7.7(3)
C(28)-Ti(1)-Ti(2)-C(33)	23.1(3)
C(3)-Ti(1)-Ti(2)-C(33)	-156.1(3)
C(29)-Ti(1)-Ti(2)-C(33)	46.7(3)
C(4)-Ti(1)-Ti(2)-C(33)	-169.2(3)
C(30)-Ti(1)-Ti(2)-C(33)	31.9(3)
C(1)-Ti(1)-Ti(2)-C(7)	-17.9(3)
C(27)-Ti(1)-Ti(2)-C(7)	-173.3(3)
C(5)-Ti(1)-Ti(2)-C(7)	-11.5(3)
C(2)-Ti(1)-Ti(2)-C(7)	17.9(3)
C(31)-Ti(1)-Ti(2)-C(7)	-169.4(3)
C(28)-Ti(1)-Ti(2)-C(7)	-138.6(3)
C(3)-Ti(1)-Ti(2)-C(7)	42.2(3)
C(29)-Ti(1)-Ti(2)-C(7)	-115.1(3)
C(4)-Ti(1)-Ti(2)-C(7)	29.1(3)
C(30)-Ti(1)-Ti(2)-C(7)	-129.8(3)
C(1)-Ti(1)-Ti(2)-C(4)	-47.0(3)
C(27)-Ti(1)-Ti(2)-C(4)	157.6(3)
C(5)-Ti(1)-Ti(2)-C(4)	-40.6(3)
C(2)-Ti(1)-Ti(2)-C(4)	-11.2(3)
C(31)-Ti(1)-Ti(2)-C(4)	161.5(3)
C(28)-Ti(1)-Ti(2)-C(4)	-167.7(3)
C(3)-Ti(1)-Ti(2)-C(4)	13.1(3)

C(29)-Ti(1)-Ti(2)-C(4)	-144.1(3)
C(30)-Ti(1)-Ti(2)-C(4)	-158.9(3)
C(1)-Ti(1)-Ti(2)-C(6)	7.3(3)
C(27)-Ti(1)-Ti(2)-C(6)	-148.1(3)
C(5)-Ti(1)-Ti(2)-C(6)	13.7(3)
C(2)-Ti(1)-Ti(2)-C(6)	43.1(3)
C(31)-Ti(1)-Ti(2)-C(6)	-144.2(3)
C(28)-Ti(1)-Ti(2)-C(6)	-113.4(3)
C(3)-Ti(1)-Ti(2)-C(6)	67.4(3)
C(29)-Ti(1)-Ti(2)-C(6)	-89.9(3)
C(4)-Ti(1)-Ti(2)-C(6)	54.3(3)
C(30)-Ti(1)-Ti(2)-C(6)	-104.6(3)
C(1)-Ti(1)-Ti(2)-C(32)	167.1(3)
C(27)-Ti(1)-Ti(2)-C(32)	11.7(3)
C(5)-Ti(1)-Ti(2)-C(32)	173.5(3)
C(2)-Ti(1)-Ti(2)-C(32)	-157.1(3)
C(31)-Ti(1)-Ti(2)-C(32)	15.5(3)
C(28)-Ti(1)-Ti(2)-C(32)	46.4(3)
C(3)-Ti(1)-Ti(2)-C(32)	-132.8(3)
C(29)-Ti(1)-Ti(2)-C(32)	69.9(3)
C(4)-Ti(1)-Ti(2)-C(32)	-145.9(3)
C(30)-Ti(1)-Ti(2)-C(32)	55.2(3)
C(1)-Ti(1)-Ti(2)-C(31)	151.5(3)
C(27)-Ti(1)-Ti(2)-C(31)	-3.9(3)
C(5)-Ti(1)-Ti(2)-C(31)	157.9(3)
C(2)-Ti(1)-Ti(2)-C(31)	-172.6(3)
C(28)-Ti(1)-Ti(2)-C(31)	30.8(3)
C(3)-Ti(1)-Ti(2)-C(31)	-148.3(3)
C(29)-Ti(1)-Ti(2)-C(31)	54.4(3)
C(4)-Ti(1)-Ti(2)-C(31)	-161.5(3)
C(30)-Ti(1)-Ti(2)-C(31)	39.6(3)
C(1)-Ti(1)-Ti(2)-C(5)	-6.4(3)
C(27)-Ti(1)-Ti(2)-C(5)	-161.8(3)
C(2)-Ti(1)-Ti(2)-C(5)	29.4(3)
C(31)-Ti(1)-Ti(2)-C(5)	-157.9(3)
C(28)-Ti(1)-Ti(2)-C(5)	-127.1(3)
C(3)-Ti(1)-Ti(2)-C(5)	53.7(3)
C(29)-Ti(1)-Ti(2)-C(5)	-103.5(3)
C(4)-Ti(1)-Ti(2)-C(5)	40.6(3)
C(30)-Ti(1)-Ti(2)-C(5)	-118.3(3)
C(7)-C(6)-Ti(2)-C(34)	122.4(5)
C(5)-C(6)-Ti(2)-C(34)	-122.0(4)
C(7)-C(6)-Ti(2)-C(8)	-35.7(4)
C(5)-C(6)-Ti(2)-C(8)	80.0(5)
C(7)-C(6)-Ti(2)-C(30)	160.7(5)
C(5)-C(6)-Ti(2)-C(30)	-83.6(5)
C(7)-C(6)-Ti(2)-C(33)	100.5(5)
C(5)-C(6)-Ti(2)-C(33)	-143.9(4)
C(5)-C(6)-Ti(2)-C(7)	115.6(7)
C(7)-C(6)-Ti(2)-C(4)	-78.6(5)

C(5)-C(6)-Ti(2)-C(4)	37.1(4)
C(7)-C(6)-Ti(2)-Ti(1)	-136.1(5)
C(5)-C(6)-Ti(2)-Ti(1)	-20.5(4)
C(7)-C(6)-Ti(2)-C(32)	138.1(7)
C(5)-C(6)-Ti(2)-C(32)	-106.2(8)
C(7)-C(6)-Ti(2)-C(31)	-178.8(4)
C(5)-C(6)-Ti(2)-C(31)	-63.1(6)
C(7)-C(6)-Ti(2)-C(5)	-115.6(7)
C(33)-C(32)-Ti(2)-C(34)	-36.6(4)
C(31)-C(32)-Ti(2)-C(34)	79.9(5)
C(33)-C(32)-Ti(2)-C(8)	117.0(5)
C(31)-C(32)-Ti(2)-C(8)	-126.4(5)
C(33)-C(32)-Ti(2)-C(30)	-80.6(5)
C(31)-C(32)-Ti(2)-C(30)	36.0(4)
C(31)-C(32)-Ti(2)-C(33)	116.6(7)
C(33)-C(32)-Ti(2)-C(7)	51.5(9)
C(31)-C(32)-Ti(2)-C(7)	168.1(6)
C(33)-C(32)-Ti(2)-C(4)	173.4(4)
C(31)-C(32)-Ti(2)-C(4)	-70.1(6)
C(33)-C(32)-Ti(2)-Ti(1)	-140.3(4)
C(31)-C(32)-Ti(2)-Ti(1)	-23.7(4)
C(33)-C(32)-Ti(2)-C(6)	-54.5(9)
C(31)-C(32)-Ti(2)-C(6)	62.0(9)
C(33)-C(32)-Ti(2)-C(31)	-116.6(7)
C(33)-C(32)-Ti(2)-C(5)	-130.5(5)
C(31)-C(32)-Ti(2)-C(5)	-13.9(7)
C(30)-C(31)-Ti(2)-C(34)	39.1(4)
C(32)-C(31)-Ti(2)-C(34)	-79.7(5)
C(27)-C(31)-Ti(2)-C(34)	136.0(7)
Ti(1)-C(31)-Ti(2)-C(34)	128.5(3)
C(30)-C(31)-Ti(2)-C(8)	-137.5(5)
C(32)-C(31)-Ti(2)-C(8)	103.7(6)
C(27)-C(31)-Ti(2)-C(8)	-40.6(9)
Ti(1)-C(31)-Ti(2)-C(8)	-48.1(5)
C(32)-C(31)-Ti(2)-C(30)	-118.8(6)
C(27)-C(31)-Ti(2)-C(30)	96.9(8)
Ti(1)-C(31)-Ti(2)-C(30)	89.4(4)
C(30)-C(31)-Ti(2)-C(33)	82.3(5)
C(32)-C(31)-Ti(2)-C(33)	-36.5(4)
C(27)-C(31)-Ti(2)-C(33)	179.2(7)
Ti(1)-C(31)-Ti(2)-C(33)	171.7(3)
C(30)-C(31)-Ti(2)-C(7)	-39.6(13)
C(32)-C(31)-Ti(2)-C(7)	-158.4(11)
C(27)-C(31)-Ti(2)-C(7)	57.3(15)
Ti(1)-C(31)-Ti(2)-C(7)	49.8(12)
C(30)-C(31)-Ti(2)-C(4)	-107.9(4)
C(32)-C(31)-Ti(2)-C(4)	133.2(5)
C(27)-C(31)-Ti(2)-C(4)	-11.1(7)
Ti(1)-C(31)-Ti(2)-C(4)	-18.6(3)
C(30)-C(31)-Ti(2)-Ti(1)	-89.4(4)

C(32)-C(31)-Ti(2)-Ti(1)	151.8(5)
C(27)-C(31)-Ti(2)-Ti(1)	7.5(5)
C(30)-C(31)-Ti(2)-C(6)	-36.5(6)
C(32)-C(31)-Ti(2)-C(6)	-155.3(5)
C(27)-C(31)-Ti(2)-C(6)	60.4(7)
Ti(1)-C(31)-Ti(2)-C(6)	52.9(4)
C(30)-C(31)-Ti(2)-C(32)	118.8(6)
C(27)-C(31)-Ti(2)-C(32)	-144.3(9)
Ti(1)-C(31)-Ti(2)-C(32)	-151.8(5)
C(30)-C(31)-Ti(2)-C(5)	-69.6(5)
C(32)-C(31)-Ti(2)-C(5)	171.6(4)
C(27)-C(31)-Ti(2)-C(5)	27.3(7)
Ti(1)-C(31)-Ti(2)-C(5)	19.8(3)
C(6)-C(5)-Ti(2)-C(34)	68.5(5)
C(4)-C(5)-Ti(2)-C(34)	-174.5(4)
C(1)-C(5)-Ti(2)-C(34)	-74.3(7)
Ti(1)-C(5)-Ti(2)-C(34)	-86.9(3)
C(6)-C(5)-Ti(2)-C(8)	-79.2(5)
C(4)-C(5)-Ti(2)-C(8)	37.8(4)
C(1)-C(5)-Ti(2)-C(8)	138.0(8)
Ti(1)-C(5)-Ti(2)-C(8)	125.5(3)
C(6)-C(5)-Ti(2)-C(30)	102.4(5)
C(4)-C(5)-Ti(2)-C(30)	-140.5(4)
C(1)-C(5)-Ti(2)-C(30)	-40.4(7)
Ti(1)-C(5)-Ti(2)-C(30)	-52.9(2)
C(6)-C(5)-Ti(2)-C(33)	74.8(7)
C(4)-C(5)-Ti(2)-C(33)	-168.2(6)
C(1)-C(5)-Ti(2)-C(33)	-68.1(9)
Ti(1)-C(5)-Ti(2)-C(33)	-80.6(6)
C(6)-C(5)-Ti(2)-C(7)	-37.2(4)
C(4)-C(5)-Ti(2)-C(7)	79.8(4)
C(1)-C(5)-Ti(2)-C(7)	179.9(8)
Ti(1)-C(5)-Ti(2)-C(7)	167.4(3)
C(6)-C(5)-Ti(2)-C(4)	-117.0(6)
C(1)-C(5)-Ti(2)-C(4)	100.1(8)
Ti(1)-C(5)-Ti(2)-C(4)	87.6(4)
C(6)-C(5)-Ti(2)-Ti(1)	155.4(5)
C(4)-C(5)-Ti(2)-Ti(1)	-87.6(4)
C(1)-C(5)-Ti(2)-Ti(1)	12.5(6)
C(4)-C(5)-Ti(2)-C(6)	117.0(6)
C(1)-C(5)-Ti(2)-C(6)	-142.8(9)
Ti(1)-C(5)-Ti(2)-C(6)	-155.4(5)
C(6)-C(5)-Ti(2)-C(32)	143.7(5)
C(4)-C(5)-Ti(2)-C(32)	-99.3(6)
C(1)-C(5)-Ti(2)-C(32)	0.8(10)
Ti(1)-C(5)-Ti(2)-C(32)	-11.7(5)
C(6)-C(5)-Ti(2)-C(31)	135.2(4)
C(4)-C(5)-Ti(2)-C(31)	-107.8(4)
C(1)-C(5)-Ti(2)-C(31)	-7.6(7)
Ti(1)-C(5)-Ti(2)-C(31)	-20.1(3)

Cartesian coordinates for optimized structures of $Ti_2(C_8H_6)_2$:

D_{2h} symmetry Imaginary wavenumber –i80 cm^{-1}

C	-0.73839508	0.00000000	1.91046605
C	0.73839508	0.00000000	1.91046605
C	1.16792315	1.38617789	2.02158907
C	0.00000000	2.18580662	2.16502157
C	-1.16792315	1.38617789	2.02158907
C	1.16792315	-1.38617789	2.02158907
C	-1.16792315	-1.38617789	2.02158907
C	0.00000000	-2.18580662	2.16502157
H	2.19225812	1.74241584	2.09725587
H	0.00000000	3.26570869	2.30532552
H	-2.19225812	1.74241584	2.09725587
H	2.19225812	-1.74241584	2.09725587
H	-2.19225812	-1.74241584	2.09725587
H	0.00000000	-3.26570869	2.30532552
C	-0.73839508	0.00000000	-1.91048192
C	0.73839508	0.00000000	-1.91048192
C	1.16792315	1.38617789	-2.02160494
C	0.00000000	2.18580662	-2.16503744
C	-1.16792315	1.38617789	-2.02160494
C	1.16792315	-1.38617789	-2.02160494
C	-1.16792315	-1.38617789	-2.02160494
C	0.00000000	-2.18580662	-2.16503744
H	2.19225812	1.74241584	-2.09727173

H	0.00000000	3.26570869	-2.30534139
H	-2.19225812	1.74241584	-2.09727173
H	2.19225812	-1.74241584	-2.09727173
H	-2.19225812	-1.74241584	-2.09727173
H	0.00000000	-3.26570869	-2.30534139
Ti	0.00000000	1.16737704	-0.00000793
Ti	0.00000000	-1.16737704	-0.00000793

C_{2v} symmetry All frequencies positive

C	0.79766479	0.57836000	0.53523236
C	1.15665999	0.57836000	-0.89165713
C	1.35902733	1.96016432	-1.27505595
C	1.21316963	2.76416565	-0.11379869
C	0.77523505	1.96393713	0.98521908
C	1.35902733	-0.80344432	-1.27505595
C	0.77523505	-0.80721713	0.98521908
C	1.21316963	-1.60744565	-0.11379869
H	1.64279336	2.31938587	-2.26255289
H	1.35068358	3.84399979	-0.08418932
H	0.62696705	2.31212651	2.00205460
H	1.64279336	-1.16266587	-2.26255289
H	0.62696705	-1.15540651	2.00205460
H	1.35068358	-2.68727979	-0.08418932
C	-2.56933366	0.57836000	0.53523236
C	-2.92832886	0.57836000	-0.89165713
C	-3.13069620	1.96016432	-1.27505595

C	-2.98483849	2.76416565	-0.11379869
C	-2.54690391	1.96393713	0.98521908
C	-3.13069620	-0.80344432	-1.27505595
C	-2.54690391	-0.80721713	0.98521908
C	-2.98483849	-1.60744565	-0.11379869
H	-3.41446223	2.31938587	-2.26255289
H	-3.12235244	3.84399979	-0.08418932
H	-2.39863591	2.31212651	2.00205460
H	-3.41446223	-1.16266587	-2.26255289
H	-2.39863591	-1.15540651	2.00205460
H	-3.12235244	-2.68727979	-0.08418932
Ti	-0.88583443	1.76374193	-0.58359737
Ti	-0.88583443	-0.60702193	-0.58359737

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