Supplementary Material (ESI) for Chemical Communications

Supplementary data

Supporting information for the paper entitled "Snapshots of an oxidatively induced α-hydrogen abstraction reaction to prepare a terminal and four-coordinate titanium imide"

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Experimental Section

General Considerations. Unless otherwise stated, all operations were performed in a M. Braun Lab Master double-dry box under an atmosphere of purified nitrogen or using high vacuum standard Schlenk techniques under an argon atmosphere.[1] Anhydrous *n*-Hexane, pentane, toluene, and benzene were purchased from Aldrich in sure-sealed reservoirs (18 L) and dried by passage through two columns of activated alumina and a Q-5 column.[2] Diethylether and CH_2Cl_2 were dried by passage through a column of activated alumina.[2] THF was distilled, under nitrogen, from purple sodium benzophenone ketyl and stored under sodium metal. Distilled THF was transferred under vacuum into bombs before being pumped into a dry box. C_6D_6, and CD_2Cl_2 were purchased from Cambridge Isotope Laboratory (CIL), degassed and dried over 4 Å molecular sieves and CaH_2, respectively. CD_2Cl_2 was vacuum transferred from the CaF_2 mixture and stored in a reaction vessel under N_2. Celite, alumina, and 4 Å molecular sieves were activated under vacuum overnight at 200ºC. Li(Nacnac) ($Nacnac^-$ = [Ar]NC(Me)CHC(Me)N[Ar], Ar = 2,6-$(CHMe_2)_2C_6H_3$),[3] and (Nacnac)$TiCl_2$(THF),[4,5] Tl(OTf),[6] $[CPh_3][B(C_6F_5)_4]$[7] were prepared according to the literature. LiNHAr was prepared by deprotonation of freshly distilled aniline at -35°C with *n*-BuLi in hexanes. The white solid was collected via filtration, washed with pentane, and dried under reduced pressure. $FeCp^*_2$ (Cp^* = $C_5Me_5^-$) was purchased from Strem chemicals and used without further purification. All other chemical were used as received. Solution infrared spectra (CaF_2 plates) were measured using a Nicolet 510P FTIR spectrometer. CHN analysis were performed by Desert Analytics, Tucson, AZ. ^1H, ^{13}C, and ^{19}F NMR spectra were recorded on a varian 400 or 300 MHz NMR spectrometers. ^1H and ^{13}C NMR are reported with reference to solvent resonances (residual C_6D_5H in C_6D_6, 7.16 ppm and 128.0 ppm; residual $CHDCl_2$ in CD_2Cl_2, 5.32 ppm 53.8ppm). ^{19}F NMR chemical shifts are reported with respect to external $HOCOCF_3$ (-78.5 ppm). ^{11}B NMR chemical shift are reported with respect to external BF_3•Et_2O (0.0 ppm). Magnetic moments were obtained by the method of Evans.[8, 9] Cyclic voltammetry were collected with the assistance of an E2 Epsilon potentiostat/galvanostat with a PC unit controlled by Bioanalytical systems (BAS) software. Room temperature and liquid helium temperature X-band EPR spectra were recorded on a Bruker EMX spectrometer. Acquisition and simulation were performed using an integrated WIN-EPR software package (Bruker). Electronic absorption spectra were recorded from 190 to 820 (HP 8452A Diode Array) UV-vis spectrophotometer. X-ray diffraction data were collected on a SMART6000 (Bruker) system under a stream of N_2(g) at low temperatures.

Synthesis of $[FeCp^*_2][B(C_6F_5)_4]$

In a 100 mL round bottom flask was dissolved $FeCp^*_2$ [188 mg, 0.576 mmol] in 10 mL of Et_2O. To the yellow solution was added dropwise an Et_2O (8 mL) solution containing $[CPh_3][(C_6F_5)_4]$[7] [524 mg, 0.568 mmol] causing an immediate color change to pale green concomitant with precipitation of a pale green solid. The mixture was allowed to react for 10 minutes, upon which the light green solid was collected via filtration, washed with pentane until washings were clear, and dried under vacuum to afford pure product $[FeCp^*_2][B(C_6F_5)_4]$[10] [400 mg, 70% yield].

Synthesis of (Nacnac)Ti(NHAr)$_2$ (1)

In a vial was suspended (Nacnac)$TiCl_2$(THF) [100 mg, 0.16 mmol] in 10 mL Et_2O and the solution cooled to -35 ºC. To the solution was added a cold Et_2O solution (5 mL) of LiNHAr [64.7 mg, 0.35 mmol]. After stirring for 4 hours the solution was filtered and dried under reduced pressure. The green powder was extracted with pentane, filtered, concentrated, and the solution cooled at -35 ºC to afford in four crops large green crystals of (Nacnac)Ti(NHAr)$_2$ **(1)** [123 mg, 0.15 mmol, 92% yield].

For **1**: ^{1}H NMR (25°C, 399.8 MHz, C_6D_6): δ 11.93 ($\Delta\nu_{1/2}$ = 44.9 Hz) , 10.23 ($\Delta\nu_{1/2}$ = 56.0 Hz), 9.25 ($\Delta\nu_{1/2}$ = 84.2 Hz), 7.94 ($\Delta\nu_{1/2}$ = 84.6 H z), 6.65 (br), 4.52 ($\Delta\nu_{1/2}$ = 70.5 Hz), 2.68 (br), 2.26 ($\Delta\nu_{1/2}$ = 206.7 Hz), 1.16 (br). IR (C_6H_6, CaF_2): 3323 (w), 3239 (w), 3098 (m), 3065 (m), 3044 (m), 3022 (m), 2963 (s), 2926 (m), 2868 (m), 1589 (m), 1523 (m), 1485 (m), 1471 (s), 1469 (s), 1431 (s), 1372 (s), 1315 (s), 1256 (s), 1195 (m), 1171 (m), 1153 (w), 1105 (m) cm^{-1}. UV-vis (Et_2O, 23°C): 642 nm (ε = 415), 360 nm (ε = 13048), 284 nm (ε = 19226). μ_{eff} = 2.20 μ_B (C_6D_6, 298 K, Evans' method). Anal. Anal. Calcd. For $C_{53}H_{77}N_4Ti$: C, 77.81; H, 9.49; N, 6.85. Found: C, 78.14; H, 9.66; N, 6.73.

Synthesis of [(Nacnac)Ti(NHAr)$_2$][OTf] (2)

In a reaction vessel was dissolved in 10 mL of THF (Nacnac)Ti(NHAr)$_2$ **(1)** [150 mg, 0.18 mmol] and the solution cooled to -100 ^{o}C. To the solution was added a cold THF solution containing AgOTf [51.82 mg, 0.20 mmol]. After stirring for 5 min the solution was filtered to remove the Ag metal and the filtrate dried under reduced pressure. Washing of the red solids with Et_2O affords pure [(Nacnac)Ti(NHAr)$_2$][OTf] **(2)** [126.20 mg,0.13 mmol, 71% yield]. Recrystallization of **2** from CH_2Cl_2 layered with hexane at -35^{o}C afford dark-red crystals.

For **2**: ^{1}H NMR (23^{o}C, 399.8 MHz, CD_2Cl_2): δ 11.05 (s, N*H*, 1H), 10.43 (s, N*H*, 1H), 7.21 (t, C_6H_3, 2H), 7.12 (d, C_6H_3, 2H), 7.04 (d, C_6H_3, 2H), 6.88 (t, C_6H_3, 1H), 6.76 (d, C_6H_3, 2H), 6.69 (t, C_6H_3, 1H), 6.54 (d, C_6H_3, 2H), 6.37 (s, ArNC(CH$_3$)C*H*C(CH$_3$)NAr, 1H), 2.66 (septet, C*H*(CH$_3$)$_2$, 2H), 2.32 (septet, C*H*(CH$_3$)$_2$, 2H), 2.25 (septet, C*H*(CH$_3$)$_2$, 1H), 1.85 (s, ArNC(C*H*$_3$)CHC(C*H*$_3$)NAr, 6H), 1.41 (septet, C*H*(CH$_3$)$_2$, 1H), 1.33 (septet, C*H*(CH$_3$)$_2$, 2H), 1.13 (d, CH(C*H*$_3$)$_2$, 6H), 0.98 (d, CH(C*H*$_3$)$_2$, 6H), 0.86 (d, CH(C*H*$_3$)$_2$, 6H), 0.75 (d, CH(C*H*$_3$)$_2$, 6H), 0.59 (d, CH(C*H*$_3$)$_2$, 6H), 0.32 (d, CH(C*H*$_3$)$_2$, 6H), 0.29 (d, CH(C*H*$_3$)$_2$, 6H), 0.03 (d, CH(C*H*$_3$)$_2$, 6H). ^{13}C NMR (25^{o}C, 100.6 MHz, CD_2Cl_2): δ 172.5 (ArN*C*(CH$_3$)CH*C*(CH$_3$)NAr), 151.1 (aryl), 149.7 (aryl), 143.3 (aryl), 141.4 (aryl), 140. 9 (aryl), 139.2 (aryl), 138.1 (aryl), 134.4 (aryl), 130.3 (aryl), 128.9 (aryl), 126.6 (aryl), 126.5 (a ryl), 126.4 (aryl), 124.2 (aryl), 123.5 (aryl), 123.3 (aryl), 107.0 (ArNC(CH$_3$)*C*HC(CH$_3$)NAr), 32.90 (*C*H(CH$_3$)$_2$), 29.96 (*C*H(CH$_3$)$_2$), 29.10 (*C*H(CH$_3$)$_2$), 28.30 (*C*H(CH$_3$)$_2$), 28.01 (*C*H(CH$_3$)$_2$), 26.90 (*C*H$_3$), 26.08 (*C*H$_3$), 25.46 (*C*H$_3$), 25.06 (*C*H$_3$), 24.59 (ArNC(*C*H$_3$)CHC(*C*H$_3$)NAr), 24.54 (*C*H$_3$), 24.01 (*C*H$_3$), 23.65 (*C*H$_3$), 21.74 (*C*H$_3$). ^{19}F NMR

(23°C, 282.3 MHz, C_6D_6): δ −79.7 (s, O_3SCF_3). IR (C_6H_6, CaF_2): 3247 (w), 3138 (w), 3059 (w), 2910 (s), 2931 (m), 2871 (w), 1539 (m), 1467 (m), 1427 (m), 1355 (m), 1309 (s), 1226 (m), 1151 (m), 1108 (w), 1032 (s) cm^{-1}. UV-vis (CH_2Cl_2, 23°C): 330 nm (ε = 51670). Anal. Calcd. For $C_{54}H_{77}N_4O_3SF_3Ti$: C, 67.06; H, 8.02; N, 5.79. Found: C, 65.11; H, 7.76; N, 6.52. Attempts to get satisfactory elemental analysis were unsuccessful, presumably because of the gradual decomposition of **2**.

Synthesis of [(Nacnac)Ti(NHAr)$_2$][B(C_6F_5)$_4$] (3)

In a vial was dissolved in 15 mL of Et_2O (Nacnac)Ti(NHAr)$_2$ [96.4 mg, 0.12 mmol] and the solution cooled to -35 ºC. To the green solution was added a cold suspension of [FeCp*$_2$][B(C_6F_5)$_4$] [117 mg, 0.12 mmol]. After stirring for 10 min the solution was filtered and dried under reduced pressure. Washing of the brick-red solid with pentane affords pure [(Nacnac)Ti(NHAr)$_2$][B(C_6F_5)$_4$] **(3)** [165 mg,0.11 mmol, 92% yield].

For **3**: ^{1}H NMR (23°C, 399.8 MHz, CD_2Cl_2): 11.42 (s, N*H*, 1H), 10.85 (s, N*H*, 1H), 7.54 (t, C_6H_3, 2H), 7.44 (d, C_6H_3, 2H), 7.38 (d, C_6H_3, 2H), 7.22 (t, C_6H_3, 1H), 7.10 (d, C_6H_3, 2H), 7.02 (t, C_6H_3, 1H), 6.86 (d, C_6H_3, 2H), 6.52 (s, ArNC(CH_3)C*H*C(CH_3)NAr, 1H), 2.98 (septet, C*H*(CH_3)$_2$, 2H), 2.62 (septet, C*H*(CH_3)$_2$, 2H), 2.55 (septet, C*H*(CH_3)$_2$, 1H), 2.15 (s, ArNC(C*H*$_3$)CHC(C*H*$_3$)NAr, 6H), 1.76 (septet, C*H*(CH_3)$_2$, 1H), 1.66 (septet, C*H*(CH_3)$_2$, 2H), 1.46 (d, CH(C*H*$_3$)$_2$, 6H), 1.30 (d, CH(C*H*$_3$)$_2$, 6H), 1.19 (d, CH(C*H*$_3$)$_2$, 6H), 1.07 (d, CH(C*H*$_3$)$_2$, 6H), 0.92 (d, CH(C*H*$_3$)$_2$, 6H), 0.66 (d, CH(C*H*$_3$)$_2$, 6H), 0.62 (d, CH(C*H*$_3$)$_2$, 6H), 0.36 (d, CH(C*H*$_3$)$_2$, 6H). ^{13}C NMR (25°C, 100.6 MHz, CD_2Cl_2): δ 172.4 (ArN*C*(CH_3)CH*C*(CH_3)NAr), 151.4 (aryl), 149.8 (aryl), 149.6 (br, B(*C*$_6$F$_5$)$_4$), 147.1 (br,B(*C*$_6$F$_5$)$_4$), 143.5 (aryl), 141.4 (aryl), 140.9 (aryl), 139.3 (aryl), 138.1 (aryl), 137.7 (br,

$B(C_6F_5)_4$), 135.3 (br,$B(C_6F_5)_4$), 134.5 (aryl), 130.5 (aryl), 129.1 (aryl), 126.7 (aryl), 126.6 (ar yl), 124.3 (aryl), 123.7 (aryl), 123.5 (aryl), 106.7 ($ArNC(CH_3)CHC(CH_3)NAr$), 32.98 ($CH(CH_3)_2$), 30.12 ($CH(CH_3)_2$), 29.24 ($CH(CH_3)_2$), 28.45 ($CH(CH_3)_2$), 28.14 ($CH(CH_3)_2$), 27.00 (CH_3), 26.24 (CH_3), 25.57 (CH_3), 25.09 (CH_3), 24.66 ($ArNC(CH_3)CHC(CH_3)NAr$), 24.08 (CH_3), 23.76 (CH_3), 21.83 (CH_3). ^{19}F NMR (23°C, 282.3 MHz, CD_2Cl_2): δ -133.8 (s, *o*-C_6F_5), -164.5 (t, *p*-C_6F_5), -168.3 (t, *m*-C_6F_5). ^{11}B NMR (70°C, 128.37 MHz, CD_2Cl_2): δ 16.94 (s, $B(C_6F_5)_4$). IR (CH_2Cl_2, CaF_2): 3247 (w), 3138 (w), 3061 (w), 2971 (m), 2930 (w), 2873 (w), 1643 (m), 1514 (s), 1465 (s), 1435 (w), 1386 (w), 1350 (w), 1314 (w), 1261 (s), 1242 (w), 1178 (w), 1085 (m), 981 (s) cm^{-1}. Anal. Calcd. For $C_{77}H_{77}N_4F_{20}B$ Ti: C, 61.77; H, 5.18; N, 3.74. Found: C, 61.44; H, 5.31; N, 3.80.

Synthesis of (Nacnac)Ti=NAr(OTf) (4)

Method A: Treatment of (Nacnac)Ti(NHAr)$_2$ (1) with AgOTf

In a vial was dissolved in 10 mL of THF (Nacnac)Ti(NHAr)$_2$ **(1)** [100 mg, 0.12 mmol] and the solution cooled to -35 ºC. To the cold solution was added a cold THF solution (5 mL) of AgOTf [34 mg, 0.13 mmol] causing formation of a silver mirror. After stirring for 2 hours the solution was filtered and dried under reduced pressure. The red solid was extracted with pentane, filtered, concentrated, and the solution cooled at -35 ºC to afford in two crops red crystals of (Nacnac)Ti=NAr(OTf) **(4)** [64.6 gm, 0.082 mmol, 67% yield]. If the reaction is carried out using CH_2Cl_2 or benzene as solvent, and the mixture is allowed to react for 5 days, complex **4** is then isolated in yields greater than 90% (quantitative by ^1H NMR spectroscopy). For **4**: ^1H NMR (23°C, 399.8 MHz, CD_2Cl_2): δ 7.28 (m, C_6H_3, 6H), 6.66 (d, C_6H_3, 2H), 6.60 (t, C_6H_3, 1H), 5.66 (s, $ArNC(CH_3)CHC(CH_3)NAr$, 1H), 3.55 (s, $CH(CH_3)_2$, 2H), 3.03 (s, C*H*(CH_3)$_2$, 2H), 2.88 (s, C*H*(CH_3)$_2$, 2H), 2.06 (s, ArNC(C*H*$_3$)CHC(C*H*$_3$)NAr, 6H), 1.30 (CH(C*H*$_3$)$_2$, 18H), 1.08 (d, CH(C*H*$_3$)$_2$, 6H), 0.82 (d, C*H*(CH_3)$_2$, 12H). ^{1}H NMR (23°C, 399.8 MHz, C_6D_6): δ 7.26-7.11 (m, C_6*H*$_3$, 6H), 6.84 (d, C_6*H*$_3$, 2H), 6.77 (t, C_6*H*$_3$, 1H), 5.22 (s, ArNC(CH_3)C*H*C(CH_3)NAr, 1H), 3.81 (s, C*H*(CH_3)$_2$, 2H), 3.32 (s, C*H*(CH_3)$_2$, 2H), 2.97 (s, C*H*(CH_3)$_2$, 2H), 1.70 (s, ArNC(C*H*$_3$)CHC(C*H*$_3$)NAr, 6H), 1.50 (CH(C*H*$_3$)$_2$, 6H), 1.40 (d, CH(C*H*$_3$)$_2$, 6H), 1.30 (d, C*H*(CH_3)$_2$, 6H), 1.10 (d, C*H*(CH_3)$_2$, 12H), 0.96 (d, C*H*(CH_3)$_2$, 6H). ^{13}C NMR (25°C, 100.6 MHz, C_6D_6): δ 168.1 (ArN*C*(CH_3)CH*C*(CH_3)NAr), 159.9 (aryl), 145.3 (aryl), 143.0 (aryl), 142.4 (aryl), 127.7 (aryl), 125.1 (aryl), 124.2 (aryl), 123.6 (aryl), 123.2 (aryl), 122.3 (aryl), 94.41 (ArNC(CH_3)*C*HC(CH_3)NAr), 30.34 (*C*H(CH_3)$_2$), 28.73 (*C*H(CH_3)$_2$), 28.12 (*C*H(CH_3)$_2$), 25.52 (CH(*C*H$_3$)$_2$), 24.62 (CH(*C*H$_3$)$_2$), 24.45 (CH(*C*H$_3$)$_2$), 24.33 (ArNC(*C*H$_3$)CHC(*C*H$_3$)NAr), 22.70 (CH(*C*H$_3$)$_2$). ^{19}F NMR (23°C, 282.3 MHz, C_6D_6): δ −78.3 (s, O_3SC*F*$_3$). IR (CH_2Cl_2, CaF_2): 3076 (m), 3060 (s), 3029 (s), 2964 (s), 2928 (m), 2869 (m), 1622 (m), 1551 (m), 1524 (m), 1486 (m), 1463 (m), 1438 (m), 1359 (s), 1318 (m), 1271 (m), 1256 (m), 1239 (m), 1202 (s), 1109 (w), 1057 (w), 1004 (s) cm^{-1}. UV-vis (Et_2O, 23°C): 323 nm (ε = 18460). Anal. Calcd. For $CHNO_3SF_3Ti$: C, 63.86; H, 7.40; N, 5.32. Found: C, 63.61; H, 7.52; N, 5.09.

Method B: Decomposition of [(Nacnac)Ti(NHAr)$_2$][OTf] (2)

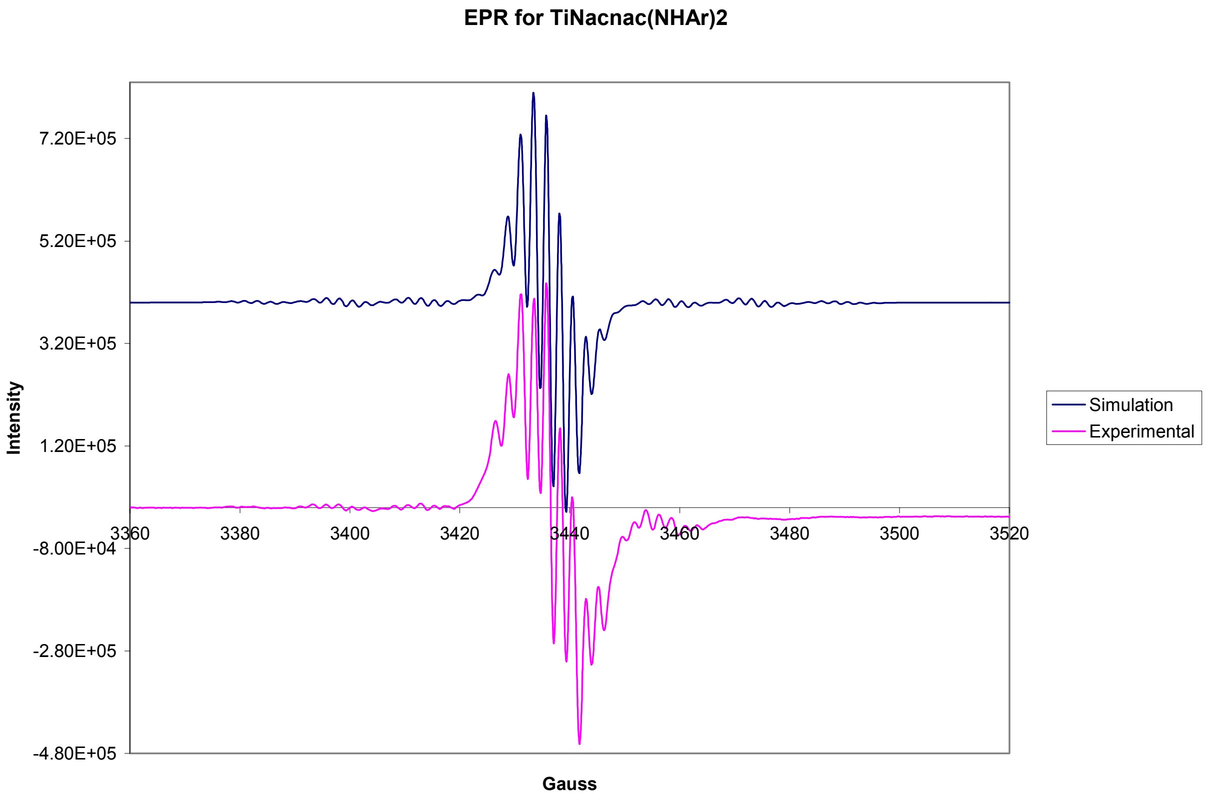
In a vial was dissolved [(Nacnac)Ti(NHAr)$_2$][OTf] **(2)** in [93 mg, 0.96 mmol] in 10 mL of THF and the solution stirred for 45 minutes. The mixture was dried under reduced pressure, extracted with pentane, filtered, concentrated, and cooled to -35°C to afford in two crops pure imido (Nacnac)Ti=NAr(OTf) **4** [56 mg, 0.70 mmol , 73 % yield]. When the reaction is carried in CH_2Cl_2, the formation of **4** and aniline is quantitative (isolated yield 82%) as evidenced by the ^{1}H NMR of the reaction mixture (CD_2Cl_2). However, the formation of **4** occurs much slower (4.5 days at 25°C, $t_{1/2} \sim 52$ hours). In both solvents the formation and characterization of **4** was determined by comparison of ^{1}H NMR and ^{19}F NMR spectra with authentic samples prepared independently by method A.

Method C: Treatment of [(Nacnac)Ti(NHAr)$_2$][B(C_6F_5)$_4$] (3) with Tl(OTf)

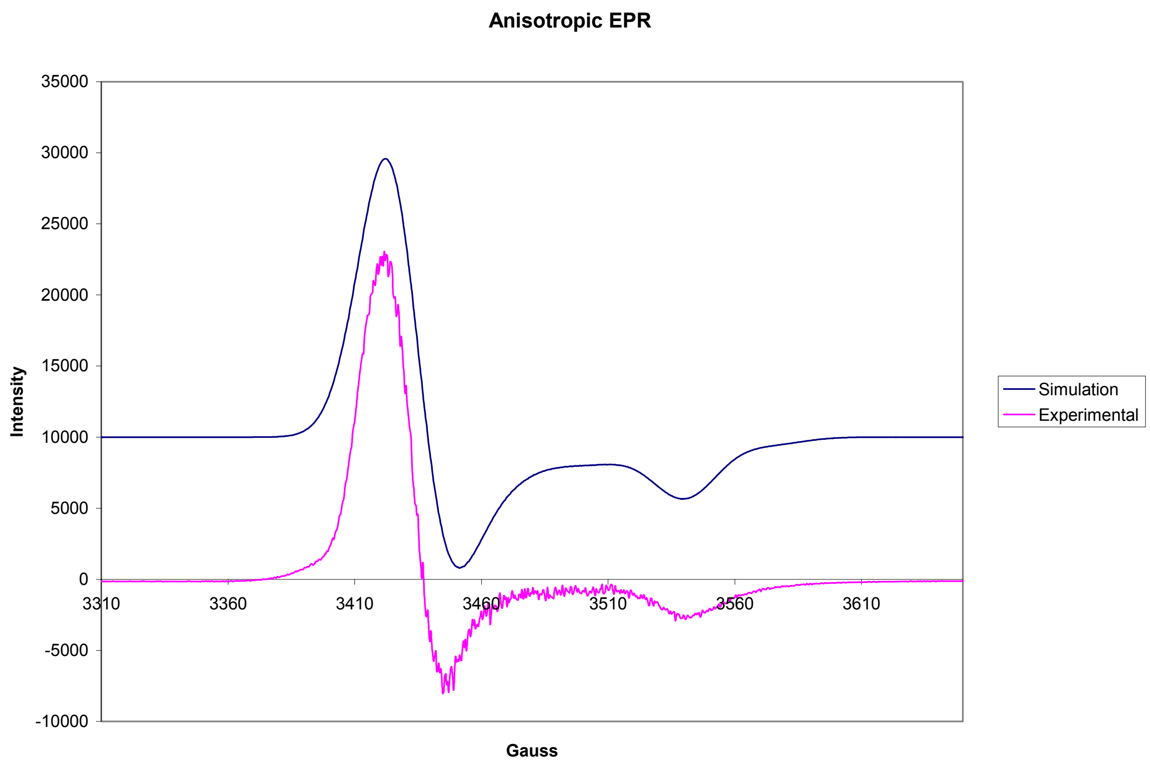
In a vial was dissolved [(Nacnac)Ti(NHAr)$_2$][B(C_6F_5)$_4$] **(3)** [78 mg, 0.052 mmol] in 5 mL of THF and to the mixture was added a THF solution (~5 mL) containing Tl(OTf)[6] [20 mg, 0.055 mmol]. The red solution gradually turned darker over the course of 2 hours and the mixture was then dried under reduced pressure. Pentane was added to the oily residue and the solution, filtered and dried under vacuum. Examination of the pentane extract by ^{1}H NMR and ^{19}F NMR spectra revealed formation of **4** along with free aniline and additional by-products. Complex **4** was observed to form by examination of ^{1}H NMR and ^{19}F NMR spectra of the reaction mixture but isolation of the product was hampered by the formation of other side products generated in the reaction. The formation and characterization of **4** was determined by comparison of ^{1}H NMR spectra with authentic sample prepared independently by method A.

EPR Measurements for 1

A 2 mmol solution of **1** in Et_2O/pentane (1:1) was used to collect the room temperature data at 278 K and the liquid helium temperature at 4.6 K. Typical EPR conditions for room temperature spectra: microwave power, 10 mW; modulation amplitude, 1 G; modulation frequency, 100 kHz; receiver gain, (2-5) x 10^{-4}. The magnitude of titanium (^{47}Ti, I = 5/2, 7.4%; ^{49}Ti, I = 7/2, 5.4%, n = 1), and the nitrogens (^{14}N, I=1, 96.63%, n = 4) coupling (A_{iso}) was found by simulation to be 15 G and 2.31 G, respectively. g_{iso} was centered at 1.97. Typical EPR conditions for room temperature spectra: microwave power, 10 mW; modulation amplitude, 1 G; modulation frequency, 100 kHz; receiver gain, (2-5) x 10^{-4}. The spectrum was determined to be axial with $g_{\perp}$ = 1.97 and $g_{\parallel}$ = 1.91. Coupling constants could not be accurately determined by simulation.



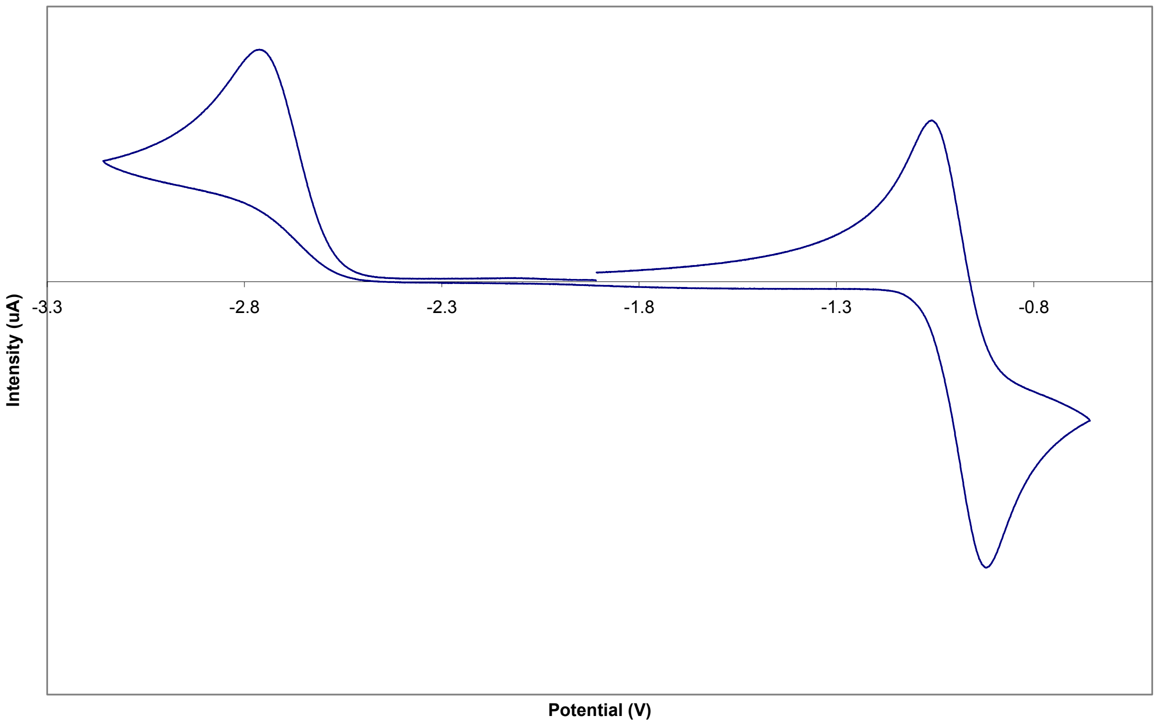
Anisotropic EPR spectrum of **1** (4.6 K).



Cyclic Voltammagram of Complex 2.

Cyclic voltammetry was peformed in pre-dried solutions of THF (0.3-0.5 M of pre-dried and recrystallized TBAH, Aldrich). A platinum disk (2.0 mm diameter, Bioanalytical Systems), a platinum wire, and silver wire were employed as the working electrode, the auxiliary, and the reference electrode, respectively. A one compartment cell was used in the CV measurement. The electrochemical response was collected with the assistance of an E2 Epsilon (BAS) autolab potentiostat/galvanostat with a BAS software. The IR drop correction was applied when significant resistance was noted. All the potentials were reported against ferrocenium/ferrocene couple (0 V) measured as an internal standard. All spectra were recorded under an N_2 atmosphere. In a typical experiment 10-15 mg of crystalline **1** was dissolved in 5 mL of a TBAH solution in THF at 26^{o}C.

Potential (V) vs. Intensity for Ti(NHAr)2 (Scan Rate=50 mV/s)



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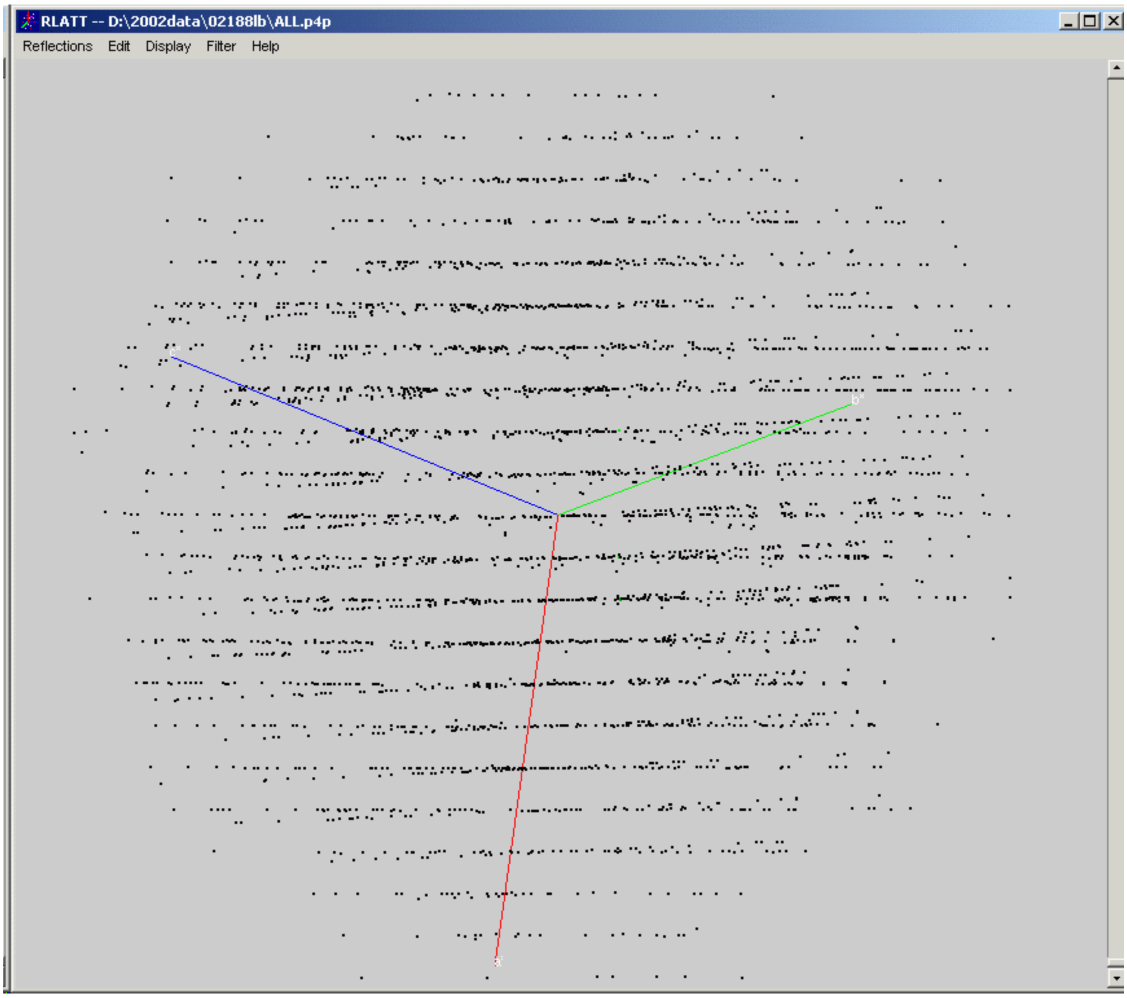
Crystallographic Experimental Section and Tables for Complex 1, 3, and 4

Crystallographic data for complex (Nacnac)Ti(NHAr)$_2$ (1)

The sample was submitted by the research group of Prof. Dan Mindiola, Department of Chemistry, Indiana University. Inert atmosphere techniques were used to place a dark green crystal of approximate dimensions 0.30 × 0.30 × 0.30 mm was placed onto the tip of a 0.2 mm diameter glass capillary and mounted on a SMART6000 (Bruker) at 138(2) K. Each of four crystals examined were badly split with varying degrees. The sample examined indicated two distinct lattices that were easily separable, as shown in the figure below.



A preliminary set of cell constants was calculated by deleting all but one set of lattice points (the horizontal component above). The resulting xyz coordinates were indexed yielding a triclinic cell. The data collection was carried out using graphite monochromated Mo Kα radiation with a frame time of 3 seconds and a detector distance of 5.0 cm. A randomly oriented region of a sphere in reciprocal space was surveyed. Six sections of 606 frames were collected with 0.30° steps in ω at different ϕ settings with the detector set at −43° in 2θ. Final cell constants were calculated from the xyz centroids of 7608 strong reflections from the actual data collection after integration (SAINT).[1]

Solution and Refinement

Intensity statistics and lack of systematic absences indicated the centrosymmetric space group P1bar, and solution and refinement confirmed this choice. The structure was solved in using SHELXS-97 and refined with SHELXL-97.[2] A direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed which located the remaining non-hydrogen atoms. All hydrogen atoms were subsequently located and refined with isotropic displacement parameters. The final full matrix least squares refinement converged to R1 = 0.0666 and wR2 = 0.1694 (F^2, all data).

[1] SAINT 6.1, Bruker Analytical X-Ray Systems, Madison, WI.
[2] SHELXTL-Plus V5.10, Bruker Analytical X-Ray Systems, Madison, WI.

Table 1

Program MU for data file labeled

MSC02188 **/12/26 12:

The following were used

At.No.	At.Wt.	Abs.	%	No.	Element
22	47.880	23.400	5.85	1	Ti
7	14.007	.845	6.85	4	N
6	12.011	.576	77.81	53	C
1	1.008	.373	9.49	77	H

The density is 1.135 g/cc.

The volume is 2392.86 cubic Angstroms

Z = 2 and the molecular wt. is 818.10

F(000) = 890

The linear absorption coefficient = 2.170 reciprocal centimeters,

and 1/4Mu = 1.1522 mm.

Table 2

Crystal Data for MSC Sample 02188

Empirical Formula	C53 H77 N4 Ti
Color of Crystal:	dark green
Crystal Dimensions were:	.3 x .3 x .3 mm.
Space Group:	P 1bar
Cell Dimensions (at 138(2) K; 7608 reflections)	
a =	11.3389(14)
b =	11.7121(15)
c =	20.010(2)
alpha =	90.265(3)
beta =	95.720(3)
gamma =	115.017(3)
Z (Molecules/cell):	2
Volume:	2392.9(5)
Calculated Density:	1.135
Wavelength:	0.71073
Molecular Weight:	818.09
F(000):	890
Linear Absorption Coefficient:	0.217

Data were collected on a Bruker SMART 6000 sealed-tube system comprising a three-circle platform goniostat, an HOG crystal monochromator, a four kilopixel by four kilopixel single-chip CCD-based detector, a K761 high voltage generator, and a PC interface running Bruker's SMART software.

Detector to sample distance = 5.0 cm.
Take off angle = 6.0 deg.

Data collected by the omega scan technique according to the following parameters:

frame width = 0.3 deg.
time per frame = 3.0 sec.

Data processing statistics for 30.1 degrees maximum theta:

Total number of intensities integrated = 26431
Number of unique intensities = 13917
Number with F > 4sigma(F) = 7605

R for averaging = 0.125

Refinement results:

Final residuals are:
R(F) (observed data) = 0.0666
Rw(F2) (refinement data) = 0.1694

Final Goodness of Fit = 0.880
Maximum delta/sigma for the last cycle = 0.01

Table 3: Fractional Coordinates and Isotropic Thermal Parameters for MSC Sample 02188

Atom	x	y	z	Uiso
Ti(1)	7573(1)	6922(1)	7520(1)	17(1)
N(2)	9475(2)	7240(2)	7383(1)	18(1)
C(3)	10525(2)	8230(2)	7687(1)	20(1)
C(4)	10477(2)	9314(2)	7955(1)	22(1)
C(5)	9437(2)	9673(2)	7878(1)	21(1)
N(6)	8215(2)	8885(2)	7642(1)	19(1)
C(7)	9738(2)	6377(2)	6966(1)	19(1)
C(8)	9490(2)	5149(2)	7181(1)	20(1)

C(9)	9732(2)	4348(2)	6747(1)	23(1)
C(11)	10174(2)	4706(2)	6133(1)	25(1)
C(12)	10392(2)	5901(2)	5929(1)	26(1)
C(13)	10184(2)	6750(2)	6336(1)	23(1)
C(14)	10449(3)	8057(2)	6077(1)	29(1)
C(15)	11873(3)	8768(3)	5918(2)	44(1)
C(16)	9504(3)	7952(3)	5456(2)	37(1)
C(17)	9002(2)	4688(2)	7844(1)	21(1)
C(18)	9978(3)	4359(3)	8298(1)	29(1)
C(19)	7665(3)	3530(2)	7740(2)	28(1)
C(20)	11853(2)	8202(3)	7759(2)	28(1)
C(21)	9780(3)	11033(2)	8081(2)	30(1)
C(22)	7243(2)	9376(2)	7500(1)	20(1)
C(23)	6988(2)	9664(2)	6837(1)	23(1)
C(24)	6020(3)	10104(2)	6697(1)	28(1)
C(25)	5335(3)	10255(2)	7198(1)	29(1)
C(26)	5591(2)	9958(2)	7842(1)	27(1)
C(27)	6549(2)	9521(2)	8015(1)	23(1)
C(28)	6828(3)	9261(3)	8742(1)	29(1)
C(29)	7184(4)	10429(4)	9213(2)	45(1)
C(30)	5680(3)	8127(3)	8976(2)	38(1)
C(31)	7766(3)	9548(2)	6281(1)	27(1)
C(32)	8978(3)	10789(3)	6235(2)	37(1)
C(33)	6959(3)	9144(3)	5594(2)	40(1)
N(34)	6765(2)	5905(2)	8265(1)	23(1)
C(35)	6908(2)	5326(2)	8861(1)	21(1)
C(36)	5912(2)	4145(2)	9012(1)	24(1)
C(37)	6135(3)	3553(3)	9578(1)	32(1)
C(38)	7286(3)	4078(3)	10005(2)	37(1)
C(39)	8227(3)	5249(3)	9875(1)	34(1)
C(40)	8068(2)	5890(2)	9315(1)	24(1)
C(41)	9095(2)	7214(2)	9228(1)	25(1)
C(42)	10494(3)	7310(3)	9299(2)	33(1)
C(43)	9014(3)	8151(3)	9737(2)	35(1)
C(44)	4573(3)	3530(2)	8600(2)	28(1)
C(45)	4203(3)	2168(3)	8354(2)	50(1)
C(46)	3527(3)	3612(4)	8995(2)	49(1)
N(47)	6631(2)	6174(2)	6635(1)	21(1)
C(48)	5478(2)	5039(2)	6525(1)	20(1)
C(49)	4347(2)	4941(2)	6810(1)	23(1)
C(50)	3235(3)	3797(3)	6736(2)	31(1)
C(51)	3202(3)	2768(3)	6373(2)	35(1)
C(52)	4297(3)	2883(2)	6075(1)	29(1)
C(53)	5436(2)	4004(2)	6138(1)	22(1)
C(54)	6604(2)	4148(2)	5775(1)	23(1)
C(55)	6590(3)	4814(3)	5116(1)	32(1)
C(56)	6698(3)	2905(3)	5629(2)	34(1)
C(57)	4295(2)	6100(2)	7133(1)	26(1)
C(58)	3991(3)	6865(3)	6582(2)	32(1)
C(59)	3323(3)	5814(3)	7650(2)	34(1)
H(132)	463(3)	707(3)	626(2)	47(9)
H(133)	399(3)	761(3)	675(2)	35(8)
H(60)	1128(3)	992(2)	819(1)	19(6)
H(61)	953(3)	356(3)	686(1)	21(7)
H(62)	1028(2)	411(2)	584(1)	20(6)
H(63)	1066(3)	614(2)	548(1)	20(6)

H(64)	1036(2)	855(2)	643(1)	17(6)
H(65)	1252(3)	891(3)	630(2)	39(8)
H(66)	1200(3)	959(3)	579(2)	53(10)
H(67)	1204(3)	838(3)	548(2)	43(9)
H(68)	968(3)	876(3)	532(2)	47(9)
H(69)	965(3)	751(3)	510(2)	29(7)
H(70)	853(4)	753(3)	555(2)	54(10)
H(71)	895(2)	539(2)	811(1)	18(6)
H(72)	971(3)	412(3)	873(2)	37(8)
H(73)	1010(3)	368(2)	809(1)	24(7)
H(74)	1084(3)	512(3)	839(1)	31(7)
H(75)	704(3)	373(3)	745(2)	31(7)
H(76)	738(2)	330(2)	818(1)	18(6)
H(77)	779(2)	282(2)	752(1)	19(6)
H(78)	1179(4)	743(4)	792(2)	62(11)
H(79)	1212(3)	826(3)	734(2)	38(9)
H(80)	1240(3)	879(3)	811(2)	56(10)
H(81)	1068(4)	1166(3)	801(2)	57(10)
H(82)	978(3)	1112(3)	853(2)	41(9)
H(83)	913(3)	1130(3)	792(2)	36(8)
H(84)	582(3)	1027(2)	625(1)	21(7)
H(85)	469(3)	1061(3)	708(2)	49(9)
H(86)	520(3)	1009(2)	821(1)	21(7)
H(87)	757(3)	906(2)	878(1)	28(7)
H(88)	740(3)	1027(3)	967(2)	48(9)
H(89)	785(4)	1115(4)	911(2)	77(14)
H(90)	641(4)	1062(3)	924(2)	58(10)
H(91)	586(3)	801(3)	943(2)	43(9)
H(92)	489(3)	831(3)	897(2)	39(8)
H(93)	547(3)	736(3)	872(2)	34(8)
H(94)	808(3)	888(3)	642(1)	28(7)
H(95)	941(3)	1072(3)	587(2)	38(8)
H(96)	945(4)	1103(3)	663(2)	57(11)
H(97)	871(3)	1148(3)	614(2)	42(9)
H(98)	740(3)	895(3)	524(2)	46(9)
H(99)	615(3)	831(3)	561(2)	50(9)
H(100)	660(3)	970(3)	544(2)	49(10)
H(101)	600(3)	549(2)	806(1)	17(6)
H(102)	546(3)	273(3)	964(2)	32(8)
H(103)	746(3)	369(3)	1039(2)	46(9)
H(104)	897(3)	560(3)	1016(2)	50(10)
H(105)	896(2)	745(2)	878(1)	18(6)
H(106)	1070(3)	712(3)	975(2)	42(9)
H(107)	1049(3)	662(3)	897(2)	47(9)
H(108)	1111(3)	814(3)	926(2)	36(8)
H(109)	814(3)	810(3)	973(2)	35(8)
H(110)	923(3)	805(3)	1019(2)	49(10)
H(111)	957(3)	898(3)	965(2)	37(8)
H(112)	456(3)	395(2)	822(1)	22(7)
H(113)	334(4)	186(3)	807(2)	60(11)
H(114)	490(4)	209(4)	806(2)	76(12)
H(115)	413(4)	172(4)	874(2)	55(11)
H(116)	262(3)	329(3)	872(2)	30(7)
H(117)	344(4)	310(4)	937(2)	74(13)
H(118)	380(3)	452(3)	914(2)	45(9)
H(119)	704(3)	627(3)	630(2)	47(10)
H(120)	250(3)	371(3)	691(2)	42(9)

H(121)	250(3)	202(3)	636(2)	32(8)
H(122)	421(3)	216(2)	580(1)	22(7)
H(123)	734(2)	467(2)	606(1)	17(6)
H(124)	741(4)	498(3)	489(2)	57(10)
H(125)	588(4)	430(3)	482(2)	54(10)
H(126)	656(3)	559(3)	521(2)	39(8)
H(127)	756(3)	310(3)	544(2)	50(9)
H(128)	665(3)	245(3)	605(2)	35(8)
H(129)	591(3)	234(3)	532(2)	34(8)
H(130)	516(3)	663(2)	738(1)	21(6)
H(131)	317(4)	640(3)	634(2)	49(9)
H(134)	338(3)	527(3)	801(2)	46(9)
H(135)	351(3)	660(3)	787(2)	35(8)
H(136)	237(3)	538(3)	741(2)	40(8)

Notes:
1) Fractional coordinates are X 10**4 for non-hydrogen atoms and X 10**3 for hydrogen atoms. Uiso values are all X 10**3.
2) Isotropic values for those atoms refined anisotropically are calculated as one third of the trace of the orthogonalized Uij tensor.
3) Parameters without standard deviations were not varied.

Table 4: Anisotropic Thermal Parameters for MSC Sample 02188

Atom	U11	U22	U33	U23	U13	U12
Ti(1)	14(1)	18(1)	19(1)	1(1)	0(1)	8(1)
N(2)	14(1)	19(1)	21(1)	-1(1)	0(1)	8(1)
C(3)	14(1)	23(1)	23(1)	1(1)	2(1)	8(1)
C(4)	16(1)	21(1)	27(1)	-5(1)	-2(1)	6(1)
C(5)	20(1)	20(1)	23(1)	0(1)	2(1)	9(1)
N(6)	17(1)	19(1)	21(1)	0(1)	-1(1)	9(1)
C(7)	13(1)	22(1)	23(1)	-3(1)	-3(1)	9(1)
C(8)	14(1)	22(1)	23(1)	-2(1)	-3(1)	9(1)
C(9)	20(1)	21(1)	29(1)	-3(1)	-4(1)	12(1)
C(11)	21(1)	29(1)	26(1)	-8(1)	-2(1)	14(1)
C(12)	24(1)	30(1)	25(1)	-1(1)	6(1)	12(1)
C(13)	21(1)	25(1)	25(1)	1(1)	3(1)	12(1)
C(14)	39(2)	26(1)	26(1)	4(1)	12(1)	14(1)
C(15)	41(2)	35(2)	51(2)	12(2)	12(2)	10(1)
C(16)	53(2)	34(2)	33(2)	9(1)	9(1)	24(1)
C(17)	22(1)	19(1)	25(1)	0(1)	0(1)	11(1)
C(18)	34(2)	29(1)	28(1)	2(1)	-1(1)	18(1)
C(19)	23(1)	24(1)	33(2)	1(1)	5(1)	8(1)
C(20)	18(1)	30(1)	37(2)	-7(1)	1(1)	12(1)
C(21)	26(1)	23(1)	42(2)	-7(1)	-4(1)	12(1)
C(22)	18(1)	14(1)	26(1)	-2(1)	-4(1)	7(1)
C(23)	23(1)	17(1)	28(1)	0(1)	0(1)	7(1)
C(24)	30(1)	22(1)	33(1)	4(1)	-4(1)	13(1)
C(25)	24(1)	24(1)	41(2)	0(1)	-3(1)	14(1)
C(26)	21(1)	26(1)	36(2)	-3(1)	2(1)	13(1)
C(27)	21(1)	21(1)	28(1)	-3(1)	-1(1)	10(1)
C(28)	27(1)	37(1)	28(1)	-2(1)	1(1)	20(1)
C(29)	46(2)	56(2)	37(2)	-14(2)	-2(2)	28(2)
C(30)	35(2)	52(2)	31(2)	8(1)	8(1)	22(1)
C(31)	32(1)	24(1)	27(1)	5(1)	4(1)	14(1)
C(32)	35(2)	35(2)	38(2)	0(1)	11(1)	11(1)
C(33)	39(2)	51(2)	27(2)	5(1)	4(1)	15(2)
N(34)	17(1)	27(1)	23(1)	3(1)	-3(1)	8(1)
C(35)	22(1)	28(1)	22(1)	5(1)	5(1)	17(1)
C(36)	25(1)	27(1)	26(1)	5(1)	9(1)	17(1)
C(37)	36(2)	33(1)	36(2)	14(1)	14(1)	21(1)
C(38)	45(2)	50(2)	30(2)	19(1)	9(1)	32(2)
C(39)	33(2)	50(2)	26(1)	5(1)	-3(1)	26(1)
C(40)	23(1)	31(1)	22(1)	1(1)	2(1)	17(1)
C(41)	20(1)	33(1)	22(1)	-3(1)	-4(1)	14(1)
C(42)	23(1)	40(2)	37(2)	-6(1)	-6(1)	16(1)
C(43)	33(2)	39(2)	36(2)	-5(1)	-1(1)	20(1)
C(44)	25(1)	27(1)	36(2)	6(1)	9(1)	13(1)
C(45)	34(2)	31(2)	83(3)	-5(2)	3(2)	11(1)
C(46)	28(2)	70(2)	56(2)	2(2)	11(2)	27(2)
N(47)	19(1)	22(1)	22(1)	1(1)	1(1)	9(1)
C(48)	18(1)	23(1)	19(1)	0(1)	-4(1)	11(1)
C(49)	19(1)	29(1)	23(1)	-2(1)	-4(1)	13(1)
C(50)	18(1)	35(1)	40(2)	-1(1)	1(1)	11(1)
C(51)	24(1)	28(1)	46(2)	-3(1)	2(1)	5(1)
C(52)	26(1)	25(1)	34(1)	-7(1)	-4(1)	11(1)

C(53)	22(1)	26(1)	22(1)	-1(1)	-5(1)	14(1)
C(54)	23(1)	25(1)	23(1)	-4(1)	-3(1)	13(1)
C(55)	34(2)	41(2)	25(1)	0(1)	-1(1)	21(1)
C(56)	31(2)	32(1)	42(2)	-7(1)	-2(1)	19(1)
C(57)	17(1)	31(1)	32(1)	-5(1)	-5(1)	13(1)
C(58)	31(2)	26(1)	40(2)	-2(1)	-1(1)	13(1)
C(59)	33(2)	43(2)	35(2)	0(1)	8(1)	25(1)

Form of the anisotropic thermal parameter:
exp{ -2 pi**2 [h**2 (a*)**2 U11 + ... + 2 h k (a*) (b*) U12] }
All values are X 10**3

Table 5a: Bond Distances for MSC Sample 02188

A	B	Distance
Ti(1)	N(34)	1.961(2)
Ti(1)	N(47)	1.966(2)
Ti(1)	N(2)	2.0746(19)
Ti(1)	N(6)	2.1027(18)
N(2)	C(3)	1.346(3)
N(2)	C(7)	1.450(3)
C(3)	C(4)	1.401(3)
C(3)	C(20)	1.512(3)
C(4)	C(5)	1.405(3)
C(5)	N(6)	1.334(3)
C(5)	C(21)	1.514(3)
N(6)	C(22)	1.449(3)
C(7)	C(13)	1.408(4)
C(7)	C(8)	1.422(3)
C(8)	C(9)	1.402(3)
C(8)	C(17)	1.503(3)
C(9)	C(11)	1.373(4)
C(11)	C(12)	1.386(4)
C(12)	C(13)	1.393(3)
C(13)	C(14)	1.533(4)
C(14)	C(16)	1.526(4)
C(14)	C(15)	1.539(4)
C(17)	C(18)	1.537(3)
C(17)	C(19)	1.542(3)
C(22)	C(23)	1.403(3)
C(22)	C(27)	1.410(3)
C(23)	C(24)	1.402(3)
C(23)	C(31)	1.527(4)
C(24)	C(25)	1.382(4)
C(25)	C(26)	1.372(4)
C(26)	C(27)	1.399(3)
C(27)	C(28)	1.517(4)
C(28)	C(30)	1.530(4)
C(28)	C(29)	1.540(4)
C(31)	C(33)	1.525(4)
C(31)	C(32)	1.532(4)
N(34)	C(35)	1.403(3)
C(35)	C(40)	1.419(3)
C(35)	C(36)	1.425(3)
C(36)	C(37)	1.387(4)
C(36)	C(44)	1.525(4)

C(37)	C(38)	1.381(4)
C(38)	C(39)	1.381(4)
C(39)	C(40)	1.390(4)
C(40)	C(41)	1.519(4)
C(41)	C(43)	1.530(4)
C(41)	C(42)	1.534(3)
C(44)	C(46)	1.524(4)
C(44)	C(45)	1.533(4)
N(47)	C(48)	1.413(3)
C(48)	C(49)	1.415(3)
C(48)	C(53)	1.417(3)
C(49)	C(50)	1.393(4)
C(49)	C(57)	1.527(3)
C(50)	C(51)	1.388(4)
C(51)	C(52)	1.387(4)
C(52)	C(53)	1.392(3)
C(53)	C(54)	1.521(3)
C(54)	C(56)	1.533(3)
C(54)	C(55)	1.536(4)
C(57)	C(59)	1.521(4)
C(57)	C(58)	1.525(4)

Symmetry transformations used to generate equivalent atoms:

Table 5b: Bond Angles for MSC Sample 02188

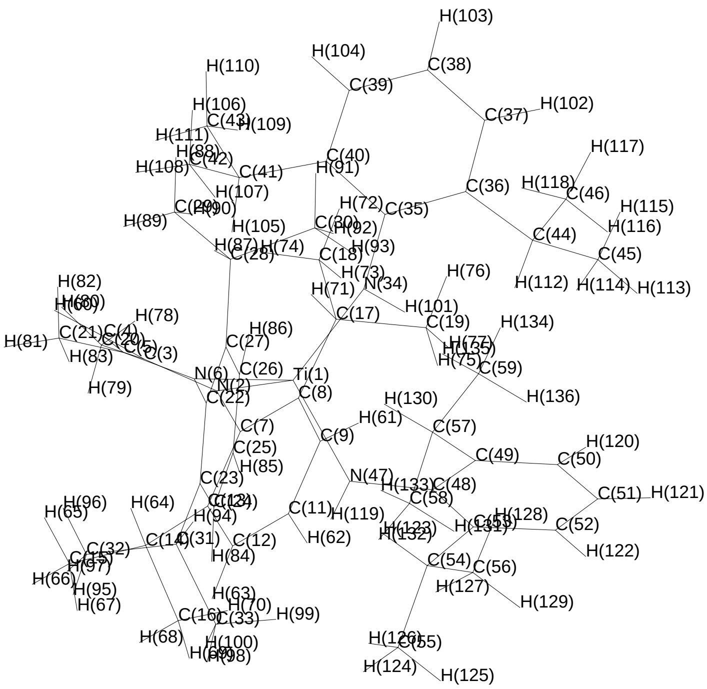
A	B	C	Angle
N(34)	Ti(1)	N(47)	112.99(9)
N(34)	Ti(1)	N(2)	118.60(8)
N(47)	Ti(1)	N(2)	101.65(8)
N(34)	Ti(1)	N(6)	117.20(8)
N(47)	Ti(1)	N(6)	114.88(8)
N(2)	Ti(1)	N(6)	88.42(7)
C(3)	N(2)	C(7)	116.52(18)
C(3)	N(2)	Ti(1)	122.29(14)
C(7)	N(2)	Ti(1)	121.16(14)
N(2)	C(3)	C(4)	124.0(2)
N(2)	C(3)	C(20)	119.8(2)
C(4)	C(3)	C(20)	116.2(2)
C(3)	C(4)	C(5)	128.3(2)
N(6)	C(5)	C(4)	123.3(2)
N(6)	C(5)	C(21)	120.9(2)
C(4)	C(5)	C(21)	115.8(2)
C(5)	N(6)	C(22)	119.33(18)
C(5)	N(6)	Ti(1)	123.31(15)
C(22)	N(6)	Ti(1)	117.23(14)
C(13)	C(7)	C(8)	120.6(2)
C(13)	C(7)	N(2)	119.3(2)
C(8)	C(7)	N(2)	120.1(2)
C(9)	C(8)	C(7)	117.3(2)
C(9)	C(8)	C(17)	119.4(2)
C(7)	C(8)	C(17)	123.3(2)
C(11)	C(9)	C(8)	122.5(2)
C(9)	C(11)	C(12)	119.4(2)
C(11)	C(12)	C(13)	121.3(2)

C(12)	C(13)	C(7)	118.9(2)
C(12)	C(13)	C(14)	118.4(2)
C(7)	C(13)	C(14)	122.7(2)
C(16)	C(14)	C(13)	110.9(2)
C(16)	C(14)	C(15)	110.1(3)
C(13)	C(14)	C(15)	111.7(2)
C(8)	C(17)	C(18)	112.1(2)
C(8)	C(17)	C(19)	111.0(2)
C(18)	C(17)	C(19)	109.5(2)
C(23)	C(22)	C(27)	121.3(2)
C(23)	C(22)	N(6)	118.4(2)
C(27)	C(22)	N(6)	120.3(2)
C(24)	C(23)	C(22)	118.3(2)
C(24)	C(23)	C(31)	120.2(2)
C(22)	C(23)	C(31)	121.5(2)
C(25)	C(24)	C(23)	121.1(3)
C(26)	C(25)	C(24)	119.8(2)
C(25)	C(26)	C(27)	122.0(2)
C(26)	C(27)	C(22)	117.6(2)
C(26)	C(27)	C(28)	119.6(2)
C(22)	C(27)	C(28)	122.7(2)
C(27)	C(28)	C(30)	111.9(2)
C(27)	C(28)	C(29)	111.4(2)
C(30)	C(28)	C(29)	110.2(3)
C(33)	C(31)	C(23)	113.4(2)
C(33)	C(31)	C(32)	109.8(3)
C(23)	C(31)	C(32)	110.6(2)
C(35)	N(34)	Ti(1)	148.64(17)
N(34)	C(35)	C(40)	120.5(2)
N(34)	C(35)	C(36)	120.8(2)
C(40)	C(35)	C(36)	118.7(2)
C(37)	C(36)	C(35)	119.1(2)
C(37)	C(36)	C(44)	118.0(2)
C(35)	C(36)	C(44)	122.8(2)
C(38)	C(37)	C(36)	122.1(3)
C(39)	C(38)	C(37)	118.8(3)
C(38)	C(39)	C(40)	121.9(3)
C(39)	C(40)	C(35)	119.3(2)
C(39)	C(40)	C(41)	119.3(2)
C(35)	C(40)	C(41)	121.3(2)
C(40)	C(41)	C(43)	110.4(2)
C(40)	C(41)	C(42)	113.0(2)
C(43)	C(41)	C(42)	109.1(2)
C(46)	C(44)	C(36)	110.3(2)
C(46)	C(44)	C(45)	111.3(3)
C(36)	C(44)	C(45)	113.2(2)
C(48)	N(47)	Ti(1)	125.11(17)
N(47)	C(48)	C(49)	119.0(2)
N(47)	C(48)	C(53)	121.2(2)
C(49)	C(48)	C(53)	119.7(2)
C(50)	C(49)	C(48)	118.9(2)
C(50)	C(49)	C(57)	120.0(2)
C(48)	C(49)	C(57)	120.8(2)
C(51)	C(50)	C(49)	121.4(3)
C(52)	C(51)	C(50)	119.4(3)
C(51)	C(52)	C(53)	121.4(2)
C(52)	C(53)	C(48)	119.0(2)

C(52)	C(53)	C(54)	121.1(2)
C(48)	C(53)	C(54)	119.8(2)
C(53)	C(54)	C(56)	114.2(2)
C(53)	C(54)	C(55)	110.3(2)
C(56)	C(54)	C(55)	109.6(2)
C(59)	C(57)	C(58)	109.7(2)
C(59)	C(57)	C(49)	114.8(2)
C(58)	C(57)	C(49)	109.1(2)

Symmetry transformations used to generate equivalent atoms:

Figure 1: VERSORT Drawing(s)



Supplementary Material (ESI) for Chemical Communications

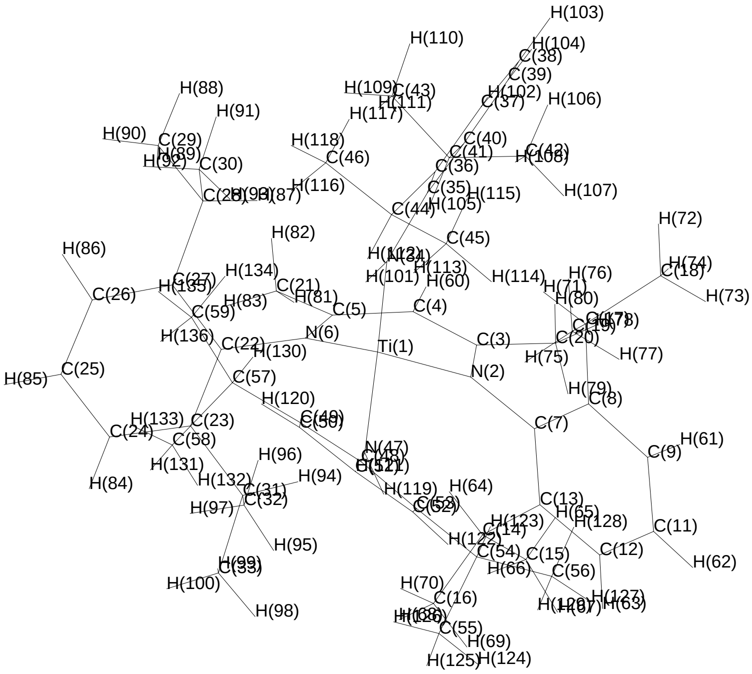
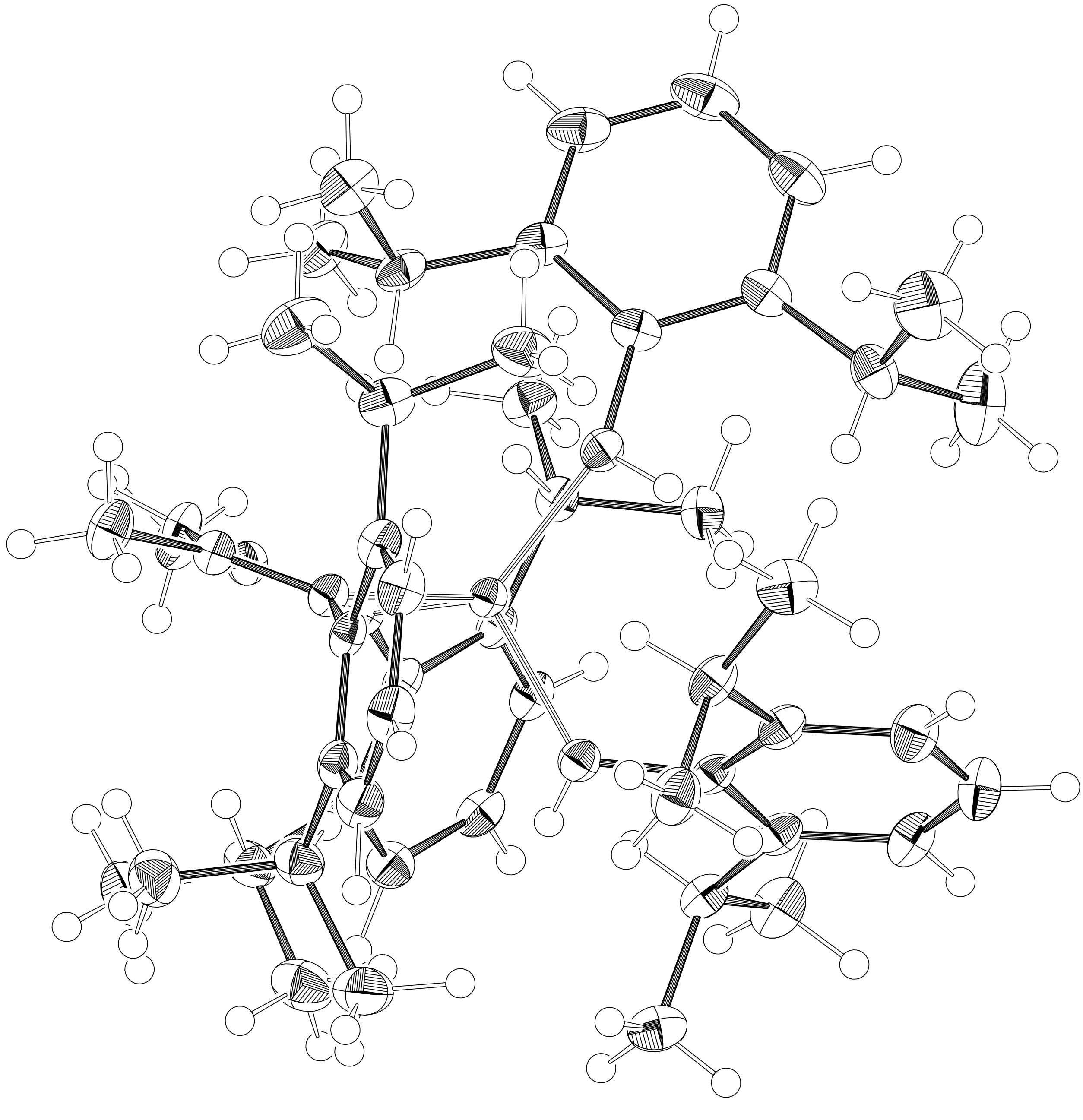


Figure 2: ORTEP Drawing(s)



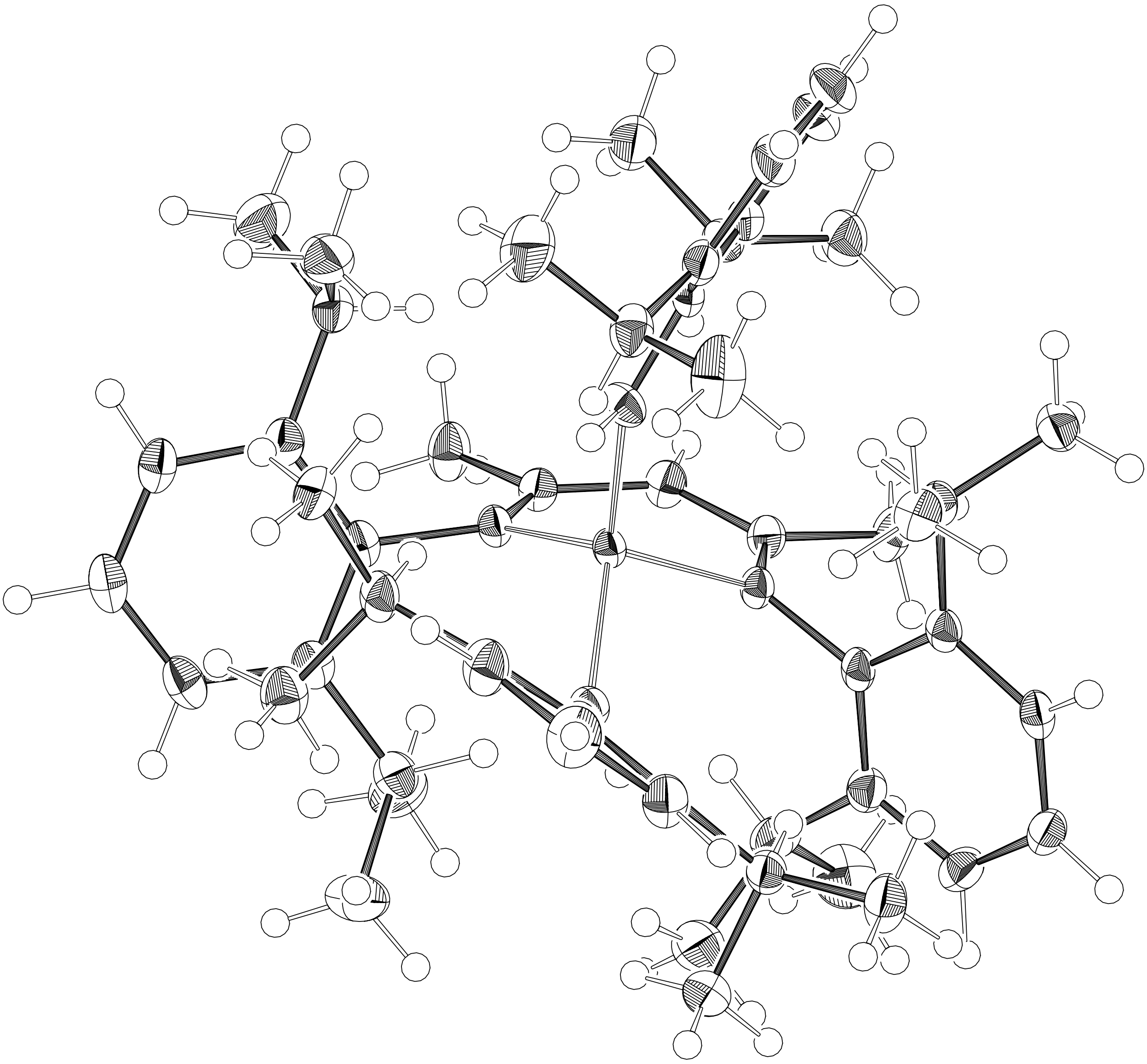
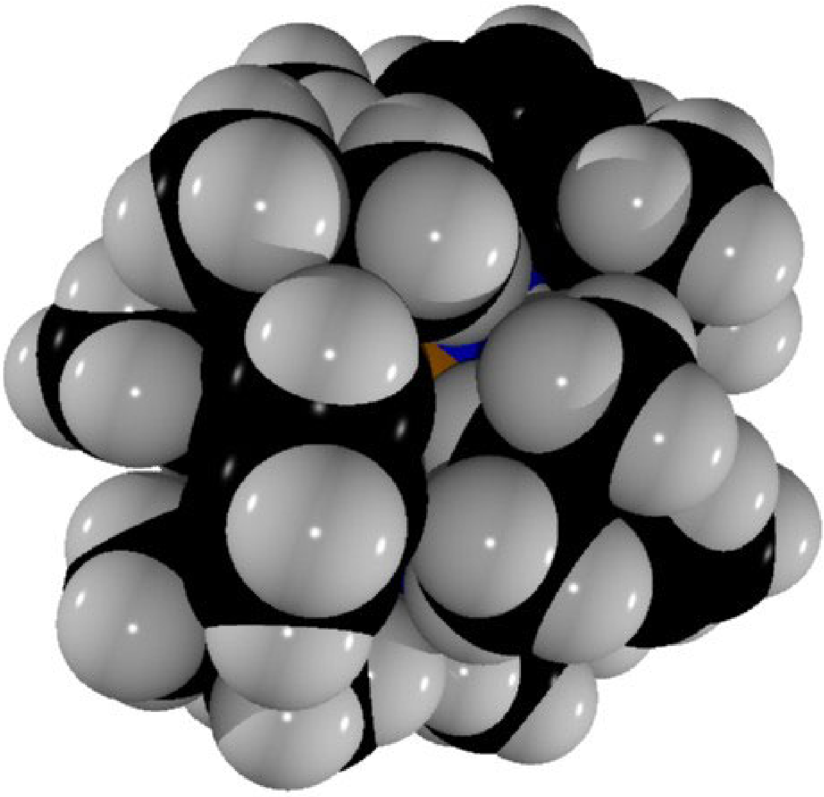


Figure 3: Space Filling Model Drawing(s)



Crystallographic data for complex ([(Nacnac)Ti(NHAr)$_2$][B(C_6F_5)$_4$] (3)

The sample was submitted by the research group of Prof. Daniel J. Mindiola, Department of Chemistry, Indiana University. Inert atmosphere techniques were used to place an orange/red crystal of approximate dimensions 0.25 × 0.25 × 0.07 mm onto the tip of a 0.1 mm diameter glass fiber which was subsequently mounted on a SMART6000 (Bruker) and cooled to 136(2) K.

Data collection
A preliminary set of cell constants was calculated from reflections obtained from three nearly orthogonal sets of 20 frames. The data collection was carried out using graphite monochromated Mo Kα radiation with a frame time of 15 seconds and a detector distance of 5.0 cm. A randomly oriented region of a sphere in reciprocal space was surveyed. Six sections of 606 frames were collected with 0.30° steps in ω at different ϕ settings with the detector set at −43° in 2θ. Final cell constants were calculated from the xyz centroids of 7190 strong reflections from the actual data collection after integration (SAINT).[1]

Structure solution and refinement
Intensity statistics and systematic absences suggested the centrosymmetric space group $P2_1/c$ and subsequent solution and refinement confirmed this choice. The structure was solved using SHELXS-97 and refined with SHELXL-97.[2] A direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were located in subsequent Fourier maps and included as isotropic contributors in the final cycles of refinement.

The final full matrix least squares refinement converged to R1 = 0.0443 and wR2 = 0.1116 (F2, all data). The remaining electron density is located on bonds.

1 SAINT 6.1, Bruker Analytical X-Ray Systems, Madison, WI.
2 SHELXTL-Plus V5.10, Bruker Analytical X-Ray Systems, Madison, WI.

Table 1

Program MU for data file labeled

MSC03054

The following were used

At.No.	At.Wt.	Abs.	%	No.	Element
22	47.880	23.400	3.05	1	Ti
9	18.998	1.630	24.18	20	F
8	15.999	1.220	1.02	1	O
7	14.007	.845	3.57	4	N
6	12.011	.576	61.92	81	C
5	10.811	.368	.69	1	B
1	1.008	.373	5.58	87	H

The density is 1.375 g/cc.

The volume is 7591.27 cubic Angstroms

Z = 4 and the molecular wt. is 1571.27

F(000) = 3264

The linear absorption coefficient = 2.103 reciprocal centimeters,

and 1/4Mu = 1.1887 mm.

Table 2

Crystal Data for MSC Sample 03054

Empirical Formula	C81H87BF20N4OTi
Color of Crystal:	orange/red
Crystal Dimensions were:	0.25 x 0.25 x 0.07 mm.
Space Group:	P2(1)/c
Cell Dimensions (at 136(2) K; 7190 reflections)	
a =	13.8639(6)
b =	39.2661(16)
c =	13.9675(6)
alpha =	90
beta =	93.2700(10)
gamma =	90
Z (Molecules/cell):	4
Volume:	7591.3(6)
Calculated Density:	1.375
Wavelength:	0.71073
Molecular Weight:	1571.26
F(000):	3264
Linear Absorption Coefficient:	0.210

Data were collected on a Bruker SMART 6000 sealed-tube system comprising a three-circle platform goniostat, an HOG crystal monochromator, a four kilopixel by four kilopixel single-chip CCD-based detector, a K761 high voltage generator, and a PC interface running Bruker's SMART software.

Detector to sample distance =	5.0 cm.
Take off angle =	6.0 deg.

Data collected by the omega scan technique according to the following parameters:

frame width =	0.3 deg.
time per frame =	15.0 sec.

Data processing statistics for 27.5 degrees maximum theta:

Total number of intensities integrated =	111677
Number of unique intensities =	17467
Number with F > 4sigma(F) =	9392
R for averaging =	0.109

Refinement results:

Final residuals are:

R(F) (observed data) =	0.0443
Rw(F2) (refinement data) =	0.1116
Final Goodness of Fit =	0.962
Maximum delta/sigma for the last cycle =	0.02

Table 3: Fractional Coordinates and Isotropic Thermal Parameters for MSC Sample 03054

Atom	x	y	z	Uiso
Ti(1)	506(1)	1166(1)	2590(1)	16(1)
N(2)	560(1)	704(1)	1968(1)	17(1)
C(3)	-256(2)	560(1)	1595(2)	17(1)
C(4)	-1117(2)	748(1)	1441(2)	19(1)
C(5)	-1261(2)	1097(1)	1416(2)	19(1)
N(6)	-554(1)	1325(1)	1679(1)	16(1)
C(7)	1469(2)	519(1)	1974(2)	17(1)
C(8)	2111(2)	600(1)	1269(2)	20(1)
C(9)	2993(2)	433(1)	1293(2)	25(1)
C(10)	3243(2)	200(1)	2002(2)	26(1)
C(11)	2603(2)	122(1)	2683(2)	24(1)
C(12)	1701(2)	276(1)	2687(2)	22(1)
C(13)	1005(2)	169(1)	3433(2)	31(1)
C(14)	1338(3)	300(1)	4425(2)	43(1)
C(15)	859(3)	-216(1)	3440(3)	41(1)
C(16)	1843(2)	855(1)	482(2)	25(1)
C(17)	2671(2)	1094(1)	277(3)	36(1)
C(18)	1434(3)	680(1)	-427(2)	35(1)
C(19)	-283(2)	191(1)	1311(2)	26(1)
C(20)	-2246(2)	1228(1)	1081(2)	25(1)
C(21)	-683(2)	1681(1)	1419(2)	18(1)
C(22)	-343(2)	1790(1)	536(2)	22(1)
C(23)	-455(2)	2132(1)	302(2)	27(1)
C(24)	-867(2)	2359(1)	911(2)	28(1)
C(25)	-1201(2)	2248(1)	1766(2)	24(1)
C(26)	-1128(2)	1908(1)	2037(2)	20(1)
C(27)	-1561(2)	1800(1)	2968(2)	25(1)
C(28)	-2634(2)	1896(1)	2964(2)	34(1)
C(29)	-1008(2)	1952(1)	3844(2)	32(1)
C(30)	108(2)	1546(1)	-155(2)	25(1)
C(31)	-645(2)	1363(1)	-811(2)	38(1)
C(32)	842(2)	1713(1)	-773(2)	38(1)
N(33)	1688(2)	1387(1)	2508(2)	24(1)
C(34)	2315(2)	1566(1)	3207(2)	26(1)
C(35)	2143(2)	1915(1)	3364(2)	28(1)
C(36)	2695(2)	2076(1)	4090(2)	39(1)
C(37)	3391(3)	1901(1)	4635(3)	52(1)
C(38)	3575(3)	1568(1)	4449(3)	53(1)
C(39)	3048(2)	1390(1)	3726(2)	39(1)
C(40)	3359(3)	1031(1)	3486(2)	46(1)
C(41)	4235(3)	1047(1)	2875(4)	70(1)
C(42)	3559(5)	809(1)	4373(4)	82(2)
C(43)	1451(2)	2114(1)	2703(2)	30(1)
C(44)	1927(3)	2193(1)	1769(2)	40(1)
C(45)	1084(2)	2442(1)	3139(3)	39(1)
N(46)	268(2)	1168(1)	3898(2)	23(1)
C(47)	-284(2)	1170(1)	4719(2)	23(1)
C(48)	103(2)	1323(1)	5575(2)	30(1)
C(49)	-461(3)	1317(1)	6365(2)	38(1)
C(50)	-1361(3)	1172(1)	6338(2)	41(1)

C(51)	-1737(2)	1029(1)	5492(2)	35(1)
C(52)	-1215(2)	1023(1)	4673(2)	25(1)
C(53)	-1623(2)	842(1)	3787(2)	27(1)
C(54)	-2691(2)	920(1)	3541(3)	41(1)
C(55)	-1484(2)	459(1)	3911(2)	33(1)
C(56)	1106(2)	1474(1)	5684(2)	38(1)
C(57)	1120(4)	1828(1)	6139(3)	58(1)
C(58)	1779(4)	1231(1)	6258(4)	74(1)
B(59)	5439(2)	1051(1)	8125(2)	19(1)
C(60)	4808(2)	770(1)	7473(2)	21(1)
C(61)	3834(2)	691(1)	7514(2)	25(1)
C(62)	3390(2)	421(1)	7022(2)	31(1)
C(63)	3920(2)	213(1)	6476(2)	33(1)
C(64)	4893(2)	275(1)	6410(2)	27(1)
C(65)	5296(2)	549(1)	6899(2)	23(1)
F(66)	3254(1)	876(1)	8059(1)	30(1)
F(67)	2441(1)	361(1)	7105(1)	46(1)
F(68)	3507(1)	-54(1)	6005(1)	51(1)
F(69)	5433(1)	71(1)	5889(1)	39(1)
F(70)	6257(1)	596(1)	6800(1)	26(1)
C(71)	4791(2)	1330(1)	8688(2)	20(1)
C(72)	4123(2)	1531(1)	8159(2)	22(1)
C(73)	3601(2)	1792(1)	8526(2)	28(1)
C(74)	3737(2)	1874(1)	9475(2)	28(1)
C(75)	4394(2)	1691(1)	10039(2)	26(1)
C(76)	4902(2)	1429(1)	9642(2)	21(1)
F(77)	3976(1)	1471(1)	7206(1)	29(1)
F(78)	2964(1)	1971(1)	7960(1)	39(1)
F(79)	3239(1)	2130(1)	9857(1)	40(1)
F(80)	4540(1)	1769(1)	10977(1)	37(1)
F(81)	5541(1)	1268(1)	10261(1)	27(1)
C(82)	6069(2)	794(1)	8863(2)	18(1)
C(83)	5586(2)	606(1)	9529(2)	19(1)
C(84)	6007(2)	365(1)	10135(2)	22(1)
C(85)	6970(2)	290(1)	10064(2)	22(1)
C(86)	7482(2)	458(1)	9400(2)	20(1)
C(87)	7035(2)	704(1)	8824(2)	18(1)
F(88)	4627(1)	658(1)	9613(1)	26(1)
F(89)	5491(1)	202(1)	10786(1)	30(1)
F(90)	7397(1)	53(1)	10643(1)	31(1)
F(91)	8417(1)	380(1)	9298(1)	29(1)
F(92)	7602(1)	856(1)	8198(1)	23(1)
C(93)	6101(2)	1306(1)	7485(2)	19(1)
C(94)	5972(2)	1363(1)	6508(2)	23(1)
C(95)	6450(2)	1614(1)	6027(2)	28(1)
C(96)	7083(2)	1825(1)	6521(2)	29(1)
C(97)	7236(2)	1782(1)	7492(2)	26(1)
C(98)	6751(2)	1529(1)	7940(2)	21(1)
F(99)	5352(1)	1171(1)	5948(1)	30(1)
F(100)	6290(1)	1650(1)	5071(1)	41(1)
F(101)	7562(1)	2065(1)	6058(1)	43(1)
F(102)	7865(1)	1988(1)	7984(1)	36(1)
F(103)	6925(1)	1501(1)	8902(1)	26(1)
C(104)	6588(3)	2231(1)	9995(3)	61(1)
C(105)	5836(3)	2448(1)	9468(3)	52(1)
O(106)	5718(2)	2329(1)	8498(2)	53(1)
C(107)	5000(3)	2521(1)	7940(3)	50(1)

C(108)	4915(3)	2376(1)	6948(3)	58(1)
H(109)	-164(2)	62(1)	127(2)	18(6)
H(110)	344(2)	49(1)	81(2)	23(7)
H(111)	383(2)	9(1)	200(2)	17(6)
H(112)	276(2)	-4(1)	318(2)	27(7)
H(113)	40(2)	28(1)	329(2)	30(7)
H(114)	198(2)	22(1)	463(2)	29(7)
H(115)	147(2)	55(1)	447(2)	30(8)
H(116)	84(3)	25(1)	490(3)	72(12)
H(117)	143(2)	-34(1)	368(2)	46(9)
H(118)	70(2)	-31(1)	274(2)	53(9)
H(119)	33(2)	-28(1)	386(2)	60(10)
H(120)	135(2)	100(1)	72(2)	17(6)
H(121)	291(2)	120(1)	89(2)	53(10)
H(122)	320(2)	96(1)	-1(2)	43(8)
H(123)	245(2)	127(1)	-17(2)	51(9)
H(124)	192(2)	53(1)	-66(2)	41(9)
H(125)	125(2)	84(1)	-96(2)	50(9)
H(126)	93(2)	54(1)	-31(2)	32(8)
H(127)	37(2)	9(1)	125(2)	43(8)
H(128)	-59(2)	17(1)	72(2)	51(9)
H(129)	-59(2)	5(1)	179(2)	50(9)
H(130)	-224(2)	141(1)	64(2)	48(9)
H(131)	-259(2)	130(1)	165(2)	42(9)
H(132)	-260(2)	104(1)	78(2)	50(9)
H(133)	-24(2)	221(1)	-27(2)	12(6)
H(134)	-90(2)	259(1)	77(2)	22(7)
H(135)	-147(2)	240(1)	219(2)	17(6)
H(136)	-152(2)	157(1)	302(2)	12(6)
H(137)	-269(2)	213(1)	297(2)	31(8)
H(138)	-294(2)	181(1)	353(2)	45(9)
H(139)	-300(2)	180(1)	237(2)	33(8)
H(140)	-106(2)	220(1)	384(2)	38(8)
H(141)	-131(2)	188(1)	443(2)	31(8)
H(142)	-31(2)	189(1)	386(2)	32(8)
H(143)	39(2)	137(1)	20(2)	18(6)
H(144)	-111(2)	122(1)	-49(2)	54(10)
H(145)	-99(2)	155(1)	-115(2)	48(9)
H(146)	-30(2)	121(1)	-126(2)	47(9)
H(147)	128(2)	184(1)	-36(2)	46(9)
H(148)	51(2)	189(1)	-123(2)	56(10)
H(149)	122(2)	155(1)	-113(2)	40(8)
H(150)	177(3)	142(1)	199(3)	84(16)
H(151)	261(2)	230(1)	424(2)	36(8)
H(152)	377(2)	202(1)	515(2)	63(10)
H(153)	408(2)	147(1)	476(2)	59(11)
H(154)	285(2)	92(1)	313(2)	32(8)
H(155)	413(2)	119(1)	229(2)	52(11)
H(156)	445(2)	81(1)	273(2)	54(10)
H(157)	478(3)	115(1)	327(3)	80(12)
H(158)	368(2)	57(1)	420(2)	64(10)
H(159)	419(3)	88(1)	464(2)	60(11)
H(160)	288(4)	79(1)	489(4)	180(30)
H(161)	92(2)	197(1)	259(2)	25(7)
H(162)	150(2)	233(1)	132(2)	59(10)
H(163)	251(2)	234(1)	190(2)	54(10)

H(164)	214(2)	199(1)	144(2)	39(8)
H(165)	166(2)	263(1)	322(2)	54(9)
H(166)	85(2)	240(1)	379(2)	33(8)
H(167)	60(2)	254(1)	271(2)	54(10)
H(168)	82(2)	123(1)	400(2)	32(9)
H(169)	-20(2)	142(1)	694(2)	34(8)
H(170)	-168(2)	118(1)	692(2)	47(9)
H(171)	-234(2)	93(1)	545(2)	28(8)
H(172)	-126(2)	91(1)	327(2)	7(6)
H(173)	-279(2)	117(1)	351(2)	40(8)
H(174)	-289(2)	82(1)	292(2)	42(9)
H(175)	-310(2)	82(1)	405(2)	52(9)
H(176)	-191(2)	38(1)	443(2)	30(7)
H(177)	-78(2)	40(1)	409(2)	49(9)
H(178)	-167(2)	36(1)	330(2)	45(9)
H(179)	136(2)	150(1)	511(2)	49(10)
H(180)	72(3)	199(1)	575(3)	86(14)
H(181)	182(3)	194(1)	612(3)	83(13)
H(182)	87(3)	182(1)	677(3)	89(14)
H(183)	237(3)	132(1)	621(3)	83(15)
H(184)	181(3)	98(1)	599(3)	80(12)
H(185)	158(3)	122(1)	695(4)	120(20)
H(186)	730(4)	224(1)	971(3)	126(17)
H(187)	670(3)	231(1)	1072(3)	84(13)
H(188)	633(3)	193(1)	1003(3)	131(17)
H(189)	515(2)	245(1)	984(2)	56(10)
H(190)	605(3)	274(1)	947(2)	81(12)
H(191)	426(3)	249(1)	832(2)	69(11)
H(192)	522(2)	280(1)	795(2)	78(12)
H(193)	438(3)	254(1)	651(3)	88(13)
H(194)	558(3)	240(1)	659(2)	69(11)
H(195)	471(3)	211(1)	698(3)	82(12)

Notes:
1) Fractional coordinates are X 10**4 for non-hydrogen atoms and X 10**3 for hydrogen atoms. Uiso values are all X 10**3.
2) Isotropic values for those atoms refined anisotropically are calculated as one third of the trace of the orthogonalized Uij tensor.
3) Parameters without standard deviations were not varied.

Table 4: Anisotropic Thermal Parameters for MSC Sample 03054

Atom	U11	U22	U33	U23	U13	U12
Ti(1)	18(1)	18(1)	13(1)	-1(1)	-2(1)	1(1)
N(2)	16(1)	20(1)	13(1)	0(1)	0(1)	1(1)
C(3)	19(1)	19(1)	14(1)	1(1)	1(1)	-2(1)
C(4)	14(1)	24(1)	19(1)	-2(1)	-3(1)	-3(1)
C(5)	18(1)	29(1)	11(1)	-2(1)	0(1)	3(1)
N(6)	18(1)	18(1)	12(1)	0(1)	0(1)	1(1)
C(7)	16(1)	15(1)	20(1)	-4(1)	-4(1)	2(1)
C(8)	23(1)	16(1)	22(1)	0(1)	1(1)	-1(1)
C(9)	22(1)	23(1)	32(2)	2(1)	7(1)	1(1)
C(10)	20(1)	24(1)	33(2)	-3(1)	-2(1)	7(1)
C(11)	24(2)	26(1)	22(1)	1(1)	-6(1)	4(1)
C(12)	23(1)	23(1)	19(1)	0(1)	-2(1)	2(1)
C(13)	28(2)	40(2)	25(2)	10(1)	3(1)	11(1)
C(14)	54(2)	49(2)	26(2)	4(2)	3(2)	20(2)
C(15)	41(2)	44(2)	39(2)	18(2)	7(2)	0(2)
C(16)	27(2)	22(1)	28(2)	6(1)	11(1)	8(1)
C(17)	36(2)	30(2)	42(2)	11(2)	14(2)	3(1)
C(18)	41(2)	33(2)	32(2)	10(1)	2(2)	4(2)
C(19)	26(2)	20(1)	30(2)	0(1)	-6(1)	1(1)
C(20)	21(1)	27(2)	27(2)	-1(1)	-4(1)	6(1)
C(21)	16(1)	20(1)	18(1)	1(1)	-3(1)	1(1)
C(22)	18(1)	25(1)	22(1)	4(1)	1(1)	4(1)
C(23)	26(2)	30(2)	24(2)	11(1)	6(1)	4(1)
C(24)	28(2)	21(1)	36(2)	8(1)	3(1)	5(1)
C(25)	24(1)	22(1)	26(2)	-2(1)	2(1)	6(1)
C(26)	20(1)	21(1)	20(1)	2(1)	-1(1)	-1(1)
C(27)	31(2)	20(1)	24(2)	1(1)	8(1)	4(1)
C(28)	35(2)	32(2)	36(2)	2(2)	13(2)	7(1)
C(29)	48(2)	27(2)	22(2)	-2(1)	4(1)	2(2)
C(30)	26(2)	30(2)	19(1)	8(1)	2(1)	11(1)
C(31)	38(2)	45(2)	30(2)	-8(2)	10(2)	2(2)
C(32)	36(2)	43(2)	37(2)	-1(2)	16(2)	4(2)
N(33)	27(1)	24(1)	19(1)	-2(1)	-3(1)	-6(1)
C(34)	30(2)	25(1)	23(1)	-2(1)	-3(1)	-10(1)
C(35)	27(2)	29(2)	30(2)	-3(1)	1(1)	-8(1)
C(36)	47(2)	25(2)	44(2)	-9(1)	-6(2)	-11(2)
C(37)	62(2)	35(2)	55(2)	-8(2)	-31(2)	-12(2)
C(38)	59(2)	34(2)	61(2)	0(2)	-40(2)	-4(2)
C(39)	45(2)	26(2)	43(2)	1(1)	-19(2)	-7(1)
C(40)	50(2)	26(2)	59(2)	-3(2)	-33(2)	-3(2)
C(41)	47(3)	45(2)	116(4)	-19(3)	-21(3)	6(2)
C(42)	124(4)	26(2)	89(3)	2(2)	-68(3)	1(2)
C(43)	22(2)	23(1)	43(2)	-6(1)	0(1)	-5(1)
C(44)	38(2)	38(2)	43(2)	5(2)	1(2)	3(2)
C(45)	33(2)	28(2)	55(2)	-9(2)	2(2)	-2(1)
N(46)	22(1)	30(1)	19(1)	-1(1)	-1(1)	2(1)
C(47)	30(1)	24(1)	15(1)	4(1)	3(1)	11(1)
C(48)	40(2)	32(2)	19(2)	-1(1)	0(1)	12(1)
C(49)	56(2)	41(2)	16(2)	-4(1)	3(1)	14(2)
C(50)	62(2)	42(2)	22(2)	6(1)	20(2)	15(2)
C(51)	37(2)	33(2)	34(2)	8(1)	13(1)	6(1)

C(52)	33(2)	22(1)	22(1)	7(1)	7(1)	5(1)
C(53)	28(2)	30(2)	24(2)	8(1)	8(1)	-3(1)
C(54)	37(2)	40(2)	45(2)	13(2)	-1(2)	0(2)
C(55)	31(2)	32(2)	35(2)	1(1)	6(2)	-2(1)
C(56)	44(2)	48(2)	21(2)	-10(1)	-9(1)	4(2)
C(57)	81(3)	50(2)	43(2)	-13(2)	6(2)	-5(2)
C(58)	58(3)	66(3)	94(4)	-8(3)	-43(3)	8(2)
B(59)	16(1)	20(1)	21(2)	2(1)	1(1)	1(1)
C(60)	20(1)	23(1)	20(1)	8(1)	-4(1)	0(1)
C(61)	21(1)	27(1)	26(2)	6(1)	0(1)	1(1)
C(62)	19(1)	35(2)	36(2)	3(1)	-5(1)	-6(1)
C(63)	32(2)	30(2)	37(2)	-5(1)	-12(1)	-7(1)
C(64)	27(2)	29(2)	25(2)	-2(1)	-5(1)	4(1)
C(65)	18(1)	27(1)	23(1)	6(1)	-5(1)	2(1)
F(66)	18(1)	35(1)	37(1)	-1(1)	3(1)	-2(1)
F(67)	22(1)	51(1)	64(1)	-5(1)	-3(1)	-14(1)
F(68)	40(1)	48(1)	64(1)	-23(1)	-12(1)	-12(1)
F(69)	35(1)	43(1)	38(1)	-17(1)	-10(1)	6(1)
F(70)	19(1)	32(1)	26(1)	-3(1)	-1(1)	4(1)
C(71)	13(1)	20(1)	27(1)	3(1)	2(1)	-3(1)
C(72)	17(1)	23(1)	26(2)	3(1)	0(1)	-1(1)
C(73)	21(1)	24(1)	38(2)	12(1)	1(1)	5(1)
C(74)	25(2)	17(1)	43(2)	4(1)	13(1)	5(1)
C(75)	30(2)	22(1)	26(2)	1(1)	8(1)	-2(1)
C(76)	19(1)	21(1)	25(1)	7(1)	1(1)	2(1)
F(77)	24(1)	32(1)	29(1)	6(1)	-6(1)	6(1)
F(78)	30(1)	35(1)	51(1)	12(1)	-1(1)	14(1)
F(79)	42(1)	27(1)	52(1)	5(1)	16(1)	14(1)
F(80)	49(1)	32(1)	30(1)	-4(1)	9(1)	8(1)
F(81)	30(1)	28(1)	24(1)	1(1)	-3(1)	6(1)
C(82)	18(1)	17(1)	18(1)	-3(1)	-1(1)	-1(1)
C(83)	13(1)	19(1)	24(1)	-1(1)	1(1)	1(1)
C(84)	23(1)	21(1)	22(1)	0(1)	2(1)	-4(1)
C(85)	28(2)	15(1)	23(1)	2(1)	-9(1)	4(1)
C(86)	13(1)	22(1)	25(1)	-5(1)	-4(1)	3(1)
C(87)	18(1)	18(1)	19(1)	-2(1)	0(1)	-3(1)
F(88)	16(1)	30(1)	31(1)	8(1)	5(1)	3(1)
F(89)	31(1)	31(1)	28(1)	12(1)	1(1)	-3(1)
F(90)	30(1)	26(1)	36(1)	8(1)	-9(1)	5(1)
F(91)	17(1)	36(1)	32(1)	-1(1)	-3(1)	8(1)
F(92)	16(1)	29(1)	26(1)	3(1)	3(1)	-1(1)
C(93)	17(1)	19(1)	22(1)	3(1)	4(1)	4(1)
C(94)	18(1)	23(1)	27(2)	1(1)	-3(1)	0(1)
C(95)	32(2)	29(2)	22(2)	9(1)	4(1)	1(1)
C(96)	28(2)	23(1)	36(2)	11(1)	9(1)	-4(1)
C(97)	20(1)	22(1)	36(2)	-1(1)	1(1)	-4(1)
C(98)	21(1)	23(1)	19(1)	1(1)	2(1)	4(1)
F(99)	30(1)	35(1)	23(1)	6(1)	-5(1)	-4(1)
F(100)	51(1)	47(1)	24(1)	14(1)	3(1)	-5(1)
F(101)	44(1)	40(1)	45(1)	14(1)	10(1)	-13(1)
F(102)	32(1)	30(1)	45(1)	1(1)	-2(1)	-12(1)
F(103)	25(1)	28(1)	23(1)	1(1)	-3(1)	-4(1)
C(104)	46(2)	71(3)	64(3)	-22(2)	-3(2)	0(2)
C(105)	51(2)	50(2)	53(2)	-19(2)	3(2)	-5(2)
O(106)	46(1)	55(1)	57(2)	-12(1)	1(1)	-1(1)
C(107)	47(2)	43(2)	61(2)	1(2)	9(2)	3(2)
C(108)	64(3)	58(3)	51(2)	7(2)	11(2)	1(2)

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Form of the anisotropic thermal parameter:
   exp{ -2 pi**2 [ h**2 (a*)**2 U11 + ... + 2 h k (a*) (b*) U12 ] }
All values are X 10**3
```

Table 5a: Bond Distances for MSC Sample 03054

A	B	Distance
Ti(1)	N(33)	1.863(2)
Ti(1)	N(46)	1.875(2)
Ti(1)	N(6)	1.9876(19)
Ti(1)	N(2)	2.0150(19)
Ti(1)	H(150)	2.22(4)
Ti(1)	H(168)	2.01(3)
N(2)	C(3)	1.343(3)
N(2)	C(7)	1.455(3)
C(3)	C(4)	1.410(3)
C(3)	C(19)	1.501(3)
C(4)	C(5)	1.385(3)
C(4)	H(109)	0.91(2)
C(5)	N(6)	1.361(3)
C(5)	C(20)	1.508(3)
N(6)	C(21)	1.454(3)
C(7)	C(8)	1.401(3)
C(7)	C(12)	1.402(3)
C(8)	C(9)	1.386(3)
C(8)	C(16)	1.517(3)
C(9)	C(10)	1.379(4)
C(9)	H(110)	0.96(2)
C(10)	C(11)	1.372(4)
C(10)	H(111)	0.93(2)
C(11)	C(12)	1.391(3)
C(11)	H(112)	0.95(3)
C(12)	C(13)	1.519(4)
C(13)	C(14)	1.524(4)
C(13)	C(15)	1.525(4)
C(13)	H(113)	0.95(3)
C(14)	H(114)	0.98(3)
C(14)	H(115)	0.98(3)
C(14)	H(116)	1.00(4)
C(15)	H(117)	0.96(3)
C(15)	H(118)	1.07(3)
C(15)	H(119)	1.00(3)
C(16)	C(18)	1.523(4)
C(16)	C(17)	1.524(4)
C(16)	H(120)	0.96(2)
C(17)	H(121)	0.99(3)
C(17)	H(122)	1.00(3)
C(17)	H(123)	0.96(3)
C(18)	H(124)	0.96(3)
C(18)	H(125)	0.99(3)
C(18)	H(126)	0.92(3)
C(19)	H(127)	0.99(3)
C(19)	H(128)	0.91(3)

C(19)	H(129)	0.98(3)
C(20)	H(130)	0.93(3)
C(20)	H(131)	0.99(3)
C(20)	H(132)	0.97(3)
C(21)	C(26)	1.407(3)
C(21)	C(22)	1.412(3)
C(22)	C(23)	1.388(3)
C(22)	C(30)	1.520(3)
C(23)	C(24)	1.379(4)
C(23)	H(133)	0.92(2)
C(24)	C(25)	1.376(4)
C(24)	H(134)	0.94(2)
C(25)	C(26)	1.389(3)
C(25)	H(135)	0.95(2)
C(26)	C(27)	1.524(3)
C(27)	C(29)	1.529(4)
C(27)	C(28)	1.535(4)
C(27)	H(136)	0.90(2)
C(28)	H(137)	0.93(3)
C(28)	H(138)	0.98(3)
C(28)	H(139)	1.02(3)
C(29)	H(140)	0.96(3)
C(29)	H(141)	0.99(3)
C(29)	H(142)	1.01(3)
C(30)	C(32)	1.520(4)
C(30)	C(31)	1.530(4)
C(30)	H(143)	0.93(2)
C(31)	H(144)	0.98(3)
C(31)	H(145)	1.00(3)
C(31)	H(146)	1.02(3)
C(32)	H(147)	0.95(3)
C(32)	H(148)	1.02(3)
C(32)	H(149)	1.00(3)
N(33)	C(34)	1.450(3)
N(33)	H(150)	0.74(4)
C(34)	C(39)	1.397(4)
C(34)	C(35)	1.410(4)
C(35)	C(36)	1.388(4)
C(35)	C(43)	1.511(4)
C(36)	C(37)	1.377(4)
C(36)	H(151)	0.93(3)
C(37)	C(38)	1.361(4)
C(37)	H(152)	0.97(3)
C(38)	C(39)	1.400(4)
C(38)	H(153)	0.90(3)
C(39)	C(40)	1.516(4)
C(40)	C(41)	1.525(6)
C(40)	C(42)	1.526(5)
C(40)	H(154)	0.94(3)
C(41)	H(155)	1.00(3)
C(41)	H(156)	0.99(3)
C(41)	H(157)	0.99(4)
C(42)	H(158)	1.00(3)
C(42)	H(159)	0.97(3)
C(42)	H(160)	1.22(6)
C(43)	C(45)	1.526(4)
C(43)	C(44)	1.527(4)

C(43)	H(161)	0.93(3)
C(44)	H(162)	0.99(3)
C(44)	H(163)	1.00(3)
C(44)	H(164)	0.99(3)
C(45)	H(165)	1.07(3)
C(45)	H(166)	1.00(3)
C(45)	H(167)	0.95(3)
N(46)	C(47)	1.414(3)
N(46)	H(168)	0.81(3)
C(47)	C(52)	1.412(4)
C(47)	C(48)	1.417(3)
C(48)	C(49)	1.389(4)
C(48)	C(56)	1.512(4)
C(49)	C(50)	1.370(5)
C(49)	H(169)	0.94(3)
C(50)	C(51)	1.383(4)
C(50)	H(170)	0.95(3)
C(51)	C(52)	1.388(4)
C(51)	H(171)	0.93(3)
C(52)	C(53)	1.509(4)
C(53)	C(55)	1.522(4)
C(53)	C(54)	1.533(4)
C(53)	H(172)	0.95(2)
C(54)	H(173)	1.00(3)
C(54)	H(174)	0.98(3)
C(54)	H(175)	1.02(3)
C(55)	H(176)	1.02(3)
C(55)	H(177)	1.03(3)
C(55)	H(178)	0.96(3)
C(56)	C(57)	1.529(5)
C(56)	C(58)	1.530(5)
C(56)	H(179)	0.89(3)
C(57)	H(180)	0.98(4)
C(57)	H(181)	1.07(4)
C(57)	H(182)	0.97(4)
C(58)	H(183)	0.90(4)
C(58)	H(184)	1.05(4)
C(58)	H(185)	1.02(5)
B(59)	C(71)	1.645(4)
B(59)	C(60)	1.650(4)
B(59)	C(93)	1.655(4)
B(59)	C(82)	1.656(4)
C(60)	C(65)	1.384(3)
C(60)	C(61)	1.390(3)
C(61)	F(66)	1.350(3)
C(61)	C(62)	1.387(4)
C(62)	F(67)	1.348(3)
C(62)	C(63)	1.363(4)
C(63)	F(68)	1.347(3)
C(63)	C(64)	1.378(4)
C(64)	F(69)	1.341(3)
C(64)	C(65)	1.375(3)
C(65)	F(70)	1.360(3)
C(71)	C(76)	1.389(3)
C(71)	C(72)	1.395(3)
C(72)	F(77)	1.356(3)
C(72)	C(73)	1.372(3)

C(73)	F(78)	1.349(3)
C(73)	C(74)	1.366(4)
C(74)	F(79)	1.348(3)
C(74)	C(75)	1.371(4)
C(75)	F(80)	1.349(3)
C(75)	C(76)	1.381(3)
C(76)	F(81)	1.357(3)
C(82)	C(83)	1.388(3)
C(82)	C(87)	1.390(3)
C(83)	F(88)	1.356(3)
C(83)	C(84)	1.378(3)
C(84)	F(89)	1.350(3)
C(84)	C(85)	1.377(3)
C(85)	F(90)	1.347(3)
C(85)	C(86)	1.368(3)
C(86)	F(91)	1.346(3)
C(86)	C(87)	1.381(3)
C(87)	F(92)	1.348(3)
C(93)	C(98)	1.385(3)
C(93)	C(94)	1.384(3)
C(94)	F(99)	1.356(3)
C(94)	C(95)	1.384(3)
C(95)	F(100)	1.348(3)
C(95)	C(96)	1.364(4)
C(96)	F(101)	1.341(3)
C(96)	C(97)	1.371(4)
C(97)	F(102)	1.349(3)
C(97)	C(98)	1.371(3)
C(98)	F(103)	1.356(3)
C(104)	C(105)	1.506(5)
C(104)	H(186)	1.09(5)
C(104)	H(187)	1.06(4)
C(104)	H(188)	1.24(5)
C(105)	O(106)	1.433(4)
C(105)	H(189)	1.11(3)
C(105)	H(190)	1.19(4)
O(106)	C(107)	1.442(4)
C(107)	C(108)	1.497(5)
C(107)	H(191)	1.18(3)
C(107)	H(192)	1.14(4)
C(108)	H(193)	1.12(4)
C(108)	H(194)	1.08(4)
C(108)	H(195)	1.07(4)

Symmetry transformations used to generate equivalent atoms:

Table 5b: Bond Angles for MSC Sample 03054

A	B	C	Angle
N(33)	Ti(1)	N(46)	105.25(11)
N(33)	Ti(1)	N(6)	115.88(9)
N(46)	Ti(1)	N(6)	117.24(9)
N(33)	Ti(1)	N(2)	109.78(9)
N(46)	Ti(1)	N(2)	115.77(9)
N(6)	Ti(1)	N(2)	92.87(8)
N(33)	Ti(1)	H(150)	18.6(10)

N(46)	Ti(1)	H(150)	123.5(10)
N(6)	Ti(1)	H(150)	101.0(10)
N(2)	Ti(1)	H(150)	101.1(10)
N(33)	Ti(1)	H(168)	82.0(8)
N(46)	Ti(1)	H(168)	23.7(8)
N(6)	Ti(1)	H(168)	134.6(8)
N(2)	Ti(1)	H(168)	121.2(8)
H(150)	Ti(1)	H(168)	100.5(13)
C(3)	N(2)	C(7)	120.03(19)
C(3)	N(2)	Ti(1)	119.79(16)
C(7)	N(2)	Ti(1)	120.07(14)
N(2)	C(3)	C(4)	121.6(2)
N(2)	C(3)	C(19)	121.2(2)
C(4)	C(3)	C(19)	117.2(2)
C(5)	C(4)	C(3)	130.0(2)
C(5)	C(4)	H(109)	115.5(15)
C(3)	C(4)	H(109)	114.2(15)
N(6)	C(5)	C(4)	122.8(2)
N(6)	C(5)	C(20)	119.1(2)
C(4)	C(5)	C(20)	118.0(2)
C(5)	N(6)	C(21)	119.21(19)
C(5)	N(6)	Ti(1)	117.52(15)
C(21)	N(6)	Ti(1)	122.46(15)
C(8)	C(7)	C(12)	121.6(2)
C(8)	C(7)	N(2)	117.9(2)
C(12)	C(7)	N(2)	120.4(2)
C(9)	C(8)	C(7)	118.1(2)
C(9)	C(8)	C(16)	120.5(2)
C(7)	C(8)	C(16)	121.4(2)
C(10)	C(9)	C(8)	121.1(3)
C(10)	C(9)	H(110)	119.7(15)
C(8)	C(9)	H(110)	119.2(15)
C(11)	C(10)	C(9)	120.0(3)
C(11)	C(10)	H(111)	119.6(14)
C(9)	C(10)	H(111)	120.3(14)
C(10)	C(11)	C(12)	121.6(2)
C(10)	C(11)	H(112)	121.3(15)
C(12)	C(11)	H(112)	117.1(15)
C(11)	C(12)	C(7)	117.5(2)
C(11)	C(12)	C(13)	119.3(2)
C(7)	C(12)	C(13)	123.2(2)
C(12)	C(13)	C(14)	111.1(3)
C(12)	C(13)	C(15)	111.6(2)
C(14)	C(13)	C(15)	111.2(3)
C(12)	C(13)	H(113)	108.4(15)
C(14)	C(13)	H(113)	104.7(15)
C(15)	C(13)	H(113)	109.6(16)
C(13)	C(14)	H(114)	112.2(15)
C(13)	C(14)	H(115)	115.6(16)
H(114)	C(14)	H(115)	98(2)
C(13)	C(14)	H(116)	111(2)
H(114)	C(14)	H(116)	113(2)
H(115)	C(14)	H(116)	106(3)
C(13)	C(15)	H(117)	112.5(18)
C(13)	C(15)	H(118)	111.6(16)
H(117)	C(15)	H(118)	105(2)
C(13)	C(15)	H(119)	111.5(18)

H(117)	C(15)	H(119)	107(2)
H(118)	C(15)	H(119)	109(3)
C(8)	C(16)	C(18)	111.8(2)
C(8)	C(16)	C(17)	112.8(2)
C(18)	C(16)	C(17)	111.7(3)
C(8)	C(16)	H(120)	106.2(14)
C(18)	C(16)	H(120)	108.3(14)
C(17)	C(16)	H(120)	105.5(14)
C(16)	C(17)	H(121)	109.3(18)
C(16)	C(17)	H(122)	108.8(16)
H(121)	C(17)	H(122)	111(2)
C(16)	C(17)	H(123)	110.0(18)
H(121)	C(17)	H(123)	109(2)
H(122)	C(17)	H(123)	109(2)
C(16)	C(18)	H(124)	109.1(17)
C(16)	C(18)	H(125)	114.4(17)
H(124)	C(18)	H(125)	106(2)
C(16)	C(18)	H(126)	112.6(17)
H(124)	C(18)	H(126)	103(2)
H(125)	C(18)	H(126)	110(2)
C(3)	C(19)	H(127)	112.9(16)
C(3)	C(19)	H(128)	109.2(19)
H(127)	C(19)	H(128)	106(2)
C(3)	C(19)	H(129)	111.0(18)
H(127)	C(19)	H(129)	106(2)
H(128)	C(19)	H(129)	112(3)
C(5)	C(20)	H(130)	114.8(19)
C(5)	C(20)	H(131)	108.5(16)
H(130)	C(20)	H(131)	109(2)
C(5)	C(20)	H(132)	107.8(18)
H(130)	C(20)	H(132)	108(2)
H(131)	C(20)	H(132)	109(2)
C(26)	C(21)	C(22)	121.6(2)
C(26)	C(21)	N(6)	120.6(2)
C(22)	C(21)	N(6)	117.9(2)
C(23)	C(22)	C(21)	117.4(2)
C(23)	C(22)	C(30)	120.3(2)
C(21)	C(22)	C(30)	122.3(2)
C(24)	C(23)	C(22)	121.7(3)
C(24)	C(23)	H(133)	119.9(14)
C(22)	C(23)	H(133)	118.4(14)
C(25)	C(24)	C(23)	120.0(3)
C(25)	C(24)	H(134)	118.9(15)
C(23)	C(24)	H(134)	121.0(15)
C(24)	C(25)	C(26)	121.3(2)
C(24)	C(25)	H(135)	120.4(14)
C(26)	C(25)	H(135)	118.3(14)
C(25)	C(26)	C(21)	118.0(2)
C(25)	C(26)	C(27)	118.4(2)
C(21)	C(26)	C(27)	123.6(2)
C(26)	C(27)	C(29)	111.7(2)
C(26)	C(27)	C(28)	110.9(2)
C(29)	C(27)	C(28)	110.4(2)
C(26)	C(27)	H(136)	108.6(14)
C(29)	C(27)	H(136)	107.7(15)
C(28)	C(27)	H(136)	107.5(15)
C(27)	C(28)	H(137)	109.4(17)

C(27)	C(28)	H(138)	111.9(17)
H(137)	C(28)	H(138)	107(2)
C(27)	C(28)	H(139)	110.9(15)
H(137)	C(28)	H(139)	109(2)
H(138)	C(28)	H(139)	109(2)
C(27)	C(29)	H(140)	110.6(17)
C(27)	C(29)	H(141)	109.2(15)
H(140)	C(29)	H(141)	106(2)
C(27)	C(29)	H(142)	110.8(15)
H(140)	C(29)	H(142)	109(2)
H(141)	C(29)	H(142)	110(2)
C(32)	C(30)	C(22)	113.7(2)
C(32)	C(30)	C(31)	108.7(2)
C(22)	C(30)	C(31)	112.7(2)
C(32)	C(30)	H(143)	110.8(15)
C(22)	C(30)	H(143)	108.2(14)
C(31)	C(30)	H(143)	102.3(15)
C(30)	C(31)	H(144)	116.1(18)
C(30)	C(31)	H(145)	102.9(17)
H(144)	C(31)	H(145)	110(3)
C(30)	C(31)	H(146)	109.0(16)
H(144)	C(31)	H(146)	107(2)
H(145)	C(31)	H(146)	113(2)
C(30)	C(32)	H(147)	107.8(18)
C(30)	C(32)	H(148)	110.7(18)
H(147)	C(32)	H(148)	106(2)
C(30)	C(32)	H(149)	113.3(16)
H(147)	C(32)	H(149)	108(2)
H(148)	C(32)	H(149)	110(2)
C(34)	N(33)	Ti(1)	132.80(19)
C(34)	N(33)	H(150)	117(3)
Ti(1)	N(33)	H(150)	109(3)
C(39)	C(34)	C(35)	121.6(2)
C(39)	C(34)	N(33)	120.0(2)
C(35)	C(34)	N(33)	118.3(2)
C(36)	C(35)	C(34)	117.7(3)
C(36)	C(35)	C(43)	121.1(3)
C(34)	C(35)	C(43)	121.0(2)
C(37)	C(36)	C(35)	121.2(3)
C(37)	C(36)	H(151)	116.4(17)
C(35)	C(36)	H(151)	122.4(18)
C(38)	C(37)	C(36)	120.4(3)
C(38)	C(37)	H(152)	119.1(19)
C(36)	C(37)	H(152)	120.5(19)
C(37)	C(38)	C(39)	121.5(3)
C(37)	C(38)	H(153)	119(2)
C(39)	C(38)	H(153)	119(2)
C(34)	C(39)	C(38)	117.5(3)
C(34)	C(39)	C(40)	123.6(2)
C(38)	C(39)	C(40)	118.7(3)
C(39)	C(40)	C(41)	109.4(3)
C(39)	C(40)	C(42)	113.1(3)
C(41)	C(40)	C(42)	111.3(4)
C(39)	C(40)	H(154)	109.2(16)
C(41)	C(40)	H(154)	108.5(16)
C(42)	C(40)	H(154)	105.2(16)

C(40)	C(41)	H(155)	113.5(19)
C(40)	C(41)	H(156)	109.3(18)
H(155)	C(41)	H(156)	113(3)
C(40)	C(41)	H(157)	108(2)
H(155)	C(41)	H(157)	108(3)
H(156)	C(41)	H(157)	104(3)
C(40)	C(42)	H(158)	111.7(19)
C(40)	C(42)	H(159)	105(2)
H(158)	C(42)	H(159)	103(3)
C(40)	C(42)	H(160)	113(3)
H(158)	C(42)	H(160)	104(3)
H(159)	C(42)	H(160)	120(3)
C(35)	C(43)	C(45)	114.1(3)
C(35)	C(43)	C(44)	109.7(2)
C(45)	C(43)	C(44)	109.8(3)
C(35)	C(43)	H(161)	104.6(15)
C(45)	C(43)	H(161)	107.4(15)
C(44)	C(43)	H(161)	111.1(15)
C(43)	C(44)	H(162)	112.6(19)
C(43)	C(44)	H(163)	110.3(18)
H(162)	C(44)	H(163)	104(2)
C(43)	C(44)	H(164)	112.7(16)
H(162)	C(44)	H(164)	109(2)
H(163)	C(44)	H(164)	108(2)
C(43)	C(45)	H(165)	110.3(16)
C(43)	C(45)	H(166)	110.7(16)
H(165)	C(45)	H(166)	107(2)
C(43)	C(45)	H(167)	109.0(19)
H(165)	C(45)	H(167)	107(2)
H(166)	C(45)	H(167)	113(3)
C(47)	N(46)	Ti(1)	157.47(19)
C(47)	N(46)	H(168)	114(2)
Ti(1)	N(46)	H(168)	88(2)
C(52)	C(47)	N(46)	119.8(2)
C(52)	C(47)	C(48)	120.8(2)
N(46)	C(47)	C(48)	119.4(2)
C(49)	C(48)	C(47)	117.5(3)
C(49)	C(48)	C(56)	118.9(3)
C(47)	C(48)	C(56)	123.6(2)
C(50)	C(49)	C(48)	122.5(3)
C(50)	C(49)	H(169)	120.0(17)
C(48)	C(49)	H(169)	117.4(17)
C(49)	C(50)	C(51)	119.4(3)
C(49)	C(50)	H(170)	115.6(18)
C(51)	C(50)	H(170)	125.0(18)
C(50)	C(51)	C(52)	121.5(3)
C(50)	C(51)	H(171)	121.8(16)
C(52)	C(51)	H(171)	116.7(16)
C(51)	C(52)	C(47)	118.3(3)
C(51)	C(52)	C(53)	119.7(3)
C(47)	C(52)	C(53)	121.9(2)
C(52)	C(53)	C(55)	109.5(2)
C(52)	C(53)	C(54)	113.7(2)
C(55)	C(53)	C(54)	109.7(2)
C(52)	C(53)	H(172)	107.5(13)
C(55)	C(53)	H(172)	108.2(13)
C(54)	C(53)	H(172)	108.1(13)

C(53)	C(54)	H(173)	110.0(16)
C(53)	C(54)	H(174)	109.7(17)
H(173)	C(54)	H(174)	109(2)
C(53)	C(54)	H(175)	109.1(17)
H(173)	C(54)	H(175)	110(2)
H(174)	C(54)	H(175)	108(2)
C(53)	C(55)	H(176)	108.5(15)
C(53)	C(55)	H(177)	111.7(17)
H(176)	C(55)	H(177)	110(2)
C(53)	C(55)	H(178)	106.2(17)
H(176)	C(55)	H(178)	111(2)
H(177)	C(55)	H(178)	109(2)
C(48)	C(56)	C(57)	112.9(3)
C(48)	C(56)	C(58)	109.7(3)
C(57)	C(56)	C(58)	110.9(3)
C(48)	C(56)	H(179)	111(2)
C(57)	C(56)	H(179)	105(2)
C(58)	C(56)	H(179)	107(2)
C(56)	C(57)	H(180)	111(2)
C(56)	C(57)	H(181)	111(2)
H(180)	C(57)	H(181)	102(3)
C(56)	C(57)	H(182)	111(2)
H(180)	C(57)	H(182)	108(3)
H(181)	C(57)	H(182)	114(3)
C(56)	C(58)	H(183)	105(3)
C(56)	C(58)	H(184)	116(2)
H(183)	C(58)	H(184)	105(3)
C(56)	C(58)	H(185)	110(3)
H(183)	C(58)	H(185)	113(4)
H(184)	C(58)	H(185)	108(3)
C(71)	B(59)	C(60)	115.0(2)
C(71)	B(59)	C(93)	100.94(19)
C(60)	B(59)	C(93)	113.5(2)
C(71)	B(59)	C(82)	113.1(2)
C(60)	B(59)	C(82)	100.33(18)
C(93)	B(59)	C(82)	114.6(2)
C(65)	C(60)	C(61)	113.2(2)
C(65)	C(60)	B(59)	118.5(2)
C(61)	C(60)	B(59)	127.7(2)
F(66)	C(61)	C(62)	115.4(2)
F(66)	C(61)	C(60)	120.9(2)
C(62)	C(61)	C(60)	123.7(2)
F(67)	C(62)	C(63)	120.2(2)
F(67)	C(62)	C(61)	120.0(3)
C(63)	C(62)	C(61)	119.8(2)
F(68)	C(63)	C(62)	120.8(3)
F(68)	C(63)	C(64)	119.8(3)
C(62)	C(63)	C(64)	119.4(2)
F(69)	C(64)	C(65)	120.9(2)
F(69)	C(64)	C(63)	120.5(2)
C(65)	C(64)	C(63)	118.5(2)
F(70)	C(65)	C(64)	115.5(2)
F(70)	C(65)	C(60)	119.2(2)
C(64)	C(65)	C(60)	125.4(2)
C(76)	C(71)	C(72)	112.6(2)
C(76)	C(71)	B(59)	127.7(2)
C(72)	C(71)	B(59)	119.2(2)

F(77)	C(72)	C(73)	116.4(2)
F(77)	C(72)	C(71)	118.7(2)
C(73)	C(72)	C(71)	124.9(2)
F(78)	C(73)	C(74)	119.9(2)
F(78)	C(73)	C(72)	120.7(2)
C(74)	C(73)	C(72)	119.4(2)
F(79)	C(74)	C(73)	120.9(2)
F(79)	C(74)	C(75)	120.1(2)
C(73)	C(74)	C(75)	119.0(2)
F(80)	C(75)	C(74)	119.9(2)
F(80)	C(75)	C(76)	120.4(2)
C(74)	C(75)	C(76)	119.8(2)
F(81)	C(76)	C(75)	114.9(2)
F(81)	C(76)	C(71)	120.9(2)
C(75)	C(76)	C(71)	124.2(2)
C(83)	C(82)	C(87)	113.2(2)
C(83)	C(82)	B(59)	118.9(2)
C(87)	C(82)	B(59)	127.3(2)
F(88)	C(83)	C(84)	115.6(2)
F(88)	C(83)	C(82)	119.4(2)
C(84)	C(83)	C(82)	125.0(2)
F(89)	C(84)	C(85)	120.1(2)
F(89)	C(84)	C(83)	121.2(2)
C(85)	C(84)	C(83)	118.7(2)
F(90)	C(85)	C(86)	120.8(2)
F(90)	C(85)	C(84)	119.9(2)
C(86)	C(85)	C(84)	119.3(2)
F(91)	C(86)	C(85)	120.2(2)
F(91)	C(86)	C(87)	120.0(2)
C(85)	C(86)	C(87)	119.9(2)
F(92)	C(87)	C(86)	115.4(2)
F(92)	C(87)	C(82)	120.8(2)
C(86)	C(87)	C(82)	123.8(2)
C(98)	C(93)	C(94)	113.2(2)
C(98)	C(93)	B(59)	120.1(2)
C(94)	C(93)	B(59)	125.9(2)
F(99)	C(94)	C(95)	114.9(2)
F(99)	C(94)	C(93)	121.4(2)
C(95)	C(94)	C(93)	123.7(2)
F(100)	C(95)	C(96)	120.2(2)
F(100)	C(95)	C(94)	119.9(2)
C(96)	C(95)	C(94)	119.9(2)
F(101)	C(96)	C(95)	120.3(2)
F(101)	C(96)	C(97)	120.6(2)
C(95)	C(96)	C(97)	119.0(2)
F(102)	C(97)	C(98)	121.5(2)
F(102)	C(97)	C(96)	119.3(2)
C(98)	C(97)	C(96)	119.2(2)
F(103)	C(98)	C(97)	116.5(2)
F(103)	C(98)	C(93)	118.6(2)
C(97)	C(98)	C(93)	124.9(2)
C(105)	C(104)	H(186)	115(2)
C(105)	C(104)	H(187)	111(2)
H(186)	C(104)	H(187)	104(3)
C(105)	C(104)	H(188)	111(2)
H(186)	C(104)	H(188)	109(3)
H(187)	C(104)	H(188)	106(3)

O(106)	C(105)	C(104)	108.4(3)
O(106)	C(105)	H(189)	112.9(16)
C(104)	C(105)	H(189)	111.9(16)
O(106)	C(105)	H(190)	109.6(17)
C(104)	C(105)	H(190)	112.4(17)
H(189)	C(105)	H(190)	102(2)
C(105)	O(106)	C(107)	112.3(3)
O(106)	C(107)	C(108)	108.5(3)
O(106)	C(107)	H(191)	106.8(16)
C(108)	C(107)	H(191)	110.6(16)
O(106)	C(107)	H(192)	108.7(18)
C(108)	C(107)	H(192)	113.0(17)
H(191)	C(107)	H(192)	109(2)
C(107)	C(108)	H(193)	107.7(19)
C(107)	C(108)	H(194)	111.7(19)
H(193)	C(108)	H(194)	105(3)
C(107)	C(108)	H(195)	109.6(19)
H(193)	C(108)	H(195)	113(3)
H(194)	C(108)	H(195)	110(3)

Symmetry transformations used to generate equivalent atoms:

Table 5c: Torsion angles for MSC Sample 03054

A - B - C - D				Torsion Angle
N(33)	Ti(1)	N(2)	C(3)	-153.14(17)
N(46)	Ti(1)	N(2)	C(3)	87.92(19)
N(6)	Ti(1)	N(2)	C(3)	-34.29(18)
N(33)	Ti(1)	N(2)	C(7)	30.51(19)
N(46)	Ti(1)	N(2)	C(7)	-88.43(18)
N(6)	Ti(1)	N(2)	C(7)	149.35(17)
C(7)	N(2)	C(3)	C(4)	-170.0(2)
Ti(1)	N(2)	C(3)	C(4)	13.6(3)
C(7)	N(2)	C(3)	C(19)	9.0(3)
Ti(1)	N(2)	C(3)	C(19)	-167.31(19)
N(2)	C(3)	C(4)	C(5)	15.8(4)
C(19)	C(3)	C(4)	C(5)	-163.2(3)
C(3)	C(4)	C(5)	N(6)	-9.4(4)
C(3)	C(4)	C(5)	C(20)	170.5(3)
C(4)	C(5)	N(6)	C(21)	165.3(2)
C(20)	C(5)	N(6)	C(21)	-14.7(3)
C(4)	C(5)	N(6)	Ti(1)	-24.8(3)
C(20)	C(5)	N(6)	Ti(1)	155.25(19)
N(33)	Ti(1)	N(6)	C(5)	152.73(17)
N(46)	Ti(1)	N(6)	C(5)	-81.93(19)
N(2)	Ti(1)	N(6)	C(5)	39.10(17)
N(33)	Ti(1)	N(6)	C(21)	-37.7(2)
N(46)	Ti(1)	N(6)	C(21)	87.68(19)
N(2)	Ti(1)	N(6)	C(21)	-151.30(17)
C(3)	N(2)	C(7)	C(8)	100.8(3)

Ti(1)	N(2)	C(7)	C(8)	-82.9(2)
C(3)	N(2)	C(7)	C(12)	-81.4(3)
Ti(1)	N(2)	C(7)	C(12)	95.0(2)
C(12)	C(7)	C(8)	C(9)	-0.2(4)
N(2)	C(7)	C(8)	C(9)	177.6(2)
C(12)	C(7)	C(8)	C(16)	178.1(2)
N(2)	C(7)	C(8)	C(16)	-4.1(3)
C(7)	C(8)	C(9)	C(10)	-1.4(4)
C(16)	C(8)	C(9)	C(10)	-179.7(2)
C(8)	C(9)	C(10)	C(11)	1.9(4)
C(9)	C(10)	C(11)	C(12)	-0.8(4)
C(10)	C(11)	C(12)	C(7)	-0.8(4)
C(10)	C(11)	C(12)	C(13)	177.4(2)
C(8)	C(7)	C(12)	C(11)	1.2(4)
N(2)	C(7)	C(12)	C(11)	-176.5(2)
C(8)	C(7)	C(12)	C(13)	-176.9(2)
N(2)	C(7)	C(12)	C(13)	5.4(4)
C(11)	C(12)	C(13)	C(14)	72.0(3)
C(7)	C(12)	C(13)	C(14)	-109.9(3)
C(11)	C(12)	C(13)	C(15)	-52.7(3)
C(7)	C(12)	C(13)	C(15)	125.4(3)
C(9)	C(8)	C(16)	C(18)	83.2(3)
C(7)	C(8)	C(16)	C(18)	-95.0(3)
C(9)	C(8)	C(16)	C(17)	-43.7(3)
C(7)	C(8)	C(16)	C(17)	138.1(3)
C(5)	N(6)	C(21)	C(26)	90.0(3)
Ti(1)	N(6)	C(21)	C(26)	-79.5(3)
C(5)	N(6)	C(21)	C(22)	-90.4(3)
Ti(1)	N(6)	C(21)	C(22)	100.1(2)
C(26)	C(21)	C(22)	C(23)	0.6(4)
N(6)	C(21)	C(22)	C(23)	-179.0(2)
C(26)	C(21)	C(22)	C(30)	-177.8(2)
N(6)	C(21)	C(22)	C(30)	2.6(3)
C(21)	C(22)	C(23)	C(24)	1.1(4)
C(30)	C(22)	C(23)	C(24)	179.6(2)
C(22)	C(23)	C(24)	C(25)	-1.6(4)
C(23)	C(24)	C(25)	C(26)	0.3(4)
C(24)	C(25)	C(26)	C(21)	1.4(4)
C(24)	C(25)	C(26)	C(27)	-176.8(2)
C(22)	C(21)	C(26)	C(25)	-1.8(4)
N(6)	C(21)	C(26)	C(25)	177.8(2)
C(22)	C(21)	C(26)	C(27)	176.2(2)
N(6)	C(21)	C(26)	C(27)	-4.2(4)
C(25)	C(26)	C(27)	C(29)	-67.8(3)
C(21)	C(26)	C(27)	C(29)	114.2(3)
C(25)	C(26)	C(27)	C(28)	55.8(3)
C(21)	C(26)	C(27)	C(28)	-122.3(3)
C(23)	C(22)	C(30)	C(32)	30.2(4)
C(21)	C(22)	C(30)	C(32)	-151.4(3)
C(23)	C(22)	C(30)	C(31)	-94.0(3)
C(21)	C(22)	C(30)	C(31)	84.4(3)
N(46)	Ti(1)	N(33)	C(34)	-6.6(3)
N(6)	Ti(1)	N(33)	C(34)	124.7(2)
N(2)	Ti(1)	N(33)	C(34)	-131.8(2)
Ti(1)	N(33)	C(34)	C(39)	91.3(3)
Ti(1)	N(33)	C(34)	C(35)	-86.7(3)
C(39)	C(34)	C(35)	C(36)	-3.3(4)

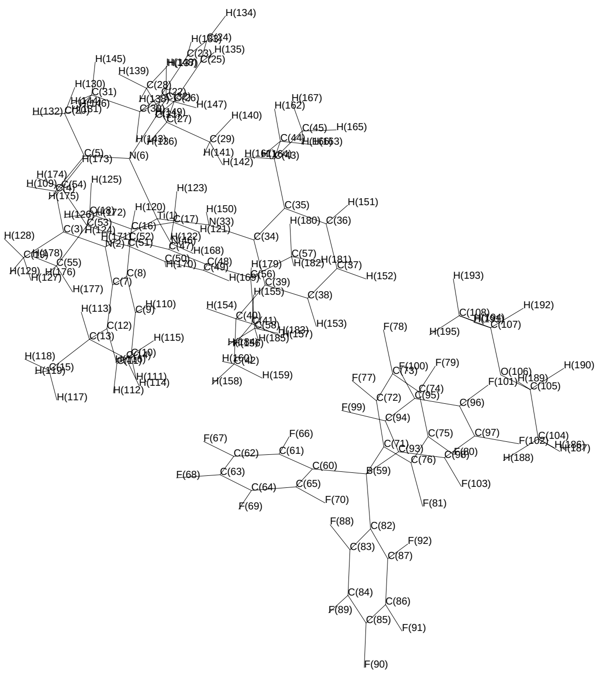
N(33)	C(34)	C(35)	C(36)	174.7(3)
C(39)	C(34)	C(35)	C(43)	170.9(3)
N(33)	C(34)	C(35)	C(43)	-11.1(4)
C(34)	C(35)	C(36)	C(37)	0.4(5)
C(43)	C(35)	C(36)	C(37)	-173.8(3)
C(35)	C(36)	C(37)	C(38)	2.3(6)
C(36)	C(37)	C(38)	C(39)	-2.1(6)
C(35)	C(34)	C(39)	C(38)	3.5(5)
N(33)	C(34)	C(39)	C(38)	-174.5(3)
C(35)	C(34)	C(39)	C(40)	-170.5(3)
N(33)	C(34)	C(39)	C(40)	11.5(5)
C(37)	C(38)	C(39)	C(34)	-0.7(6)
C(37)	C(38)	C(39)	C(40)	173.6(4)
C(34)	C(39)	C(40)	C(41)	96.1(4)
C(38)	C(39)	C(40)	C(41)	-77.8(4)
C(34)	C(39)	C(40)	C(42)	-139.2(4)
C(38)	C(39)	C(40)	C(42)	46.9(5)
C(36)	C(35)	C(43)	C(45)	-25.7(4)
C(34)	C(35)	C(43)	C(45)	160.2(3)
C(36)	C(35)	C(43)	C(44)	97.9(3)
C(34)	C(35)	C(43)	C(44)	-76.1(3)
N(33)	Ti(1)	N(46)	C(47)	150.6(5)
N(6)	Ti(1)	N(46)	C(47)	20.2(5)
N(2)	Ti(1)	N(46)	C(47)	-88.0(5)
Ti(1)	N(46)	C(47)	C(52)	28.6(6)
Ti(1)	N(46)	C(47)	C(48)	-150.6(4)
C(52)	C(47)	C(48)	C(49)	1.0(4)
N(46)	C(47)	C(48)	C(49)	-179.7(2)
C(52)	C(47)	C(48)	C(56)	177.9(2)
N(46)	C(47)	C(48)	C(56)	-2.8(4)
C(47)	C(48)	C(49)	C(50)	-0.2(4)
C(56)	C(48)	C(49)	C(50)	-177.2(3)
C(48)	C(49)	C(50)	C(51)	-1.0(5)
C(49)	C(50)	C(51)	C(52)	1.3(5)
C(50)	C(51)	C(52)	C(47)	-0.5(4)
C(50)	C(51)	C(52)	C(53)	175.6(3)
N(46)	C(47)	C(52)	C(51)	-180.0(2)
C(48)	C(47)	C(52)	C(51)	-0.7(4)
N(46)	C(47)	C(52)	C(53)	4.1(4)
C(48)	C(47)	C(52)	C(53)	-176.7(2)
C(51)	C(52)	C(53)	C(55)	-77.9(3)
C(47)	C(52)	C(53)	C(55)	98.0(3)
C(51)	C(52)	C(53)	C(54)	45.2(3)
C(47)	C(52)	C(53)	C(54)	-138.9(3)
C(49)	C(48)	C(56)	C(57)	-50.8(4)
C(47)	C(48)	C(56)	C(57)	132.4(3)
C(49)	C(48)	C(56)	C(58)	73.5(4)
C(47)	C(48)	C(56)	C(58)	-103.4(4)
C(71)	B(59)	C(60)	C(65)	173.3(2)
C(93)	B(59)	C(60)	C(65)	57.7(3)
C(82)	B(59)	C(60)	C(65)	-65.0(3)
C(71)	B(59)	C(60)	C(61)	-16.2(3)
C(93)	B(59)	C(60)	C(61)	-131.8(3)
C(82)	B(59)	C(60)	C(61)	105.5(3)
C(65)	C(60)	C(61)	F(66)	178.5(2)
B(59)	C(60)	C(61)	F(66)	7.6(4)
C(65)	C(60)	C(61)	C(62)	-0.6(4)

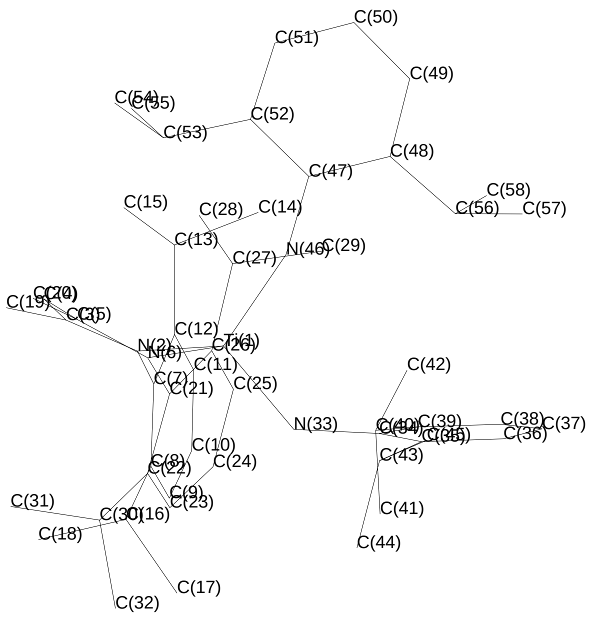
B(59)	C(60)	C(61)	C(62)	-171.5(2)
F(66)	C(61)	C(62)	F(67)	0.4(4)
C(60)	C(61)	C(62)	F(67)	179.6(2)
F(66)	C(61)	C(62)	C(63)	-178.0(2)
C(60)	C(61)	C(62)	C(63)	1.2(4)
F(67)	C(62)	C(63)	F(68)	0.6(4)
C(61)	C(62)	C(63)	F(68)	179.0(2)
F(67)	C(62)	C(63)	C(64)	-179.1(2)
C(61)	C(62)	C(63)	C(64)	-0.7(4)
F(68)	C(63)	C(64)	F(69)	-0.7(4)
C(62)	C(63)	C(64)	F(69)	178.9(2)
F(68)	C(63)	C(64)	C(65)	-180.0(2)
C(62)	C(63)	C(64)	C(65)	-0.3(4)
F(69)	C(64)	C(65)	F(70)	0.9(3)
C(63)	C(64)	C(65)	F(70)	-179.8(2)
F(69)	C(64)	C(65)	C(60)	-178.3(2)
C(63)	C(64)	C(65)	C(60)	0.9(4)
C(61)	C(60)	C(65)	F(70)	-179.7(2)
B(59)	C(60)	C(65)	F(70)	-7.8(3)
C(61)	C(60)	C(65)	C(64)	-0.5(4)
B(59)	C(60)	C(65)	C(64)	171.4(2)
C(60)	B(59)	C(71)	C(76)	132.5(3)
C(93)	B(59)	C(71)	C(76)	-104.9(3)
C(82)	B(59)	C(71)	C(76)	18.0(3)
C(60)	B(59)	C(71)	C(72)	-56.5(3)
C(93)	B(59)	C(71)	C(72)	66.1(3)
C(82)	B(59)	C(71)	C(72)	-171.0(2)
C(76)	C(71)	C(72)	F(77)	177.2(2)
B(59)	C(71)	C(72)	F(77)	5.0(3)
C(76)	C(71)	C(72)	C(73)	-1.8(4)
B(59)	C(71)	C(72)	C(73)	-174.0(2)
F(77)	C(72)	C(73)	F(78)	1.6(4)
C(71)	C(72)	C(73)	F(78)	-179.4(2)
F(77)	C(72)	C(73)	C(74)	-177.9(2)
C(71)	C(72)	C(73)	C(74)	1.2(4)
F(78)	C(73)	C(74)	F(79)	0.3(4)
C(72)	C(73)	C(74)	F(79)	179.7(2)
F(78)	C(73)	C(74)	C(75)	-179.5(2)
C(72)	C(73)	C(74)	C(75)	-0.1(4)
F(79)	C(74)	C(75)	F(80)	0.1(4)
C(73)	C(74)	C(75)	F(80)	179.9(2)
F(79)	C(74)	C(75)	C(76)	180.0(2)
C(73)	C(74)	C(75)	C(76)	-0.2(4)
F(80)	C(75)	C(76)	F(81)	-0.8(3)
C(74)	C(75)	C(76)	F(81)	179.3(2)
F(80)	C(75)	C(76)	C(71)	179.4(2)
C(74)	C(75)	C(76)	C(71)	-0.5(4)
C(72)	C(71)	C(76)	F(81)	-178.4(2)
B(59)	C(71)	C(76)	F(81)	-6.9(4)
C(72)	C(71)	C(76)	C(75)	1.4(4)
B(59)	C(71)	C(76)	C(75)	172.9(2)
C(71)	B(59)	C(82)	C(83)	55.7(3)
C(60)	B(59)	C(82)	C(83)	-67.4(3)
C(93)	B(59)	C(82)	C(83)	170.7(2)
C(71)	B(59)	C(82)	C(87)	-133.5(2)
C(60)	B(59)	C(82)	C(87)	103.4(3)
C(93)	B(59)	C(82)	C(87)	-18.5(3)

C(87)	C(82)	C(83)	F(88)	-177.2(2)
B(59)	C(82)	C(83)	F(88)	-5.2(3)
C(87)	C(82)	C(83)	C(84)	2.9(4)
B(59)	C(82)	C(83)	C(84)	175.0(2)
F(88)	C(83)	C(84)	F(89)	-2.1(3)
C(82)	C(83)	C(84)	F(89)	177.8(2)
F(88)	C(83)	C(84)	C(85)	177.6(2)
C(82)	C(83)	C(84)	C(85)	-2.5(4)
F(89)	C(84)	C(85)	F(90)	0.2(4)
C(83)	C(84)	C(85)	F(90)	-179.5(2)
F(89)	C(84)	C(85)	C(86)	179.9(2)
C(83)	C(84)	C(85)	C(86)	0.2(4)
F(90)	C(85)	C(86)	F(91)	1.9(3)
C(84)	C(85)	C(86)	F(91)	-177.8(2)
F(90)	C(85)	C(86)	C(87)	-179.0(2)
C(84)	C(85)	C(86)	C(87)	1.3(4)
F(91)	C(86)	C(87)	F(92)	-1.4(3)
C(85)	C(86)	C(87)	F(92)	179.5(2)
F(91)	C(86)	C(87)	C(82)	178.3(2)
C(85)	C(86)	C(87)	C(82)	-0.8(4)
C(83)	C(82)	C(87)	F(92)	178.5(2)
B(59)	C(82)	C(87)	F(92)	7.3(4)
C(83)	C(82)	C(87)	C(86)	-1.2(3)
B(59)	C(82)	C(87)	C(86)	-172.5(2)
C(71)	B(59)	C(93)	C(98)	63.7(3)
C(60)	B(59)	C(93)	C(98)	-172.7(2)
C(82)	B(59)	C(93)	C(98)	-58.3(3)
C(71)	B(59)	C(93)	C(94)	-105.2(3)
C(60)	B(59)	C(93)	C(94)	18.5(3)
C(82)	B(59)	C(93)	C(94)	132.9(2)
C(98)	C(93)	C(94)	F(99)	-179.2(2)
B(59)	C(93)	C(94)	F(99)	-9.7(4)
C(98)	C(93)	C(94)	C(95)	0.7(4)
B(59)	C(93)	C(94)	C(95)	170.2(2)
F(99)	C(94)	C(95)	F(100)	-0.8(4)
C(93)	C(94)	C(95)	F(100)	179.2(2)
F(99)	C(94)	C(95)	C(96)	179.3(2)
C(93)	C(94)	C(95)	C(96)	-0.7(4)
F(100)	C(95)	C(96)	F(101)	-1.0(4)
C(94)	C(95)	C(96)	F(101)	178.9(2)
F(100)	C(95)	C(96)	C(97)	-179.7(2)
C(94)	C(95)	C(96)	C(97)	0.2(4)
F(101)	C(96)	C(97)	F(102)	1.0(4)
C(95)	C(96)	C(97)	F(102)	179.7(2)
F(101)	C(96)	C(97)	C(98)	-178.6(2)
C(95)	C(96)	C(97)	C(98)	0.1(4)
F(102)	C(97)	C(98)	F(103)	1.1(4)
C(96)	C(97)	C(98)	F(103)	-179.4(2)
F(102)	C(97)	C(98)	C(93)	-179.6(2)
C(96)	C(97)	C(98)	C(93)	0.0(4)
C(94)	C(93)	C(98)	F(103)	178.9(2)
B(59)	C(93)	C(98)	F(103)	8.8(3)
C(94)	C(93)	C(98)	C(97)	-0.4(4)
B(59)	C(93)	C(98)	C(97)	-170.6(2)
C(104)	C(105)	O(106)	C(107)	179.4(3)
C(105)	O(106)	C(107)	C(108)	-179.1(3)

Symmetry transformations used to generate equivalent atoms:

Figure 1: VERSORT Drawing(s)





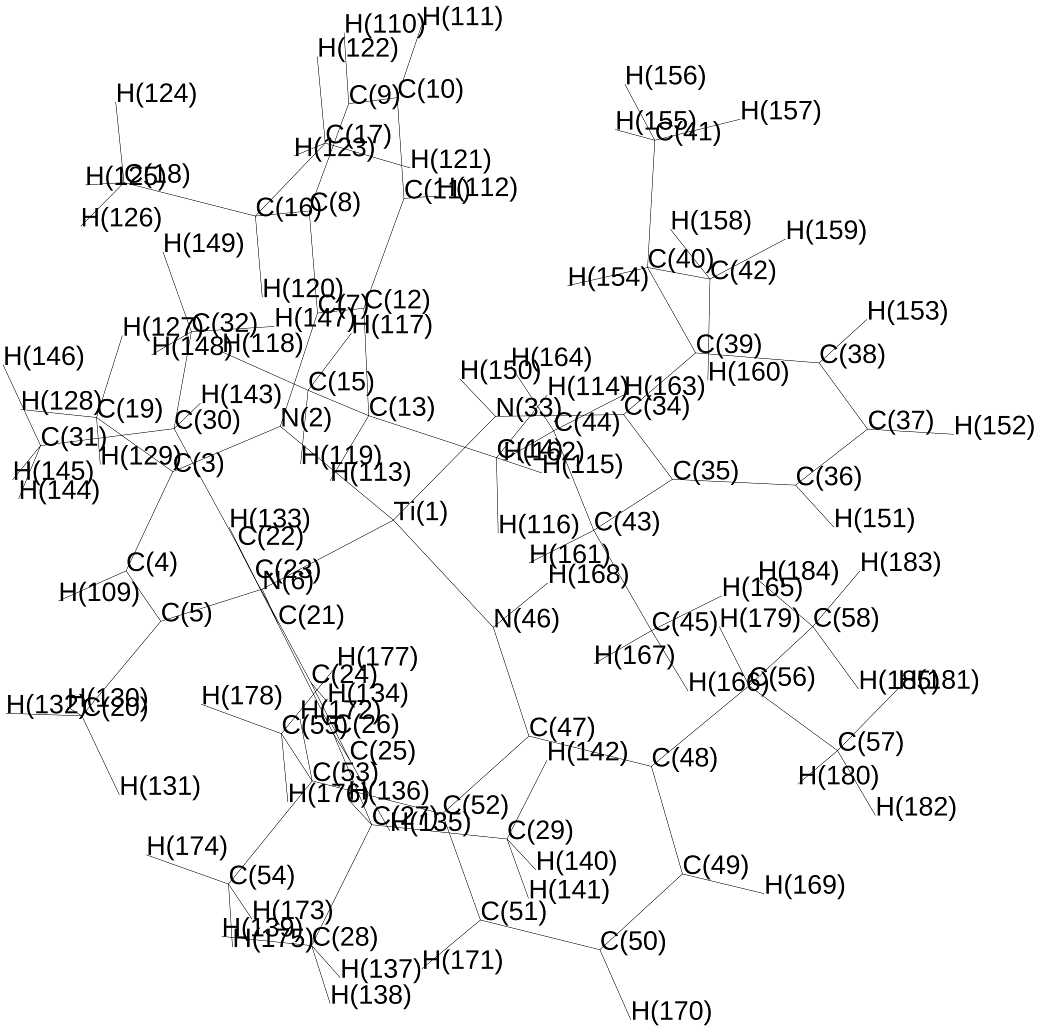
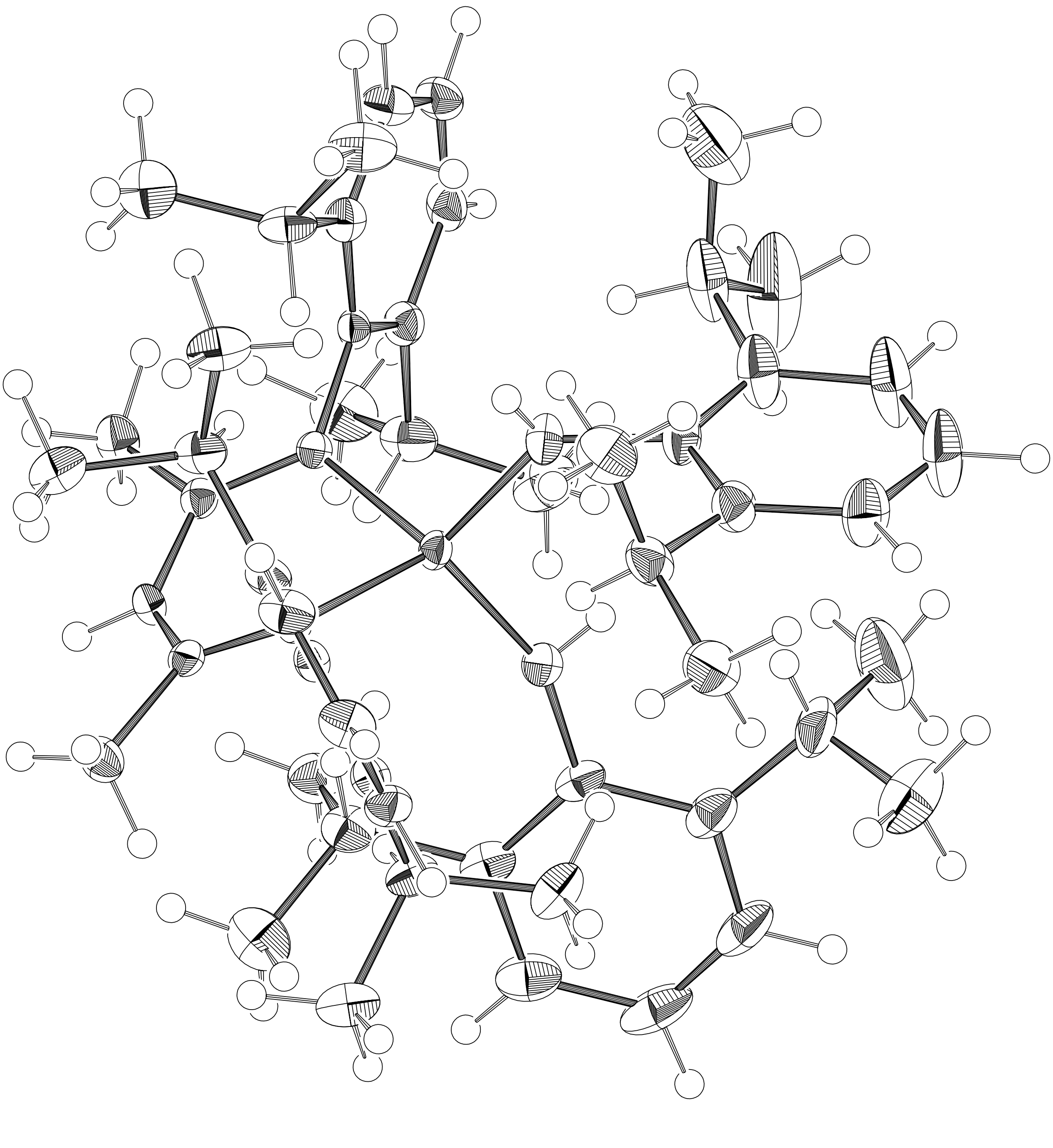
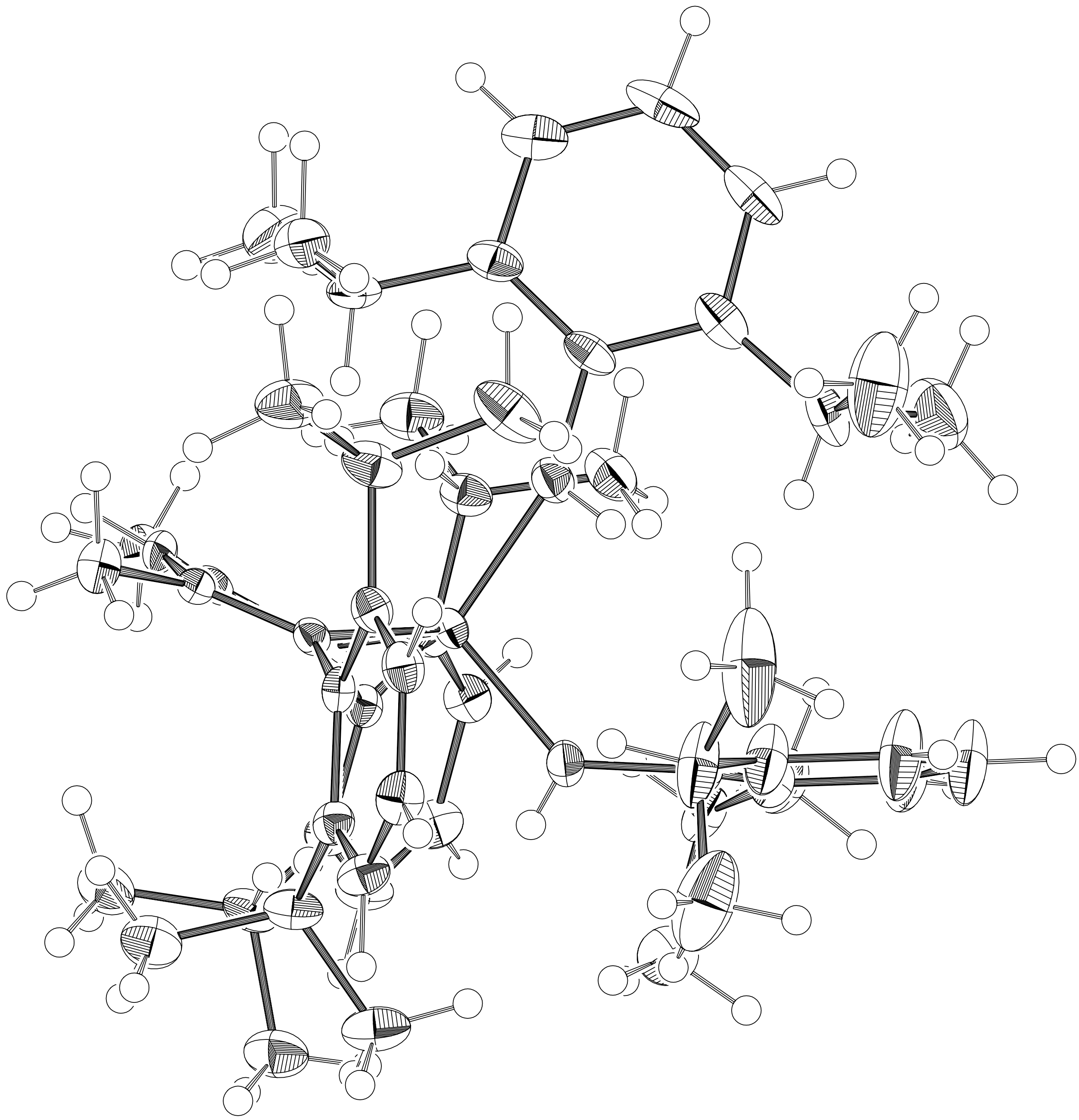

H(110)
H(111)
H(122)
H(124)
C(10)
H(156)
H(157)
C(41)
H(121)
H(126)
C(16)
C(8)
H(149)
H(158)
H(159)
H(154)
C(40)
C(42)
H(120)
C(12)
H(117)
H(153)
H(146)
C(39)
C(38)
H(160)
H(150)
H(164)
H(114)
H(163)
C(15)
H(143)
C(13)
C(34)
H(128)
C(19)
C(30)
N(2)
N(33)
C(44)
C(37)
H(152)
C(31)
H(129)
C(3)
H(119)
H(113)
H(115)
C(35)
C(36)
H(145)
H(144)
Ti(1)
H(116)
C(43)
H(151)
H(133)
C(22)
H(161)
H(168)
H(184)
H(183)
C(4)
H(109)
C(23)
N(6)
H(165)
C(5)
C(21)
N(46)
C(45)
H(179)
C(58)
H(177)
H(167)
C(24)
H(178)
C(56)
C(20)
H(134)
C(26)
C(25)
C(47)
H(142)
C(48)
C(57)
H(180)
H(131)
C(53)
H(136)
C(52)
H(182)
C(29)
H(174)
H(140)
C(54)
C(49)
H(169)
H(141)
H(173)
C(51)
C(28)
C(50)
H(137)
H(171)
H(138)
H(170)

Figure 2: ORTEP Drawing(s)



Supplementary Material (ESI) for Chemical Communications



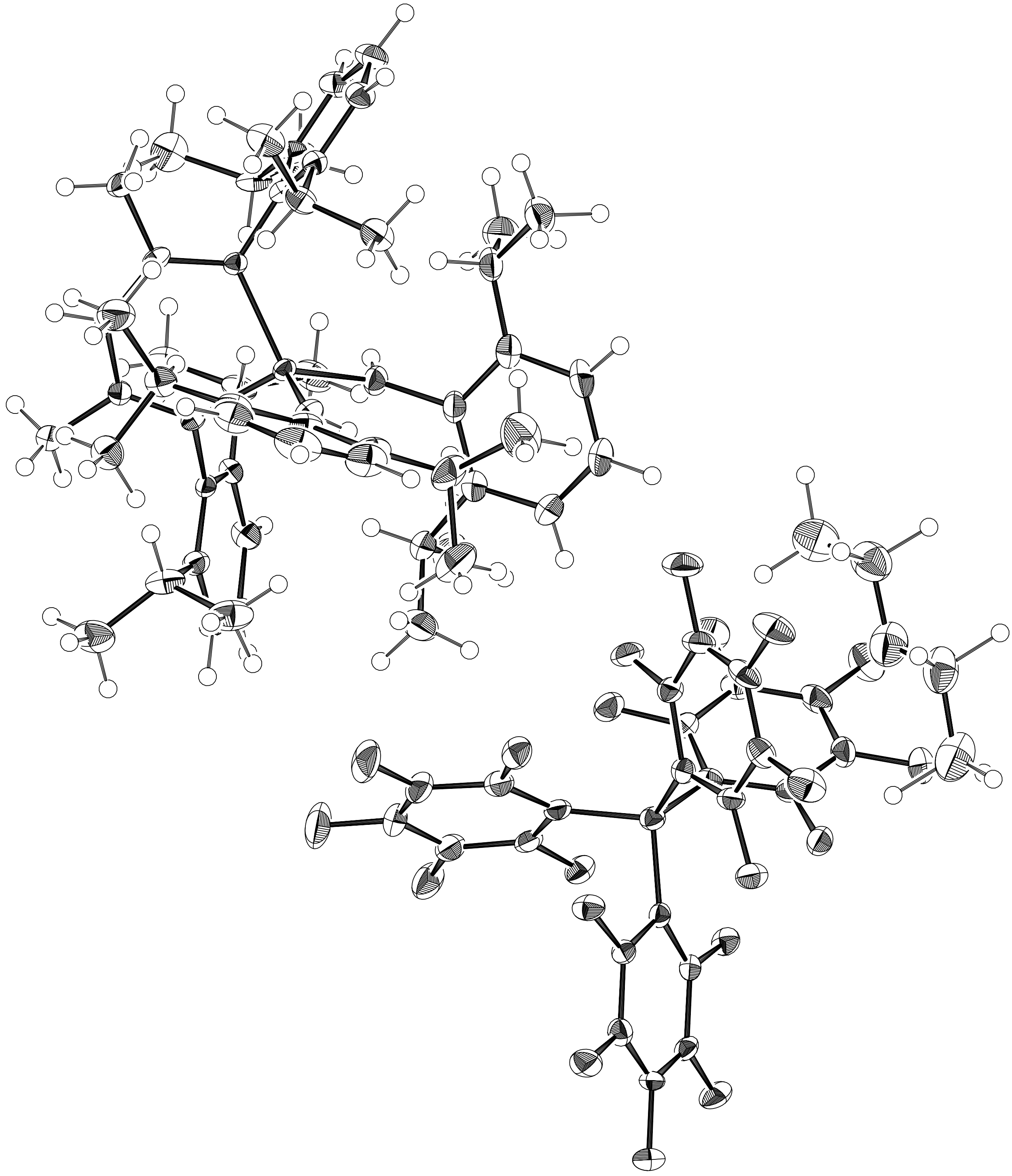
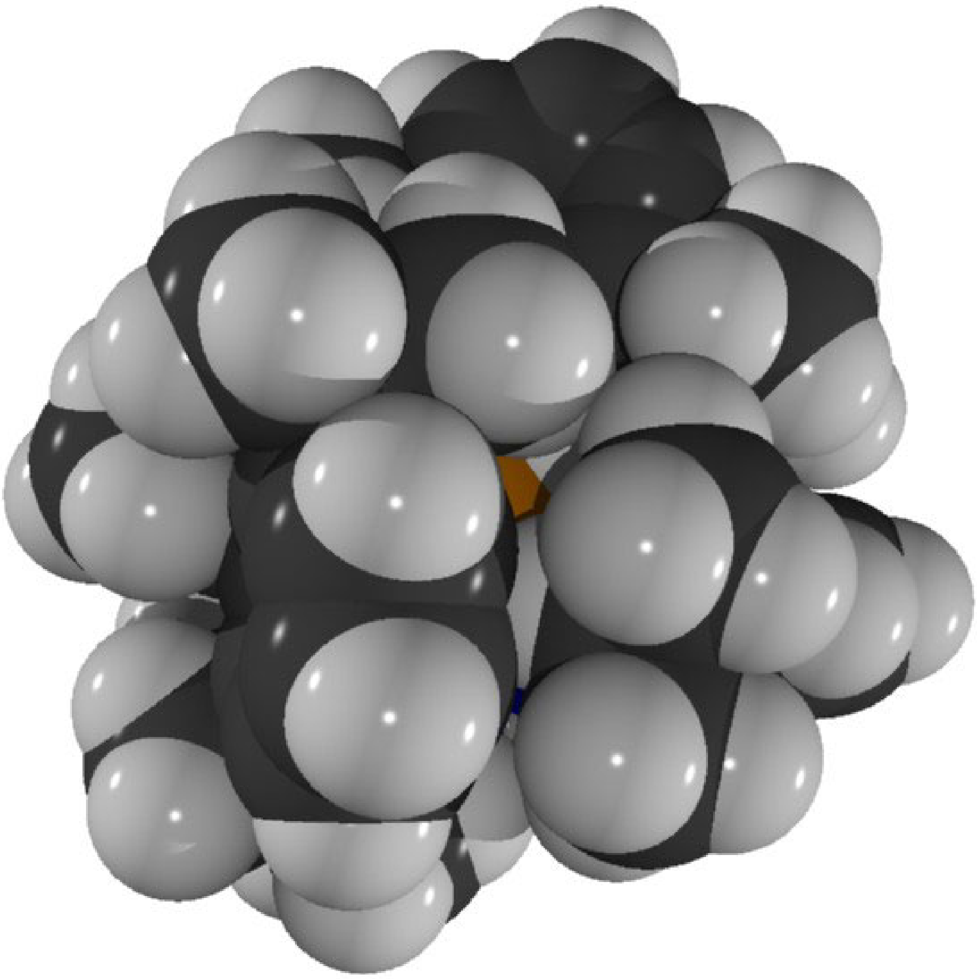


Figure 3: Space Filling Model Drawing(s)



Crystallographic data for complex (Nacnac)Ti=NAr(OTf) (4)

The sample was submitted by the research group of Prof. Daniel J. Mindiola, Department of Chemistry, Indiana University. Inert atmosphere techniques were used to place an orange crystal of approximate dimensions 0.30 × 0.25 × 0.25 mm was placed onto the tip of a 0.2 mm diameter glass capillary and mounted on a SMART6000 (Bruker) at 128(2) K.

Data collection

A preliminary set of cell constants was calculated from reflections obtained from three nearly orthogonal sets of 30 frames. The data collection was carried out using graphite monochromated Mo Kα radiation with a frame time of 15 seconds and a detector distance of 5.0 cm. A randomly oriented region of a sphere in reciprocal space was surveyed. Two sections of 606 frames were collected with 0.30° steps in ω at two different ϕ settings with the detector set at −43° in 2θ. Final cell constants were calculated from the xyz centroids of 7572 strong reflections from the actual data collection after integration (SAINT).1

Structure solution and refinement

Intensity statistics and lack of systematic absences indicated the centrosymmetric space group P1bar., and solution and refinement yielded satisfactory results. The structure was solve using SHELXS-97 and refined with SHELXL-97.2 A direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed which located the remaining non-hydrogen atoms including a disordered pentane solvent. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms not associated with the solvent were located and and refined with isotropic displacement parameters. The final full matrix least squares refinement converged to R1 = 0.0400 and wR2 = 0.0978 (F2, all data). The remaining electron density is located on bonds. The structure shows a pseudo-inversion center and is merohedrally twinned (domain ratio 57:43).

1 SAINT 6.1, Bruker Analytical X-Ray Systems, Madison, WI.
2 SHELXTL-Plus V5.10, Bruker Analytical X-Ray Systems, Madison, WI.

Table 1

Program MU for data file labeled

MSC02190 **/12/25 21:

The following were used

At.No.	At.Wt.	Abs.	%	No.	Element
22	47.880	23.400	5.55	1	Ti
16	32.066	9.990	3.72	1	S
9	18.998	1.630	6.61	3	F
8	15.999	1.220	5.57	3	O
7	14.007	.845	4.87	3	N
6	12.011	.576	65.49	47	C
1	1.008	.373	8.18	70	H

The density is 1.228 g/cc.

The volume is 2330.94 cubic Angstroms

Z = 2 and the molecular wt. is 862.03

F(000) = 924

The linear absorption coefficient = 2.820 reciprocal centimeters,

and 1/4Mu = .8865 mm.

Table 2

Crystal Data for MSC Sample 02190

Empirical Formula	C47 H70 F3 N3 O3 S Ti
Color of Crystal:	orange
Crystal Dimensions were:	0.30 x 0.25 x 0.25 mm.
Space Group:	P 1bar
Cell Dimensions (at 138(2) K; 7572 reflections)	
a =	10.2710(14)
b =	12.9651(17)
c =	18.451(3)
alpha =	93.783(7)
beta =	106.097(9)
gamma =	96.880(9)
Z (Molecules/cell):	2
Volume:	2330.9(6)
Calculated Density:	1.228
Wavelength:	0.71073
Molecular Weight:	862.02
F(000):	924
Linear Absorption Coefficient:	0.282

Data were collected on a Bruker SMART 6000 sealed-tube system comprising a three-circle platform goniostat, an HOG crystal monochromator, a four kilopixel by four kilopixel single-chip CCD-based detector, a K761 high voltage generator, and a PC interface running Bruker's SMART software.

Detector to sample distance = 5.0 cm.
Take off angle = 6.0 deg.

Data collected by the omega scan technique according to the following parameters:

frame width = 0.3 deg.
time per frame = 15.0 sec.

Data processing statistics for 27.6 degrees maximum theta:

Total number of intensities integrated = 51577
Number of unique intensities = 10763
Number with F > 4sigma(F) = 7221

R for averaging = 0.083

Refinement results:

Final residuals are:
R(F) (observed data) = 0.0400
Rw(F2) (refinement data) = 0.0978

Final Goodness of Fit = 0.933
Maximum delta/sigma for the last cycle = 0.50

Table 3: Fractional Coordinates and Isotropic Thermal Parameters for MSC Sample 02190

Atom	x	y	z	Uiso
Ti(1)	2410(1)	3116(1)	2980(1)	15(1)
N(2)	3788(2)	3717(1)	2501(1)	17(1)
C(3)	4966(2)	4037(1)	3072(1)	19(1)
C(4)	5363(2)	3507(2)	3709(1)	21(1)
C(5)	4818(2)	2531(2)	3893(1)	18(1)
N(6)	3534(1)	2090(1)	3559(1)	16(1)
C(7)	3621(2)	4102(1)	1772(1)	17(1)

C(8)	2672(2)	4796(1)	1534(1)	20(1)
C(9)	2454(2)	5092(2)	801(1)	24(1)
C(10)	3149(2)	4729(2)	321(1)	25(1)
C(11)	4103(2)	4066(2)	571(1)	24(1)
C(12)	4364(2)	3738(2)	1294(1)	20(1)
C(13)	5381(2)	2975(2)	1524(1)	24(1)
C(14)	6738(2)	3313(2)	1359(1)	31(1)
C(15)	4749(2)	1882(2)	1130(2)	34(1)
C(16)	1914(2)	5262(2)	2045(1)	24(1)
C(17)	2314(3)	6447(2)	2198(2)	34(1)
C(18)	359(2)	4967(2)	1724(1)	31(1)
C(19)	5892(3)	4997(2)	3016(1)	32(1)
C(20)	5789(2)	2036(2)	4487(1)	25(1)
C(21)	2998(2)	1094(1)	3759(1)	18(1)
C(22)	2714(2)	223(2)	3223(1)	20(1)
C(23)	2170(2)	-728(2)	3409(1)	25(1)
C(24)	1901(2)	-805(2)	4099(1)	29(1)
C(25)	2174(2)	63(2)	4613(1)	28(1)
C(26)	2723(2)	1034(2)	4464(1)	21(1)
C(27)	2965(2)	1962(2)	5058(1)	25(1)
C(28)	1605(2)	2229(2)	5158(1)	33(1)
C(29)	3901(3)	1763(2)	5829(1)	35(1)
C(30)	3071(2)	284(2)	2480(1)	22(1)
C(31)	4532(2)	54(2)	2592(2)	36(1)
C(32)	2066(2)	-432(2)	1820(1)	30(1)
N(33)	1039(2)	2419(1)	2311(1)	17(1)
C(34)	-121(2)	1761(1)	1863(1)	17(1)
C(35)	-423(2)	1627(1)	1064(1)	18(1)
C(36)	-1567(2)	930(2)	654(1)	23(1)
C(37)	-2394(2)	364(2)	1005(1)	26(1)
C(38)	-2111(2)	511(2)	1788(1)	24(1)
C(39)	-998(2)	1209(2)	2230(1)	20(1)
C(40)	-753(2)	1431(2)	3077(1)	23(1)
C(41)	-1249(2)	507(2)	3451(2)	36(1)
C(42)	-1403(2)	2393(2)	3239(1)	32(1)
C(43)	451(2)	2228(2)	644(1)	20(1)
C(44)	-388(2)	2913(2)	107(1)	30(1)
C(45)	1076(2)	1498(2)	196(1)	29(1)
O(46)	1817(1)	4032(1)	3708(1)	24(1)
S(47)	2312(1)	4963(1)	4281(1)	24(1)
O(48)	3278(2)	5704(1)	4095(1)	37(1)
O(49)	2590(2)	4681(1)	5035(1)	33(1)
C(50)	758(2)	5575(2)	4129(1)	33(1)
F(51)	-291(1)	4915(1)	4179(1)	42(1)
F(52)	428(2)	5927(1)	3454(1)	56(1)
F(53)	976(1)	6382(1)	4653(1)	47(1)
C(54S)	4444(3)	-2082(3)	936(2)	44(1)
C(55A)	5742(8)	-2609(9)	1256(5)	70(2)
C(55S)	5881(9)	-2209(6)	1181(5)	44(2)
C(56A)	6443(6)	-2400(4)	2068(3)	40(1)
C(56S)	6210(5)	-3092(4)	1630(3)	41(1)
C(57A)	7673(6)	-3249(5)	1882(4)	50(2)
C(57S)	7763(6)	-2896(5)	2311(4)	43(1)
C(58A)	8641(12)	-2359(9)	2391(8)	86(4)
C(58S)	8899(10)	-2367(8)	2011(6)	53(2)
H(1S)	388(4)	-206(3)	128(2)	112(13)

H(2S)	447(5)	-140(4)	77(3)	156(19)
H(3S)	396(4)	-255(3)	52(2)	100(13)
H(4S)	648(4)	-230(3)	89(2)	13(9)
H(5S)	628(5)	-167(5)	184(3)	63(16)
H(6S)	573(4)	-269(3)	215(2)	107(14)
H(7S)	565(4)	-369(3)	135(2)	12(9)
H(8S)	774(4)	-379(3)	222(2)	18(10)
H(9S)	797(4)	-273(3)	281(3)	21(12)
H(10S)	821(7)	-291(6)	147(4)	90(20)
H(11S)	971(5)	-260(3)	233(2)	27(11)
H(12S)	891(3)	-180(3)	213(2)	69(11)
H(59)	620(2)	382(2)	407(1)	21(5)
H(60)	183(2)	558(2)	64(1)	20(5)
H(61)	302(2)	492(2)	-16(1)	33(6)
H(62)	459(2)	382(2)	24(1)	19(5)
H(63)	553(2)	293(2)	204(1)	18(5)
H(64)	714(2)	399(2)	162(1)	32(6)
H(65)	742(2)	283(2)	156(1)	29(6)
H(66)	663(2)	331(2)	81(1)	29(6)
H(67)	539(2)	140(2)	128(1)	39(6)
H(68)	400(3)	165(2)	131(1)	46(7)
H(69)	453(2)	187(2)	57(1)	41(7)
H(70)	218(2)	501(2)	252(1)	29(6)
H(71)	200(2)	680(2)	173(1)	33(6)
H(72)	187(2)	677(2)	258(1)	39(6)
H(73)	330(3)	663(2)	240(2)	63(9)
H(74)	1(2)	523(2)	122(1)	35(6)
H(75)	-9(2)	528(2)	205(1)	44(7)
H(76)	7(2)	418(2)	166(1)	28(6)
H(77)	638(3)	488(2)	265(2)	67(9)
H(78)	539(3)	551(2)	287(2)	55(8)
H(79)	650(3)	522(2)	348(2)	55(8)
H(80)	664(2)	205(2)	437(1)	35(6)
H(81)	597(2)	241(2)	499(1)	36(6)
H(82)	549(2)	135(2)	453(1)	31(6)
H(83)	202(2)	-135(2)	305(1)	20(5)
H(84)	155(2)	-145(2)	423(1)	32(6)
H(85)	199(2)	1(2)	507(1)	30(6)
H(86)	337(2)	257(1)	489(1)	14(5)
H(87)	111(2)	164(2)	533(1)	39(7)
H(88)	178(2)	284(2)	554(1)	35(6)
H(89)	103(2)	243(2)	470(1)	39(7)
H(90)	345(2)	122(2)	608(1)	43(7)
H(91)	413(2)	237(2)	616(1)	41(7)
H(92)	474(3)	152(2)	579(1)	49(7)
H(93)	305(2)	99(2)	235(1)	17(5)
H(94)	514(2)	55(2)	298(1)	42(7)
H(95)	477(2)	10(2)	214(1)	44(7)
H(96)	462(2)	-66(2)	274(1)	42(7)
H(97)	231(2)	-32(2)	135(1)	27(6)
H(98)	211(2)	-116(2)	188(1)	46(7)
H(99)	112(3)	-28(2)	174(1)	42(7)
H(100)	-175(2)	84(1)	14(1)	16(5)
H(101)	-315(2)	-13(2)	70(1)	39(6)
H(102)	-269(2)	13(2)	204(1)	25(5)
H(103)	24(2)	161(1)	332(1)	17(5)
H(104)	-89(2)	-14(2)	333(1)	32(6)

H(105)	-223(3)	35(2)	330(1)	53(8)
H(106)	-97(2)	69(2)	401(2)	47(7)
H(107)	-241(2)	226(2)	303(1)	39(6)
H(108)	-120(2)	261(2)	378(1)	43(7)
H(109)	-105(2)	302(2)	302(1)	41(7)
H(110)	115(2)	267(2)	100(1)	18(5)
H(111)	-84(2)	339(2)	37(1)	40(7)
H(112)	-106(3)	245(2)	-31(1)	46(7)
H(113)	18(2)	334(2)	-15(1)	31(6)
H(114)	160(2)	102(2)	52(1)	34(6)
H(115)	38(2)	103(2)	-18(1)	38(6)
H(116)	168(2)	190(2)	-6(1)	35(6)

Notes:
1) Fractional coordinates are X 10**4 for non-hydrogen atoms and X 10**3 for hydrogen atoms. Uiso values are all X 10**3.
2) Isotropic values for those atoms refined anisotropically are calculated as one third of the trace of the orthogonalized Uij tensor.
3) Parameters without standard deviations were not varied.

Table 4: Anisotropic Thermal Parameters for MSC Sample 02190

Atom	U11	U22	U33	U23	U13	U12
Ti(1)	15(1)	17(1)	14(1)	4(1)	5(1)	4(1)
N(2)	17(1)	17(1)	17(1)	5(1)	4(1)	3(1)
C(3)	19(1)	20(1)	19(1)	2(1)	5(1)	1(1)
C(4)	19(1)	24(1)	16(1)	3(1)	0(1)	-3(1)
C(5)	19(1)	23(1)	14(1)	1(1)	5(1)	3(1)
N(6)	15(1)	18(1)	15(1)	5(1)	3(1)	2(1)
C(7)	19(1)	16(1)	16(1)	5(1)	4(1)	-1(1)
C(8)	19(1)	18(1)	23(1)	5(1)	7(1)	2(1)
C(9)	22(1)	23(1)	28(1)	12(1)	6(1)	7(1)
C(10)	26(1)	30(1)	19(1)	12(1)	5(1)	3(1)
C(11)	25(1)	30(1)	23(1)	7(1)	11(1)	7(1)
C(12)	18(1)	22(1)	20(1)	6(1)	6(1)	3(1)
C(13)	23(1)	33(1)	20(1)	11(1)	9(1)	13(1)
C(14)	23(1)	38(1)	33(1)	9(1)	10(1)	9(1)
C(15)	31(1)	30(1)	48(2)	13(1)	15(1)	12(1)
C(16)	29(1)	23(1)	26(1)	9(1)	12(1)	11(1)
C(17)	42(1)	26(1)	38(1)	5(1)	16(1)	8(1)
C(18)	28(1)	33(1)	39(1)	9(1)	16(1)	12(1)
C(19)	33(1)	29(1)	26(1)	9(1)	1(1)	-9(1)
C(20)	18(1)	28(1)	25(1)	10(1)	2(1)	2(1)
C(21)	13(1)	20(1)	20(1)	10(1)	3(1)	3(1)
C(22)	15(1)	21(1)	23(1)	8(1)	3(1)	4(1)
C(23)	25(1)	20(1)	29(1)	5(1)	5(1)	3(1)
C(24)	26(1)	24(1)	37(1)	16(1)	8(1)	0(1)
C(25)	28(1)	34(1)	25(1)	16(1)	10(1)	7(1)
C(26)	17(1)	26(1)	20(1)	8(1)	3(1)	6(1)
C(27)	29(1)	32(1)	17(1)	8(1)	8(1)	4(1)
C(28)	37(1)	38(1)	28(1)	7(1)	12(1)	10(1)
C(29)	37(1)	46(2)	20(1)	9(1)	5(1)	6(1)
C(30)	25(1)	18(1)	22(1)	4(1)	6(1)	4(1)
C(31)	28(1)	53(2)	30(1)	6(1)	12(1)	8(1)
C(32)	36(1)	26(1)	25(1)	1(1)	2(1)	5(1)

N(33)	17(1)	19(1)	17(1)	6(1)	6(1)	5(1)
C(34)	16(1)	14(1)	22(1)	4(1)	4(1)	7(1)
C(35)	17(1)	18(1)	21(1)	4(1)	4(1)	7(1)
C(36)	24(1)	26(1)	18(1)	1(1)	3(1)	5(1)
C(37)	20(1)	23(1)	33(1)	-2(1)	5(1)	0(1)
C(38)	19(1)	21(1)	34(1)	7(1)	10(1)	2(1)
C(39)	16(1)	21(1)	24(1)	7(1)	6(1)	8(1)
C(40)	15(1)	33(1)	24(1)	10(1)	6(1)	4(1)
C(41)	27(1)	50(2)	34(1)	22(1)	9(1)	2(1)
C(42)	29(1)	46(2)	23(1)	3(1)	10(1)	11(1)
C(43)	20(1)	22(1)	17(1)	3(1)	2(1)	1(1)
C(44)	31(1)	32(1)	27(1)	11(1)	6(1)	8(1)
C(45)	28(1)	32(1)	28(1)	5(1)	11(1)	7(1)
O(46)	25(1)	26(1)	22(1)	0(1)	8(1)	6(1)
S(47)	26(1)	25(1)	22(1)	-1(1)	8(1)	5(1)
O(48)	36(1)	32(1)	43(1)	-1(1)	18(1)	-3(1)
O(49)	40(1)	36(1)	19(1)	-1(1)	5(1)	6(1)
C(50)	39(1)	36(1)	29(1)	4(1)	16(1)	13(1)
F(51)	30(1)	51(1)	46(1)	-6(1)	16(1)	6(1)
F(52)	64(1)	78(1)	43(1)	28(1)	23(1)	45(1)
F(53)	55(1)	34(1)	59(1)	-6(1)	28(1)	14(1)
C(54S)	38(1)	52(2)	42(2)	4(1)	13(1)	7(1)
C(55A)	38(4)	93(8)	73(5)	29(6)	3(3)	5(5)
C(56A)	43(3)	39(3)	44(3)	9(3)	22(3)	2(2)
C(56S)	39(3)	26(3)	46(3)	8(3)	-5(2)	0(2)
C(57S)	33(3)	54(4)	46(4)	26(3)	13(3)	11(3)
C(58A)	49(7)	41(5)	141(12)	30(7)	-23(6)	4(5)
C(58S)	31(4)	24(4)	100(8)	15(5)	13(4)	3(3)

Form of the anisotropic thermal parameter:
exp{ -2 pi**2 [h**2 (a*)**2 U11 + ... + 2 h k (a*) (b*) U12] }
All values are X 10**3

Table 5a: Bond Distances for MSC Sample 02190

A	B	Distance
Ti(1)	N(33)	1.7049(15)
Ti(1)	N(2)	1.9783(15)
Ti(1)	O(46)	1.9991(13)
Ti(1)	N(6)	2.0289(15)
N(2)	C(3)	1.365(2)
N(2)	C(7)	1.438(2)
C(3)	C(4)	1.388(3)
C(3)	C(19)	1.501(3)
C(4)	C(5)	1.421(3)
C(5)	N(6)	1.330(2)
C(5)	C(20)	1.500(3)
N(6)	C(21)	1.453(2)
C(7)	C(8)	1.407(3)
C(7)	C(12)	1.408(3)
C(8)	C(9)	1.396(3)
C(8)	C(16)	1.518(3)
C(9)	C(10)	1.374(3)
C(10)	C(11)	1.384(3)
C(11)	C(12)	1.393(3)

C(12)	C(13)	1.518(3)
C(13)	C(14)	1.528(3)
C(13)	C(15)	1.530(3)
C(16)	C(17)	1.528(3)
C(16)	C(18)	1.532(3)
C(21)	C(22)	1.397(3)
C(21)	C(26)	1.410(3)
C(22)	C(23)	1.395(3)
C(22)	C(30)	1.520(3)
C(23)	C(24)	1.383(3)
C(24)	C(25)	1.372(3)
C(25)	C(26)	1.393(3)
C(26)	C(27)	1.521(3)
C(27)	C(28)	1.535(3)
C(27)	C(29)	1.537(3)
C(30)	C(31)	1.525(3)
C(30)	C(32)	1.528(3)
N(33)	C(34)	1.396(2)
C(34)	C(35)	1.414(3)
C(34)	C(39)	1.425(2)
C(35)	C(36)	1.390(3)
C(35)	C(43)	1.522(3)
C(36)	C(37)	1.378(3)
C(37)	C(38)	1.388(3)
C(38)	C(39)	1.388(3)
C(39)	C(40)	1.514(3)
C(40)	C(41)	1.525(3)
C(40)	C(42)	1.534(3)
C(43)	C(45)	1.525(3)
C(43)	C(44)	1.529(3)
O(46)	S(47)	1.4901(14)
S(47)	O(49)	1.4227(15)
S(47)	O(48)	1.4252(15)
S(47)	C(50)	1.828(2)
C(50)	F(51)	1.322(2)
C(50)	F(52)	1.323(2)
C(50)	F(53)	1.330(2)
C(54S)	C(55S)	1.453(9)
C(54S)	C(55A)	1.558(9)
C(55A)	C(55S)	0.558(11)
C(55A)	C(56S)	1.022(9)
C(55A)	C(56A)	1.463(10)
C(55S)	C(56S)	1.473(8)
C(55S)	C(56A)	1.624(10)
C(56A)	C(56S)	1.123(7)
C(56A)	C(57S)	1.537(7)
C(56A)	C(57A)	1.859(9)
C(56S)	C(57A)	1.488(8)
C(56S)	C(57S)	1.714(8)
C(57A)	C(57S)	0.865(7)
C(57A)	C(58A)	1.506(14)
C(57A)	C(58S)	1.550(12)
C(57S)	C(58A)	1.040(11)
C(57S)	C(58S)	1.533(10)
C(58A)	C(58S)	0.814(15)

Symmetry transformations used to generate equivalent atoms:

Table 5b: Bond Angles for MSC Sample 02190

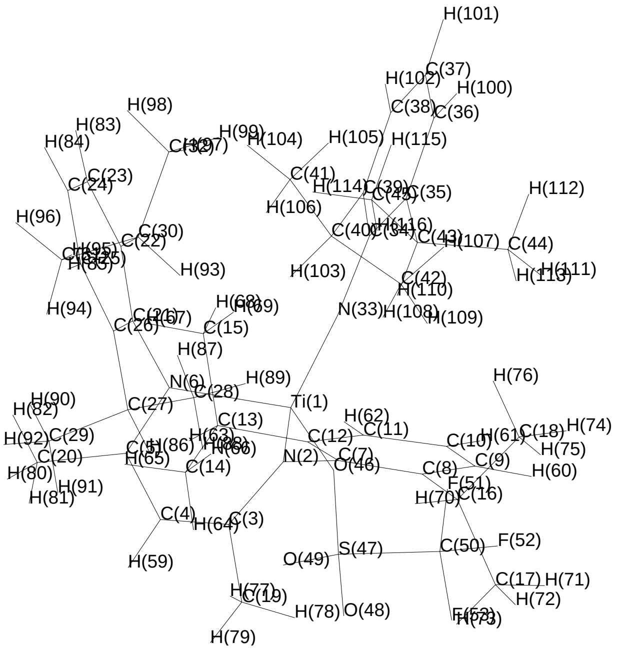
A	B	C	Angle
N(33)	Ti(1)	N(2)	110.31(7)
N(33)	Ti(1)	O(46)	111.46(6)
N(2)	Ti(1)	O(46)	119.46(6)
N(33)	Ti(1)	N(6)	108.06(7)
N(2)	Ti(1)	N(6)	97.10(6)
O(46)	Ti(1)	N(6)	109.07(6)
C(3)	N(2)	C(7)	119.92(15)
C(3)	N(2)	Ti(1)	106.63(11)
C(7)	N(2)	Ti(1)	130.58(12)
N(2)	C(3)	C(4)	122.88(17)
N(2)	C(3)	C(19)	119.33(17)
C(4)	C(3)	C(19)	117.78(17)
C(3)	C(4)	C(5)	131.72(18)
N(6)	C(5)	C(4)	122.10(17)
N(6)	C(5)	C(20)	122.45(17)
C(4)	C(5)	C(20)	115.45(16)
C(5)	N(6)	C(21)	121.10(15)
C(5)	N(6)	Ti(1)	111.22(12)
C(21)	N(6)	Ti(1)	126.05(11)
C(8)	C(7)	C(12)	121.19(16)
C(8)	C(7)	N(2)	119.40(16)
C(12)	C(7)	N(2)	119.34(16)
C(9)	C(8)	C(7)	118.08(18)
C(9)	C(8)	C(16)	118.81(17)
C(7)	C(8)	C(16)	123.08(17)
C(10)	C(9)	C(8)	121.58(19)
C(9)	C(10)	C(11)	119.57(19)
C(10)	C(11)	C(12)	121.65(19)
C(11)	C(12)	C(7)	117.90(17)
C(11)	C(12)	C(13)	119.19(17)
C(7)	C(12)	C(13)	122.87(16)
C(12)	C(13)	C(14)	112.74(17)
C(12)	C(13)	C(15)	109.99(17)
C(14)	C(13)	C(15)	110.37(18)
C(8)	C(16)	C(17)	111.12(17)
C(8)	C(16)	C(18)	112.00(18)
C(17)	C(16)	C(18)	110.97(18)
C(22)	C(21)	C(26)	121.77(17)
C(22)	C(21)	N(6)	118.07(16)
C(26)	C(21)	N(6)	120.11(17)
C(23)	C(22)	C(21)	118.04(18)
C(23)	C(22)	C(30)	120.45(18)
C(21)	C(22)	C(30)	121.38(16)
C(24)	C(23)	C(22)	121.1(2)
C(25)	C(24)	C(23)	119.84(19)
C(24)	C(25)	C(26)	121.9(2)
C(25)	C(26)	C(21)	117.33(19)
C(25)	C(26)	C(27)	118.53(18)
C(21)	C(26)	C(27)	124.13(17)
C(26)	C(27)	C(28)	110.92(18)

C(26)	C(27)	C(29)	111.91(18)
C(28)	C(27)	C(29)	109.34(18)
C(22)	C(30)	C(31)	109.18(17)
C(22)	C(30)	C(32)	113.39(17)
C(31)	C(30)	C(32)	111.18(19)
C(34)	N(33)	Ti(1)	170.47(13)
N(33)	C(34)	C(35)	121.45(16)
N(33)	C(34)	C(39)	118.42(16)
C(35)	C(34)	C(39)	120.13(16)
C(36)	C(35)	C(34)	118.54(17)
C(36)	C(35)	C(43)	119.31(17)
C(34)	C(35)	C(43)	122.14(16)
C(37)	C(36)	C(35)	121.78(19)
C(36)	C(37)	C(38)	119.60(19)
C(37)	C(38)	C(39)	121.47(18)
C(38)	C(39)	C(34)	118.41(17)
C(38)	C(39)	C(40)	121.38(17)
C(34)	C(39)	C(40)	120.12(16)
C(39)	C(40)	C(41)	114.09(18)
C(39)	C(40)	C(42)	109.61(16)
C(41)	C(40)	C(42)	110.79(19)
C(35)	C(43)	C(45)	111.70(16)
C(35)	C(43)	C(44)	110.91(16)
C(45)	C(43)	C(44)	109.44(17)
S(47)	O(46)	Ti(1)	142.36(9)
O(49)	S(47)	O(48)	119.16(9)
O(49)	S(47)	O(46)	111.94(8)
O(48)	S(47)	O(46)	112.61(8)
O(49)	S(47)	C(50)	105.05(10)
O(48)	S(47)	C(50)	104.98(10)
O(46)	S(47)	C(50)	100.76(9)
F(51)	C(50)	F(52)	108.38(19)
F(51)	C(50)	F(53)	108.50(17)
F(52)	C(50)	F(53)	108.09(18)
F(51)	C(50)	S(47)	111.62(15)
F(52)	C(50)	S(47)	111.03(15)
F(53)	C(50)	S(47)	109.13(15)
C(55S)	C(54S)	C(55A)	21.0(4)
C(55S)	C(55A)	C(56S)	135.7(19)
C(55S)	C(55A)	C(56A)	96.5(18)
C(56S)	C(55A)	C(56A)	50.0(5)
C(55S)	C(55A)	C(54S)	68.8(15)
C(56S)	C(55A)	C(54S)	147.1(8)
C(56A)	C(55A)	C(54S)	117.7(7)
C(55A)	C(55S)	C(54S)	90.2(16)
C(55A)	C(55S)	C(56S)	29.0(13)
C(54S)	C(55S)	C(56S)	115.8(6)
C(55A)	C(55S)	C(56A)	63.6(15)
C(54S)	C(55S)	C(56A)	114.3(6)
C(56S)	C(55S)	C(56A)	42.2(3)
C(56S)	C(56A)	C(55A)	44.2(5)
C(56S)	C(56A)	C(57S)	78.5(5)
C(55A)	C(56A)	C(57S)	113.2(6)
C(56S)	C(56A)	C(55S)	61.7(5)
C(55A)	C(56A)	C(55S)	20.0(5)
C(57S)	C(56A)	C(55S)	117.4(5)
C(56S)	C(56A)	C(57A)	53.2(4)

C(55A)	C(56A)	C(57A)	85.9(5)
C(57S)	C(56A)	C(57A)	27.5(3)
C(55S)	C(56A)	C(57A)	92.8(5)
C(55A)	C(56S)	C(56A)	85.9(7)
C(55A)	C(56S)	C(55S)	15.3(7)
C(56A)	C(56S)	C(55S)	76.1(5)
C(55A)	C(56S)	C(57A)	129.9(7)
C(56A)	C(56S)	C(57A)	89.6(5)
C(55S)	C(56S)	C(57A)	117.1(6)
C(55A)	C(56S)	C(57S)	131.0(7)
C(56A)	C(56S)	C(57S)	61.5(5)
C(55S)	C(56S)	C(57S)	115.7(5)
C(57A)	C(56S)	C(57S)	30.3(3)
C(57S)	C(57A)	C(56S)	89.4(7)
C(57S)	C(57A)	C(58A)	42.1(7)
C(56S)	C(57A)	C(58A)	115.6(7)
C(57S)	C(57A)	C(58S)	72.7(7)
C(56S)	C(57A)	C(58S)	124.3(6)
C(58A)	C(57A)	C(58S)	30.8(6)
C(57S)	C(57A)	C(56A)	55.1(6)
C(56S)	C(57A)	C(56A)	37.2(3)
C(58A)	C(57A)	C(56A)	79.2(6)
C(58S)	C(57A)	C(56A)	96.4(5)
C(57A)	C(57S)	C(58A)	104.1(11)
C(57A)	C(57S)	C(58S)	74.8(7)
C(58A)	C(57S)	C(58S)	29.7(10)
C(57A)	C(57S)	C(56A)	97.4(7)
C(58A)	C(57S)	C(56A)	112.7(8)
C(58S)	C(57S)	C(56A)	112.2(6)
C(57A)	C(57S)	C(56S)	60.3(6)
C(58A)	C(57S)	C(56S)	132.3(8)
C(58S)	C(57S)	C(56S)	111.5(6)
C(56A)	C(57S)	C(56S)	40.0(3)
C(58S)	C(58A)	C(57S)	111(2)
C(58S)	C(58A)	C(57A)	77.6(16)
C(57S)	C(58A)	C(57A)	33.8(6)
C(58A)	C(58S)	C(57S)	39.3(12)
C(58A)	C(58S)	C(57A)	71.6(13)
C(57S)	C(58S)	C(57A)	32.6(3)

Symmetry transformations used to generate equivalent atoms:

Figure 1: VERSORT Drawing(s)



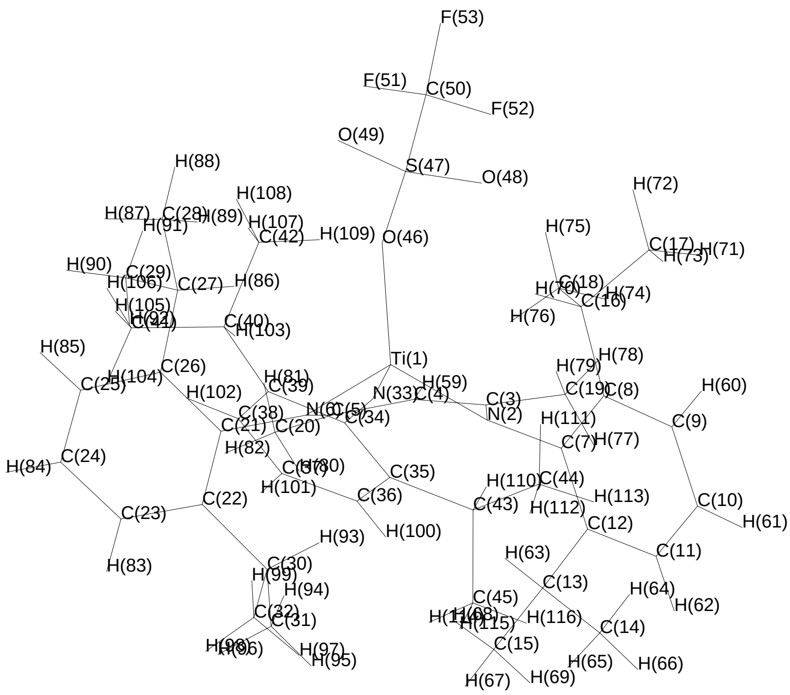
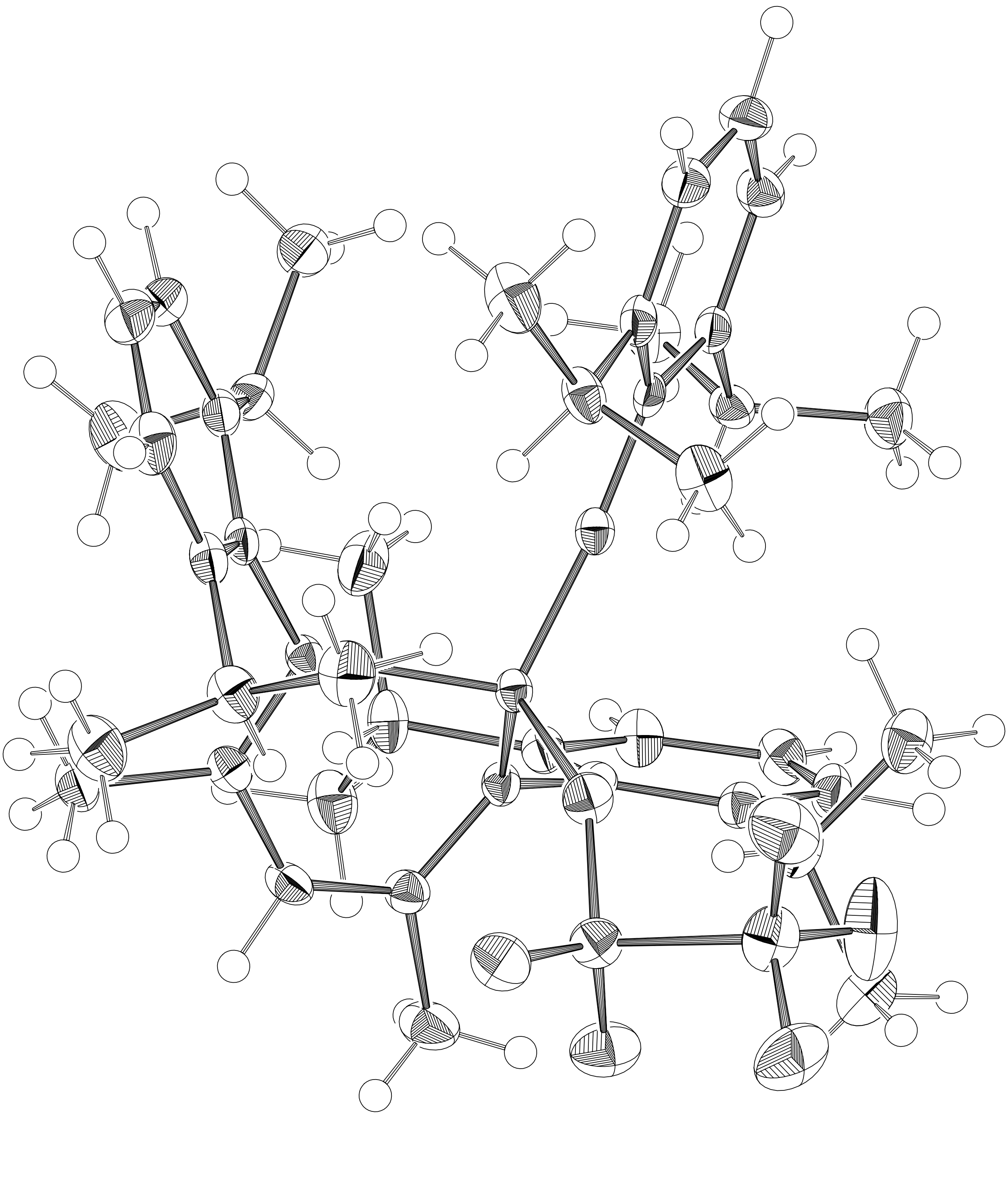


Figure 2: ORTEP Drawing(s)



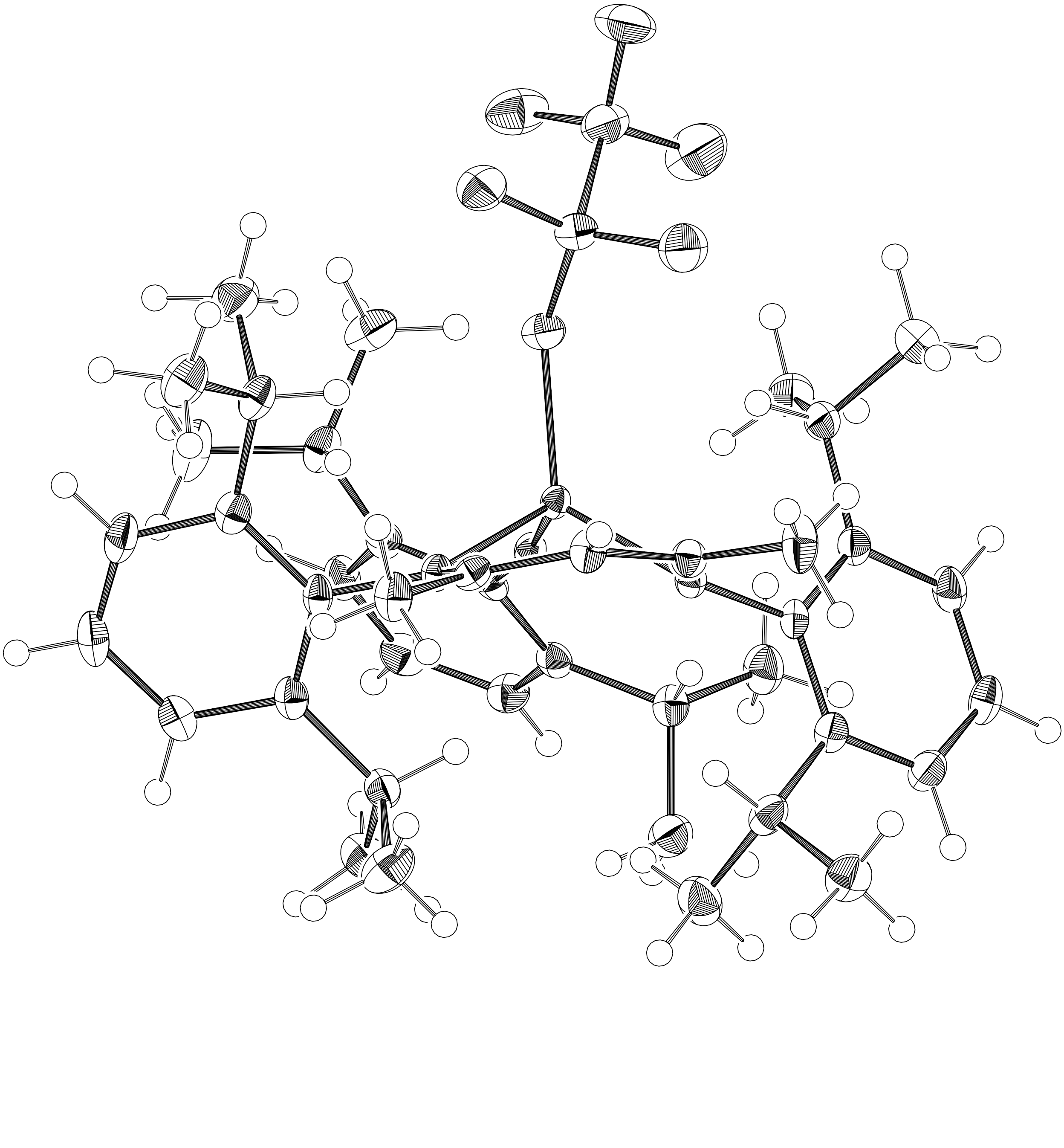


Figure 3: Space Filling Model Drawing(s)