Supplementary Material (ESI) for Dalton Transactions

Supporting Information for the Paper Entitled "Phosphaazaallene and phosphinylimide complexes stemming from terminal and four-coordinate titanium phosphinidene"

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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 pentane and hexane 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 $C_6D_5CD_3$ were purchased from Cambridge Isotope Laboratory (CIL), degassed and dried over CaH_2, then vacuum transferred to 4 Å molecular sieves. Celite, alumina, and 4 Å molecular sieves were activated under vacuum overnight at 200 ºC. Li(Nacnac) (Nacnac$^-$ = [Ar]NC(Me)CHC(Me)N[Ar], Ar = 2,6-$(CHMe_2)_2C_6H_3$),[3] $LiCH_2{}^tBu$,[4] (Nacnac)$TiCl_2$(THF),[5,6] (Nacnac)Ti=CH^tBu(OTf),[6] LiPHMes* (Mes* = 2, 4, 6-$(Me_3C)_3C_6H_2$),[7,8] (Nacnac)Ti=PMes*$(CH_2{}^tBu)$,[9] and N_2CPh_2[10] were prepared according to the literature. All other chemical were used as received. CHN analyses were performed by Desert Analytics, Tucson, AZ. ^1H, ^{13}C, and ^{31}P NMR spectra were recorded on Varian 500 or 400 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 proteo-toluene in d_8-toluene 137.9, 129.2, 128.3, 125.5, and 20.4 ppm). ^{31}P NMR chemical shifts are reported with respect to external H_3PO_4 (aqueous solution, δ 0.0 ppm). X-ray diffraction data were collected on a SMART6000 (Bruker) system under a stream of N_2 (g) at low temperatures.

Synthesis of (η^1-Nacnac)Ti(CN^{t}Bu)(η^2-(*N,C*)-^{t}BuN=CCH$_2{}^t$Bu)(η^2-(*N,C*)-^{t}BuN=C=PMes*) (2)

In a vial was loaded (Nacnac)Ti=PMes*(CH$_2{}^t$Bu),[9] [100 mg, 0.12 mmol] and dissolved in 10 mL of pentane and the solution cooled to –35 ºC. To the cold solution was added a cold pentane solution (~5 mL) containing 3 equiv of CN^{t}Bu [31.2 mg, 0.37 mmol]. After stirring for 2 hours the solution was filtered, concentrated, and cooled to –35 ^{o}C to give dark crystals of (η^1-Nacnac)Ti(CN^{t}Bu)(η^2-(*N,C*)-^{t}BuN=CCH$_2{}^t$Bu)(η^2-(*N,C*)-^{t}BuN=C=PMes*) (**2**) [79 mg, 0.07 mmol, 60% yield]. Both ^{1}H and ^{13}C NMR spectra are consistent with two isomers being present in solution. Complex **2** decomposes in solution (~$t_{1/2}$ = 2 h, 25 ^{o}C, approx.) and in the solid state (24 h, 25 ^{o}C).

For **2**: ^{1}H NMR (23 ^{o}C, 399.8 MHz, C_6D_6): δ 7.52-7.08 (m, aryl), 4.01 (s, MeCC*H*CMe, isomer), 4.25 (s, MeCC*H*CMe), 3.94 (septet, C*H*Me$_2$), 3.82 (b, C*H*Me$_2$), 3.53 (septet, C*H*Me$_2$), 3.46 (septet, C*H*(Me)$_2$), 3.29 (septet, C*H*(Me)$_2$), 3.25 (septet, C*H*(Me)$_2$), 3.11 (s, ^{t}BuNCC*H*$_2{}^t$Bu), 2.95 (s, ^{t}BuNCC*H*$_2{}^t$Bu, isomer), 1.97 (s, C*Me*$_3$), 1.92 (s, C*Me*$_3$), 1.89 (*Me*), 1.86 (*Me*), 1.84 (*Me*), 1.82 (s, C*Me*$_3$), 1.77 (s, C*Me*$_3$), 1.58 (*Me*), 1.50 (s, C*Me*$_3$), 1.48 (s, C*Me*$_3$), 1.46 (*Me*), 1.42 (s, C*Me*$_3$), 1.39 (s, C*Me*$_3$), 1.35 (*Me*), 1.28 (*Me*), 1.26 (*Me*), 1.24 (*Me*), 1.22 (*Me*), 1.19 (s, C*Me*$_3$), 1.12 (s, C*Me*$_3$), 1.03 (s, C*Me*$_3$), 0.96 (s, C*Me*$_3$), 0.88 (s, C*Me*$_3$), 0.87 (s, C*Me*$_3$).

^{13}C NMR (0 ^{o}C, 125.7 MHz, $C_6D_5CD_3$): δ 250.2 (^{t}BuN=*C*CH$_2{}^t$Bu, isomer), 246.3 (^{t}BuN=*C*CH$_2{}^t$Bu), 217.6 (d, ^{t}BuN*C*PMes*, $J_{C\text{-}P}$ = 166 Hz, isomer), 213.8 (d, ^{t}BuN*C*PMes*, $J_{C\text{-}P}$ = 172 Hz), 164.7 (Me*C*CHCMe), 164.4 (Me*C*CHCMe), 161.3, 161.1, 160.8, 158.1, 157.7, 155.1, 154.6, 154.5, 154.0, 149.6, 149.5, 147.9, 147.7, 147.6, 147.1,

147.0, 146.9, 146.8, 145.8, 145.0, 142.9, 141.9, 136.9, 136.7, 136.1, 126.3, 125.8, 124.6, 123.4, 123.2 ($J_{C\text{-}P}$ = 4 Hz), 123.0 ($J_{C\text{-}P}$ = 6Hz), 122.8, 122.7, 122.3, 122.2, 120.9, 120.7, 103.3 ((Me)C*C*HC(Me)), 100.3 ((Me)C*C*HC(Me)), 64.8 (Me_3CN), 63.1 (Me_3CN), 62.6 (Me_3CN), 61.1 (Me_3CN), 57.4 (Me_3CN), 57.1 (Me_3CN), 51.9 (^{t}BuN=C*C*H_2CMe_3, isomer), 51.2 (^{t}BuN=C*C*H_2CMe_3), 38.9, 34.9, 34.7, 34.5, 33.8 ($J_{C\text{-}P}$ = 9 Hz), 33.5, 33.4, 32.2, 32.0, 31.9, 30.9 ($J_{C\text{-}P}$ = 10 Hz), 30.6, 29.9, 29.5, 29.1, 28.9, 28.5, 28.4, 28.0, 27.7, 27.6, 27.2, 26.8, 26.4, 26.1, 24.3, 24.0, 23.8, 23.4, 23.2, 23.1, 23.0, 22.8. ^{31}P NMR (25 ^{o}C, 161.9 MHz, C_6D_6): δ -8.5 (s, ^{t}BuNC*P*Mes*, isomer), -17.5 (s, ^{t}BuNC*P*Mes*). IR (C_6H_6, CaF_2): 3022 (m), 2962 (s), 2868 (m), 2210 (w, ν_{CN}), 2187 (w, ν_{CN}), 1958 (m), 1813 (m), 1621 (m), 1551 (m, ν_{CP}), 1528 (m, ν_{CP}), 1476 (s),1363 (m) cm^{-1}. Anal. Calcd. for $C_{67}H_{108}N_5PTi$: C, 75.74; H, 10.24; N, 6.59. Found: C, 75.76; H, 10.31; N, 6.77. Complex **3** decomposes in solution (~$t_{1/2}$ = 6 h, 25 ^{o}C, approx.) and in the solid state (48 h, 25 ^{o}C).

Synthesis of (Nacnac)Ti=N[P($CH_2{}^t$Bu)(Mes*)](N=CPh_2) (3)

In a vial was loaded (Nacnac)Ti=PMes*($CH_2{}^t$Bu),[9] [100 mg, 0.12 mmol] and dissolved in 10 mL of pentane and the solution cooled to –35 ºC. To the cold solution was added a cold pentane solution (~5 mL) containing 1 equiv of N_2CPh_2[10] [24.12 mg, 0.12 mmol] causing an immediate color change to brown. After stirring for 1 hour the solution was filtered, concentrated, and cooled to –35 ^{o}C to give dark brown blocks of (Nacnac)Ti=N[P($CH_2{}^t$Bu)(Mes*)](N=CPh_2) (**3**) [84 mg, 0.08 mmol, 68% yield].

For **3**: ^{1}H NMR (23 ^{o}C, 399.8 MHz, C_6D_6): δ 7.7-6.9 (m, aryl, 18H), 5.14 (s, C(Me)C*H*C(Me), 1H), 3.45 (septet, C*H*Me_2, 1H), 3.27 (septet, C*H*Me_2, 1H), 3.20 (septet, C*H*Me_2, 1H), 3.13 (septet, C*H*Me_2, 1H), 2.35 (d, Ti=N-PC*H*$_2{}^t$Bu(Mes*), $J_{H\text{-}P}$ = 13 Hz,

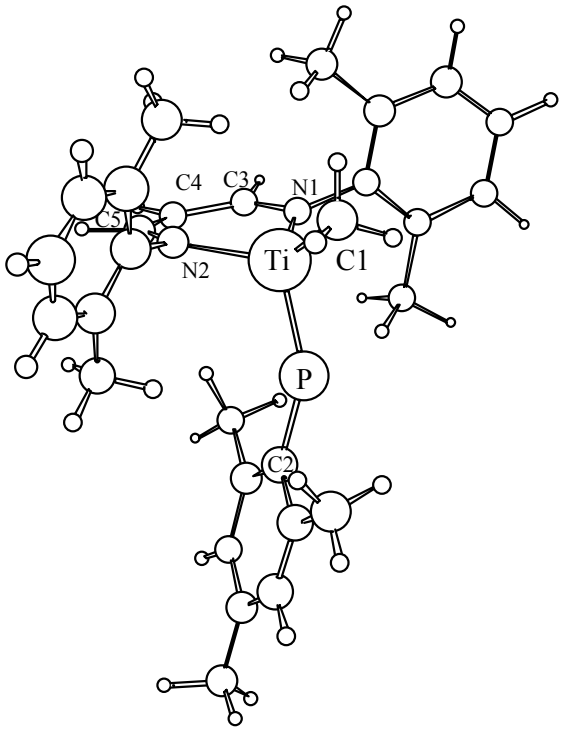
2H), 1.86 (s, C*Me*$_3$, 9H), 1.60-1.51 (m, C(*Me*)CHC(*Me*) and CH*Me*$_2$, 12H), 1.46 (s, C*Me*$_3$, 9H), 1.39 (d, CH*Me*$_2$, 3H), 1.36 (d, CH*Me*$_2$, 3H), 1.26 (s, C*Me*$_3$, 9H), 1.18 (d, CH*Me*$_2$, 3H), 1.16 (d, CH*Me*$_2$, 3H), 0.59 (d, CH*Me*$_2$, 3H), 0.57 (s, C*Me*$_3$, 9H), 0.52 (d, CH*Me*$_2$, 3H).

^{13}C NMR (0 ^{o}C, 125.7 MHz, $C_6D_5CD_3$): δ 179.0 (N*C*Ph$_2$), 167.4 (*C*(Me)CHC(Me)), 167.1 (C(Me)CH*C*(Me)), 158.2, 155.6, 148.7, 146.0 (ipso, *C*$_6$H$_2$^{t}Bu$_3$, $J_{C\text{-}P}$ = 28 Hz), 142.7, 142.6, 142.5, 141.1 (*C*$_6$H$_2$^{t}Bu$_3$, $J_{C\text{-}P}$ = 7 Hz), 136.8, 130.1, 127.3, 127.1, 126.8, 126.6, 124.4, 124.3, 124.1, 123.1, 121.4, 52.2 (Ti=N-P*C*H$_2$CMe$_3$(Mes*), $J_{C\text{-}P}$ = 52 Hz), 39.7 (Ti=N-PCH$_2$*C*Me$_3$(Mes*), $J_{C\text{-}P}$ = 8 Hz), 34.8, 34.6, 34.5, 31.4, 31.2, 30.5, 30.4, 29.1, 28.8, 28.6, 28.4, 25.3, 25.1, 24.8, 24.7, 24.5, 24.3, 24.2, 23.9, 23.6. ^{31}P NMR (25 ^{o}C, 161.9 MHz, C_6D_6): δ 99.7 (s, Ti=N-*P*CH$_2$^{t}Bu(Mes*)). IR (C_6H_6, CaF_2): 2962 (m), 1958 (m), 1813 (m), 1527 (m), 1485 (m), 1389 (w) cm^{-1}. Anal. Calcd. for $C_{65}H_{91}N_4PTi$: C, 77.51; H, 9.11; N, 5.90. Found: C, 75.88; H, 8.49; N, 5.03. Attempts to obtain satisfactory elemental analysis failed, presumably due to the thermal decomposition of **3** in the solid state.

Computational Details:

All calculations were performed with the Gaussian 98 package[11] at the B3PW91[12] level of theory. Basis sets used included LANL2DZ for Ti and P, 6-31G* for C and N, and 6-31G** for all hydrogens.[13] The basis set LANL2DZ is the Los Alamos National Laboratory ECP plus a double zeta valence on Ti and P;[14] additional d polarization functions[15] were added to all phosphorus atoms in all DFT calculations. All optimizations were performed with C_1 symmetry and all minima were confirmed by analytical calculation of frequencies, which were also used to compute zero point energy

corrections without scaling. The initial geometry was adapted from the refined crystal structure of the analogous compound. (Nacnac*)Ti=PMes(Me) (Nacnac*$^-$ = ArNCHCHCHNAr, Ar = 2,6-$Me_2C_6H_3$, and Mes = 2,4,6-$Me_3C_6H_2$) was used as the model.



Selected Bond Distances (Å) and Angles(°):
Ti-C: 2.083
Ti-P: 2.188
Ti-N1: 2.046
Ti-N2: 2.035
N-C(ipso): 1.437
∠Ti-P-C2 148.1
∠P-Ti-C1: 105.1
∠N1-Ti-P: 114.1
∠N2-Ti-P: 111.5

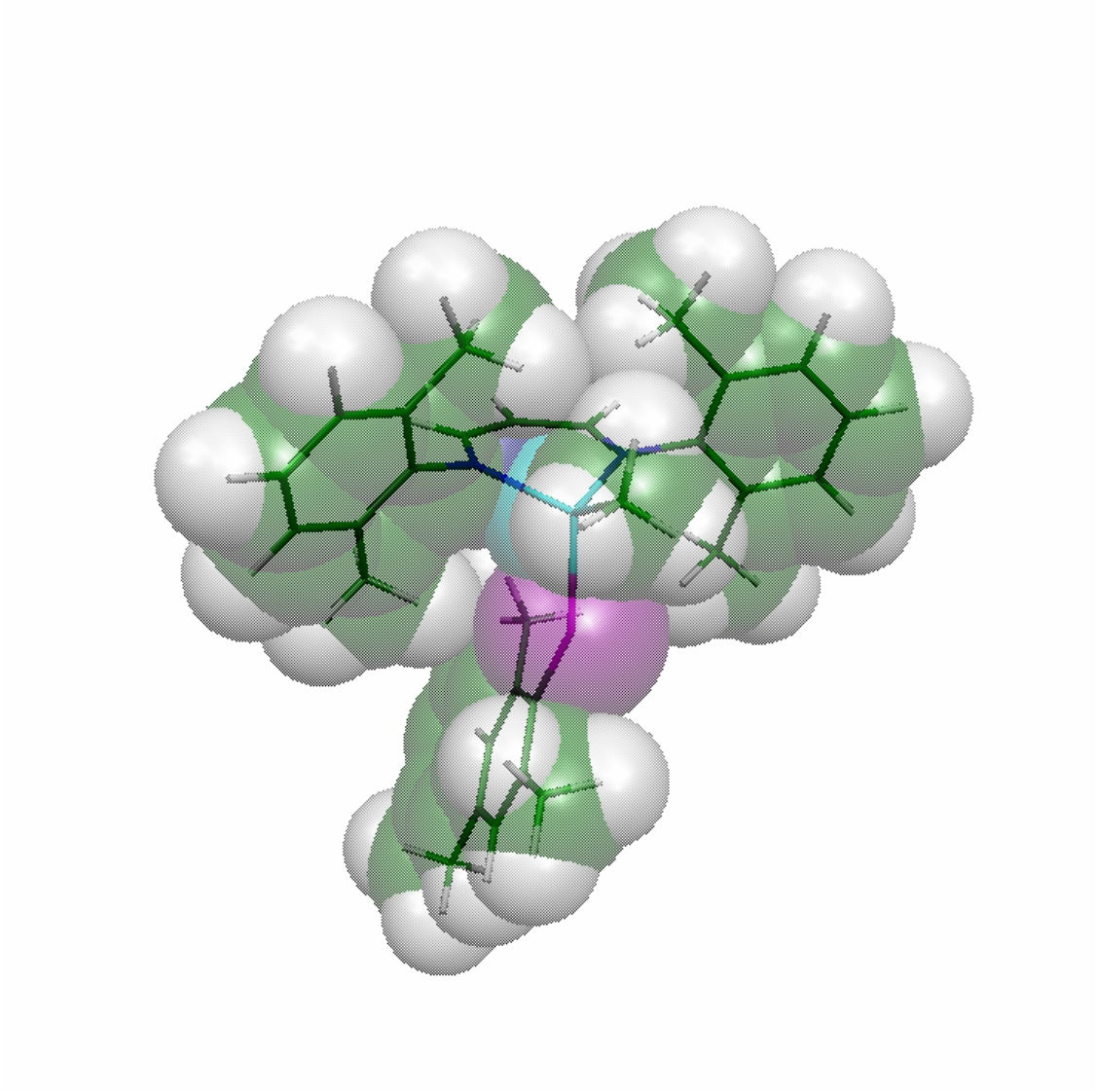
Atomic Coordinates (XYZ)

Ti -0.86521 0.23925 -0.56390
N -0.62897 1.74625 0.78354
C -0.79586 1.56229 2.09321
C -1.36971 0.44990 2.71059
C -2.01615 -0.60352 2.05506
N -2.03077 -0.81816 0.74422
C -0.16082 3.03403 0.34942
C -1.09237 3.95706 -0.16480
C -0.62411 5.19495 -0.61298
C 0.72660 5.51712 -0.54822
C 1.62912 4.60252 -0.01737

C 1.20971 3.35134 0.44348
H -2.78503 2.90435 -1.00176
H -2.92999 3.23496 0.72333
H -3.13853 4.54313 -0.45184
H -1.33621 5.91328 -1.01128
H 1.07444 6.48285 -0.90390
H 2.68459 4.85487 0.04445
H 3.22439 2.74972 0.87407
H 2.11385 1.39794 0.57804
H 2.06174 2.26716 2.11102
C -2.96388 -1.78449 0.23382
C -2.57447 -3.12703 0.06145
C -3.50757 -4.01997 -0.47419
C -4.78745 -3.60507 -0.82302
C -5.16165 -2.28027 -0.62593
C -4.26498 -1.35122 -0.09375
C 2.20452 2.39039 1.03106
C -2.56300 3.64233 -0.22344
C -4.69834 0.07031 0.14345
H -4.03015 0.78570 -0.34497
H -4.70123 0.31954 1.21049
H -5.70822 0.23432 -0.24073
H -6.16570 -1.95426 -0.88506
H -5.49512 -4.31479 -1.24204
H -3.21657 -5.05790 -0.61356
C -1.21181 -3.61011 0.46827
H -1.07569 -3.54714 1.55432
H -0.42336 -3.00278 0.01073
H -1.06804 -4.65261 0.17386
C 3.00241 -1.58276 0.85382
C 2.71907 -1.19888 -0.48163
C 3.76633 -1.18482 -1.43606
C 5.05763 -1.53583 -1.03712
C 5.35470 -1.90731 0.27351
C 4.30928 -1.92382 1.20023
H 4.51721 -2.21374 2.22898
H 5.85560 -1.51663 -1.77699
C 6.75277 -2.28528 0.68344
H 7.45710 -2.17310 -0.14526
H 7.10797 -1.66188 1.51197
H 6.80086 -3.32651 1.02327
C 3.52447 -0.79105 -2.86876
H 4.43601 -0.90525 -3.46261
H 3.19271 0.25029 -2.94830
H 2.73609 -1.40159 -3.32263
C 1.92949 -1.65227 1.90417

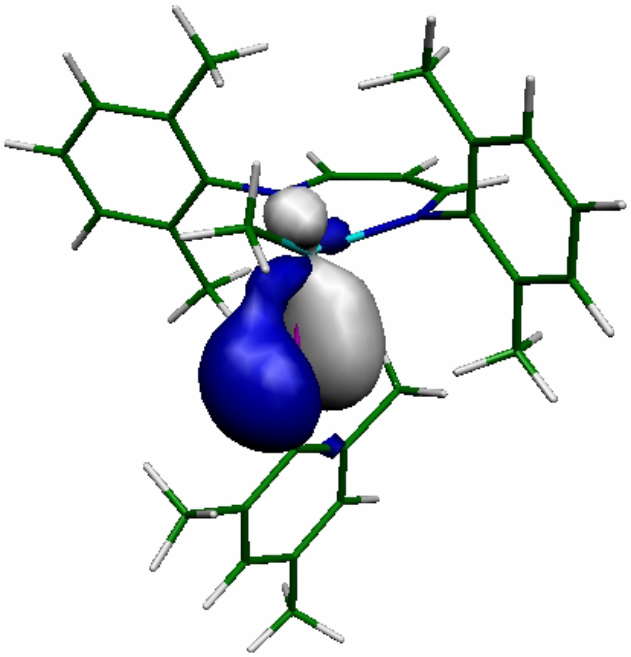
H 2.36474 -1.76865 2.90121
H 1.26277 -2.50300 1.72723
H 1.29814 -0.75895 1.89747
P 1.04345 -0.72012 -1.03508
C -1.72323 0.67462 -2.41127
H -1.43415 0.46894 3.79236
H -2.60661 -1.28638 2.67124
H -0.49363 2.38775 2.74204
H -2.75682 1.04166 -2.32742
H -1.12017 1.44171 -2.91819
H -1.72599 -0.21026 -3.06058

Space filling model

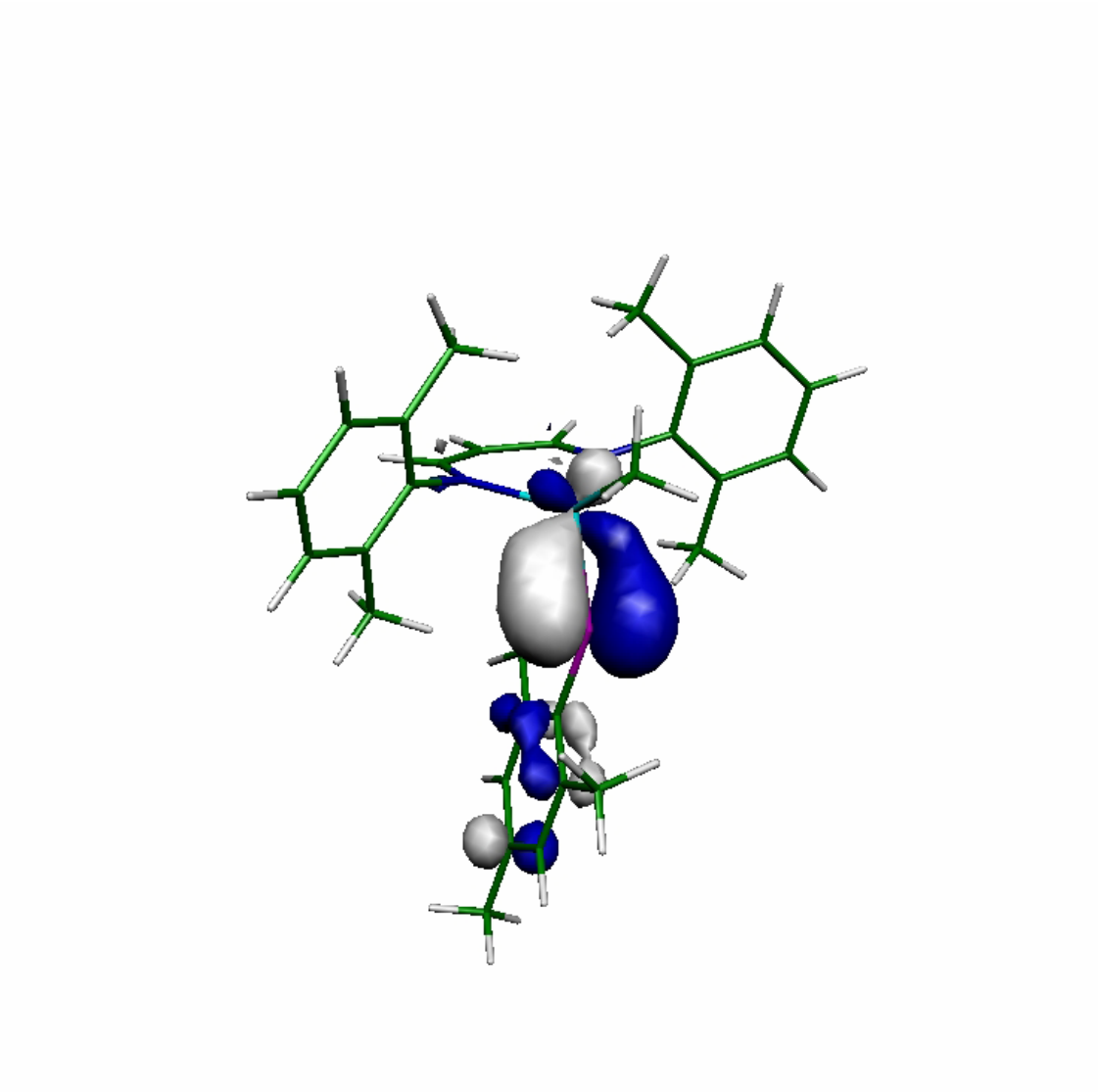


Frontier Orbitals (HOMO-1, HOMO, and LUMO)

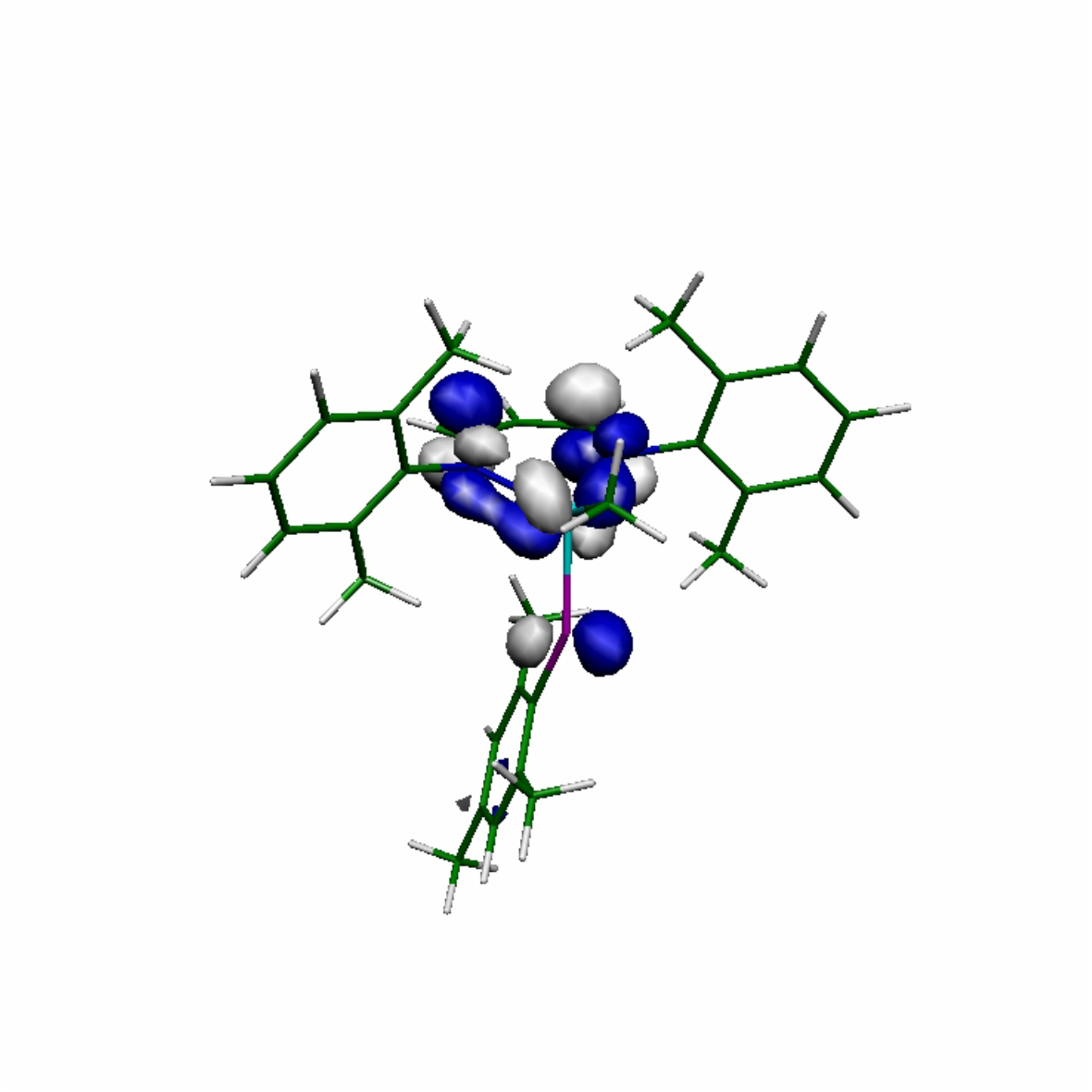
HOMO-1



HOMO



LUMO



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Supplementary Material (ESI) for Dalton Transactions

Crystallographic Experimental Section and Tables for Complexes 2 and 3

Crystallographic data for complex (η^1-Nacnac)Ti(CN^{t}Bu)(η^2-(*N,C*)-^{t}BuN=CCH$_2{}^t$Bu)(η^2-(*N,C*)-^{t}BuN=C=PMes*) (2)

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 cleaved fragment of a large red/purple crystal of approximate dimensions 0.35 × 0.30 × 0.30 mm onto the tip of a 0.15 mm diameter glass fiber which was subsequently mounted on a SMART6000 (Bruker) and cooled to 127(2) K. Several crystals were examined and were all found to have poorly defined spot shapes on the CCD detector.

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 10 seconds and a detector distance of 5.0 cm. A randomly oriented region of a sphere in reciprocal space was surveyed. Four sections of 606 frames were collected with 0.30º 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 966 strong reflections from the actual data collection after integration (SAINT).

Structure solution and refinement
Intensity statistics and systematic absences suggested the centrosymmetric space group P1bar and subsequent solution and refinement confirmed this choice. The structure was solved using SHELXS-97 and refined with SHELXL-97. 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 placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters.

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Figure 3: Space Filling Model Drawing(s)

Table 1

Program MU for data file labeled

MSC03118

The following were used

At.No.	At.Wt.	Abs.	%	No.	Element
22	47.880	23.400	3.97	1	Ti
15	30.974	7.970	2.57	1	P
7	14.007	.845	5.80	5	N
6	12.011	.576	76.64	77	C
1	1.008	.373	11.03	132	H

The density is 1.025 g/cc.

The volume is 3908.77 cubic Angstroms

Z = 2 and the molecular wt. is 1206.78

F(000) = 1332

The linear absorption coefficient = 1.707 reciprocal centimeters,

and 1/4Mu = 1.4647 mm.

Table 2

Crystal Data for MSC Sample 03118

Empirical Formula	C77H132N5PTi
Color of Crystal:	red/purple?
Crystal Dimensions were:	0.35 x 0.30 x 0.30 mm.
Space Group:	P-1
Cell Dimensions (at 127(2) K; 957 reflections)	
a =	12.297(2)
b =	13.182(3)
c =	24.843(5)
alpha =	103.400(5)
beta =	92.806(6)
gamma =	91.863(6)
Z (Molecules/cell):	2
Volume:	3908.8(13)
Calculated Density:	1.025
Wavelength:	0.71073
Molecular Weight:	1206.75
F(000):	1332
Linear Absorption Coefficient:	0.171

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 =	10.0 sec.

Data processing statistics for 25.0 degrees maximum theta:

Total number of intensities integrated =	47023
Number of unique intensities =	13721
Number with F > 4sigma(F) =	9219
R for averaging =	0.116

Refinement results:

Final residuals are:	
R(F) (observed data) =	0.0869
Rw(F2) (refinement data) =	0.2567
Final Goodness of Fit =	1.022
Maximum delta/sigma for the last cycle =	0.03

Table 3: Fractional Coordinates and Isotropic Thermal Parameters for MSC Sample 03118

Atom	x	y	z	Uiso
Ti(1)	10711(1)	-59(1)	-2225(1)	22(1)
C(2)	8909(3)	-35(3)	-2271(2)	27(1)
N(3)	7980(3)	-42(3)	-2357(1)	31(1)
C(4)	6818(3)	66(3)	-2472(2)	36(1)
C(5)	6279(4)	260(5)	-1918(2)	62(2)
C(6)	6714(4)	1007(5)	-2724(3)	60(2)
C(7)	6371(4)	-925(4)	-2875(2)	53(1)
N(8)	10638(3)	13(2)	-3038(1)	24(1)
C(9)	10094(3)	757(3)	-3243(2)	28(1)
C(10)	9782(4)	643(3)	-3793(2)	34(1)
C(11)	9300(4)	1411(3)	-4050(2)	36(1)
N(12)	8920(3)	2261(3)	-3762(2)	41(1)
C(13)	8577(4)	3053(3)	-4024(2)	38(1)
C(14)	7465(4)	3210(4)	-4073(2)	45(1)
C(15)	7129(4)	4040(4)	-4289(2)	47(1)
C(16)	7893(4)	4677(3)	-4472(2)	43(1)
C(17)	8966(4)	4531(3)	-4406(2)	41(1)
C(18)	9351(4)	3732(3)	-4174(2)	37(1)
C(19)	10557(4)	3624(4)	-4062(2)	48(1)
C(20)	11263(6)	3923(7)	-4493(3)	87(2)
C(21)	10936(5)	4295(5)	-3495(3)	67(2)
C(22)	6645(4)	2497(4)	-3868(3)	55(1)
C(23)	5584(5)	3018(6)	-3697(3)	76(2)
C(24)	6428(5)	1464(5)	-4302(3)	72(2)
C(25)	9294(5)	1160(4)	-4677(2)	47(1)
C(26)	9898(4)	1736(3)	-2820(2)	31(1)
C(27)	11078(3)	-814(3)	-3450(2)	26(1)
C(28)	10541(3)	-1797(3)	-3620(2)	29(1)
C(29)	11032(4)	-2580(3)	-4001(2)	35(1)
C(30)	11998(4)	-2394(3)	-4218(2)	38(1)
C(31)	12505(4)	-1398(3)	-4062(2)	36(1)
C(32)	12066(3)	-594(3)	-3682(2)	29(1)
C(33)	12617(3)	491(3)	-3548(2)	35(1)
C(34)	12606(5)	944(4)	-4064(2)	53(1)
C(35)	13779(4)	500(4)	-3302(2)	40(1)
C(36)	9406(4)	-2018(3)	-3443(2)	44(1)
C(37)	8571(4)	-2111(5)	-3924(3)	66(2)
C(38)	9307(5)	-2984(4)	-3216(2)	57(1)
N(40)	11515(3)	-1342(2)	-2138(1)	27(1)
C(41)	10601(3)	-1411(3)	-1933(2)	27(1)
C(42)	10126(4)	-2247(3)	-1673(2)	36(1)
C(43)	9641(4)	-1824(3)	-1109(2)	38(1)
C(44)	8714(5)	-1116(5)	-1159(2)	58(2)
C(45)	10536(5)	-1237(4)	-693(2)	52(1)
C(47)	12496(3)	-2005(3)	-2178(2)	33(1)
C(48)	13319(3)	-1536(3)	-2501(2)	35(1)
C(49)	12175(4)	-3122(3)	-2498(2)	41(1)
C(50)	12962(4)	-1964(4)	-1596(2)	46(1)
N(51)	10752(3)	1205(2)	-1615(1)	24(1)
C(52)	11776(3)	1029(3)	-1702(2)	25(1)

P(53)	13152(1)	1235(1)	-1628(1)	26(1)
C(54)	13426(3)	2532(3)	-1103(2)	24(1)
C(55)	13515(3)	2564(3)	-525(2)	26(1)
C(56)	13329(3)	3512(3)	-159(2)	28(1)
C(57)	13139(3)	4425(3)	-327(2)	29(1)
C(58)	13273(3)	4405(3)	-878(2)	30(1)
C(59)	13444(3)	3476(3)	-1273(2)	28(1)
C(60)	9201(4)	-2782(4)	-909(2)	48(1)
C(61)	14691(4)	2959(4)	-2057(2)	38(1)
C(62)	12714(4)	3196(4)	-2297(2)	42(1)
C(63)	13962(5)	4718(4)	-1889(2)	49(1)
C(64)	12801(3)	5401(3)	87(2)	35(1)
C(65)	11716(4)	5135(4)	307(3)	61(2)
C(66)	13665(5)	5742(4)	562(2)	54(1)
C(67)	12627(5)	6329(4)	-186(2)	58(1)
C(68)	13876(3)	1633(3)	-280(2)	31(1)
C(69)	12987(4)	763(3)	-333(2)	35(1)
C(70)	14894(4)	1178(3)	-572(2)	35(1)
C(71)	14225(4)	1993(4)	337(2)	41(1)
C(72)	10225(3)	2071(3)	-1219(2)	28(1)
C(73)	8994(3)	1915(3)	-1311(2)	35(1)
C(74)	10563(4)	2029(4)	-627(2)	36(1)
C(75)	10587(3)	3117(3)	-1328(2)	34(1)
C(76)	15869(7)	-1687(9)	-4592(4)	116(3)
C(77)	15450(9)	-2771(8)	-4648(4)	116(3)
C(78)	15127(6)	-3045(6)	-4123(3)	82(2)
C(79)	14589(7)	-4084(6)	-4182(4)	93(3)
C(80)	14270(9)	-4333(8)	-3641(5)	130(4)
C(81)	18162(12)	4102(11)	-2337(6)	174(5)
C(82)	17917(15)	4933(14)	-2510(8)	200(6)
C(83)	17097(12)	5517(11)	-2241(6)	154(4)
C(84)	16758(12)	6452(11)	-2310(6)	170(5)
C(85)	15877(9)	6926(9)	-1994(5)	129(3)
C(93)	13678(4)	3567(3)	-1874(2)	33(1)
H(5A)	638	-34	-175	93
H(5B)	550	36	-198	93
H(5C)	662	89	-167	93
H(6A)	700	164	-246	90
H(6B)	595	109	-282	90
H(6C)	713	90	-306	90
H(7A)	673	-101	-323	79
H(7B)	558	-88	-294	79
H(7C)	651	-153	-272	79
H(10)	990	-2	-403	41
H(15)	638	418	-431	57
H(16)	765	521	-464	51
H(17)	948	498	-452	49
H(19)	1068	288	-406	58
H(20A)	1107	346	-486	131
H(20B)	1203	386	-439	131
H(20C)	1114	465	-451	131
H(21A)	1092	503	-350	100
H(21B)	1168	413	-340	100
H(21C)	1045	415	-322	100
H(22)	700	233	-353	67
H(23A)	575	372	-346	114

H(23B)	518	260	-349	114
H(23C)	515	307	-403	114
H(24A)	611	161	-465	109
H(24B)	592	101	-416	109
H(24C)	712	112	-438	109
H(25A)	884	165	-482	70
H(25B)	900	44	-483	70
H(25C)	1004	122	-479	70
H(26A)	1025	234	-292	46
H(26B)	1021	168	-246	46
H(26C)	911	183	-280	46
H(29)	1068	-326	-411	41
H(30)	1232	-294	-447	45
H(31)	1317	-127	-422	43
H(33)	1219	95	-327	42
H(34A)	1302	51	-435	79
H(34B)	1294	165	-396	79
H(34C)	1185	96	-421	79
H(35A)	1378	20	-298	60
H(35B)	1408	122	-319	60
H(35C)	1423	9	-358	60
H(36)	922	-141	-314	53
H(37A)	874	-270	-423	98
H(37B)	860	-147	-406	98
H(37C)	784	-223	-380	98
H(38A)	859	-302	-306	85
H(38B)	988	-295	-292	85
H(38C)	939	-361	-352	85
H(42A)	1071	-273	-162	43
H(42B)	955	-266	-193	43
H(44A)	837	-93	-81	87
H(44B)	818	-148	-145	87
H(44C)	900	-48	-125	87
H(45A)	1081	-63	-82	77
H(45B)	1113	-170	-67	77
H(45C)	1024	-100	-33	77
H(48A)	1301	-157	-288	53
H(48B)	1398	-193	-253	53
H(48C)	1350	-81	-231	53
H(49A)	1161	-342	-231	62
H(49B)	1282	-355	-252	62
H(49C)	1189	-312	-287	62
H(50A)	1312	-123	-140	69
H(50B)	1364	-234	-162	69
H(50C)	1243	-229	-140	69
H(56)	1333	353	23	34
H(58)	1325	504	-100	36
H(60A)	981	-321	-84	73
H(60B)	868	-320	-119	73
H(60C)	883	-254	-56	73
H(61A)	1453	221	-210	57
H(61B)	1529	319	-178	57
H(61C)	1490	309	-241	57
H(62A)	1290	331	-266	63
H(62B)	1208	359	-218	63
H(62C)	1255	245	-233	63
H(63A)	1426	474	-225	74

H(63B)	1451	502	-159	74
H(63C)	1330	512	-184	74
H(65A)	1116	495	0	91
H(65B)	1149	574	58	91
H(65C)	1180	454	48	91
H(66A)	1340	632	84	82
H(66B)	1434	597	42	82
H(66C)	1381	516	73	82
H(67A)	1205	614	-48	87
H(67B)	1331	651	-34	87
H(67C)	1241	693	9	87
H(69A)	1329	18	-21	53
H(69B)	1272	53	-72	53
H(69C)	1239	103	-10	53
H(70A)	1518	65	-39	53
H(70B)	1545	174	-55	53
H(70C)	1469	86	-96	53
H(71A)	1359	221	55	62
H(71B)	1475	259	39	62
H(71C)	1456	142	46	62
H(73A)	878	194	-169	53
H(73B)	865	247	-105	53
H(73C)	877	123	-125	53
H(74A)	1035	134	-57	55
H(74B)	1020	257	-37	55
H(74C)	1136	214	-57	55
H(75A)	1138	320	-128	51
H(75B)	1027	368	-106	51
H(75C)	1035	314	-171	51
H(76A)	1537	-120	-438	173
H(76B)	1593	-155	-496	173
H(76C)	1659	-159	-440	173
H(77A)	1602	-325	-481	139
H(77B)	1481	-290	-491	139
H(78A)	1579	-300	-387	99
H(86)	1463	-251	-394	99
H(79A)	1508	-462	-436	112
H(79B)	1393	-414	-443	112
H(80A)	1493	-441	-342	195
H(80B)	1382	-499	-372	195
H(80C)	1385	-377	-344	195
H(81A)	1895	411	-226	261
H(81B)	1793	348	-262	261
H(81C)	1778	410	-200	261
H(82A)	1769	471	-291	240
H(82B)	1858	539	-247	240
H(83A)	1644	504	-231	185
H(83B)	1730	563	-184	185
H(84A)	1654	637	-271	204
H(84B)	1739	695	-223	204
H(85A)	1519	656	-215	194
H(85B)	1585	766	-201	194
H(85C)	1600	689	-161	194

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.

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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.
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Table 4: Anisotropic Thermal Parameters for MSC Sample 03118

Atom	U11	U22	U33	U23	U13	U12
Ti(1)	22(1)	21(1)	21(1)	3(1)	6(1)	2(1)
C(2)	24(2)	28(2)	28(2)	3(2)	8(2)	0(2)
N(3)	31(2)	28(2)	31(2)	1(1)	10(2)	3(1)
C(4)	24(2)	41(2)	41(3)	4(2)	9(2)	1(2)
C(5)	32(3)	92(4)	58(4)	4(3)	18(2)	8(3)
C(6)	34(3)	63(4)	88(4)	29(3)	-5(3)	3(2)
C(7)	31(3)	54(3)	64(3)	-4(3)	2(2)	-7(2)
N(8)	27(2)	24(2)	21(2)	2(1)	4(1)	3(1)
C(9)	26(2)	27(2)	28(2)	3(2)	8(2)	0(2)
C(10)	46(3)	23(2)	29(2)	0(2)	0(2)	8(2)
C(11)	42(3)	32(2)	33(2)	3(2)	2(2)	7(2)
N(12)	54(2)	34(2)	38(2)	10(2)	7(2)	18(2)
C(13)	51(3)	32(2)	32(2)	7(2)	5(2)	16(2)
C(14)	48(3)	39(3)	51(3)	17(2)	3(2)	7(2)
C(15)	40(3)	44(3)	60(3)	16(2)	4(2)	15(2)
C(16)	57(3)	26(2)	46(3)	12(2)	0(2)	5(2)
C(17)	50(3)	31(2)	41(3)	6(2)	0(2)	2(2)
C(18)	49(3)	29(2)	30(2)	-1(2)	6(2)	8(2)
C(19)	49(3)	42(3)	54(3)	13(2)	-1(2)	7(2)
C(20)	57(4)	143(7)	70(4)	34(5)	20(3)	32(4)
C(21)	61(4)	75(4)	61(4)	17(3)	-15(3)	-10(3)
C(22)	50(3)	54(3)	72(4)	32(3)	8(3)	11(2)
C(23)	66(4)	84(5)	94(5)	46(4)	31(4)	17(3)
C(24)	58(4)	61(4)	107(5)	36(4)	7(4)	2(3)
C(25)	70(3)	41(3)	28(2)	3(2)	-5(2)	19(2)
C(26)	40(2)	28(2)	24(2)	4(2)	5(2)	5(2)
C(27)	28(2)	27(2)	20(2)	1(2)	0(2)	7(2)
C(28)	33(2)	30(2)	22(2)	1(2)	4(2)	3(2)
C(29)	41(3)	27(2)	31(2)	-1(2)	0(2)	5(2)
C(30)	41(3)	36(2)	34(2)	2(2)	7(2)	13(2)
C(31)	33(2)	41(2)	34(2)	7(2)	6(2)	8(2)
C(32)	26(2)	34(2)	27(2)	8(2)	-1(2)	4(2)
C(33)	31(2)	37(2)	37(2)	8(2)	8(2)	-2(2)
C(34)	61(3)	47(3)	54(3)	23(3)	-3(3)	-11(2)
C(35)	34(2)	48(3)	39(3)	12(2)	5(2)	-7(2)
C(36)	46(3)	32(2)	48(3)	-10(2)	18(2)	-4(2)
C(37)	35(3)	61(4)	106(5)	29(3)	8(3)	4(3)
C(38)	55(3)	63(3)	46(3)	7(3)	3(2)	-24(3)
N(40)	28(2)	26(2)	27(2)	5(1)	5(1)	1(1)
C(41)	29(2)	21(2)	29(2)	3(2)	4(2)	-1(2)
C(42)	39(3)	34(2)	34(2)	8(2)	11(2)	1(2)
C(43)	50(3)	36(2)	31(2)	9(2)	15(2)	-1(2)
C(44)	65(4)	66(4)	51(3)	24(3)	34(3)	16(3)
C(45)	75(4)	48(3)	29(3)	3(2)	15(2)	-14(3)
C(47)	31(2)	35(2)	33(2)	6(2)	6(2)	7(2)
C(48)	29(2)	34(2)	43(3)	9(2)	10(2)	8(2)
C(49)	48(3)	29(2)	47(3)	5(2)	16(2)	7(2)
C(50)	50(3)	54(3)	36(3)	10(2)	8(2)	12(2)
N(51)	22(2)	24(2)	25(2)	0(1)	5(1)	2(1)
C(52)	33(2)	23(2)	18(2)	4(2)	4(2)	3(2)
P(53)	22(1)	25(1)	27(1)	-1(1)	7(1)	2(1)

C(54)	17(2)	26(2)	24(2)	-2(2)	5(2)	1(2)
C(55)	18(2)	27(2)	30(2)	1(2)	6(2)	-2(2)
C(56)	26(2)	32(2)	24(2)	-1(2)	6(2)	-1(2)
C(57)	23(2)	25(2)	34(2)	-4(2)	8(2)	-2(2)
C(58)	25(2)	26(2)	37(2)	3(2)	3(2)	-1(2)
C(59)	22(2)	29(2)	30(2)	2(2)	3(2)	-1(2)
C(60)	59(3)	52(3)	35(3)	12(2)	11(2)	-11(2)
C(61)	37(2)	46(3)	32(2)	11(2)	11(2)	-2(2)
C(62)	45(3)	51(3)	32(2)	14(2)	4(2)	1(2)
C(63)	64(3)	40(3)	47(3)	16(2)	11(2)	-5(2)
C(64)	30(2)	25(2)	44(3)	-7(2)	11(2)	1(2)
C(65)	49(3)	37(3)	85(4)	-15(3)	38(3)	-1(2)
C(66)	59(3)	44(3)	48(3)	-14(2)	7(3)	3(2)
C(67)	70(4)	35(3)	61(4)	-7(2)	17(3)	9(2)
C(68)	32(2)	30(2)	31(2)	6(2)	5(2)	3(2)
C(69)	43(3)	32(2)	33(2)	11(2)	9(2)	3(2)
C(70)	35(2)	36(2)	34(2)	7(2)	3(2)	9(2)
C(71)	49(3)	39(2)	36(3)	8(2)	6(2)	4(2)
C(72)	25(2)	26(2)	26(2)	-7(2)	7(2)	5(2)
C(73)	30(2)	34(2)	37(2)	-5(2)	12(2)	5(2)
C(74)	37(2)	42(2)	28(2)	-2(2)	13(2)	6(2)
C(75)	28(2)	30(2)	39(2)	-1(2)	9(2)	3(2)
C(76)	91(6)	160(10)	104(7)	56(7)	-18(5)	-18(6)
C(77)	162(10)	115(7)	72(6)	28(5)	-13(6)	11(7)
C(78)	63(4)	100(6)	74(5)	2(4)	-6(3)	5(4)
C(79)	78(5)	76(5)	112(7)	-2(4)	-16(4)	30(4)
C(80)	144(9)	117(8)	136(9)	32(7)	60(7)	22(7)
C(93)	34(2)	35(2)	31(2)	8(2)	4(2)	-1(2)

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 03118

A	B	Distance
Ti(1)	N(51)	1.973(3)
Ti(1)	N(40)	2.036(3)
Ti(1)	N(8)	2.041(3)
Ti(1)	C(52)	2.077(4)
Ti(1)	C(41)	2.078(4)
Ti(1)	C(2)	2.214(4)
C(2)	N(3)	1.151(5)
N(3)	C(4)	1.462(6)
C(4)	C(7)	1.518(7)
C(4)	C(6)	1.519(7)
C(4)	C(5)	1.527(7)
N(8)	C(9)	1.382(5)
N(8)	C(27)	1.450(5)
C(9)	C(10)	1.373(6)
C(9)	C(26)	1.498(5)
C(10)	C(11)	1.445(6)
C(11)	N(12)	1.295(6)
C(11)	C(25)	1.515(6)
N(12)	C(13)	1.416(6)
C(13)	C(14)	1.393(7)
C(13)	C(18)	1.408(7)
C(14)	C(15)	1.392(7)
C(14)	C(22)	1.539(7)
C(15)	C(16)	1.400(7)
C(16)	C(17)	1.347(7)
C(17)	C(18)	1.397(6)
C(18)	C(19)	1.513(7)
C(19)	C(21)	1.521(8)
C(19)	C(20)	1.524(8)
C(22)	C(23)	1.527(8)
C(22)	C(24)	1.535(9)
C(27)	C(28)	1.399(6)
C(27)	C(32)	1.421(6)
C(28)	C(29)	1.404(6)
C(28)	C(36)	1.523(6)
C(29)	C(30)	1.366(6)
C(30)	C(31)	1.396(6)
C(31)	C(32)	1.388(6)
C(32)	C(33)	1.520(6)
C(33)	C(35)	1.526(6)
C(33)	C(34)	1.533(7)
C(36)	C(38)	1.511(7)
C(36)	C(37)	1.517(8)
N(40)	C(41)	1.267(5)
N(40)	C(47)	1.506(5)
C(41)	C(42)	1.514(6)
C(42)	C(43)	1.540(6)
C(43)	C(44)	1.514(7)

C(43)	C(45)	1.530(7)
C(43)	C(60)	1.551(6)
C(47)	C(50)	1.519(6)
C(47)	C(48)	1.523(6)
C(47)	C(49)	1.531(6)
N(51)	C(52)	1.308(5)
N(51)	C(72)	1.510(5)
C(52)	P(53)	1.698(4)
P(53)	C(54)	1.903(4)
C(54)	C(59)	1.403(6)
C(54)	C(55)	1.427(6)
C(55)	C(56)	1.398(5)
C(55)	C(68)	1.558(6)
C(56)	C(57)	1.385(6)
C(57)	C(58)	1.380(6)
C(57)	C(64)	1.532(5)
C(58)	C(59)	1.409(6)
C(59)	C(93)	1.565(6)
C(61)	C(93)	1.534(6)
C(62)	C(93)	1.535(7)
C(63)	C(93)	1.555(6)
C(64)	C(66)	1.524(7)
C(64)	C(65)	1.526(6)
C(64)	C(67)	1.546(7)
C(68)	C(71)	1.531(6)
C(68)	C(69)	1.536(6)
C(68)	C(70)	1.546(6)
C(72)	C(73)	1.519(6)
C(72)	C(74)	1.521(6)
C(72)	C(75)	1.523(6)
C(76)	C(77)	1.477(12)
C(77)	C(78)	1.499(11)
C(78)	C(79)	1.474(11)
C(79)	C(80)	1.521(12)
C(81)	C(82)	1.305(17)
C(82)	C(83)	1.390(18)
C(83)	C(84)	1.359(15)
C(84)	C(85)	1.443(15)

Symmetry transformations used to generate equivalent atoms:

Table 5b: Bond Angles for MSC Sample 03118

A	B	C	Angle
N(51)	Ti(1)	N(40)	120.78(14)
N(51)	Ti(1)	N(8)	122.17(13)
N(40)	Ti(1)	N(8)	109.53(13)
N(51)	Ti(1)	C(52)	37.56(14)
N(40)	Ti(1)	C(52)	96.28(14)
N(8)	Ti(1)	C(52)	115.55(14)
N(51)	Ti(1)	C(41)	111.68(15)
N(40)	Ti(1)	C(41)	35.85(14)
N(8)	Ti(1)	C(41)	125.90(14)
C(52)	Ti(1)	C(41)	109.67(15)
N(51)	Ti(1)	C(2)	88.90(14)
N(40)	Ti(1)	C(2)	122.35(14)
N(8)	Ti(1)	C(2)	86.97(14)
C(52)	Ti(1)	C(2)	126.39(15)
C(41)	Ti(1)	C(2)	89.31(15)
N(3)	C(2)	Ti(1)	172.5(3)
C(2)	N(3)	C(4)	173.8(4)
N(3)	C(4)	C(7)	108.3(4)
N(3)	C(4)	C(6)	107.1(4)
C(7)	C(4)	C(6)	111.2(4)
N(3)	C(4)	C(5)	107.3(4)
C(7)	C(4)	C(5)	112.6(4)
C(6)	C(4)	C(5)	110.2(4)
C(9)	N(8)	C(27)	115.6(3)
C(9)	N(8)	Ti(1)	124.3(2)
C(27)	N(8)	Ti(1)	119.8(2)
C(10)	C(9)	N(8)	123.7(4)
C(10)	C(9)	C(26)	121.4(4)
N(8)	C(9)	C(26)	114.8(3)
C(9)	C(10)	C(11)	127.3(4)
N(12)	C(11)	C(10)	122.2(4)
N(12)	C(11)	C(25)	122.7(4)
C(10)	C(11)	C(25)	115.0(4)
C(11)	N(12)	C(13)	120.4(4)
C(14)	C(13)	C(18)	121.1(4)
C(14)	C(13)	N(12)	118.4(4)
C(18)	C(13)	N(12)	120.2(4)
C(15)	C(14)	C(13)	118.6(5)
C(15)	C(14)	C(22)	121.7(5)
C(13)	C(14)	C(22)	119.7(4)
C(14)	C(15)	C(16)	120.5(5)
C(17)	C(16)	C(15)	120.0(4)
C(16)	C(17)	C(18)	121.9(4)
C(17)	C(18)	C(13)	117.8(4)
C(17)	C(18)	C(19)	121.5(4)
C(13)	C(18)	C(19)	120.6(4)
C(18)	C(19)	C(21)	110.2(4)
C(18)	C(19)	C(20)	113.6(4)
C(21)	C(19)	C(20)	108.4(5)
C(23)	C(22)	C(24)	111.4(5)
C(23)	C(22)	C(14)	113.4(4)

C(24)	C(22)	C(14)	110.4(5)
C(28)	C(27)	C(32)	120.7(3)
C(28)	C(27)	N(8)	121.2(3)
C(32)	C(27)	N(8)	118.1(3)
C(27)	C(28)	C(29)	118.5(4)
C(27)	C(28)	C(36)	122.3(3)
C(29)	C(28)	C(36)	119.0(4)
C(30)	C(29)	C(28)	121.7(4)
C(29)	C(30)	C(31)	119.2(4)
C(32)	C(31)	C(30)	121.9(4)
C(31)	C(32)	C(27)	117.9(4)
C(31)	C(32)	C(33)	119.9(4)
C(27)	C(32)	C(33)	122.2(4)
C(32)	C(33)	C(35)	112.2(4)
C(32)	C(33)	C(34)	110.8(4)
C(35)	C(33)	C(34)	110.3(4)
C(38)	C(36)	C(37)	109.1(4)
C(38)	C(36)	C(28)	114.1(4)
C(37)	C(36)	C(28)	110.3(4)
C(41)	N(40)	C(47)	132.6(3)
C(41)	N(40)	Ti(1)	73.9(2)
C(47)	N(40)	Ti(1)	153.4(3)
N(40)	C(41)	C(42)	130.2(4)
N(40)	C(41)	Ti(1)	70.3(2)
C(42)	C(41)	Ti(1)	159.6(3)
C(41)	C(42)	C(43)	114.3(3)
C(44)	C(43)	C(45)	110.2(4)
C(44)	C(43)	C(42)	111.5(4)
C(45)	C(43)	C(42)	109.5(4)
C(44)	C(43)	C(60)	109.2(4)
C(45)	C(43)	C(60)	109.3(4)
C(42)	C(43)	C(60)	107.0(4)
N(40)	C(47)	C(50)	108.5(3)
N(40)	C(47)	C(48)	107.0(3)
C(50)	C(47)	C(48)	110.4(4)
N(40)	C(47)	C(49)	109.9(4)
C(50)	C(47)	C(49)	112.0(4)
C(48)	C(47)	C(49)	108.8(3)
C(52)	N(51)	C(72)	131.3(3)
C(52)	N(51)	Ti(1)	75.5(2)
C(72)	N(51)	Ti(1)	153.1(3)
N(51)	C(52)	P(53)	158.1(3)
N(51)	C(52)	Ti(1)	66.9(2)
P(53)	C(52)	Ti(1)	135.0(2)
C(52)	P(53)	C(54)	106.36(17)
C(59)	C(54)	C(55)	118.8(3)
C(59)	C(54)	P(53)	120.9(3)
C(55)	C(54)	P(53)	120.1(3)
C(56)	C(55)	C(54)	117.3(4)
C(56)	C(55)	C(68)	118.6(4)
C(54)	C(55)	C(68)	124.0(3)
C(57)	C(56)	C(55)	123.6(4)
C(58)	C(57)	C(56)	116.7(3)
C(58)	C(57)	C(64)	122.6(4)
C(56)	C(57)	C(64)	120.6(4)
C(57)	C(58)	C(59)	122.5(4)

C(54)	C(59)	C(58)	118.5(4)
C(54)	C(59)	C(93)	123.8(3)
C(58)	C(59)	C(93)	117.6(4)
C(66)	C(64)	C(65)	110.5(4)
C(66)	C(64)	C(57)	110.6(4)
C(65)	C(64)	C(57)	107.9(3)
C(66)	C(64)	C(67)	108.1(4)
C(65)	C(64)	C(67)	107.5(4)
C(57)	C(64)	C(67)	112.2(4)
C(71)	C(68)	C(69)	106.6(3)
C(71)	C(68)	C(70)	106.1(4)
C(69)	C(68)	C(70)	109.7(3)
C(71)	C(68)	C(55)	111.5(3)
C(69)	C(68)	C(55)	114.0(3)
C(70)	C(68)	C(55)	108.5(3)
N(51)	C(72)	C(73)	109.0(3)
N(51)	C(72)	C(74)	109.0(3)
C(73)	C(72)	C(74)	109.6(3)
N(51)	C(72)	C(75)	109.2(3)
C(73)	C(72)	C(75)	109.6(3)
C(74)	C(72)	C(75)	110.4(3)
C(76)	C(77)	C(78)	115.8(8)
C(79)	C(78)	C(77)	116.4(7)
C(78)	C(79)	C(80)	114.9(7)
C(81)	C(82)	C(83)	116.1(16)
C(84)	C(83)	C(82)	127.5(14)
C(83)	C(84)	C(85)	118.9(13)
C(61)	C(93)	C(62)	110.5(4)
C(61)	C(93)	C(63)	105.9(4)
C(62)	C(93)	C(63)	106.3(4)
C(61)	C(93)	C(59)	109.0(3)
C(62)	C(93)	C(59)	113.8(3)
C(63)	C(93)	C(59)	111.1(4)

Symmetry transformations used to generate equivalent atoms:

Table 5c: Torsion angles for MSC Sample 03118

A	B	C	D	Torsion Angle
N(51)	Ti(1)	C(2)	N(3)	134(3)
N(40)	Ti(1)	C(2)	N(3)	-99(3)
N(8)	Ti(1)	C(2)	N(3)	12(3)
C(52)	Ti(1)	C(2)	N(3)	132(3)
C(41)	Ti(1)	C(2)	N(3)	-114(3)
Ti(1)	C(2)	N(3)	C(4)	-81(5)
C(2)	N(3)	C(4)	C(7)	137(4)
C(2)	N(3)	C(4)	C(6)	17(4)
C(2)	N(3)	C(4)	C(5)	-101(4)
N(51)	Ti(1)	N(8)	C(9)	-33.9(4)
N(40)	Ti(1)	N(8)	C(9)	176.3(3)
C(52)	Ti(1)	N(8)	C(9)	-76.4(3)
C(41)	Ti(1)	N(8)	C(9)	139.9(3)
C(2)	Ti(1)	N(8)	C(9)	52.9(3)
N(51)	Ti(1)	N(8)	C(27)	152.8(3)
N(40)	Ti(1)	N(8)	C(27)	2.9(3)
C(52)	Ti(1)	N(8)	C(27)	110.3(3)
C(41)	Ti(1)	N(8)	C(27)	-33.5(3)
C(2)	Ti(1)	N(8)	C(27)	-120.4(3)
C(27)	N(8)	C(9)	C(10)	12.8(6)
Ti(1)	N(8)	C(9)	C(10)	-160.8(3)
C(27)	N(8)	C(9)	C(26)	-165.0(3)
Ti(1)	N(8)	C(9)	C(26)	21.4(5)
N(8)	C(9)	C(10)	C(11)	-174.2(4)
C(26)	C(9)	C(10)	C(11)	3.5(7)
C(9)	C(10)	C(11)	N(12)	-12.9(8)
C(9)	C(10)	C(11)	C(25)	165.8(4)
C(10)	C(11)	N(12)	C(13)	172.2(4)
C(25)	C(11)	N(12)	C(13)	-6.5(7)
C(11)	N(12)	C(13)	C(14)	109.0(5)
C(11)	N(12)	C(13)	C(18)	-77.8(6)
C(18)	C(13)	C(14)	C(15)	1.8(7)
N(12)	C(13)	C(14)	C(15)	175.0(4)
C(18)	C(13)	C(14)	C(22)	-175.8(5)
N(12)	C(13)	C(14)	C(22)	-2.7(7)
C(13)	C(14)	C(15)	C(16)	2.3(8)
C(22)	C(14)	C(15)	C(16)	179.9(5)
C(14)	C(15)	C(16)	C(17)	-4.3(8)
C(15)	C(16)	C(17)	C(18)	2.1(7)
C(16)	C(17)	C(18)	C(13)	1.9(7)
C(16)	C(17)	C(18)	C(19)	-175.4(4)
C(14)	C(13)	C(18)	C(17)	-3.9(7)
N(12)	C(13)	C(18)	C(17)	-177.0(4)
C(14)	C(13)	C(18)	C(19)	173.4(4)
N(12)	C(13)	C(18)	C(19)	0.4(6)

C(17)	C(18)	C(19)	C(21)	86.6(6)
C(13)	C(18)	C(19)	C(21)	-90.7(5)
C(17)	C(18)	C(19)	C(20)	-35.2(7)
C(13)	C(18)	C(19)	C(20)	147.5(5)
C(15)	C(14)	C(22)	C(23)	-24.3(8)
C(13)	C(14)	C(22)	C(23)	153.3(5)
C(15)	C(14)	C(22)	C(24)	101.5(6)
C(13)	C(14)	C(22)	C(24)	-80.9(6)
C(9)	N(8)	C(27)	C(28)	-100.7(4)
Ti(1)	N(8)	C(27)	C(28)	73.2(4)
C(9)	N(8)	C(27)	C(32)	78.6(4)
Ti(1)	N(8)	C(27)	C(32)	-107.5(3)
C(32)	C(27)	C(28)	C(29)	3.7(6)
N(8)	C(27)	C(28)	C(29)	-177.1(4)
C(32)	C(27)	C(28)	C(36)	-171.2(4)
N(8)	C(27)	C(28)	C(36)	8.0(6)
C(27)	C(28)	C(29)	C(30)	-1.8(6)
C(36)	C(28)	C(29)	C(30)	173.3(4)
C(28)	C(29)	C(30)	C(31)	-0.8(7)
C(29)	C(30)	C(31)	C(32)	1.5(7)
C(30)	C(31)	C(32)	C(27)	0.4(6)
C(30)	C(31)	C(32)	C(33)	-176.8(4)
C(28)	C(27)	C(32)	C(31)	-3.0(6)
N(8)	C(27)	C(32)	C(31)	177.7(4)
C(28)	C(27)	C(32)	C(33)	174.1(4)
N(8)	C(27)	C(32)	C(33)	-5.1(6)
C(31)	C(32)	C(33)	C(35)	-60.7(5)
C(27)	C(32)	C(33)	C(35)	122.2(4)
C(31)	C(32)	C(33)	C(34)	63.0(5)
C(27)	C(32)	C(33)	C(34)	-114.1(5)
C(27)	C(28)	C(36)	C(38)	-130.4(4)
C(29)	C(28)	C(36)	C(38)	54.6(6)
C(27)	C(28)	C(36)	C(37)	106.3(5)
C(29)	C(28)	C(36)	C(37)	-68.6(5)
N(51)	Ti(1)	N(40)	C(41)	84.8(3)
N(8)	Ti(1)	N(40)	C(41)	-124.8(2)
C(52)	Ti(1)	N(40)	C(41)	115.2(2)
C(2)	Ti(1)	N(40)	C(41)	-25.7(3)
N(51)	Ti(1)	N(40)	C(47)	-89.7(6)
N(8)	Ti(1)	N(40)	C(47)	60.6(6)
C(52)	Ti(1)	N(40)	C(47)	-59.3(6)
C(41)	Ti(1)	N(40)	C(47)	-174.5(7)
C(2)	Ti(1)	N(40)	C(47)	159.7(6)
C(47)	N(40)	C(41)	C(42)	-3.9(7)
Ti(1)	N(40)	C(41)	C(42)	179.4(5)
C(47)	N(40)	C(41)	Ti(1)	176.7(4)
N(51)	Ti(1)	C(41)	N(40)	-113.0(2)
N(8)	Ti(1)	C(41)	N(40)	72.7(3)
C(52)	Ti(1)	C(41)	N(40)	-72.8(3)
C(2)	Ti(1)	C(41)	N(40)	158.5(2)
N(51)	Ti(1)	C(41)	C(42)	68.3(9)
N(40)	Ti(1)	C(41)	C(42)	-178.8(10)
N(8)	Ti(1)	C(41)	C(42)	-106.0(9)
C(52)	Ti(1)	C(41)	C(42)	108.5(9)
C(2)	Ti(1)	C(41)	C(42)	-20.3(9)
N(40)	C(41)	C(42)	C(43)	131.0(5)

Ti(1)	C(41)	C(42)	C(43)	-50.5(11)
C(41)	C(42)	C(43)	C(44)	60.7(5)
C(41)	C(42)	C(43)	C(45)	-61.5(5)
C(41)	C(42)	C(43)	C(60)	-179.9(4)
C(41)	N(40)	C(47)	C(50)	-63.8(6)
Ti(1)	N(40)	C(47)	C(50)	109.1(6)
C(41)	N(40)	C(47)	C(48)	177.1(4)
Ti(1)	N(40)	C(47)	C(48)	-10.0(8)
C(41)	N(40)	C(47)	C(49)	59.0(6)
Ti(1)	N(40)	C(47)	C(49)	-128.1(5)
N(40)	Ti(1)	N(51)	C(52)	55.5(3)
N(8)	Ti(1)	N(51)	C(52)	-91.0(2)
C(41)	Ti(1)	N(51)	C(52)	94.4(2)
C(2)	Ti(1)	N(51)	C(52)	-176.8(2)
N(40)	Ti(1)	N(51)	C(72)	-128.3(6)
N(8)	Ti(1)	N(51)	C(72)	85.1(6)
C(52)	Ti(1)	N(51)	C(72)	176.2(7)
C(41)	Ti(1)	N(51)	C(72)	-89.4(6)
C(2)	Ti(1)	N(51)	C(72)	-0.6(6)
C(72)	N(51)	C(52)	P(53)	-1.8(11)
Ti(1)	N(51)	C(52)	P(53)	175.9(8)
C(72)	N(51)	C(52)	Ti(1)	-177.7(4)
N(40)	Ti(1)	C(52)	N(51)	-134.5(2)
N(8)	Ti(1)	C(52)	N(51)	110.3(2)
C(41)	Ti(1)	C(52)	N(51)	-100.3(2)
C(2)	Ti(1)	C(52)	N(51)	4.0(3)
N(51)	Ti(1)	C(52)	P(53)	-177.8(4)
N(40)	Ti(1)	C(52)	P(53)	47.6(3)
N(8)	Ti(1)	C(52)	P(53)	-67.5(3)
C(41)	Ti(1)	C(52)	P(53)	81.9(3)
C(2)	Ti(1)	C(52)	P(53)	-173.8(2)
N(51)	C(52)	P(53)	C(54)	-2.2(9)
Ti(1)	C(52)	P(53)	C(54)	172.4(3)
C(52)	P(53)	C(54)	C(59)	-86.9(3)
C(52)	P(53)	C(54)	C(55)	87.3(3)
C(59)	C(54)	C(55)	C(56)	16.5(5)
P(53)	C(54)	C(55)	C(56)	-157.8(3)
C(59)	C(54)	C(55)	C(68)	-159.6(4)
P(53)	C(54)	C(55)	C(68)	26.2(5)
C(54)	C(55)	C(56)	C(57)	-4.6(6)
C(68)	C(55)	C(56)	C(57)	171.7(4)
C(55)	C(56)	C(57)	C(58)	-7.8(6)
C(55)	C(56)	C(57)	C(64)	172.3(4)
C(56)	C(57)	C(58)	C(59)	8.7(6)
C(64)	C(57)	C(58)	C(59)	-171.5(4)
C(55)	C(54)	C(59)	C(58)	-15.8(5)
P(53)	C(54)	C(59)	C(58)	158.5(3)
C(55)	C(54)	C(59)	C(93)	162.3(4)
P(53)	C(54)	C(59)	C(93)	-23.5(5)
C(57)	C(58)	C(59)	C(54)	3.0(6)
C(57)	C(58)	C(59)	C(93)	-175.2(4)
C(58)	C(57)	C(64)	C(66)	-120.4(5)
C(56)	C(57)	C(64)	C(66)	59.4(5)
C(58)	C(57)	C(64)	C(65)	118.7(5)
C(56)	C(57)	C(64)	C(65)	-61.5(6)
C(58)	C(57)	C(64)	C(67)	0.4(6)

C(56)	C(57)	C(64)	C(67)	-179.8(4)
C(56)	C(55)	C(68)	C(71)	-13.3(5)
C(54)	C(55)	C(68)	C(71)	162.7(4)
C(56)	C(55)	C(68)	C(69)	107.6(4)
C(54)	C(55)	C(68)	C(69)	-76.4(5)
C(56)	C(55)	C(68)	C(70)	-129.8(4)
C(54)	C(55)	C(68)	C(70)	46.2(5)
C(52)	N(51)	C(72)	C(73)	177.4(4)
Ti(1)	N(51)	C(72)	C(73)	2.4(7)
C(52)	N(51)	C(72)	C(74)	-62.9(5)
Ti(1)	N(51)	C(72)	C(74)	122.0(5)
C(52)	N(51)	C(72)	C(75)	57.7(5)
Ti(1)	N(51)	C(72)	C(75)	-117.3(5)
C(76)	C(77)	C(78)	C(79)	173.1(8)
C(77)	C(78)	C(79)	C(80)	-179.8(8)
C(81)	C(82)	C(83)	C(84)	173.9(16)
C(82)	C(83)	C(84)	C(85)	179.1(16)
C(54)	C(59)	C(93)	C(61)	-47.7(5)
C(58)	C(59)	C(93)	C(61)	130.3(4)
C(54)	C(59)	C(93)	C(62)	76.0(5)
C(58)	C(59)	C(93)	C(62)	-105.9(4)
C(54)	C(59)	C(93)	C(63)	-164.0(4)
C(58)	C(59)	C(93)	C(63)	14.1(5)

Symmetry transformations used to generate equivalent atoms:

Table 6: Listing of Final SHELX Results File

```
REM  MSC03118
REM R1 =  0.0873 for   9219 Fo > 4sig(Fo)  and  0.1245 for all  13721 data
REM    767 parameters refined using      0 restraints
REM Highest difference peak  1.646,  deepest hole -0.576,  1-sigma level
0.088
REM  MSC03118
REM R1 =  0.0871 for   9219 Fo > 4sig(Fo)  and  0.1243 for all  13721 data
REM    767 parameters refined using      0 restraints
REM Highest difference peak  1.631,  deepest hole -0.585,  1-sigma level
0.088
TITL MSC03118
CELL 0.71073 12.2970 13.1823 24.8428 103.400 92.806 91.863
ZERR 2.0000 0.0023 0.0027 0.0046 0.005 0.006 0.006
LATT 1
SFAC TI  P  N  C  H
UNIT 2 2 10 154 264
MERG 2
FMAP 2
GRID
PLAN 20
TEMP -146
SIZE 0.35 0.3 0.3
BOND
CONF
L.S. 4
ACTA
WGHT    0.147300    3.712800
FVAR       0.26972
TI1   1    1.071053   -0.005901   -0.222483    11.00000    0.02185
0.02106 =
         0.02139    0.00251    0.00606    0.00175
C2    4    0.890938   -0.003469   -0.227128    11.00000    0.02383
0.02847 =
         0.02823    0.00331    0.00814    0.00023
N3    3    0.798050   -0.004157   -0.235725    11.00000    0.03135
0.02844 =
         0.03060    0.00142    0.01016    0.00339
C4    4    0.681759    0.006635   -0.247186    11.00000    0.02448
0.04147 =
         0.04067    0.00366    0.00871    0.00092
C5    4    0.627916    0.026023   -0.191819    11.00000    0.03158
0.09177 =
         0.05836    0.00435    0.01806    0.00830
AFIX 137
H5A   5    0.637597   -0.033983   -0.175289    11.00000   -1.50000
H5B   5    0.549942    0.035568   -0.197884    11.00000   -1.50000
H5C   5    0.661661    0.088925   -0.166759    11.00000   -1.50000
AFIX   0
C6    4    0.671418    0.100672   -0.272374    11.00000    0.03382
0.06312 =
         0.08797    0.02924   -0.00500    0.00317
AFIX 137
H6A   5    0.700278    0.163534   -0.245465    11.00000   -1.50000
H6B   5    0.594503    0.108714   -0.282116    11.00000   -1.50000
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```
H6C   5    0.712801    0.090450   -0.305794    11.00000   -1.50000
AFIX   0
C7    4    0.637101   -0.092485   -0.287465    11.00000    0.03089
0.05395 =
         0.06362   -0.00365    0.00248   -0.00675
AFIX 137
H7A   5    0.672885   -0.100603   -0.322509    11.00000   -1.50000
H7B   5    0.558390   -0.088178   -0.294233    11.00000   -1.50000
H7C   5    0.651193   -0.152674   -0.271660    11.00000   -1.50000
AFIX   0
N8    3    1.063784    0.001254   -0.303755    11.00000    0.02659
0.02429 =
         0.02090    0.00176    0.00375    0.00247
C9    4    1.009425    0.075679   -0.324284    11.00000    0.02583
0.02745 =
         0.02785    0.00270    0.00801    0.00015
C10   4    0.978241    0.064267   -0.379274    11.00000    0.04564
0.02327 =
         0.02946   -0.00023   -0.00013    0.00749
AFIX  43
H10   5    0.989701   -0.001598   -0.403126    11.00000   -1.20000
AFIX   0
C11   4    0.929960    0.141143   -0.404954    11.00000    0.04214
0.03159 =
         0.03265    0.00270    0.00173    0.00731
N12   3    0.891985    0.226093   -0.376212    11.00000    0.05377
0.03380 =
         0.03768    0.01009    0.00739    0.01799
C13   4    0.857660    0.305255   -0.402352    11.00000    0.05126
0.03232 =
         0.03219    0.00650    0.00522    0.01566
C14   4    0.746489    0.321024   -0.407274    11.00000    0.04820
0.03933 =
         0.05065    0.01680    0.00337    0.00740
C15   4    0.712909    0.404001   -0.428942    11.00000    0.04039
0.04394 =
         0.06020    0.01582    0.00434    0.01539
AFIX  43
H15   5    0.637630    0.417523   -0.431340    11.00000   -1.20000
AFIX   0
C16   4    0.789257    0.467672   -0.447227    11.00000    0.05747
0.02593 =
         0.04566    0.01183   -0.00020    0.00507
AFIX  43
H16   5    0.765422    0.521134   -0.464308    11.00000   -1.20000
AFIX   0
C17   4    0.896565    0.453091   -0.440587    11.00000    0.05011
0.03098 =
         0.04095    0.00636    0.00026    0.00154
AFIX  43
H17   5    0.947536    0.498413   -0.452033    11.00000   -1.20000
AFIX   0
C18   4    0.935058    0.373234   -0.417352    11.00000    0.04927
0.02854 =
         0.03041   -0.00055    0.00648    0.00820
C19   4    1.055681    0.362395   -0.406178    11.00000    0.04853
0.04201 =
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```
         0.05423    0.01330   -0.00076    0.00701
AFIX  13
H19   5    1.067776    0.287820   -0.406003    11.00000   -1.20000
AFIX   0
C20   4    1.126251    0.392343   -0.449298    11.00000    0.05673
0.14298 =
         0.06978    0.03431    0.01954    0.03165
AFIX 137
H20A  5    1.106802    0.346077   -0.485693    11.00000   -1.50000
H20B  5    1.203196    0.385455   -0.439109    11.00000   -1.50000
H20C  5    1.114147    0.464759   -0.450829    11.00000   -1.50000
AFIX   0
C21   4    1.093593    0.429505   -0.349493    11.00000    0.06138
0.07535 =
         0.06106    0.01674   -0.01450   -0.00957
AFIX 137
H21A  5    1.091590    0.503407   -0.350280    11.00000   -1.50000
H21B  5    1.168272    0.413073   -0.340073    11.00000   -1.50000
H21C  5    1.045339    0.415264   -0.321611    11.00000   -1.50000
AFIX   0
C22   4    0.664523    0.249736   -0.386771    11.00000    0.05011
0.05367 =
         0.07188    0.03168    0.00761    0.01075
AFIX  13
H22   5    0.699569    0.232470   -0.353020    11.00000   -1.20000
AFIX   0
C23   4    0.558355    0.301820   -0.369697    11.00000    0.06646
0.08388 =
         0.09353    0.04631    0.03124    0.01665
AFIX 137
H23A  5    0.574937    0.371932   -0.346322    11.00000   -1.50000
H23B  5    0.517561    0.260046   -0.348922    11.00000   -1.50000
H23C  5    0.514455    0.306897   -0.402895    11.00000   -1.50000
AFIX   0
C24   4    0.642839    0.146439   -0.430204    11.00000    0.05814
0.06051 =
         0.10692    0.03630    0.00741    0.00196
AFIX 137
H24A  5    0.610910    0.160517   -0.464514    11.00000   -1.50000
H24B  5    0.592170    0.101171   -0.416132    11.00000   -1.50000
H24C  5    0.711595    0.111690   -0.437693    11.00000   -1.50000
AFIX   0
C25   4    0.929372    0.115958   -0.467663    11.00000    0.06972
0.04055 =
         0.02797    0.00274   -0.00524    0.01917
AFIX 137
H25A  5    0.883811    0.164750   -0.481825    11.00000   -1.50000
H25B  5    0.899956    0.044434   -0.482656    11.00000   -1.50000
H25C  5    1.003968    0.122401   -0.479063    11.00000   -1.50000
AFIX   0
C26   4    0.989834    0.173617   -0.281989    11.00000    0.03971
0.02799 =
         0.02365    0.00398    0.00529    0.00472
AFIX 137
H26A  5    1.024813    0.233474   -0.292507    11.00000   -1.50000
H26B  5    1.020600    0.168354   -0.245646    11.00000   -1.50000
H26C  5    0.911274    0.183079   -0.280150    11.00000   -1.50000
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AFIX   0
C27   4    1.107769   -0.081378   -0.344968    11.00000    0.02753
0.02691 =
         0.01987    0.00084   -0.00031    0.00729
C28   4    1.054068   -0.179705   -0.362010    11.00000    0.03268
0.03022 =
         0.02198    0.00131    0.00427    0.00263
C29   4    1.103244   -0.257964   -0.400140    11.00000    0.04089
0.02711 =
         0.03147   -0.00127    0.00004    0.00542
AFIX  43
H29   5    1.068424   -0.325540   -0.411157    11.00000   -1.20000
AFIX   0
C30   4    1.199841   -0.239445   -0.421800    11.00000    0.04125
0.03592 =
         0.03352    0.00157    0.00653    0.01335
AFIX  43
H30   5    1.232224   -0.293707   -0.447207    11.00000   -1.20000
AFIX   0
C31   4    1.250467   -0.139814   -0.406166    11.00000    0.03338
0.04111 =
         0.03421    0.00744    0.00586    0.00753
AFIX  43
H31   5    1.316794   -0.126696   -0.421951    11.00000   -1.20000
AFIX   0
C32   4    1.206640   -0.059429   -0.368227    11.00000    0.02569
0.03373 =
         0.02740    0.00774   -0.00088    0.00410
C33   4    1.261665    0.049111   -0.354820    11.00000    0.03081
0.03714 =
         0.03712    0.00760    0.00765   -0.00197
AFIX  13
H33   5    1.218833    0.095263   -0.326543    11.00000   -1.20000
AFIX   0
C34   4    1.260648    0.094386   -0.406359    11.00000    0.06140
0.04712 =
         0.05367    0.02272   -0.00331   -0.01069
AFIX 137
H34A  5    1.302217    0.050503   -0.434803    11.00000   -1.50000
H34B  5    1.293788    0.165349   -0.396476    11.00000   -1.50000
H34C  5    1.185288    0.096257   -0.420753    11.00000   -1.50000
AFIX   0
C35   4    1.377949    0.050026   -0.330236    11.00000    0.03423
0.04772 =
         0.03918    0.01240    0.00546   -0.00681
AFIX 137
H35A  5    1.377553    0.020100   -0.297625    11.00000   -1.50000
H35B  5    1.408148    0.122035   -0.319337    11.00000   -1.50000
H35C  5    1.422837    0.008530   -0.357957    11.00000   -1.50000
AFIX   0
C36   4    0.940576   -0.201847   -0.344310    11.00000    0.04560
0.03165 =
         0.04767   -0.00973    0.01798   -0.00439
AFIX  13
H36   5    0.922333   -0.140828   -0.314417    11.00000   -1.20000
AFIX   0
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C37   4    0.857060   -0.211108   -0.392413    11.00000    0.03544
0.06106 =
         0.10590    0.02945    0.00798    0.00440
AFIX 137
H37A  5    0.873464   -0.270025   -0.422568    11.00000   -1.50000
H37B  5    0.859647   -0.146594   -0.405616    11.00000   -1.50000
H37C  5    0.784123   -0.222688   -0.380128    11.00000   -1.50000
AFIX   0
C38   4    0.930660   -0.298431   -0.321610    11.00000    0.05518
0.06339 =
         0.04627    0.00667    0.00324   -0.02353
AFIX 137
H38A  5    0.859110   -0.302166   -0.306274    11.00000   -1.50000
H38B  5    0.987968   -0.295244   -0.292354    11.00000   -1.50000
H38C  5    0.938471   -0.360522   -0.351480    11.00000   -1.50000
AFIX   0
N40   3    1.151541   -0.134223   -0.213797    11.00000    0.02831
0.02576 =
         0.02694    0.00478    0.00506    0.00075
C41   4    1.060055   -0.141143   -0.193279    11.00000    0.02915
0.02139 =
         0.02909    0.00248    0.00369   -0.00049
C42   4    1.012612   -0.224675   -0.167321    11.00000    0.03922
0.03405 =
         0.03433    0.00820    0.01102    0.00078
AFIX  23
H42A  5    1.070571   -0.272696   -0.162418    11.00000   -1.20000
H42B  5    0.954873   -0.265725   -0.193231    11.00000   -1.20000
AFIX   0
C43   4    0.964057   -0.182445   -0.110935    11.00000    0.04976
0.03588 =
         0.03123    0.00907    0.01465   -0.00146
C44   4    0.871447   -0.111643   -0.115866    11.00000    0.06527
0.06591 =
         0.05119    0.02373    0.03434    0.01569
AFIX 137
H44A  5    0.836561   -0.093088   -0.080488    11.00000   -1.50000
H44B  5    0.817802   -0.147931   -0.145011    11.00000   -1.50000
H44C  5    0.900022   -0.048074   -0.125292    11.00000   -1.50000
AFIX   0
C45   4    1.053558   -0.123680   -0.069335    11.00000    0.07468
0.04800 =
         0.02910    0.00313    0.01492   -0.01440
AFIX 137
H45A  5    1.081177   -0.062936   -0.081817    11.00000   -1.50000
H45B  5    1.113221   -0.170090   -0.066644    11.00000   -1.50000
H45C  5    1.023594   -0.100378   -0.032904    11.00000   -1.50000
AFIX   0

C47   4    1.249615   -0.200468   -0.217829    11.00000    0.03145
0.03453 =
         0.03312    0.00597    0.00593    0.00664
C48   4    1.331930   -0.153607   -0.250145    11.00000    0.02878
0.03438 =
         0.04288    0.00876    0.00958    0.00764
AFIX 137
H48A  5    1.300551   -0.156453   -0.287523    11.00000   -1.50000
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H48B  5    1.398171   -0.193415   -0.252646    11.00000   -1.50000
H48C  5    1.350034   -0.080798   -0.231059    11.00000   -1.50000
AFIX   0
C49   4    1.217469   -0.312175   -0.249764    11.00000    0.04773
0.02901 =
         0.04710    0.00497    0.01564    0.00723
AFIX 137
H49A  5    1.161047   -0.341491   -0.230505    11.00000   -1.50000
H49B  5    1.281525   -0.354961   -0.251960    11.00000   -1.50000
H49C  5    1.189257   -0.311574   -0.287267    11.00000   -1.50000
AFIX   0
C50   4    1.296240   -0.196372   -0.159568    11.00000    0.04968
0.05366 =
         0.03570    0.01014    0.00841    0.01165
AFIX 137
H50A  5    1.311889   -0.123485   -0.139878    11.00000   -1.50000
H50B  5    1.363673   -0.234362   -0.161552    11.00000   -1.50000
H50C  5    1.243242   -0.228626   -0.139684    11.00000   -1.50000
AFIX   0
N51   3    1.075187    0.120519   -0.161484    11.00000    0.02229
0.02348 =
         0.02465   -0.00009    0.00447    0.00173
C52   4    1.177638    0.102949   -0.170155    11.00000    0.03318
0.02260 =
         0.01831    0.00379    0.00423    0.00329
P53   2    1.315159    0.123503   -0.162746    11.00000    0.02152
0.02510 =
         0.02680   -0.00121    0.00651    0.00170
C54   4    1.342552    0.253228   -0.110323    11.00000    0.01730
0.02629 =
         0.02441   -0.00233    0.00540    0.00070
C55   4    1.351532    0.256363   -0.052470    11.00000    0.01764
0.02696 =
         0.03019    0.00090    0.00621   -0.00165
C56   4    1.332857    0.351239   -0.015886    11.00000    0.02574
0.03159 =
         0.02368   -0.00140    0.00567   -0.00126
AFIX  43
H56   5    1.333188    0.353195    0.022590    11.00000   -1.20000
AFIX   0
C57   4    1.313899    0.442535   -0.032702    11.00000    0.02276
0.02500 =
         0.03377   -0.00408    0.00805   -0.00170
C58   4    1.327341    0.440476   -0.087746    11.00000    0.02525
0.02638 =
         0.03698    0.00328    0.00281   -0.00065
AFIX  43
H58   5    1.325024    0.504092   -0.099455    11.00000   -1.20000
AFIX   0
C59   4    1.344373    0.347643   -0.127263    11.00000    0.02178
0.02872 =
         0.02984    0.00238    0.00268   -0.00053
C60   4    0.920097   -0.278204   -0.090898    11.00000    0.05926
0.05156 =
         0.03543    0.01204    0.01138   -0.01087
AFIX 137
H60A  5    0.980916   -0.320856   -0.084300    11.00000   -1.50000
```

```
H60B  5    0.868331   -0.320029   -0.119316    11.00000   -1.50000
H60C  5    0.883274   -0.254218   -0.056420    11.00000   -1.50000
AFIX   0
C61   4    1.469074    0.295874   -0.205733    11.00000    0.03681
0.04631 =
         0.03159    0.01088    0.01137   -0.00198
AFIX 137
H61A  5    1.452745    0.221091   -0.209937    11.00000   -1.50000
H61B  5    1.529236    0.319075   -0.177754    11.00000   -1.50000
H61C  5    1.489932    0.308588   -0.241252    11.00000   -1.50000
AFIX   0
C62   4    1.271403    0.319620   -0.229738    11.00000    0.04543
0.05078 =
         0.03213    0.01415    0.00429    0.00084
AFIX 137
H62A  5    1.290376    0.330569   -0.265892    11.00000   -1.50000
H62B  5    1.207547    0.359402   -0.217489    11.00000   -1.50000
H62C  5    1.254720    0.245194   -0.232904    11.00000   -1.50000
AFIX   0
C63   4    1.396156    0.471820   -0.188856    11.00000    0.06394
0.04020 =
         0.04706    0.01628    0.01060   -0.00536
AFIX 137
H63A  5    1.425715    0.473742   -0.224548    11.00000   -1.50000
H63B  5    1.450495    0.502372   -0.158803    11.00000   -1.50000
H63C  5    1.330124    0.511880   -0.184166    11.00000   -1.50000
AFIX   0
C64   4    1.280051    0.540059    0.008721    11.00000    0.03013
0.02512 =
         0.04382   -0.00720    0.01119    0.00081
C65   4    1.171614    0.513520    0.030678    11.00000    0.04913
0.03666 =
         0.08460   -0.01532    0.03831   -0.00069
AFIX 137
H65A  5    1.116018    0.495292   -0.000030    11.00000   -1.50000
H65B  5    1.149354    0.574024    0.058282    11.00000   -1.50000
H65C  5    1.179813    0.454195    0.047887    11.00000   -1.50000
AFIX   0
C66   4    1.366520    0.574172    0.056167    11.00000    0.05902
0.04448 =
         0.04800   -0.01384    0.00650    0.00272

AFIX 137
H66A  5    1.340345    0.632170    0.084053    11.00000   -1.50000
H66B  5    1.433728    0.596809    0.041855    11.00000   -1.50000
H66C  5    1.381089    0.515471    0.073102    11.00000   -1.50000
AFIX   0
C67   4    1.262659    0.632857   -0.018582    11.00000    0.06995
0.03494 =
         0.06102   -0.00699    0.01667    0.00883
AFIX 137
H67A  5    1.205119    0.613545   -0.048295    11.00000   -1.50000
H67B  5    1.330591    0.650526   -0.034067    11.00000   -1.50000
H67C  5    1.241242    0.693330    0.009307    11.00000   -1.50000
AFIX   0
C68   4    1.387607    0.163296   -0.027994    11.00000    0.03232
0.02980 =
```

```
         0.03093    0.00601    0.00526    0.00310
C69   4    1.298748    0.076350   -0.033254    11.00000    0.04322
0.03201 =
         0.03320    0.01102    0.00875    0.00272
AFIX 137
H69A  5    1.329372    0.017496   -0.020709    11.00000   -1.50000
H69B  5    1.271570    0.052972   -0.072066    11.00000   -1.50000
H69C  5    1.238614    0.103115   -0.010340    11.00000   -1.50000
AFIX   0
C70   4    1.489424    0.117810   -0.057229    11.00000    0.03543
0.03604 =
         0.03358    0.00669    0.00292    0.00848
AFIX 137
H70A  5    1.518168    0.064564   -0.039341    11.00000   -1.50000
H70B  5    1.545231    0.173829   -0.054537    11.00000   -1.50000
H70C  5    1.469408    0.086207   -0.096337    11.00000   -1.50000
AFIX   0
C71   4    1.422509    0.199269    0.033719    11.00000    0.04911
0.03916 =
         0.03595    0.00825    0.00625    0.00401
AFIX 137
H71A  5    1.358540    0.220554    0.054882    11.00000   -1.50000
H71B  5    1.475425    0.258526    0.039398    11.00000   -1.50000
H71C  5    1.455897    0.141748    0.046371    11.00000   -1.50000
AFIX   0
C72   4    1.022467    0.207054   -0.121862    11.00000    0.02545
0.02602 =
         0.02622   -0.00662    0.00714    0.00456
C73   4    0.899439    0.191544   -0.131117    11.00000    0.02952
0.03392 =
         0.03691   -0.00493    0.01235    0.00497
AFIX 137
H73A  5    0.877837    0.194256   -0.169238    11.00000   -1.50000
H73B  5    0.864597    0.246889   -0.105184    11.00000   -1.50000
H73C  5    0.876513    0.123481   -0.124900    11.00000   -1.50000
AFIX   0
C74   4    1.056275    0.202942   -0.062708    11.00000    0.03683
0.04160 =
         0.02751   -0.00160    0.01325    0.00630
AFIX 137
H74A  5    1.034899    0.134336   -0.056691    11.00000   -1.50000
H74B  5    1.020219    0.257300   -0.036749    11.00000   -1.50000
H74C  5    1.135487    0.214542   -0.056574    11.00000   -1.50000
AFIX   0
C75   4    1.058689    0.311668   -0.132806    11.00000    0.02775
0.03034 =
         0.03938   -0.00097    0.00912    0.00302
AFIX 137
H75A  5    1.138334    0.320137   -0.128395    11.00000   -1.50000
H75B  5    1.026499    0.368195   -0.106396    11.00000   -1.50000
H75C  5    1.034540    0.313985   -0.170668    11.00000   -1.50000
AFIX   0
C76   4    1.586858   -0.168668   -0.459213    11.00000    0.09107
0.16011 =
         0.10399    0.05585   -0.01834   -0.01773
AFIX 137
H76A  5    1.536866   -0.120317   -0.438149    11.00000   -1.50000
```

```
H76B  5    1.592489   -0.154877   -0.496105    11.00000   -1.50000
H76C  5    1.658994   -0.158847   -0.439679    11.00000   -1.50000
AFIX   0
C77   4    1.544999   -0.277123   -0.464802    11.00000    0.16219
0.11477 =
         0.07227    0.02793   -0.01267    0.01099
AFIX  23
H77A  5    1.601692   -0.324822   -0.480868    11.00000   -1.20000
H77B  5    1.480844   -0.290317   -0.491541    11.00000   -1.20000
AFIX   0
C78   4    1.512662   -0.304471   -0.412342    11.00000    0.06272
0.09975 =
         0.07440    0.00247   -0.00572    0.00504
AFIX  23
H78A  5    1.578882   -0.299515   -0.387386    11.00000   -1.20000
H86   5    1.463003   -0.251310   -0.393913    11.00000   -1.20000
AFIX   0
C79   4    1.458902   -0.408387   -0.418218    11.00000    0.07840
0.07603 =
         0.11247   -0.00218   -0.01633    0.02988
AFIX  23
H79A  5    1.508488   -0.461918   -0.436343    11.00000   -1.20000
H79B  5    1.392501   -0.413729   -0.443088    11.00000   -1.20000
AFIX   0
C80   4    1.426955   -0.433251   -0.364140    11.00000    0.14422
0.11731 =
         0.13573    0.03198    0.05973    0.02221
AFIX 137
H80A  5    1.492839   -0.440761   -0.341817    11.00000   -1.50000
H80B  5    1.382371   -0.498554   -0.372194    11.00000   -1.50000
H80C  5    1.385075   -0.376456   -0.343571    11.00000   -1.50000
AFIX   0
C81   4    1.816232    0.410212   -0.233693    11.00000    0.17390
AFIX 137
H81A  5    1.895135    0.411095   -0.225688    11.00000   -1.50000
H81B  5    1.793501    0.347667   -0.262436    11.00000   -1.50000
H81C  5    1.778504    0.409504   -0.199927    11.00000   -1.50000
AFIX   0
C82   4    1.791667    0.493281   -0.251042    11.00000    0.19998
AFIX  23
H82A  5    1.769394    0.471412   -0.291021    11.00000   -1.20000
H82B  5    1.858361    0.539095   -0.247249    11.00000   -1.20000
AFIX   0
C83   4    1.709750    0.551725   -0.224110    11.00000    0.15405
AFIX  23
H83A  5    1.643707    0.504521   -0.231247    11.00000   -1.20000
H83B  5    1.730083    0.562855   -0.184049    11.00000   -1.20000
AFIX   0
C84   4    1.675792    0.645191   -0.230986    11.00000    0.16977
AFIX  23
H84A  5    1.653939    0.636646   -0.270727    11.00000   -1.20000
H84B  5    1.739448    0.695359   -0.222493    11.00000   -1.20000
AFIX   0
C85   4    1.587665    0.692620   -0.199374    11.00000    0.12939
AFIX 137
H85A  5    1.518615    0.655562   -0.214756    11.00000   -1.50000
H85B  5    1.584747    0.765939   -0.201237    11.00000   -1.50000
```

```
H85C  5    1.599777    0.688574   -0.160657    11.00000   -1.50000
AFIX   0
C93   4    1.367803    0.356721   -0.187347    11.00000    0.03400
0.03501 =
         0.03138    0.00843    0.00442   -0.00137
HKLF 4

REM  MSC03118
REM R1 =  0.0869 for   9219 Fo > 4sig(Fo)  and  0.1241 for all  13721 data
REM    767 parameters refined using      0 restraints

END

WGHT      0.1472      3.5090
REM Highest difference peak  1.629,  deepest hole -0.586,  1-sigma level
0.088
Q1    1   0.9926  0.0010 -0.2284  11.00000  0.05    1.63
Q2    1   1.2407  0.1350 -0.1675  11.00000  0.05    1.07
Q3    1   1.9246  0.4858 -0.2233  11.00000  0.05    1.07
Q4    1   1.0623 -0.0806 -0.2177  11.00000  0.05    0.65
Q5    1   0.8134  0.2257 -0.3946  11.00000  0.05    0.57
Q6    1   0.9057  0.0727 -0.3903  11.00000  0.05    0.56
Q7    1   1.1571 -0.0265 -0.2139  11.00000  0.05    0.53
Q8    1   1.7387  0.4818 -0.2086  11.00000  0.05    0.52
Q9    1   0.6423  0.3945 -0.4558  11.00000  0.05    0.50
Q10   1   1.6432  0.5078 -0.2881  11.00000  0.05    0.48
Q11   1   1.6866  0.5223 -0.2714  11.00000  0.05    0.48
Q12   1   0.9847  0.0067 -0.3074  11.00000  0.05    0.46
Q13   1   0.7149  0.4622 -0.4663  11.00000  0.05    0.46
Q14   1   1.7772  0.4377 -0.1829  11.00000  0.05    0.46
Q15   1   1.1007  0.3164 -0.4660  11.00000  0.05    0.45
Q16   1   1.7634  0.5997 -0.2183  11.00000  0.05    0.45
Q17   1   0.7843 -0.2178 -0.4085  11.00000  0.05    0.44
Q18   1   1.1332 -0.0575 -0.3691  11.00000  0.05    0.44
Q19   1   1.5577  0.6088 -0.2970  11.00000  0.05    0.43
Q20   1   0.8652  0.3838 -0.4301  11.00000  0.05    0.43
```

```
MSC03118                                    03/09/1911:31:45.8
 12.297000 13.182300 24.842800 -0.231750 -0.048950 -0.032510  0.710730
   0.00230   0.00270   0.00460   0.00008   0.00010   0.00010   3908.77
P 1BAR
   5   2   0   1   2   4   7111111001111   0   0   0   0   0   0
TI   RHF  9.7595 7.8508 7.3558  .5000 1.699135.6338 1.9021116.105 1.2807
      .248      .446             TI   MO K ALPHA 1
 P   RHF  6.4345 1.9067 4.179127.1570 1.7800  .5260 1.490868.1645 1.1149
      .090      .095             P    MO K ALPHA 1
 N   RHF 12.2126  .0057 3.1322 9.8933 2.012528.9975 1.1663  .5826-11.529
      .004      .003             N    MO K ALPHA 1
CVAL  HF 2.2606922.69071.56165.6566651.050759.75618.83925955.5949.286977
      .002      .002             C    MO K ALPHA 1
 H  SDS  .49300210.5109.32291226.1257.1401913.14236.04081057.7997.003038
      .000      .000             H    MO K ALPHA 1
  22   1  15   1   7   5   6  77   1 132   0   0   0   0   0   0
         1         0       290         0         0         0         0
         0         0         0         0         0
   0.0000000000  1  0  0   0.0000000000  0  1  0   0.0000000000  0  0  1
   0.0000000000 -1  0  0   0.0000000000  0 -1  0   0.0000000000  0  0 -1
TI(1)       1000  100000        0.000000  1.071053 -0.005901 -0.222483
155501
  0.002865  0.002533  0.000725  0.000220  0.000404  0.000160
155501
C(2)        4000  100000        0.000000  0.890938 -0.003469 -0.227128
255501
  0.003125  0.003424  0.000957  0.000029  0.000543  0.000211
255501
N(3)        3000  100000        0.000000  0.798050 -0.004157 -0.235725
355501
  0.004111  0.003421  0.001038  0.000426  0.000677  0.000091
355501
C(4)        4000  100000        0.000000  0.681759  0.006635 -0.247186
455501
  0.003210  0.004988  0.001379  0.000116  0.000581  0.000234
455501
C(5)        4000  100000        0.000000  0.627916  0.026023 -0.191819
555501
  0.004141  0.011038  0.001979  0.001042  0.001204  0.000278
555501
C(6)        4000  100000        0.000000  0.671418  0.100672 -0.272374
655501
  0.004434  0.007592  0.002983  0.000398 -0.000333  0.001868
655501
C(7)        4000  100000        0.000000  0.637101 -0.092485 -0.287465
755501
  0.004050  0.006489  0.002158 -0.000848  0.000165 -0.000233
755501
N(8)        3000  100000        0.000000  1.063784  0.001254 -0.303755
855501
  0.003486  0.002922  0.000709  0.000310  0.000250  0.000112
855501
C(9)        4000  100000        0.000000  1.009425  0.075679 -0.324284
955501
  0.003387  0.003302  0.000944  0.000019  0.000534  0.000172
955501
```

```
C(10)       4000  100000        0.000000  0.978241  0.064267 -0.379274
1055501
  0.005984  0.002799  0.000999  0.000941 -0.000009 -0.000015
1055501
C(11)       4000  100000        0.000000  0.929960  0.141143 -0.404954
1155501
  0.005525  0.003800  0.001107  0.000918  0.000115  0.000172
1155501
N(12)       3000  100000        0.000000  0.891985  0.226093 -0.376212
1255501
  0.007050  0.004066  0.001278  0.002259  0.000493  0.000644
1255501
C(13)       4000  100000        0.000000  0.857660  0.305255 -0.402352
1355501
  0.006721  0.003888  0.001092  0.001967  0.000348  0.000415
1355501
C(14)       4000  100000        0.000000  0.746489  0.321024 -0.407274
1455501
  0.006320  0.004731  0.001718  0.000929  0.000225  0.001073
1455501
C(15)       4000  100000        0.000000  0.712909  0.404001 -0.428942
1555501
  0.005296  0.005285  0.002042  0.001933  0.000289  0.001010
1555501
C(16)       4000  100000        0.000000  0.789257  0.467672 -0.447227
1655501
  0.007535  0.003119  0.001548  0.000637 -0.000013  0.000756
1655501
C(17)       4000  100000        0.000000  0.896565  0.453091 -0.440587
1755501
  0.006570  0.003726  0.001389  0.000193  0.000017  0.000406
1755501
C(18)       4000  100000        0.000000  0.935058  0.373234 -0.417352
1855501
  0.006460  0.003433  0.001031  0.001030  0.000432 -0.000035
1855501
C(19)       4000  100000        0.000000  1.055681  0.362395 -0.406178
1955501
  0.006363  0.005053  0.001839  0.000880 -0.000051  0.000849
1955501
C(20)       4000  100000        0.000000  1.126251  0.392343 -0.449298
2055501
  0.007438  0.017198  0.002366  0.003975  0.001303  0.002191
2055501
C(21)       4000  100000        0.000000  1.093593  0.429505 -0.349493
2155501
  0.008048  0.009063  0.002071 -0.001202 -0.000967  0.001069
2155501
C(22)       4000  100000        0.000000  0.664523  0.249736 -0.386771
2255501
  0.006570  0.006456  0.002438  0.001350  0.000507  0.002023
2255501
C(23)       4000  100000        0.000000  0.558355  0.301820 -0.369697
2355501
  0.008714  0.010089  0.003172  0.002091  0.002083  0.002958
2355501
```

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C(24)       4000  100000        0.000000  0.642839  0.146439 -0.430204
2455501
  0.007623  0.007278  0.003626  0.000246  0.000494  0.002318
2455501
C(25)       4000  100000        0.000000  0.929372  0.115958 -0.467663
2555501

  0.009141  0.004878  0.000949  0.002407 -0.000349  0.000175
2555501
C(26)       4000  100000        0.000000  0.989834  0.173617 -0.281989
2655501
  0.005207  0.003367  0.000802  0.000593  0.000353  0.000254
2655501
C(27)       4000  100000        0.000000  1.107769 -0.081378 -0.344968
2755501
  0.003610  0.003237  0.000674  0.000916 -0.000021  0.000054
2755501
C(28)       4000  100000        0.000000  1.054068 -0.179705 -0.362010
2855501
  0.004285  0.003635  0.000745  0.000330  0.000285  0.000084
2855501
C(29)       4000  100000        0.000000  1.103244 -0.257964 -0.400140
2955501
  0.005361  0.003261  0.001067  0.000681  0.000003 -0.000081
2955501
C(30)       4000  100000        0.000000  1.199841 -0.239445 -0.421800
3055501
  0.005409  0.004321  0.001137  0.001677  0.000435  0.000100
3055501
C(31)       4000  100000        0.000000  1.250467 -0.139814 -0.406166
3155501
  0.004377  0.004945  0.001160  0.000946  0.000391  0.000475
3155501
C(32)       4000  100000        0.000000  1.206640 -0.059429 -0.368227
3255501
  0.003368  0.004057  0.000929  0.000515 -0.000059  0.000494
3255501
C(33)       4000  100000        0.000000  1.261665  0.049111 -0.354820
3355501
  0.004040  0.004467  0.001259 -0.000247  0.000510  0.000485
3355501
C(34)       4000  100000        0.000000  1.260648  0.094386 -0.406359
3455501
  0.008051  0.005668  0.001820 -0.001342 -0.000221  0.001451
3455501
C(35)       4000  100000        0.000000  1.377949  0.050026 -0.330236
3555501
  0.004488  0.005740  0.001329 -0.000855  0.000364  0.000792
3555501
C(36)       4000  100000        0.000000  0.940576 -0.201847 -0.344310
3655501
  0.005979  0.003807  0.001617 -0.000551  0.001199 -0.000621
3655501
C(37)       4000  100000        0.000000  0.857060 -0.211108 -0.392413
3755501
  0.004647  0.007345  0.003591  0.000553  0.000532  0.001881
3755501
```

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C(38)       4000  100000        0.000000  0.930660 -0.298431 -0.321610
3855501
  0.007235  0.007625  0.001569 -0.002955  0.000216  0.000426
3855501
N(40)       3000  100000        0.000000  1.151541 -0.134223 -0.213797
3955501
  0.003712  0.003099  0.000914  0.000094  0.000337  0.000305
3955501
C(41)       4000  100000        0.000000  1.060055 -0.141143 -0.193279
4055501
  0.003822  0.002573  0.000987 -0.000062  0.000246  0.000158
4055501
C(42)       4000  100000        0.000000  1.012612 -0.224675 -0.167321
4155501
  0.005142  0.004096  0.001164  0.000098  0.000735  0.000524
4155501
C(43)       4000  100000        0.000000  0.964057 -0.182445 -0.110935
4255501
  0.006524  0.004316  0.001059 -0.000183  0.000977  0.000579
4255501
C(44)       4000  100000        0.000000  0.871447 -0.111643 -0.115866
4355501
  0.008558  0.007928  0.001736  0.001970  0.002290  0.001516
4355501
C(45)       4000  100000        0.000000  1.053558 -0.123680 -0.069335
4455501
  0.009792  0.005774  0.000987 -0.001808  0.000995  0.000200
4455501
C(47)       4000  100000        0.000000  1.249615 -0.200468 -0.217829
4555501
  0.004124  0.004153  0.001123  0.000834  0.000395  0.000381
4555501
C(48)       4000  100000        0.000000  1.331930 -0.153607 -0.250145
4655501
  0.003774  0.004135  0.001454  0.000959  0.000639  0.000559
4655501
C(49)       4000  100000        0.000000  1.217469 -0.312175 -0.249764
4755501
  0.006258  0.003489  0.001597  0.000908  0.001043  0.000317
4755501
C(50)       4000  100000        0.000000  1.296240 -0.196372 -0.159568
4855501
  0.006514  0.006454  0.001211  0.001463  0.000561  0.000648
4855501
N(51)       3000  100000        0.000000  1.075187  0.120519 -0.161484
4955501
  0.002923  0.002824  0.000836  0.000217  0.000298 -0.000006
4955501
C(52)       4000  100000        0.000000  1.177638  0.102949 -0.170155
5055501
  0.004350  0.002718  0.000621  0.000413  0.000282  0.000242
5055501
P(53)       2000  100000        0.000000  1.315159  0.123503 -0.162746
5155501
  0.002822  0.003019  0.000909  0.000213  0.000434 -0.000077
5155501
```

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C(54)       4000  100000        0.000000  1.342552  0.253228 -0.110323
5255501
  0.002268  0.003162  0.000828  0.000088  0.000360 -0.000149
5255501
C(55)       4000  100000        0.000000  1.351532  0.256363 -0.052470
5355501
  0.002313  0.003243  0.001024 -0.000207  0.000414  0.000057
5355501
C(56)       4000  100000        0.000000  1.332857  0.351239 -0.015886
5455501
  0.003375  0.003800  0.000803 -0.000158  0.000378 -0.000089
5455501
C(57)       4000  100000        0.000000  1.313899  0.442535 -0.032702
5555501
  0.002984  0.003007  0.001145 -0.000213  0.000537 -0.000261
5555501
C(58)       4000  100000        0.000000  1.327341  0.440476 -0.087746
5655501
  0.003311  0.003173  0.001254 -0.000082  0.000187  0.000209
5655501
C(59)       4000  100000        0.000000  1.344373  0.347643 -0.127263
5755501
  0.002856  0.003455  0.001012 -0.000067  0.000179  0.000152
5755501
C(60)       4000  100000        0.000000  0.920097 -0.278204 -0.090898
5855501
  0.007770  0.006202  0.001202 -0.001365  0.000759  0.000769
5855501
C(61)       4000  100000        0.000000  1.469074  0.295874 -0.205733
5955501
  0.004826  0.005570  0.001071 -0.000249  0.000758  0.000695
5955501
C(62)       4000  100000        0.000000  1.271403  0.319620 -0.229738
6055501
  0.005957  0.006108  0.001090  0.000105  0.000286  0.000904
6055501
C(63)       4000  100000        0.000000  1.396156  0.471820 -0.188856
6155501
  0.008384  0.004835  0.001596 -0.000673  0.000707  0.001040
6155501
C(64)       4000  100000        0.000000  1.280051  0.540059  0.008721
6255501
  0.003951  0.003022  0.001486  0.000102  0.000746 -0.000460
6255501
C(65)       4000  100000        0.000000  1.171614  0.513520  0.030678
6355501
  0.006442  0.004410  0.002869 -0.000087  0.002555 -0.000978
6355501
C(66)       4000  100000        0.000000  1.366520  0.574172  0.056167
6455501
  0.007739  0.005350  0.001628  0.000342  0.000433 -0.000884
6455501
C(67)       4000  100000        0.000000  1.262659  0.632857 -0.018582
6555501
  0.009172  0.004203  0.002069  0.001109  0.001112 -0.000446
6555501
```

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C(68)       4000  100000        0.000000  1.387607  0.163296 -0.027994
6655501
  0.004238  0.003584  0.001049  0.000389  0.000351  0.000384
6655501
C(69)       4000  100000        0.000000  1.298748  0.076350 -0.033254
6755501
  0.005667  0.003850  0.001126  0.000342  0.000583  0.000704
6755501
C(70)       4000  100000        0.000000  1.489424  0.117810 -0.057229
6855501
  0.004645  0.004335  0.001139  0.001065  0.000195  0.000427
6855501
C(71)       4000  100000        0.000000  1.422509  0.199269  0.033719
6955501
  0.006439  0.004710  0.001219  0.000504  0.000417  0.000527
6955501
C(72)       4000  100000        0.000000  1.022467  0.207054 -0.121862
7055501
  0.003337  0.003130  0.000889  0.000573  0.000476 -0.000423
7055501
C(73)       4000  100000        0.000000  0.899439  0.191544 -0.131117
7155501
  0.003871  0.004080  0.001252  0.000624  0.000824 -0.000315
7155501
C(74)       4000  100000        0.000000  1.056275  0.202942 -0.062708
7255501
  0.004829  0.005004  0.000933  0.000791  0.000884 -0.000102
7255501
C(75)       4000  100000        0.000000  1.058689  0.311668 -0.132806
7355501
  0.003638  0.003649  0.001336  0.000379  0.000608 -0.000062
7355501
C(76)       4000  100000        0.000000  1.586858 -0.168668 -0.459213
7455501
  0.011941  0.019259  0.003527 -0.002227 -0.001223  0.003567
7455501
C(77)       4000  100000        0.000000  1.544999 -0.277123 -0.464802
7555501
  0.021266  0.013805  0.002451  0.001380 -0.000845  0.001784
7555501
C(78)       4000  100000        0.000000  1.512662 -0.304471 -0.412342
7655501
  0.008224  0.011998  0.002523  0.000633 -0.000381  0.000158
7655501
C(79)       4000  100000        0.000000  1.458902 -0.408387 -0.418218
7755501
  0.010280  0.009145  0.003814  0.003752 -0.001089 -0.000139
7755501
C(80)       4000  100000        0.000000  1.426955 -0.433251 -0.364140
7855501
  0.018910  0.014111  0.004603  0.002789  0.003983  0.002043
7855501
C(81)       4000       0        0.000000  1.816232  0.410212 -0.233693
7955501
 13.730594
7955501
```

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C(82)       4000       0        0.000000  1.791667  0.493281 -0.251042
8055501
 15.789789
8055501
C(83)       4000       0        0.000000  1.709750  0.551725 -0.224110
8155501
 12.163301
8155501
C(84)       4000       0        0.000000  1.675792  0.645191 -0.230986
8255501
 13.404503
8255501
C(85)       4000       0        0.000000  1.587665  0.692620 -0.199374
8355501
 10.216226
8355501
C(93)       4000  100000        0.000000  1.367803  0.356721 -0.187347
8455501
  0.004458  0.004211  0.001064 -0.000172  0.000295  0.000538
8455501
H(5A)       5000       0        0.000000  0.637597 -0.033983 -0.175289
8555501
  7.353257
8555501
H(5B)       5000       0        0.000000  0.549942  0.035568 -0.197884
8655501
  7.353257
8655501
H(5C)       5000       0        0.000000  0.661661  0.088925 -0.166759
8755501
  7.353257
8755501
H(6A)       5000       0        0.000000  0.700278  0.163534 -0.245465
8855501
  7.106849
8855501
H(6B)       5000       0        0.000000  0.594503  0.108714 -0.282116
8955501

  7.106849
8955501
H(6C)       5000       0        0.000000  0.712801  0.090450 -0.305794
9055501
  7.106849
9055501
H(7A)       5000       0        0.000000  0.672885 -0.100603 -0.322509
9155501
  6.222148
9155501
H(7B)       5000       0        0.000000  0.558390 -0.088178 -0.294233
9255501
  6.222148
9255501
H(7C)       5000       0        0.000000  0.651193 -0.152674 -0.271660
9355501
  6.222148
9355501
```

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H(10)       5000       0        0.000000  0.989701 -0.001598 -0.403126
9455501
  3.200759
9455501
H(15)       5000       0        0.000000  0.637630  0.417523 -0.431340
9555501
  4.474964
9555501
H(16)       5000       0        0.000000  0.765422  0.521134 -0.464308
9655501
  4.025797
9655501
H(17)       5000       0        0.000000  0.947536  0.498413 -0.452033
9755501
  3.894327
9755501
H(19)       5000       0        0.000000  1.067776  0.287820 -0.406003
9855501
  4.541831
9855501
H(20A)      5000       0        0.000000  1.106802  0.346077 -0.485693
9955501
 10.320779
9955501
H(20B)      5000       0        0.000000  1.203196  0.385455 -0.439109
10055501
 10.320779
10055501
H(20C)      5000       0        0.000000  1.114147  0.464759 -0.450829
10155501
 10.320779
10155501
H(21A)      5000       0        0.000000  1.091590  0.503407 -0.350280
10255501
  7.898503
10255501
H(21B)      5000       0        0.000000  1.168272  0.413073 -0.340073
10355501
  7.898503
10355501
H(21C)      5000       0        0.000000  1.045339  0.415264 -0.321611
10455501
  7.898503
10455501
H(22)       5000       0        0.000000  0.699569  0.232470 -0.353020
10555501
  5.253243
10555501
H(23A)      5000       0        0.000000  0.574937  0.371932 -0.346322
10655501
  8.990538
10655501
H(23B)      5000       0        0.000000  0.517561  0.260046 -0.348922
10755501
  8.990538
10755501
```

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H(23C)      5000       0        0.000000  0.514455  0.306897 -0.402895
10855501
  8.990538
10855501
H(24A)      5000       0        0.000000  0.610910  0.160517 -0.464514
10955501
  8.572192
10955501
H(24B)      5000       0        0.000000  0.592170  0.101171 -0.416132
11055501
  8.572192
11055501
H(24C)      5000       0        0.000000  0.711595  0.111690 -0.437693
11155501
  8.572192
11155501
H(25A)      5000       0        0.000000  0.883811  0.164750 -0.481825
11255501
  5.547700
11255501
H(25B)      5000       0        0.000000  0.899956  0.044434 -0.482656
11355501
  5.547700
11355501
H(25C)      5000       0        0.000000  1.003968  0.122401 -0.479063
11455501
  5.547700
11455501
H(26A)      5000       0        0.000000  1.024813  0.233474 -0.292507
11555501
  3.623992
11555501
H(26B)      5000       0        0.000000  1.020600  0.168354 -0.245646
11655501
  3.623992
11655501
H(26C)      5000       0        0.000000  0.911274  0.183079 -0.280150
11755501
  3.623992
11755501
H(29)       5000       0        0.000000  1.068424 -0.325540 -0.411157
11855501
  3.265781
11855501
H(30)       5000       0        0.000000  1.232224 -0.293707 -0.447207
11955501
  3.558931
11955501
H(31)       5000       0        0.000000  1.316794 -0.126696 -0.421951
12055501
  3.429360
12055501
H(33)       5000       0        0.000000  1.218833  0.095263 -0.326543
12155501
  3.324437
12155501
```

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H(34A)      5000       0        0.000000  1.302217  0.050503 -0.434803
12255501
  6.252198
12255501
H(34B)      5000       0        0.000000  1.293788  0.165349 -0.396476
12355501
  6.252198
12355501
H(34C)      5000       0        0.000000  1.185288  0.096257 -0.420753
12455501
  6.252198
12455501
H(35A)      5000       0        0.000000  1.377553  0.020100 -0.297625
12555501
  4.748164
12555501
H(35B)      5000       0        0.000000  1.408148  0.122035 -0.319337
12655501
  4.748164
12655501
H(35C)      5000       0        0.000000  1.422837  0.008530 -0.357957
12755501
  4.748164
12755501
H(36)       5000       0        0.000000  0.922333 -0.140828 -0.314417
12855501
  4.204290
12855501
H(37A)      5000       0        0.000000  0.873464 -0.270025 -0.422568
12955501
  7.776422
12955501
H(37B)      5000       0        0.000000  0.859647 -0.146594 -0.405616
13055501
  7.776422
13055501
H(37C)      5000       0        0.000000  0.784123 -0.222688 -0.380128
13155501
  7.776422
13155501
H(38A)      5000       0        0.000000  0.859110 -0.302166 -0.306274
13255501
  6.694994
13255501
H(38B)      5000       0        0.000000  0.987968 -0.295244 -0.292354
13355501
  6.694994
13355501
H(38C)      5000       0        0.000000  0.938471 -0.360522 -0.351480
13455501
  6.694994
13455501
H(42A)      5000       0        0.000000  1.070571 -0.272696 -0.162418
13555501
  3.368572
13555501
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H(42B)      5000       0        0.000000  0.954873 -0.265725 -0.193231
13655501
  3.368572
13655501
H(44A)      5000       0        0.000000  0.836561 -0.093088 -0.080488
13755501
  6.847742
13755501
H(44B)      5000       0        0.000000  0.817802 -0.147931 -0.145011
13855501
  6.847742
13855501
H(44C)      5000       0        0.000000  0.900022 -0.048074 -0.125292
13955501
  6.847742
13955501
H(45A)      5000       0        0.000000  1.081177 -0.062936 -0.081817
14055501
  6.104016
14055501
H(45B)      5000       0        0.000000  1.113221 -0.170090 -0.066644
14155501
  6.104016
14155501
H(45C)      5000       0        0.000000  1.023594 -0.100378 -0.032904
14255501
  6.104016
14255501
H(48A)      5000       0        0.000000  1.300551 -0.156453 -0.287523
14355501
  4.145154
14355501
H(48B)      5000       0        0.000000  1.398171 -0.193415 -0.252646
14455501
  4.145154
14455501
H(48C)      5000       0        0.000000  1.350034 -0.080798 -0.231059
14555501
  4.145154
14555501
H(49A)      5000       0        0.000000  1.161047 -0.341491 -0.230505
14655501
  4.899156
14655501
H(49B)      5000       0        0.000000  1.281525 -0.354961 -0.251960
14755501
  4.899156
14755501
H(49C)      5000       0        0.000000  1.189257 -0.311574 -0.287267
14855501
  4.899156
14855501
H(50A)      5000       0        0.000000  1.311889 -0.123485 -0.139878
14955501
  5.446645
14955501
```

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H(50B)      5000       0        0.000000  1.363673 -0.234362 -0.161552
15055501
  5.446645
15055501
H(50C)      5000       0        0.000000  1.243242 -0.228626 -0.139684
15155501
  5.446645
15155501
H(56)       5000       0        0.000000  1.333188  0.353195  0.022590
15255501
  2.672323
15255501
H(58)       5000       0        0.000000  1.325024  0.504092 -0.099455
15355501

  2.863175
15355501
H(60A)      5000       0        0.000000  0.980916 -0.320856 -0.084300
15455501
  5.738369
15455501
H(60B)      5000       0        0.000000  0.868331 -0.320029 -0.119316
15555501
  5.738369
15555501
H(60C)      5000       0        0.000000  0.883274 -0.254218 -0.056420
15655501
  5.738369
15655501
H(61A)      5000       0        0.000000  1.452745  0.221091 -0.209937
15755501
  4.466918
15755501
H(61B)      5000       0        0.000000  1.529236  0.319075 -0.177754
15855501
  4.466918
15855501
H(61C)      5000       0        0.000000  1.489932  0.308588 -0.241252
15955501
  4.466918
15955501
H(62A)      5000       0        0.000000  1.290376  0.330569 -0.265892
16055501
  4.975580
16055501
H(62B)      5000       0        0.000000  1.207547  0.359402 -0.217489
16155501
  4.975580
16155501
H(62C)      5000       0        0.000000  1.254720  0.245194 -0.232904
16255501
  4.975580
16255501
H(63A)      5000       0        0.000000  1.425715  0.473742 -0.224548
16355501
  5.842206
16355501
```

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H(63B)      5000       0        0.000000  1.450495  0.502372 -0.158803
16455501
  5.842206
16455501
H(63C)      5000       0        0.000000  1.330124  0.511880 -0.184166
16555501
  5.842206
16555501
H(65A)      5000       0        0.000000  1.116018  0.495292 -0.000030
16655501
  7.168176
16655501
H(65B)      5000       0        0.000000  1.149354  0.574024  0.058282
16755501
  7.168176
16755501
H(65C)      5000       0        0.000000  1.179813  0.454195  0.047887
16855501
  7.168176
16855501
H(66A)      5000       0        0.000000  1.340345  0.632170  0.084053
16955501
  6.444342
16955501
H(66B)      5000       0        0.000000  1.433728  0.596809  0.041855
17055501
  6.444342
17055501
H(66C)      5000       0        0.000000  1.381089  0.515471  0.073102
17155501
  6.444342
17155501
H(67A)      5000       0        0.000000  1.205119  0.613545 -0.048295
17255501
  6.834413
17255501
H(67B)      5000       0        0.000000  1.330591  0.650526 -0.034067
17355501
  6.834413
17355501
H(67C)      5000       0        0.000000  1.241242  0.693330  0.009307
17455501
  6.834413
17455501
H(69A)      5000       0        0.000000  1.329372  0.017496 -0.020709
17555501
  4.185990
17555501
H(69B)      5000       0        0.000000  1.271570  0.052972 -0.072066
17655501
  4.185990
17655501
H(69C)      5000       0        0.000000  1.238614  0.103115 -0.010340
17755501
  4.185990
17755501
```

```
H(70A)      5000       0        0.000000  1.518168  0.064564 -0.039341
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  4.153425
17855501
H(70B)      5000       0        0.000000  1.545231  0.173829 -0.054537
17955501
  4.153425
17955501
H(70C)      5000       0        0.000000  1.469408  0.086207 -0.096337
18055501
  4.153425
18055501
H(71A)      5000       0        0.000000  1.358540  0.220554  0.054882
18155501
  4.893833
18155501
H(71B)      5000       0        0.000000  1.475425  0.258526  0.039398
18255501
  4.893833
18255501
H(71C)      5000       0        0.000000  1.455897  0.141748  0.046371
18355501
  4.893833
18355501
H(73A)      5000       0        0.000000  0.877837  0.194256 -0.169238
18455501
  4.166816
18455501
H(73B)      5000       0        0.000000  0.864597  0.246889 -0.105184
18555501
  4.166816
18555501
H(73C)      5000       0        0.000000  0.876513  0.123481 -0.124900
18655501
  4.166816
18655501
H(74A)      5000       0        0.000000  1.034899  0.134336 -0.056691
18755501
  4.312580
18755501
H(74B)      5000       0        0.000000  1.020219  0.257300 -0.036749
18855501
  4.312580
18855501
H(74C)      5000       0        0.000000  1.135487  0.214542 -0.056574
18955501
  4.312580
18955501
H(75A)      5000       0        0.000000  1.138334  0.320137 -0.128395
19055501
  3.991631
19055501
H(75B)      5000       0        0.000000  1.026499  0.368195 -0.106396
19155501
  3.991631
19155501
```

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H(75C)      5000       0        0.000000  1.034540  0.313985 -0.170668
19255501
  3.991631
19255501
H(76A)      5000       0        0.000000  1.536866 -0.120317 -0.438149
19355501
 13.694830
19355501
H(76B)      5000       0        0.000000  1.592489 -0.154877 -0.496105
19455501
 13.694830
19455501
H(76C)      5000       0        0.000000  1.658994 -0.158847 -0.439679
19555501
 13.694830
19555501
H(77A)      5000       0        0.000000  1.601692 -0.324822 -0.480868
19655501
 10.987609
19655501
H(77B)      5000       0        0.000000  1.480844 -0.290317 -0.491541
19755501
 10.987609
19755501
H(78A)      5000       0        0.000000  1.578882 -0.299515 -0.387386
19855501
  7.786448
19855501
H(86)       5000       0        0.000000  1.463003 -0.251310 -0.393913
19955501
  7.786448
19955501
H(79A)      5000       0        0.000000  1.508488 -0.461918 -0.436343
20055501
  8.818871
20055501
H(79B)      5000       0        0.000000  1.392501 -0.413729 -0.443088
20155501
  8.818871
20155501
H(80A)      5000       0        0.000000  1.492839 -0.440761 -0.341817
20255501
 15.387534
20255501
H(80B)      5000       0        0.000000  1.382371 -0.498554 -0.372194
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 15.387534
20355501
H(80C)      5000       0        0.000000  1.385075 -0.376456 -0.343571
20455501
 15.387534
20455501
H(81A)      5000       0        0.000000  1.895135  0.411095 -0.225688
20555501
 20.595890
20555501
```

```
H(81B)      5000       0        0.000000  1.793501  0.347667 -0.262436
20655501
 20.595890
20655501
H(81C)      5000       0        0.000000  1.778504  0.409504 -0.199927
20755501
 20.595890
20755501
H(82A)      5000       0        0.000000  1.769394  0.471412 -0.291021
20855501
 18.947748
20855501
H(82B)      5000       0        0.000000  1.858361  0.539095 -0.247249
20955501
 18.947748
20955501
H(83A)      5000       0        0.000000  1.643707  0.504521 -0.231247
21055501
 14.595962
21055501
H(83B)      5000       0        0.000000  1.730083  0.562855 -0.184049
21155501
 14.595962
21155501
H(84A)      5000       0        0.000000  1.653939  0.636646 -0.270727
21255501
 16.085403
21255501
H(84B)      5000       0        0.000000  1.739448  0.695359 -0.222493
21355501
 16.085403
21355501
H(85A)      5000       0        0.000000  1.518615  0.655562 -0.214756
21455501
 15.324339
21455501
H(85B)      5000       0        0.000000  1.584747  0.765939 -0.201237
21555501
 15.324339
21555501
H(85C)      5000       0        0.000000  1.599777  0.688574 -0.160657
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 15.324339
21655501
         1000000
    0.2697
0.0000E+00
```

Figure 1: VERSORT Drawing(s)

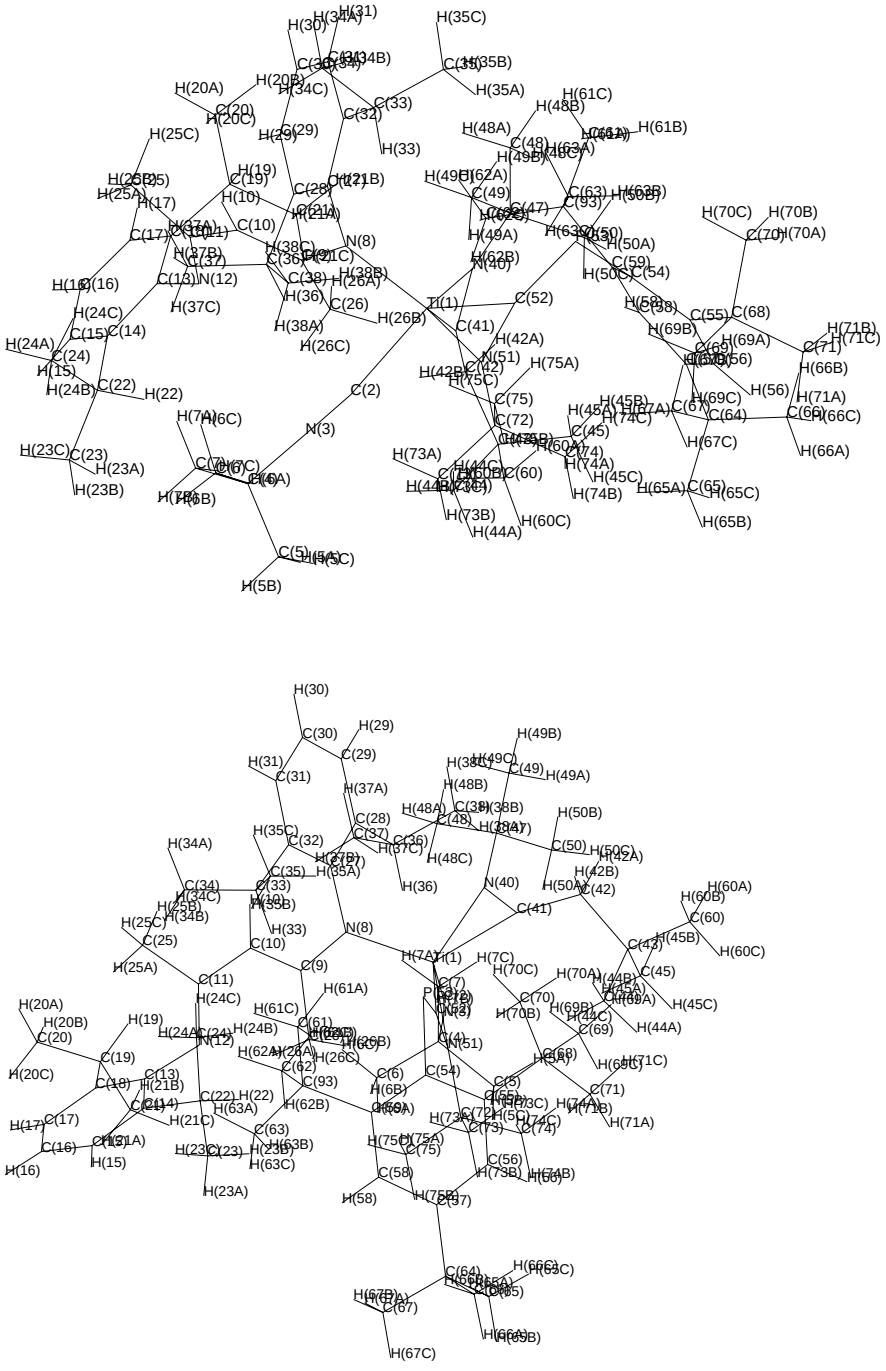
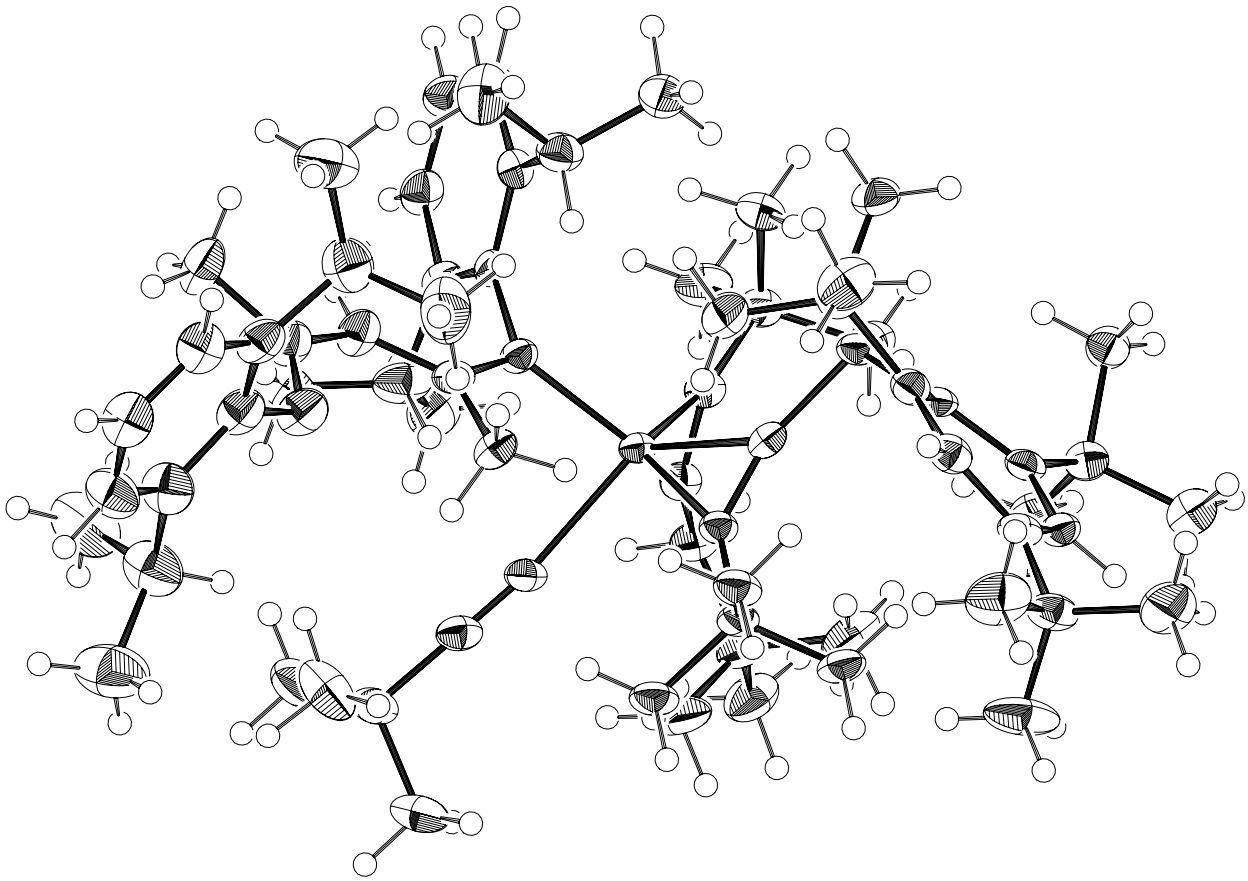


Figure 2: ORTEP Drawing(s)



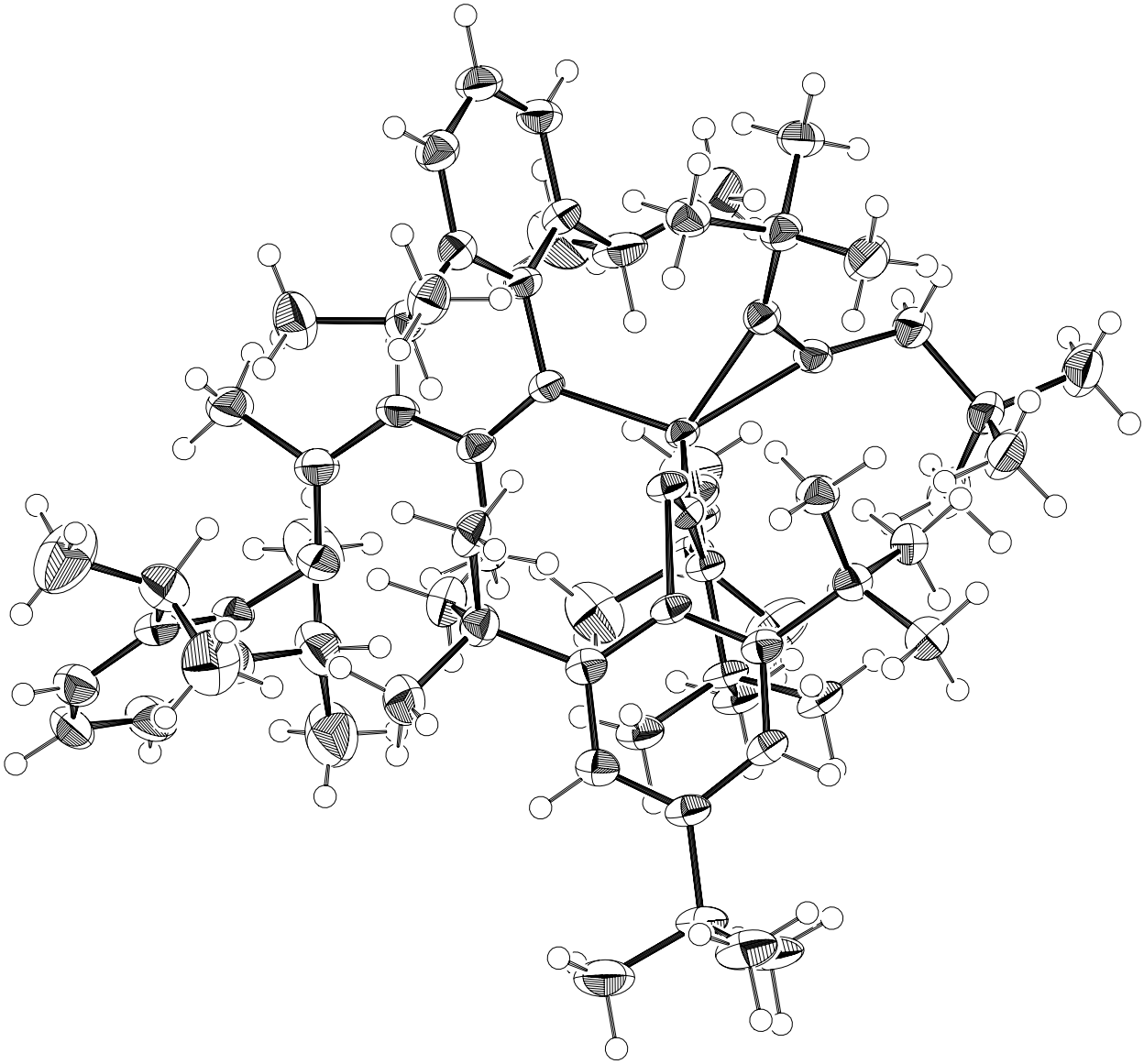
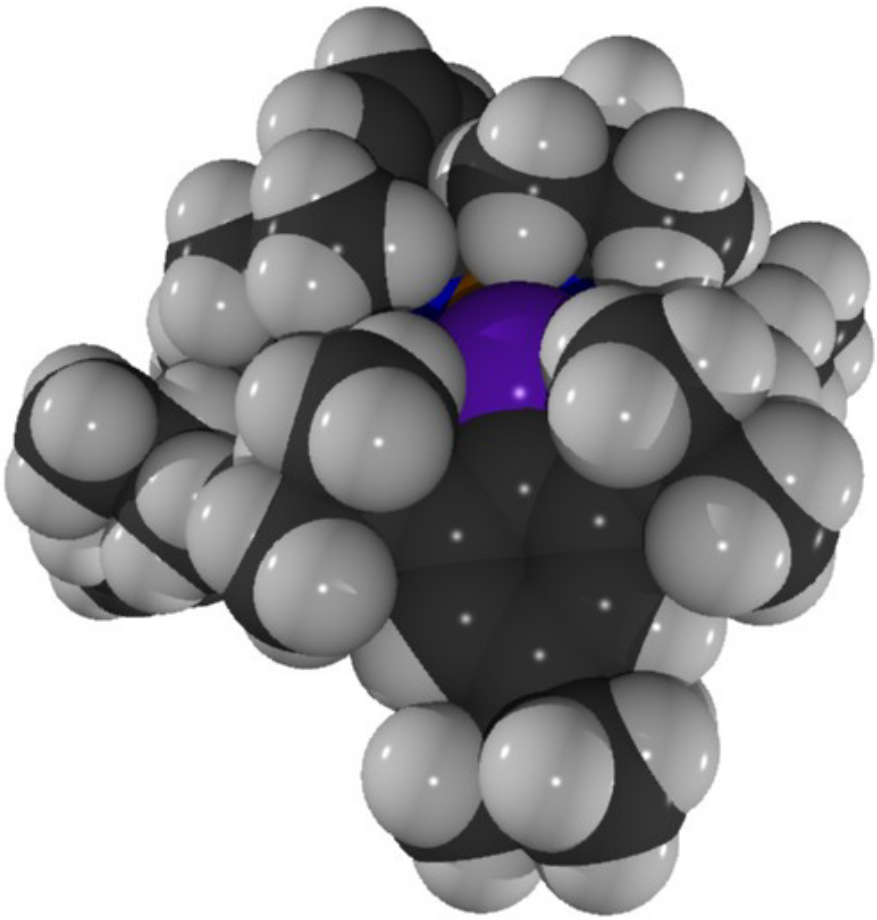


Figure 3: Space Filling Model Drawing(s)



Crystallographic data for complex (Nacnac)Ti=N[P(CH_2^{t}Bu)(Mes*)](N=CPh_2) (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 a dark red crystal of approximate dimensions 0.25 × 0.25 × 0.25 mm onto the tip of a 0.15 mm diameter glass fiber which was subsequently mounted on a SMART6000 (Bruker) and cooled to 115(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. Two sections of 606 frames were collected with 0.30º 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 727 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 P1bar 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. There is some disorder present in the molecule. The major discrepancy appears to be a "flip" of the phosphorous with an approximate ratio of 84:16. This leads to disorder in several other parts of the molecule. In addition, there is a rotational disorder about C(8)-C(16) so that the two methyl groups of the iPr ligand having alternate positions. 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. Several of those associated with the disorder tended to drift to unreasonable positions and were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters.

The final full matrix least squares refinement converged to R1 = 0.0646 and wR2 = 0.1530 (F^2, 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

MSC03117

The following were used

At.No.	At.Wt.	Abs.	%	No.	Element
22	47.880	23.400	4.75	1	Ti
15	30.974	7.970	3.07	1	P
7	14.007	.845	5.56	4	N
6	12.011	.576	77.50	65	C
1	1.008	.373	9.11	91	H

The density is 1.125 g/cc.

The volume is 2974.12 cubic Angstroms

Z = 2 and the molecular wt. is 1007.32

F(000) = 1092

The linear absorption coefficient = 2.120 reciprocal centimeters,

and 1/4Mu = 1.1792 mm.

Table 2

Crystal Data for MSC Sample 03117

Empirical Formula	C65H91N4PTi

Color of Crystal:	deep red
Crystal Dimensions were:	0.25 x 0.25 x 0.25 mm.
Space Group:	P-1

Cell Dimensions (at 115(2) K; 727 reflections)

a =	11.696(2)
b =	13.078(4)
c =	20.218(4)
alpha =	81.562(6)
beta =	78.932(5)
gamma =	80.736(5)

Z (Molecules/cell):	2
Volume:	2974.1(11)
Calculated Density:	1.125
Wavelength:	0.71073
Molecular Weight:	1007.29
F(000):	1092
Linear Absorption Coefficient:	0.212

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 =	12447
Number of unique intensities =	11628
Number with F > 4sigma(F) =	6497
R for averaging =	0.053

Refinement results:

Final residuals are:
R(F) (observed data) = 0.0624
Rw(F2) (refinement data) = 0.1530

Final Goodness of Fit = 0.915
Maximum delta/sigma for the last cycle = 2.50

Table 3: Fractional Coordinates and Isotropic Thermal Parameters for MSC Sample 03117

Atom	x	y	z	Uiso
Ti(1)	3117(1)	1967(1)	7078(1)	18(1)
N(2)	2906(2)	581(2)	7666(1)	19(1)
C(3)	3784(3)	-123(3)	7410(2)	22(1)
C(4)	4880(3)	128(3)	7052(2)	23(1)
C(5)	5420(3)	1032(3)	7019(2)	22(1)
N(6)	4819(2)	1927(2)	7205(1)	18(1)
C(7)	1949(3)	204(3)	8153(2)	22(1)
C(8)	864(3)	189(3)	7956(2)	28(1)
C(9)	-18(3)	-219(3)	8438(2)	36(1)
C(10)	152(3)	-594(3)	9094(2)	35(1)
C(11)	1208(3)	-539(3)	9282(2)	29(1)
C(12)	2124(3)	-141(3)	8821(2)	23(1)
C(13)	3254(3)	-85(3)	9068(2)	26(1)
C(14)	3047(4)	620(4)	9624(2)	40(1)
C(15)	3831(4)	-1158(4)	9329(3)	51(1)
C(16)	616(3)	586(3)	7248(2)	35(1)
C(17)	-451(5)	1520(5)	7280(3)	29(1)
C(18)	345(6)	-246(5)	6897(3)	45(2)
C(19)	3637(4)	-1257(3)	7510(2)	40(1)
C(20)	6722(3)	943(4)	6748(2)	32(1)
C(21)	5438(3)	2772(3)	7274(2)	21(1)
C(22)	5792(3)	3478(3)	6706(2)	23(1)
C(23)	6420(3)	4256(3)	6795(2)	33(1)
C(24)	6686(3)	4334(3)	7423(2)	40(1)
C(25)	6295(3)	3654(3)	7972(2)	36(1)
C(26)	5671(3)	2864(3)	7917(2)	26(1)
C(27)	5253(3)	2124(3)	8536(2)	30(1)
C(28)	4966(5)	2647(4)	9191(2)	44(1)
C(29)	6142(4)	1153(4)	8613(2)	44(1)
C(30)	5477(3)	3448(3)	6016(2)	24(1)
C(31)	4435(3)	4265(3)	5903(2)	31(1)
C(32)	6513(4)	3581(4)	5434(2)	34(1)
N(33)	3046(2)	1955(2)	6140(1)	22(1)
C(34)	3074(3)	1872(3)	5521(2)	23(1)
C(35)	4166(3)	1955(3)	5003(2)	24(1)
C(36)	4158(3)	2670(3)	4424(2)	30(1)
C(37)	5179(4)	2777(3)	3962(2)	38(1)
C(38)	6216(4)	2152(3)	4063(2)	42(1)
C(39)	6230(4)	1421(3)	4625(2)	38(1)

C(40)	5215(3)	1335(3)	5100(2)	29(1)
C(41)	2011(3)	1698(3)	5255(2)	24(1)
C(42)	2119(3)	1165(3)	4693(2)	30(1)
C(43)	1127(4)	993(3)	4470(2)	39(1)
C(44)	32(4)	1373(3)	4784(2)	40(1)
C(45)	-89(3)	1912(3)	5338(2)	37(1)
C(46)	899(3)	2066(3)	5577(2)	28(1)
N(47)	2277(2)	3043(2)	7414(1)	23(1)
P(48)	1845(1)	4322(1)	7507(1)	20(1)
C(49)	2416(3)	4497(3)	8277(2)	38(1)
C(50)	2683(3)	5597(3)	8307(2)	33(1)
C(51)	3160(5)	5568(4)	8966(3)	54(1)
C(52)	3613(5)	5908(4)	7710(3)	56(1)
C(53)	1579(4)	6386(4)	8326(3)	45(1)
C(54)	221(3)	4624(3)	7798(2)	26(1)
C(55)	-438(3)	4449(3)	8464(2)	25(1)
C(56)	-1376(3)	5200(3)	8675(2)	25(1)
C(57)	-1729(3)	6082(3)	8261(2)	27(1)
C(58)	-1208(3)	6147(3)	7580(2)	28(1)
C(59)	-273(3)	5423(3)	7331(2)	25(1)
C(60)	-297(3)	3459(3)	8989(2)	32(1)
C(61)	652(3)	2586(3)	8747(2)	41(1)
C(62)	-43(4)	3706(4)	9664(2)	45(1)
C(63)	-1456(3)	3020(3)	9131(2)	47(1)
C(64)	-2699(3)	6929(3)	8541(2)	34(1)
C(65)	-2276(4)	7411(4)	9073(3)	63(1)
C(66)	-3793(4)	6417(4)	8888(3)	72(2)
C(67)	-3039(5)	7779(4)	8002(2)	77(2)
C(68)	140(3)	5549(3)	6545(2)	35(1)
C(69)	1067(4)	6296(4)	6318(2)	42(1)
C(70)	526(5)	4499(4)	6276(2)	52(1)
C(71)	-912(4)	6043(5)	6178(2)	51(1)
C(17A)	-517(12)	925(12)	7204(7)	55(3)
C(18A)	1180(14)	-333(13)	6736(8)	68(4)
P(48A)	1720(6)	3805(6)	8013(3)	43(2)
H(86)	-114	128	758	43
H(85)	-64	174	682	43
H(84)	-23	211	745	43
H(87)	96	-85	692	68
H(89)	30	2	642	68
H(88)	-41	-46	712	68
H(138)	56	194	906	61
H(137)	143	278	874	61
H(136)	58	247	829	61
H(142)	-165	289	870	71
H(143)	-208	352	935	71
H(144)	-139	237	944	71
H(145)	-159	775	886	95
H(147)	-207	686	943	95
H(146)	-290	793	927	95
H(149)	-440	694	909	107
H(148)	-358	586	924	107
H(150)	-410	612	855	107
H(151)	-361	832	821	115
H(152)	-338	749	768	115
H(153)	-234	809	776	115

H(72)	539(2)	-43(2)	688(1)	9(7)
H(73)	-73(3)	-19(3)	831(2)	30(10)
H(74)	-44(3)	-88(3)	937(2)	33(10)
H(75)	138(2)	-79(2)	973(2)	11(7)
H(76)	379(3)	15(2)	873(2)	19(8)
H(77)	269(3)	130(3)	944(2)	41(12)
H(78)	253(3)	34(3)	1002(2)	38(11)
H(79)	377(4)	62(3)	976(2)	50(12)
H(80)	455(3)	-109(3)	944(2)	34(10)
H(81)	332(4)	-145(4)	970(3)	76(17)
H(82)	399(4)	-164(3)	896(2)	58(13)
H(83)	127(3)	91(3)	703(2)	26(9)
H(90)	361(5)	-159(4)	803(3)	100(18)
H(91)	292(4)	-132(4)	738(2)	73(16)
H(92)	420(3)	-168(3)	723(2)	41(11)
H(93)	709(4)	27(4)	678(2)	54(14)
H(94)	681(3)	116(3)	633(2)	35(11)
H(95)	710(3)	139(3)	697(2)	43(11)
H(96)	660(3)	470(3)	643(2)	21(9)
H(97)	712(3)	489(3)	747(2)	48(12)
H(98)	641(3)	377(3)	838(2)	47(12)
H(99)	454(3)	193(2)	847(1)	7(7)
H(100)	462(4)	223(3)	955(2)	52(13)
H(101)	439(5)	337(4)	922(3)	96(19)
H(102)	578(4)	280(3)	928(2)	60(13)
H(103)	689(3)	135(3)	867(2)	25(9)
H(104)	592(3)	65(3)	898(2)	48(12)
H(105)	628(3)	76(3)	824(2)	29(10)
H(106)	531(3)	273(3)	600(2)	23(9)
H(107)	417(3)	417(3)	549(2)	25(9)
H(108)	376(3)	418(3)	629(2)	40(11)
H(109)	461(3)	493(3)	587(2)	31(10)
H(110)	676(4)	425(4)	543(2)	58(13)
H(111)	629(3)	350(3)	499(2)	40(11)
H(112)	716(4)	307(3)	550(2)	54(14)
H(113)	342(3)	312(2)	433(2)	16(8)
H(114)	515(3)	323(3)	360(2)	37(11)
H(115)	687(3)	220(3)	380(2)	43(12)
H(116)	689(3)	102(3)	470(2)	19(9)
H(117)	519(3)	83(2)	549(2)	17(8)
H(118)	296(4)	89(3)	442(2)	52(12)
H(119)	121(3)	56(3)	409(2)	41(11)
H(120)	-67(3)	129(3)	465(2)	40(11)
H(121)	-82(3)	220(2)	555(2)	12(8)
H(122)	79(3)	247(3)	594(2)	22(9)
H(123)	184(3)	429(3)	878(2)	35(10)
H(124)	330(4)	400(4)	821(2)	71(14)
H(125)	260(4)	526(4)	941(2)	80(16)
H(126)	335(5)	637(5)	903(3)	130(20)
H(127)	392(4)	498(4)	897(2)	80(16)
H(128)	439(5)	533(5)	771(3)	110(20)
H(129)	312(5)	614(4)	724(3)	107(19)
H(130)	379(3)	651(3)	791(2)	48(12)
H(131)	128(4)	646(3)	788(2)	62(14)
H(132)	96(4)	617(4)	863(2)	78(17)
H(133)	170(3)	708(3)	846(2)	20(8)
H(134)	-175(3)	513(3)	912(2)	38(11)

H(135)	-151(3)	671(3)	727(2)	22(9)
H(139)	74(4)	409(3)	963(2)	58(13)
H(140)	-79(4)	432(4)	989(2)	84(16)
H(141)	2(3)	299(3)	1000(2)	44(11)
H(154)	125(3)	642(3)	581(2)	50(12)
H(155)	75(4)	702(4)	652(2)	63(14)
H(156)	179(4)	599(3)	653(2)	60(13)
H(157)	131(2)	432(2)	644(1)	0(7)
H(158)	76(4)	462(3)	573(2)	57(12)
H(159)	-31(4)	406(4)	644(2)	89(17)
H(160)	-65(4)	596(3)	565(2)	67(14)
H(161)	-155(4)	565(4)	635(2)	66(14)
H(162)	-118(4)	685(4)	627(2)	70(15)

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 03117

Atom	U11	U22	U33	U23	U13	U12
Ti(1)	15(1)	21(1)	16(1)	-1(1)	-3(1)	-2(1)
N(2)	20(1)	22(2)	16(1)	-1(1)	-3(1)	-4(1)
C(3)	25(2)	23(2)	19(2)	0(1)	-6(1)	-3(2)
C(4)	23(2)	20(2)	22(2)	-2(2)	-2(1)	7(2)
C(5)	19(2)	27(2)	18(2)	0(2)	-4(1)	0(2)
N(6)	17(1)	22(2)	15(1)	1(1)	-4(1)	-2(1)
C(7)	22(2)	20(2)	21(2)	-1(1)	2(1)	-5(2)
C(8)	23(2)	35(2)	25(2)	-4(2)	-1(1)	-8(2)
C(9)	27(2)	49(3)	36(2)	-3(2)	-4(2)	-17(2)
C(10)	31(2)	37(2)	32(2)	3(2)	6(2)	-14(2)
C(11)	33(2)	29(2)	20(2)	2(2)	2(2)	-6(2)
C(12)	24(2)	18(2)	24(2)	-3(1)	0(1)	-1(2)
C(13)	25(2)	33(2)	16(2)	5(2)	-3(1)	0(2)
C(14)	36(2)	52(3)	37(2)	-9(2)	-14(2)	-2(2)
C(15)	40(3)	53(3)	60(3)	-8(3)	-19(2)	8(3)
C(16)	29(2)	54(3)	27(2)	2(2)	-8(2)	-17(2)
C(19)	51(3)	27(2)	38(2)	-13(2)	10(2)	-9(2)
C(20)	20(2)	40(3)	34(2)	-4(2)	-2(2)	1(2)
C(21)	15(2)	27(2)	22(2)	-2(1)	-5(1)	-2(2)
C(22)	19(2)	27(2)	24(2)	-1(2)	-4(1)	-5(2)
C(23)	36(2)	34(2)	30(2)	3(2)	-5(2)	-16(2)
C(24)	41(2)	47(3)	38(2)	-8(2)	-10(2)	-23(2)
C(25)	40(2)	47(3)	28(2)	-6(2)	-15(2)	-15(2)
C(26)	25(2)	30(2)	26(2)	-4(2)	-9(1)	-7(2)
C(27)	32(2)	35(2)	26(2)	3(2)	-13(2)	-9(2)
C(28)	58(3)	54(3)	25(2)	-3(2)	-9(2)	-17(3)
C(29)	51(3)	50(3)	34(2)	1(2)	-13(2)	-14(2)
C(30)	27(2)	23(2)	22(2)	2(2)	-2(1)	-8(2)
C(31)	33(2)	32(2)	27(2)	-2(2)	-5(2)	-5(2)
C(32)	31(2)	44(3)	26(2)	-4(2)	2(2)	-8(2)

N(33)	23(1)	22(2)	20(1)	0(1)	-5(1)	0(1)
C(34)	27(2)	18(2)	21(2)	0(1)	-6(1)	0(2)
C(35)	28(2)	26(2)	18(2)	-4(1)	0(1)	-8(2)
C(36)	38(2)	30(2)	21(2)	-1(2)	-4(2)	-5(2)
C(37)	54(3)	36(3)	22(2)	-6(2)	3(2)	-14(2)
C(38)	40(2)	52(3)	35(2)	-16(2)	12(2)	-22(2)
C(39)	31(2)	42(3)	41(2)	-15(2)	0(2)	-1(2)
C(40)	34(2)	26(2)	27(2)	-4(2)	-6(2)	-3(2)
C(41)	29(2)	23(2)	20(2)	2(1)	-7(1)	-5(2)
C(42)	35(2)	29(2)	28(2)	-3(2)	-10(2)	-4(2)
C(43)	49(2)	38(3)	36(2)	-9(2)	-18(2)	-11(2)
C(44)	40(2)	41(3)	44(2)	7(2)	-26(2)	-14(2)
C(45)	25(2)	43(3)	40(2)	2(2)	-7(2)	-1(2)
C(46)	27(2)	29(2)	27(2)	0(2)	-8(2)	-2(2)
N(47)	20(1)	26(2)	22(1)	-4(1)	-2(1)	0(1)
P(48)	18(1)	18(1)	20(1)	2(1)	2(1)	-1(1)
C(49)	33(2)	39(3)	44(2)	-11(2)	-6(2)	-7(2)
C(50)	35(2)	33(2)	34(2)	-6(2)	-3(2)	-12(2)
C(51)	51(3)	61(3)	52(3)	-9(3)	-8(2)	-11(3)
C(52)	51(3)	52(3)	61(3)	0(3)	4(3)	-19(3)
C(53)	41(2)	36(3)	61(3)	-17(2)	-6(2)	-7(2)
C(54)	24(2)	24(2)	31(2)	-10(2)	1(2)	-3(2)
C(55)	23(2)	22(2)	30(2)	-4(2)	-10(1)	1(2)
C(56)	22(2)	26(2)	25(2)	-3(2)	-4(2)	0(2)
C(57)	21(2)	26(2)	37(2)	-11(2)	-5(2)	-2(2)
C(58)	28(2)	22(2)	34(2)	-1(2)	-10(2)	-4(2)
C(59)	23(2)	23(2)	29(2)	3(2)	-2(2)	-8(2)
C(60)	31(2)	31(2)	29(2)	1(2)	-5(2)	3(2)
C(61)	42(2)	37(2)	36(2)	6(2)	-1(2)	-3(2)
C(62)	51(3)	60(3)	25(2)	3(2)	-9(2)	-12(3)
C(63)	43(2)	36(3)	61(3)	14(2)	-14(2)	-11(2)
C(64)	26(2)	28(2)	45(2)	-10(2)	-6(2)	8(2)
C(65)	55(3)	53(3)	88(4)	-41(3)	-19(3)	14(2)
C(66)	34(2)	58(3)	114(4)	-26(3)	8(3)	9(2)
C(67)	85(4)	67(4)	62(3)	-13(3)	-12(3)	41(3)
C(68)	39(2)	34(2)	28(2)	2(2)	2(2)	-5(2)
C(69)	38(2)	43(3)	41(2)	10(2)	-5(2)	-7(2)
C(70)	63(3)	60(3)	33(2)	-8(2)	-7(2)	-7(3)
C(71)	45(3)	73(4)	34(2)	-2(2)	-4(2)	-16(3)
P(48A)	41(4)	43(4)	42(4)	-2(3)	-1(3)	-5(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 03117

A	B	Distance
Ti(1)	N(47)	1.727(3)
Ti(1)	N(33)	1.918(3)
Ti(1)	N(2)	2.039(3)
Ti(1)	N(6)	2.048(3)
N(2)	C(3)	1.343(4)
N(2)	C(7)	1.441(4)
C(3)	C(4)	1.409(4)

C(3)	C(19)	1.500(5)
C(4)	C(5)	1.415(5)
C(4)	H(72)	0.93(3)
C(5)	N(6)	1.330(4)
C(5)	C(20)	1.508(5)
N(6)	C(21)	1.450(4)
C(7)	C(12)	1.403(4)
C(7)	C(8)	1.405(4)
C(8)	C(9)	1.391(5)
C(8)	C(16)	1.516(5)
C(9)	C(10)	1.385(5)
C(9)	H(73)	0.91(3)
C(10)	C(11)	1.374(5)
C(10)	H(74)	0.90(3)
C(11)	C(12)	1.393(4)
C(11)	H(75)	0.97(3)
C(12)	C(13)	1.515(5)
C(13)	C(14)	1.518(5)
C(13)	C(15)	1.522(6)
C(13)	H(76)	0.90(3)
C(14)	H(77)	0.97(4)
C(14)	H(78)	0.97(4)
C(14)	H(79)	0.94(4)
C(15)	H(80)	0.94(4)
C(15)	H(81)	0.94(5)
C(15)	H(82)	1.01(5)
C(16)	C(18)	1.488(7)
C(16)	C(17)	1.598(7)
C(16)	H(83)	0.93(3)
C(17)	H(86)	0.9800
C(17)	H(85)	0.9800
C(17)	H(84)	0.9800
C(18)	H(87)	0.9800
C(18)	H(89)	0.9800
C(18)	H(88)	0.9800
C(19)	H(90)	1.07(6)
C(19)	H(91)	0.95(5)
C(19)	H(92)	0.94(4)
C(20)	H(93)	0.91(4)
C(20)	H(94)	0.85(4)
C(20)	H(95)	0.98(4)
C(21)	C(22)	1.404(4)
C(21)	C(26)	1.405(4)
C(22)	C(23)	1.396(5)
C(22)	C(30)	1.518(4)
C(23)	C(24)	1.387(5)
C(23)	H(96)	0.88(3)
C(24)	C(25)	1.371(5)
C(24)	H(97)	0.98(4)
C(25)	C(26)	1.385(5)
C(25)	H(98)	0.89(4)
C(26)	C(27)	1.518(5)
C(27)	C(29)	1.515(6)
C(27)	C(28)	1.535(5)
C(27)	H(99)	0.94(3)
C(28)	H(100)	0.91(4)
C(28)	H(101)	1.08(6)

C(28)	H(102)	1.06(4)
C(29)	H(103)	0.98(3)
C(29)	H(104)	0.95(4)
C(29)	H(105)	0.96(4)
C(30)	C(31)	1.514(5)
C(30)	C(32)	1.530(5)
C(30)	H(106)	0.99(3)
C(31)	H(107)	0.97(3)
C(31)	H(108)	1.00(4)
C(31)	H(109)	0.92(4)
C(32)	H(110)	0.96(5)
C(32)	H(111)	1.01(4)
C(32)	H(112)	0.94(4)
N(33)	C(34)	1.264(4)
C(34)	C(35)	1.496(4)
C(34)	C(41)	1.509(4)
C(35)	C(36)	1.388(5)
C(35)	C(40)	1.388(5)
C(36)	C(37)	1.379(5)
C(36)	H(113)	0.99(3)
C(37)	C(38)	1.382(6)
C(37)	H(114)	0.88(4)
C(38)	C(39)	1.373(6)
C(38)	H(115)	0.85(4)
C(39)	C(40)	1.385(5)
C(39)	H(116)	0.89(3)
C(40)	H(117)	0.95(3)
C(41)	C(46)	1.383(5)
C(41)	C(42)	1.393(5)
C(42)	C(43)	1.383(5)
C(42)	H(118)	1.07(4)
C(43)	C(44)	1.367(6)
C(43)	H(119)	1.00(4)
C(44)	C(45)	1.382(6)
C(44)	H(120)	0.94(4)
C(45)	C(46)	1.389(5)
C(45)	H(121)	0.93(3)
C(46)	H(122)	0.94(3)
N(47)	P(48)	1.695(3)
P(48)	C(49)	1.865(4)
P(48)	C(54)	1.872(3)
C(49)	C(50)	1.532(5)
C(49)	H(123)	1.12(3)
C(49)	H(124)	1.12(5)
C(50)	C(53)	1.516(6)
C(50)	C(52)	1.516(5)
C(50)	C(51)	1.532(6)
C(51)	H(125)	1.08(5)
C(51)	H(126)	1.14(7)
C(51)	H(127)	1.08(5)
C(52)	H(128)	1.08(6)
C(52)	H(129)	1.18(6)
C(52)	H(130)	1.00(4)
C(53)	H(131)	1.02(5)
C(53)	H(132)	0.91(5)
C(53)	H(133)	1.02(3)
C(54)	C(55)	1.425(4)

C(54)	C(59)	1.429(5)
C(55)	C(56)	1.395(5)
C(55)	C(60)	1.557(5)
C(56)	C(57)	1.377(5)
C(56)	H(134)	0.92(4)
C(57)	C(58)	1.392(5)
C(57)	C(64)	1.538(5)
C(58)	C(59)	1.393(5)
C(58)	H(135)	0.97(3)
C(59)	C(68)	1.562(5)
C(60)	C(63)	1.517(5)
C(60)	C(61)	1.523(5)
C(60)	C(62)	1.541(5)
C(61)	H(138)	0.9800
C(61)	H(137)	0.9800
C(61)	H(136)	0.9800
C(62)	H(139)	1.10(4)
C(62)	H(140)	1.17(5)
C(62)	H(141)	1.08(4)
C(63)	H(142)	0.9800
C(63)	H(143)	0.9800
C(63)	H(144)	0.9800
C(64)	C(67)	1.500(6)
C(64)	C(65)	1.517(6)
C(64)	C(66)	1.541(6)
C(65)	H(145)	0.9800
C(65)	H(147)	0.9800
C(65)	H(146)	0.9800
C(66)	H(149)	0.9800
C(66)	H(148)	0.9800
C(66)	H(150)	0.9800
C(67)	H(151)	0.9800
C(67)	H(152)	0.9800
C(67)	H(153)	0.9800
C(68)	C(70)	1.519(6)
C(68)	C(69)	1.536(5)
C(68)	C(71)	1.562(6)
C(69)	H(154)	1.01(4)
C(69)	H(155)	1.07(5)
C(69)	H(156)	1.02(4)
C(70)	H(157)	1.01(3)
C(70)	H(158)	1.08(4)
C(70)	H(159)	1.18(5)
C(71)	H(160)	1.07(5)
C(71)	H(161)	0.95(5)
C(71)	H(162)	1.09(5)
P(48A)	H(123)	1.78(4)

Symmetry transformations used to generate equivalent atoms:

Table 5b: Bond Angles for MSC Sample 03117

A	B	C	Angle
N(47)	Ti(1)	N(33)	112.97(12)

N(47)	Ti(1)	N(2)	114.50(11)
N(33)	Ti(1)	N(2)	114.30(11)
N(47)	Ti(1)	N(6)	108.72(12)
N(33)	Ti(1)	N(6)	110.46(10)
N(2)	Ti(1)	N(6)	94.18(10)
C(3)	N(2)	C(7)	118.1(3)
C(3)	N(2)	Ti(1)	106.4(2)
C(7)	N(2)	Ti(1)	133.9(2)
N(2)	C(3)	C(4)	123.9(3)
N(2)	C(3)	C(19)	120.0(3)
C(4)	C(3)	C(19)	116.1(3)
C(3)	C(4)	C(5)	130.3(3)
C(3)	C(4)	H(72)	115.0(18)
C(5)	C(4)	H(72)	113.4(18)
N(6)	C(5)	C(4)	122.4(3)
N(6)	C(5)	C(20)	120.8(3)
C(4)	C(5)	C(20)	116.7(3)
C(5)	N(6)	C(21)	120.1(3)
C(5)	N(6)	Ti(1)	107.8(2)
C(21)	N(6)	Ti(1)	129.7(2)
C(12)	C(7)	C(8)	121.1(3)
C(12)	C(7)	N(2)	118.8(3)
C(8)	C(7)	N(2)	120.1(3)
C(9)	C(8)	C(7)	117.9(3)
C(9)	C(8)	C(16)	118.9(3)
C(7)	C(8)	C(16)	123.2(3)
C(10)	C(9)	C(8)	121.7(3)
C(10)	C(9)	H(73)	121(2)
C(8)	C(9)	H(73)	117(2)
C(11)	C(10)	C(9)	119.4(3)
C(11)	C(10)	H(74)	123(2)
C(9)	C(10)	H(74)	117(2)
C(10)	C(11)	C(12)	121.5(3)
C(10)	C(11)	H(75)	123.1(17)
C(12)	C(11)	H(75)	115.4(17)
C(11)	C(12)	C(7)	118.3(3)
C(11)	C(12)	C(13)	118.5(3)
C(7)	C(12)	C(13)	123.1(3)
C(12)	C(13)	C(14)	111.5(3)
C(12)	C(13)	C(15)	112.0(3)
C(14)	C(13)	C(15)	108.9(3)
C(12)	C(13)	H(76)	111(2)
C(14)	C(13)	H(76)	109(2)
C(15)	C(13)	H(76)	105(2)
C(13)	C(14)	H(77)	107(2)
C(13)	C(14)	H(78)	110(2)
H(77)	C(14)	H(78)	110(3)
C(13)	C(14)	H(79)	108(3)
H(77)	C(14)	H(79)	115(3)
H(78)	C(14)	H(79)	106(3)
C(13)	C(15)	H(80)	109(2)
C(13)	C(15)	H(81)	110(3)
H(80)	C(15)	H(81)	112(4)
C(13)	C(15)	H(82)	110(2)
H(80)	C(15)	H(82)	108(3)
H(81)	C(15)	H(82)	108(4)
C(18)	C(16)	C(8)	112.6(4)

C(18)	C(16)	C(17)	109.5(4)
C(8)	C(16)	C(17)	110.0(3)
C(18)	C(16)	H(83)	115(2)
C(8)	C(16)	H(83)	105(2)
C(17)	C(16)	H(83)	104(2)
C(16)	C(17)	H(86)	109.5
C(16)	C(17)	H(85)	109.5
H(86)	C(17)	H(85)	109.5
C(16)	C(17)	H(84)	109.5
H(86)	C(17)	H(84)	109.5
H(85)	C(17)	H(84)	109.5
C(16)	C(18)	H(87)	109.5
C(16)	C(18)	H(89)	109.5
H(87)	C(18)	H(89)	109.5
C(16)	C(18)	H(88)	109.5
H(87)	C(18)	H(88)	109.5
H(89)	C(18)	H(88)	109.5
C(3)	C(19)	H(90)	112(3)
C(3)	C(19)	H(91)	108(3)
H(90)	C(19)	H(91)	109(4)
C(3)	C(19)	H(92)	115(2)
H(90)	C(19)	H(92)	109(4)
H(91)	C(19)	H(92)	103(4)
C(5)	C(20)	H(93)	113(3)
C(5)	C(20)	H(94)	108(3)
H(93)	C(20)	H(94)	106(4)
C(5)	C(20)	H(95)	111(2)
H(93)	C(20)	H(95)	112(3)
H(94)	C(20)	H(95)	108(3)
C(22)	C(21)	C(26)	121.2(3)
C(22)	C(21)	N(6)	120.3(3)
C(26)	C(21)	N(6)	118.6(3)
C(23)	C(22)	C(21)	118.0(3)
C(23)	C(22)	C(30)	119.5(3)
C(21)	C(22)	C(30)	122.5(3)
C(24)	C(23)	C(22)	121.3(3)
C(24)	C(23)	H(96)	123(2)
C(22)	C(23)	H(96)	115(2)
C(25)	C(24)	C(23)	119.3(4)
C(25)	C(24)	H(97)	121(2)
C(23)	C(24)	H(97)	119(2)
C(24)	C(25)	C(26)	122.1(4)
C(24)	C(25)	H(98)	117(3)
C(26)	C(25)	H(98)	120(3)
C(25)	C(26)	C(21)	118.0(3)
C(25)	C(26)	C(27)	120.7(3)
C(21)	C(26)	C(27)	121.3(3)
C(29)	C(27)	C(26)	111.2(3)
C(29)	C(27)	C(28)	110.2(3)
C(26)	C(27)	C(28)	112.5(3)
C(29)	C(27)	H(99)	109.5(18)
C(26)	C(27)	H(99)	107.1(17)
C(28)	C(27)	H(99)	106.1(17)
C(27)	C(28)	H(100)	112(3)
C(27)	C(28)	H(101)	121(3)
H(100)	C(28)	H(101)	102(4)
C(27)	C(28)	H(102)	106(2)

H(100)	C(28)	H(102)	110(3)
H(101)	C(28)	H(102)	105(4)
C(27)	C(29)	H(103)	110(2)
C(27)	C(29)	H(104)	115(3)
H(103)	C(29)	H(104)	108(3)
C(27)	C(29)	H(105)	113(2)
H(103)	C(29)	H(105)	109(3)
H(104)	C(29)	H(105)	101(3)
C(31)	C(30)	C(22)	110.3(3)
C(31)	C(30)	C(32)	110.7(3)
C(22)	C(30)	C(32)	112.8(3)
C(31)	C(30)	H(106)	112.0(19)
C(22)	C(30)	H(106)	107.5(19)
C(32)	C(30)	H(106)	103.5(18)
C(30)	C(31)	H(107)	110(2)
C(30)	C(31)	H(108)	111(2)
H(107)	C(31)	H(108)	107(3)
C(30)	C(31)	H(109)	112(2)
H(107)	C(31)	H(109)	109(3)
H(108)	C(31)	H(109)	108(3)
C(30)	C(32)	H(110)	109(3)
C(30)	C(32)	H(111)	110(2)
H(110)	C(32)	H(111)	112(3)
C(30)	C(32)	H(112)	111(2)
H(110)	C(32)	H(112)	107(4)
H(111)	C(32)	H(112)	107(3)
C(34)	N(33)	Ti(1)	174.5(3)
N(33)	C(34)	C(35)	122.1(3)
N(33)	C(34)	C(41)	122.4(3)
C(35)	C(34)	C(41)	115.5(3)
C(36)	C(35)	C(40)	118.6(3)
C(36)	C(35)	C(34)	120.8(3)
C(40)	C(35)	C(34)	120.6(3)
C(37)	C(36)	C(35)	120.6(4)
C(37)	C(36)	H(113)	118.4(17)
C(35)	C(36)	H(113)	121.0(17)
C(36)	C(37)	C(38)	120.2(4)
C(36)	C(37)	H(114)	119(3)
C(38)	C(37)	H(114)	121(3)
C(39)	C(38)	C(37)	119.9(4)
C(39)	C(38)	H(115)	117(3)
C(37)	C(38)	H(115)	124(3)
C(38)	C(39)	C(40)	120.0(4)
C(38)	C(39)	H(116)	121(2)
C(40)	C(39)	H(116)	119(2)
C(39)	C(40)	C(35)	120.7(3)
C(39)	C(40)	H(117)	121.9(19)
C(35)	C(40)	H(117)	117.3(19)
C(46)	C(41)	C(42)	118.9(3)
C(46)	C(41)	C(34)	119.5(3)
C(42)	C(41)	C(34)	121.6(3)
C(43)	C(42)	C(41)	120.4(4)
C(43)	C(42)	H(118)	118(2)
C(41)	C(42)	H(118)	122(2)
C(44)	C(43)	C(42)	120.4(4)
C(44)	C(43)	H(119)	120(2)
C(42)	C(43)	H(119)	120(2)

C(43)	C(44)	C(45)	119.9(4)
C(43)	C(44)	H(120)	124(2)
C(45)	C(44)	H(120)	116(2)
C(44)	C(45)	C(46)	120.2(4)
C(44)	C(45)	H(121)	121.1(19)
C(46)	C(45)	H(121)	118.6(19)
C(41)	C(46)	C(45)	120.2(4)
C(41)	C(46)	H(122)	121(2)
C(45)	C(46)	H(122)	118(2)
P(48)	N(47)	Ti(1)	157.41(17)
N(47)	P(48)	C(49)	103.94(16)
N(47)	P(48)	C(54)	112.59(14)
C(49)	P(48)	C(54)	101.11(17)
C(50)	C(49)	P(48)	115.5(3)
C(50)	C(49)	H(123)	105.3(18)
P(48)	C(49)	H(123)	115.3(18)
C(50)	C(49)	H(124)	105(2)
P(48)	C(49)	H(124)	102(2)
H(123)	C(49)	H(124)	114(3)
C(53)	C(50)	C(52)	110.6(4)
C(53)	C(50)	C(51)	108.4(4)
C(52)	C(50)	C(51)	108.9(4)
C(53)	C(50)	C(49)	111.2(3)
C(52)	C(50)	C(49)	110.5(4)
C(51)	C(50)	C(49)	107.2(4)
C(50)	C(51)	H(125)	114(3)
C(50)	C(51)	H(126)	112(3)
H(125)	C(51)	H(126)	110(4)
C(50)	C(51)	H(127)	109(3)
H(125)	C(51)	H(127)	99(3)
H(126)	C(51)	H(127)	112(4)
C(50)	C(52)	H(128)	109(3)
C(50)	C(52)	H(129)	106(3)
H(128)	C(52)	H(129)	123(4)
C(50)	C(52)	H(130)	95(2)
H(128)	C(52)	H(130)	106(4)
H(129)	C(52)	H(130)	115(4)
C(50)	C(53)	H(131)	110(3)
C(50)	C(53)	H(132)	113(3)
H(131)	C(53)	H(132)	102(4)
C(50)	C(53)	H(133)	111.7(18)
H(131)	C(53)	H(133)	113(3)
H(132)	C(53)	H(133)	107(4)
C(55)	C(54)	C(59)	117.7(3)
C(55)	C(54)	P(48)	128.7(3)
C(59)	C(54)	P(48)	110.0(2)
C(56)	C(55)	C(54)	118.4(3)
C(56)	C(55)	C(60)	114.1(3)
C(54)	C(55)	C(60)	127.4(3)
C(57)	C(56)	C(55)	123.3(3)
C(57)	C(56)	H(134)	117(2)
C(55)	C(56)	H(134)	119(2)
C(56)	C(57)	C(58)	117.1(3)
C(56)	C(57)	C(64)	120.9(3)
C(58)	C(57)	C(64)	122.0(3)
C(57)	C(58)	C(59)	122.3(3)
C(57)	C(58)	H(135)	118.7(19)

C(59)	C(58)	H(135)	118.9(19)
C(58)	C(59)	C(54)	119.0(3)
C(58)	C(59)	C(68)	116.0(3)
C(54)	C(59)	C(68)	125.0(3)
C(63)	C(60)	C(61)	106.7(3)
C(63)	C(60)	C(62)	108.3(3)
C(61)	C(60)	C(62)	107.1(3)
C(63)	C(60)	C(55)	106.7(3)
C(61)	C(60)	C(55)	115.1(3)
C(62)	C(60)	C(55)	112.5(3)
C(60)	C(61)	H(138)	109.5
C(60)	C(61)	H(137)	109.5
H(138)	C(61)	H(137)	109.5
C(60)	C(61)	H(136)	109.5
H(138)	C(61)	H(136)	109.5
H(137)	C(61)	H(136)	109.5
C(60)	C(62)	H(139)	116(2)
C(60)	C(62)	H(140)	110(2)
H(139)	C(62)	H(140)	102(3)
C(60)	C(62)	H(141)	108(2)
H(139)	C(62)	H(141)	111(3)
H(140)	C(62)	H(141)	111(3)
C(60)	C(63)	H(142)	109.5
C(60)	C(63)	H(143)	109.5
H(142)	C(63)	H(143)	109.5
C(60)	C(63)	H(144)	109.5
H(142)	C(63)	H(144)	109.5
H(143)	C(63)	H(144)	109.5
C(67)	C(64)	C(65)	108.8(4)
C(67)	C(64)	C(57)	113.0(3)
C(65)	C(64)	C(57)	109.1(3)
C(67)	C(64)	C(66)	109.0(4)
C(65)	C(64)	C(66)	108.0(4)
C(57)	C(64)	C(66)	108.9(3)
C(64)	C(65)	H(145)	109.5
C(64)	C(65)	H(147)	109.5
H(145)	C(65)	H(147)	109.5
C(64)	C(65)	H(146)	109.5
H(145)	C(65)	H(146)	109.5
H(147)	C(65)	H(146)	109.5
C(64)	C(66)	H(149)	109.5
C(64)	C(66)	H(148)	109.5
H(149)	C(66)	H(148)	109.5
C(64)	C(66)	H(150)	109.5
H(149)	C(66)	H(150)	109.5
H(148)	C(66)	H(150)	109.5
C(64)	C(67)	H(151)	109.5
C(64)	C(67)	H(152)	109.5
H(151)	C(67)	H(152)	109.5
C(64)	C(67)	H(153)	109.5
H(151)	C(67)	H(153)	109.5
H(152)	C(67)	H(153)	109.5
C(70)	C(68)	C(69)	112.9(4)
C(70)	C(68)	C(71)	103.6(4)
C(69)	C(68)	C(71)	105.5(3)
C(70)	C(68)	C(59)	111.8(3)
C(69)	C(68)	C(59)	112.2(3)

C(71)	C(68)	C(59)	110.3(3)
C(68)	C(69)	H(154)	110(2)
C(68)	C(69)	H(155)	110(2)
H(154)	C(69)	H(155)	110(3)
C(68)	C(69)	H(156)	109(2)
H(154)	C(69)	H(156)	112(3)
H(155)	C(69)	H(156)	106(3)
C(68)	C(70)	H(157)	98.4(16)
C(68)	C(70)	H(158)	109(2)
H(157)	C(70)	H(158)	104(3)
C(68)	C(70)	H(159)	105(2)
H(157)	C(70)	H(159)	128(3)
H(158)	C(70)	H(159)	111(3)
C(68)	C(71)	H(160)	108(2)
C(68)	C(71)	H(161)	108(3)
H(160)	C(71)	H(161)	107(4)
C(68)	C(71)	H(162)	110(2)
H(160)	C(71)	H(162)	113(3)
H(161)	C(71)	H(162)	110(4)

Symmetry transformations used to generate equivalent atoms:

Table 5c: Torsion angles for MSC Sample 03117

A	B	C	D	Torsion Angle
N(47)	Ti(1)	N(2)	C(3)	-167.1(2)
N(33)	Ti(1)	N(2)	C(3)	60.3(2)
N(6)	Ti(1)	N(2)	C(3)	-54.3(2)
N(47)	Ti(1)	N(2)	C(7)	28.5(3)
N(33)	Ti(1)	N(2)	C(7)	-104.0(3)
N(6)	Ti(1)	N(2)	C(7)	141.3(3)
C(7)	N(2)	C(3)	C(4)	-165.6(3)
Ti(1)	N(2)	C(3)	C(4)	27.1(4)
C(7)	N(2)	C(3)	C(19)	13.1(5)
Ti(1)	N(2)	C(3)	C(19)	-154.2(3)
N(2)	C(3)	C(4)	C(5)	17.2(6)
C(19)	C(3)	C(4)	C(5)	-161.5(4)
C(3)	C(4)	C(5)	N(6)	-17.4(6)
C(3)	C(4)	C(5)	C(20)	163.7(3)
C(4)	C(5)	N(6)	C(21)	169.3(3)
C(20)	C(5)	N(6)	C(21)	-11.8(5)
C(4)	C(5)	N(6)	Ti(1)	-26.8(4)
C(20)	C(5)	N(6)	Ti(1)	152.0(3)
N(47)	Ti(1)	N(6)	C(5)	172.7(2)
N(33)	Ti(1)	N(6)	C(5)	-62.9(2)
N(2)	Ti(1)	N(6)	C(5)	55.0(2)
N(47)	Ti(1)	N(6)	C(21)	-25.6(3)
N(33)	Ti(1)	N(6)	C(21)	98.9(3)
N(2)	Ti(1)	N(6)	C(21)	-143.2(2)
C(3)	N(2)	C(7)	C(12)	76.4(4)

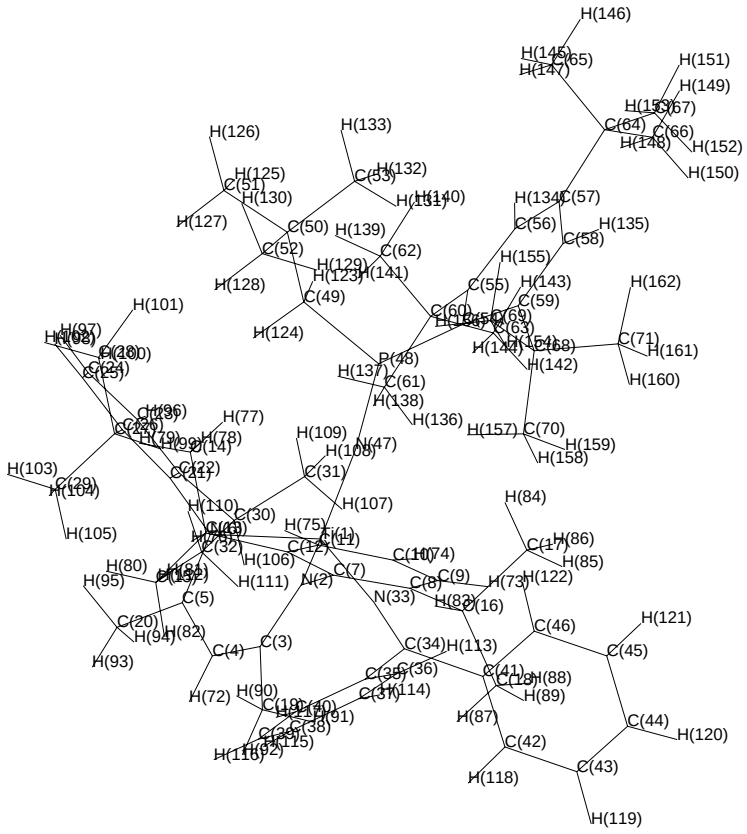
Ti(1)	N(2)	C(7)	C(12)	-120.7(3)
C(3)	N(2)	C(7)	C(8)	-103.9(4)
Ti(1)	N(2)	C(7)	C(8)	59.1(4)
C(12)	C(7)	C(8)	C(9)	-2.6(5)
N(2)	C(7)	C(8)	C(9)	177.6(3)
C(12)	C(7)	C(8)	C(16)	177.8(3)
N(2)	C(7)	C(8)	C(16)	-1.9(5)
C(7)	C(8)	C(9)	C(10)	0.5(6)
C(16)	C(8)	C(9)	C(10)	-179.9(4)
C(8)	C(9)	C(10)	C(11)	1.6(6)
C(9)	C(10)	C(11)	C(12)	-1.7(6)
C(10)	C(11)	C(12)	C(7)	-0.3(5)
C(10)	C(11)	C(12)	C(13)	178.8(4)
C(8)	C(7)	C(12)	C(11)	2.5(5)
N(2)	C(7)	C(12)	C(11)	-177.7(3)
C(8)	C(7)	C(12)	C(13)	-176.6(3)
N(2)	C(7)	C(12)	C(13)	3.2(5)
C(11)	C(12)	C(13)	C(14)	-61.6(4)
C(7)	C(12)	C(13)	C(14)	117.5(4)
C(11)	C(12)	C(13)	C(15)	60.7(4)
C(7)	C(12)	C(13)	C(15)	-120.2(4)
C(9)	C(8)	C(16)	C(18)	-61.8(5)
C(7)	C(8)	C(16)	C(18)	117.8(4)
C(9)	C(8)	C(16)	C(17)	60.7(5)
C(7)	C(8)	C(16)	C(17)	-119.7(4)
C(5)	N(6)	C(21)	C(22)	85.8(4)
Ti(1)	N(6)	C(21)	C(22)	-74.0(4)
C(5)	N(6)	C(21)	C(26)	-94.2(4)
Ti(1)	N(6)	C(21)	C(26)	106.0(3)
C(26)	C(21)	C(22)	C(23)	2.1(5)
N(6)	C(21)	C(22)	C(23)	-177.9(3)
C(26)	C(21)	C(22)	C(30)	-175.4(3)
N(6)	C(21)	C(22)	C(30)	4.5(5)
C(21)	C(22)	C(23)	C(24)	-0.1(6)
C(30)	C(22)	C(23)	C(24)	177.5(4)
C(22)	C(23)	C(24)	C(25)	-2.0(6)
C(23)	C(24)	C(25)	C(26)	2.2(6)
C(24)	C(25)	C(26)	C(21)	-0.2(6)
C(24)	C(25)	C(26)	C(27)	179.9(4)
C(22)	C(21)	C(26)	C(25)	-2.0(5)
N(6)	C(21)	C(26)	C(25)	178.0(3)
C(22)	C(21)	C(26)	C(27)	177.9(3)
N(6)	C(21)	C(26)	C(27)	-2.1(5)
C(25)	C(26)	C(27)	C(29)	-92.6(4)
C(21)	C(26)	C(27)	C(29)	87.5(4)
C(25)	C(26)	C(27)	C(28)	31.6(5)
C(21)	C(26)	C(27)	C(28)	-148.3(4)
C(23)	C(22)	C(30)	C(31)	-78.0(4)
C(21)	C(22)	C(30)	C(31)	99.5(4)
C(23)	C(22)	C(30)	C(32)	46.2(5)
C(21)	C(22)	C(30)	C(32)	-136.2(4)
N(47)	Ti(1)	N(33)	C(34)	173(3)
N(2)	Ti(1)	N(33)	C(34)	-54(3)
N(6)	Ti(1)	N(33)	C(34)	51(3)
Ti(1)	N(33)	C(34)	C(35)	-60(3)
Ti(1)	N(33)	C(34)	C(41)	121(3)
N(33)	C(34)	C(35)	C(36)	-125.0(4)

C(41)	C(34)	C(35)	C(36)	54.2(4)
N(33)	C(34)	C(35)	C(40)	53.3(5)
C(41)	C(34)	C(35)	C(40)	-127.4(3)
C(40)	C(35)	C(36)	C(37)	-1.4(5)
C(34)	C(35)	C(36)	C(37)	177.0(3)
C(35)	C(36)	C(37)	C(38)	1.7(6)
C(36)	C(37)	C(38)	C(39)	0.0(6)
C(37)	C(38)	C(39)	C(40)	-2.1(6)
C(38)	C(39)	C(40)	C(35)	2.4(6)
C(36)	C(35)	C(40)	C(39)	-0.7(5)
C(34)	C(35)	C(40)	C(39)	-179.1(3)
N(33)	C(34)	C(41)	C(46)	28.4(5)
C(35)	C(34)	C(41)	C(46)	-150.8(3)
N(33)	C(34)	C(41)	C(42)	-150.9(3)
C(35)	C(34)	C(41)	C(42)	29.9(4)
C(46)	C(41)	C(42)	C(43)	-1.0(5)
C(34)	C(41)	C(42)	C(43)	178.3(3)
C(41)	C(42)	C(43)	C(44)	2.1(6)
C(42)	C(43)	C(44)	C(45)	-1.5(6)
C(43)	C(44)	C(45)	C(46)	-0.2(6)
C(42)	C(41)	C(46)	C(45)	-0.7(5)
C(34)	C(41)	C(46)	C(45)	-180.0(3)
C(44)	C(45)	C(46)	C(41)	1.3(6)
N(33)	Ti(1)	N(47)	P(48)	-62.9(5)
N(2)	Ti(1)	N(47)	P(48)	163.9(4)
N(6)	Ti(1)	N(47)	P(48)	60.0(5)
Ti(1)	N(47)	P(48)	C(49)	-102.5(5)
Ti(1)	N(47)	P(48)	C(54)	148.9(4)
N(47)	P(48)	C(49)	C(50)	152.5(3)
C(54)	P(48)	C(49)	C(50)	-90.7(3)
P(48)	C(49)	C(50)	C(53)	62.7(4)
P(48)	C(49)	C(50)	C(52)	-60.5(4)
P(48)	C(49)	C(50)	C(51)	-178.9(3)
N(47)	P(48)	C(54)	C(55)	78.7(3)
C(49)	P(48)	C(54)	C(55)	-31.7(3)
N(47)	P(48)	C(54)	C(59)	-123.9(2)
C(49)	P(48)	C(54)	C(59)	125.8(3)
C(59)	C(54)	C(55)	C(56)	-14.4(5)
P(48)	C(54)	C(55)	C(56)	141.6(3)
C(59)	C(54)	C(55)	C(60)	160.8(3)
P(48)	C(54)	C(55)	C(60)	-43.1(5)
C(54)	C(55)	C(56)	C(57)	2.8(5)
C(60)	C(55)	C(56)	C(57)	-173.1(3)
C(55)	C(56)	C(57)	C(58)	8.2(5)
C(55)	C(56)	C(57)	C(64)	-174.6(3)
C(56)	C(57)	C(58)	C(59)	-7.4(5)
C(64)	C(57)	C(58)	C(59)	175.4(3)
C(57)	C(58)	C(59)	C(54)	-4.3(5)
C(57)	C(58)	C(59)	C(68)	174.9(3)
C(55)	C(54)	C(59)	C(58)	15.2(5)
P(48)	C(54)	C(59)	C(58)	-145.1(3)
C(55)	C(54)	C(59)	C(68)	-163.9(3)
P(48)	C(54)	C(59)	C(68)	35.9(4)
C(56)	C(55)	C(60)	C(63)	56.7(4)
C(54)	C(55)	C(60)	C(63)	-118.7(4)
C(56)	C(55)	C(60)	C(61)	174.9(3)
C(54)	C(55)	C(60)	C(61)	-0.6(5)

C(56)	C(55)	C(60)	C(62)	-62.0(4)
C(54)	C(55)	C(60)	C(62)	122.6(4)
C(56)	C(57)	C(64)	C(67)	-174.7(4)
C(58)	C(57)	C(64)	C(67)	2.4(5)
C(56)	C(57)	C(64)	C(65)	64.2(5)
C(58)	C(57)	C(64)	C(65)	-118.7(4)
C(56)	C(57)	C(64)	C(66)	-53.5(5)
C(58)	C(57)	C(64)	C(66)	123.7(4)
C(58)	C(59)	C(68)	C(70)	-144.1(4)
C(54)	C(59)	C(68)	C(70)	34.9(5)
C(58)	C(59)	C(68)	C(69)	87.8(4)
C(54)	C(59)	C(68)	C(69)	-93.1(4)
C(58)	C(59)	C(68)	C(71)	-29.5(5)
C(54)	C(59)	C(68)	C(71)	149.6(4)

Symmetry transformations used to generate equivalent atoms:

Figure 1: VERSORT Drawing(s)



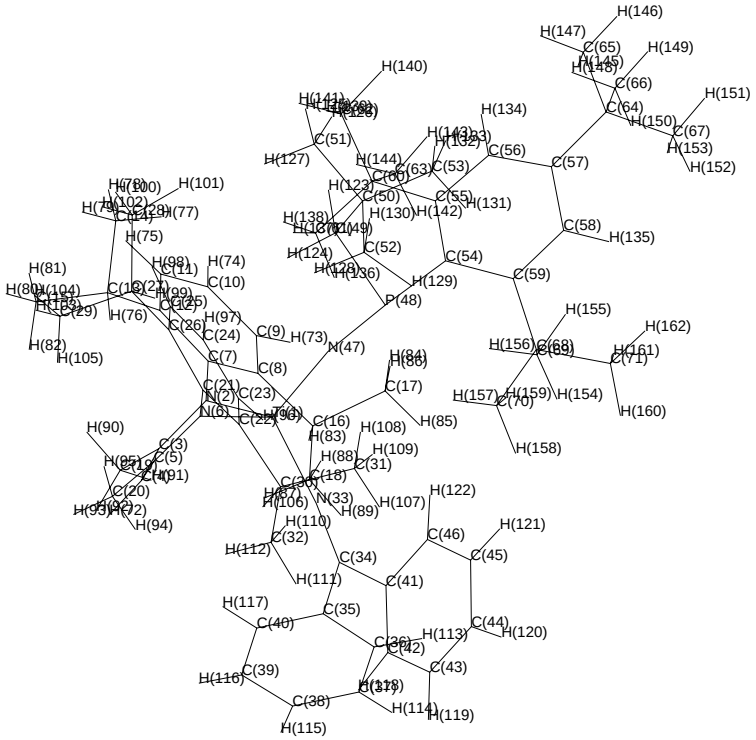
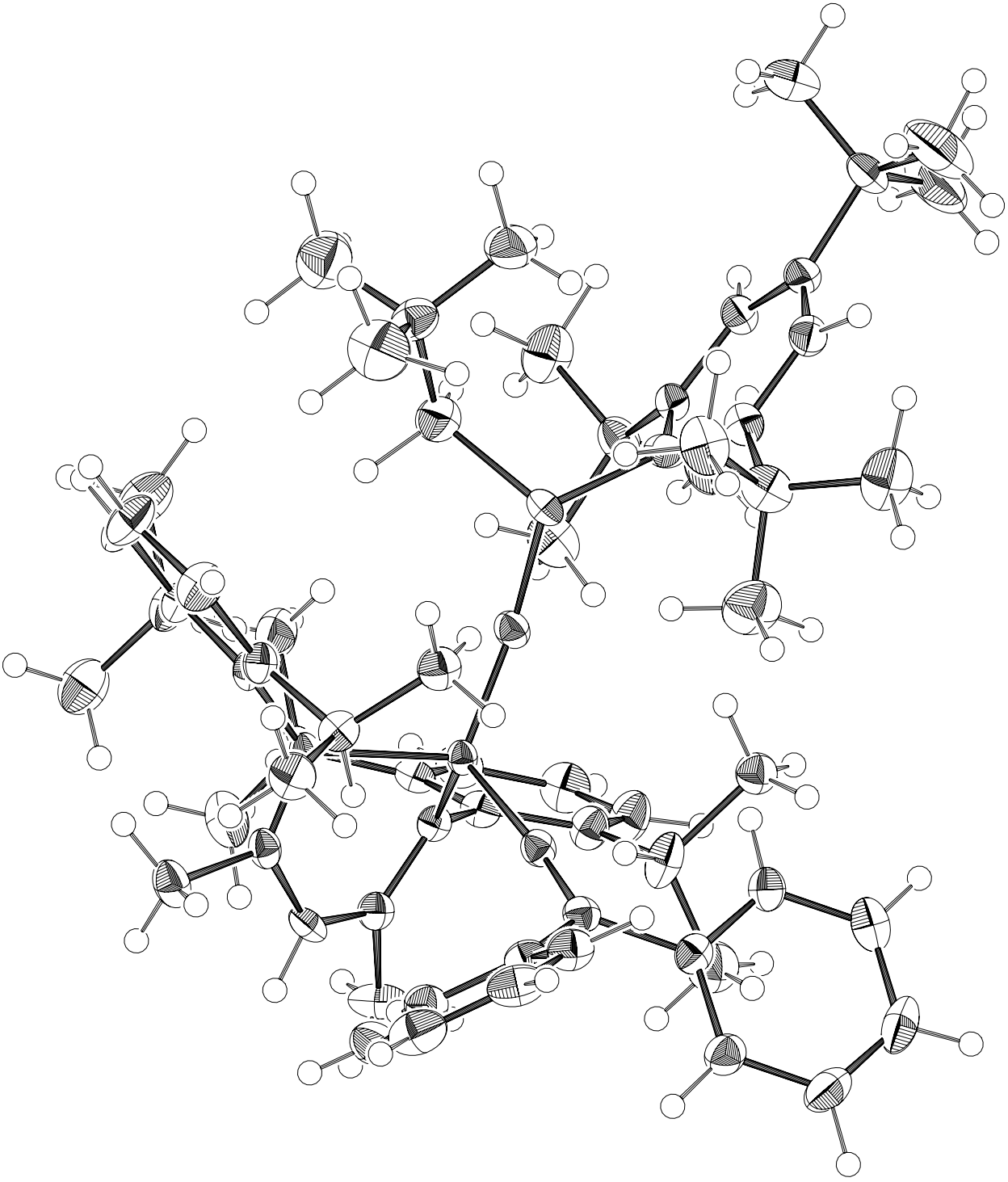


Figure 2: ORTEP Drawing(s)



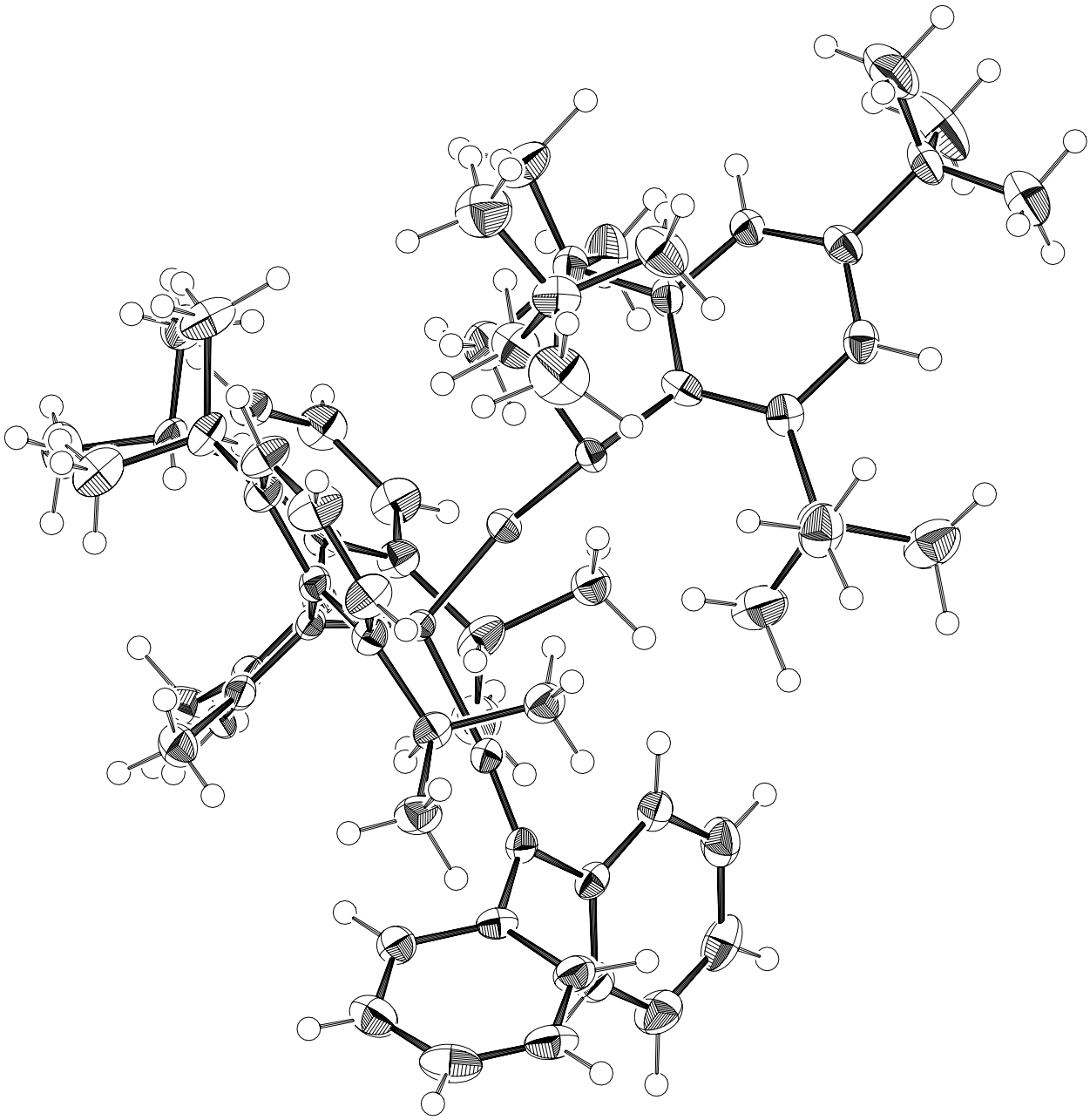


Figure 3: Space Filling Model Drawing(s)