SUPPORTING INFORMATION

New Types of Constrained Geometry Group 4 Metal Complexes Derived from Aminomethyldicarbollyl Ligand System: Synthesis and Structural Characterization of Mono- and Bis-dicarbollylamino Group 4 Metal Complexes

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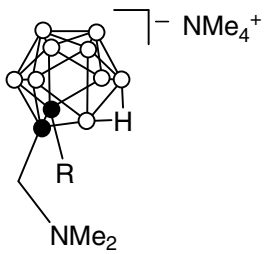
[*nido*-7-NMe_2CH_2-7,8-$C_2B_9H_{11}$]$^-$ [NMe4]$^+$ 2a

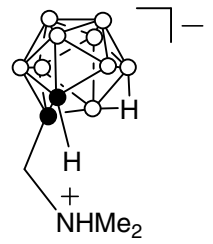


^{1}H NMR (300.1 MHz, DMSO-d_6) δ -2.61 (brs, 1H, B-H-B), 2.11 (s, 6H, CH_2NMe_2), 2.25 (s, 1H, C_{cab}-*H*), 2. 38 (d, 1H, CH_2N, $^2J_{HH}$ = 16 Hz), 2.43 (d, 1H, CH_2N, $^2J_{HH}$ = 16 Hz), 3.45 (s, 12H, NMe_4)

^{13}C NMR (75.4 MHz, DMSO-d_6) δ 45.74 (CH_2NMe_2), 55.79 (NMe_4), 69.57 (CH_2NMe_2)

^{11}B NMR (96.3 MHz, DMSO-d_6) δ -9.65 (1B), -10.32 (1B), -13.54 (1B), -16.71 (1B), -17.70 (1B), -19.32 (1B), -22.31 (1B), -33.12 (1B), -36.66 (1B)

[*nido*-7-$HNMe_2CH_2$-7,8-$C_2B_9H_{11}$] 3a

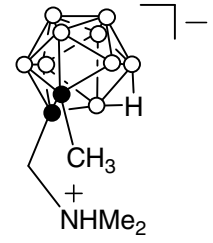


^{1}H NMR (300.1 MHz, DMSO-d_6) δ -3.01 (brs, 1H, B-H-B), 2.01 (s, 1H, C_{cab}-*H*), 2.70 (s, 6H, CH_2NHMe_2), 2. 92 (d, 1H, CH_2NH, $^2J_{HH}$ = 13 Hz), 3.31 (d, 1H, CH_2NH, $^2J_{HH}$ = 13 Hz), 8.67 (br,1H, CH_2NH)

^{13}C NMR (75.4 MHz, DMSO-d_6) δ 43.48 (CH_2NHMe_2), 44.63 (CH_2NHMe_2), 54.96 (CH_2NH)

^{11}B NMR (96.3 MHz, DMSO-d_6) δ -12.52 (2B), -15.40 (2B), -21.47 (3B), -33.99 (1B), -38.23 (1B)

[*nido*-7-$HNMe_2CH_2$-7,8-CH_3-$C_2B_9H_{11}$] 3b

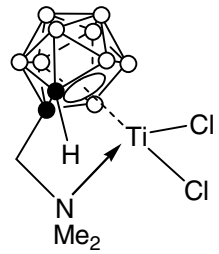


^{1}H NMR (300.1 MHz, DMSO-d_6) δ -2.82 (br, 1H, B-*H*-B), 1.45 (s, 3H, C_{cab}-*Me*), 2.50 (s, 6H, CH_2NHMe_2), 2. 72 (d, 1H, CH_2NH, $^2J_{HH}$ = 5 Hz), 2.80 (d, 1H, CH_2NH, $^2J_{HH}$ = 5 Hz), 8.33 (br, 1H,CH_2NH)

^{13}C NMR (75.4 MHz, DMSO-d_6) δ 22.32 (C_{cab}-*Me*), 43.01 (CH_2NHMe_2), 47.79 (CH_2NHMe_2), 57.53 (CH_2NH)

^{11}B NMR (96.3 MHz, DMSO-d_6) δ -11.54 (3B), -16.29 (2B), -20.90 (2B), -34.85 (1B), -37.85 (1B)

[η^5:η^1-$C_2B_9H_9$-7,8-CH_2NMe_2]$TiCl_2$ 4a

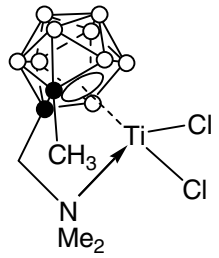


^{1}H NMR (300.1 MHz, $CDCl_3$) δ 1.68 (s, 3H, N*Me*$_2$), 1.74 (s, 3H, N*Me*$_2$), 2.70 (d, 1H, NC*H*$_2$, $^2J_{HH}$ = 14 Hz), 3.43 (d, 1H, NC*H*$_2$, $^2J_{HH}$ = 14 Hz), 4.22 (s, 1H, C_{cab}-*H*)

^{13}C NMR (75.4 MHz, $CDCl_3$) δ 54.36 (N*Me*$_2$), 58.63 (N*Me*$_2$), 69.76 (N*C*H$_2$)

^{11}B NMR (96.3 MHz, $CDCl_3$) δ -9.63 (1B), -3.34 (1B), -1.63 (1B), 0.83 (1B), 2.63 (1B), 4.78 (1B), 6.39 (1B), 8.32 (1B), 26.33 (1B)

[η^5:η^1-2-CH_3-$C_2B_9H_9$-7,8-CH_2NMe_2]$TiCl_2$ 4b

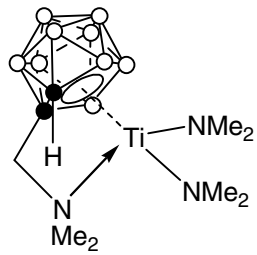


^{1}H NMR (300.1 MHz, $CDCl_3$) δ 1.52 (s, 3H, C_{cab}-*Me*), 2.09 (s, 3H, N*Me*$_2$), 2.11 (s, 3H, N*Me*$_2$), 3.20 (d, 1H, NC*H*$_2$, $^2J_{HH}$ = 14 Hz), 3.36 (d, 1H, NC*H*$_2$, $^2J_{HH}$ = 14 Hz)

^{13}C NMR (75.4 MHz, $CDCl_3$) δ 34.47 (C_{cab}-*Me*), 53.25 (N*Me*$_2$), 57.86 (N*Me*$_2$), 69.85 (N*C*H$_2$)

^{11}B NMR (96.3 MHz, $CDCl_3$) δ -8.43 (1B), -2.37 (1B), -0.67 (1B), 1.93 (1B), 4.44 (1B), 7.89 (1B), 10.17 (1B), 11.22 (1B), 28.14 (1B)

[η^5:η^1-$C_2B_9H_9$-CH_2NMe_2]$Ti(NMe_2)_2$ 5a

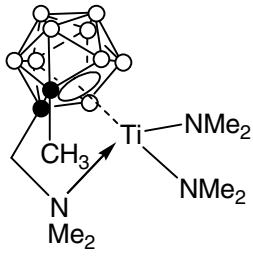


^{1}H NMR (300.1 MHz, $CDCl_3$) δ 2.34 (s,3H, N*Me*$_2$), 2.42 (s,3H, N*Me*$_2$), 2.59 (s,1H, C_{cab}-*H*), 2.81 (d, 1H, NC*H*$_2$,$^2J_{HH}$=15 Hz), 3.59 (d, 1H, NC*H*$_2$,$^2J_{HH}$=15 Hz), 3.57 (s, 6H, TiN*Me*$_2$), 3.61 (s, 6H, TiN*Me*$_2$)

^{13}C NMR (75.4 MHz, $CDCl_3$) δ 46.91 (N*Me*$_2$), 48.67 (N*Me*$_2$), 49.73 (TiN*Me*$_2$), 51.52 (TiN*Me*$_2$), 57.89 (N*C*H$_2$)

^{11}B NMR (96.3 MHz, $CDCl_3$) δ -25.19 (1B), -18.57 (2B), -13.97 (1B), -9.19 (2B), -3.89 (1B), 1.71 (1B), 12.13 (1B)

[η^5:η^1-2-CH_3-$C_2B_9H_9$-CH_2NMe_2]Ti(NMe_2)$_2$ 5b

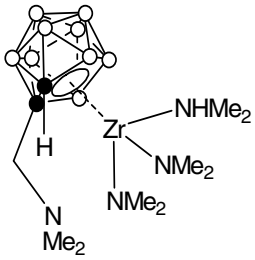


^{1}H NMR (300.1 MHz, $CDCl_3$) δ 2.17 (s,3H, C_{cab}-*Me*), 2.50 (s,3H, N*Me*$_2$), 2.78 (d,1H, NC*H*$_2$,$^2J_{HH}$ =17 Hz), 2.85 (s,3H, N*Me*$_2$), 3.51 (s,6H,TiN*Me*$_2$), 3.63 (s,6H,TiN*Me*$_2$), 3.71 (d,1H, NC*H*$_2$,$^2J_{HH}$ =17 Hz)

^{13}C NMR (75.4 MHz, $CDCl_3$) δ 26.14 (C_{cab}-*Me*), 47.66 (N*Me*$_2$), 49.01 (N*Me*$_2$), 50.66 (TiN*Me*$_2$), 52.39 (TiN*Me*$_2$), 59.63 (N*C*H$_2$)

^{11}B NMR (96.3 MHz, $CDCl_3$) δ -26.26 (1B), -14.18 (2B), -10.49 (3B), -7.01 (2B), 0.43 (1B)

[η^5:η^1-$C_2B_9H_9$-CH_2NMe_2]Zr(NMe_2)$_2$ 6a

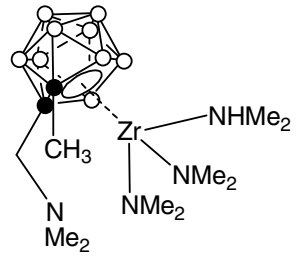


^{1}H NMR (300.1 MHz, $CDCl_3$) δ 2.44 (br,1H, C_{cab}-*H*), 2.69 (s, 6H, ZrN*Me*$_2$H), 2.71 (s, 3H, N*Me*$_2$), 2.85 (s, 3H, N*Me*$_2$), 3.20 (d, 1H, NC*H*$_2$, $^2J_{HH}$ = 15 Hz), 3.24 (s, 6H, ZrN*Me*$_2$), 3.40 (s, 6H, ZrN*Me*$_2$), 3.45 (d, 1H, NC*H*$_2$, $^2J_{HH}$ = 15 Hz), 3.57 (br, 1H, ZrNMe$_2$*H*)

^{13}C NMR (75.4 MHz, $CDCl_3$) δ 40.41 (N*Me*$_2$), 41.54 (N*Me*$_2$), 42.92 (ZrN*Me*$_2$H), 49.27 (ZrN*Me*$_2$), 50.50 (ZrN*Me*$_2$), 60.03 (N*C*H$_2$)

^{11}B NMR (96.3 MHz, $CDCl_3$) δ -26.06 (1B), -16.94 (2B), -12.66 (3B), -9.13 (1B), -7.58 (1B), -1.21 (1B)

[η^5:η^1-2-CH_3-$C_2B_9H_9$-CH_2NMe_2]Zr(NMe_2)$_2$ 6b

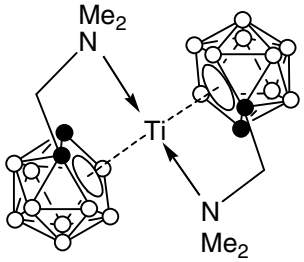


^{1}H NMR (300.1 MHz, $CDCl_3$) δ 2.00 (s, 3H, C_{cab}-*Me*), 2.54 (s, 3H, N*Me*$_2$), 2.55 (s, 6H, ZrN*Me*$_2$H), 2.73 (s, 3H, N*Me*$_2$), 3.14 (s, 6H,ZrN*Me*$_2$), 3.26 (s, 6H,ZrN*Me*$_2$), 3.43 (d, 1H, NC*H*$_2$, $^2J_{HH}$ = 15 Hz), 3.49 (br, 1H, ZrNMe$_2$*H*), 3.55 (d, 1H, NC*H*$_2$, $^2J_{HH}$ = 15 Hz)

^{13}C NMR (75.4 MHz, $CDCl_3$) δ 25.02 (C_{cab}-*Me*), 39.82 (N*Me*$_2$), 41.61 (N*Me*$_2$), 43.95 (ZrN*Me*$_2$H), 45.18 (ZrN*Me*$_2$), 46.38 (ZrN*Me*$_2$), 58.57 (N*C*H$_2$)

^{11}B NMR (96.3 MHz, $CDCl_3$) δ -31.03 (1B), -31.03 (1B), -26.62 (1B), -18.06 (1B), -13.07 (2B), -11.60 (2B), -7.91 (1B), -2.61 (1B)

[Ti(η^5:η^1-$C_2B_9H_{10}$-CH_2NMe_2)$_2$] 7

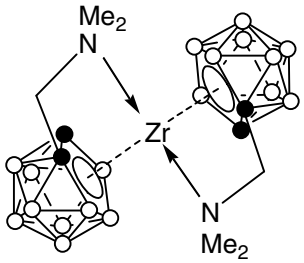


^{1}H NMR (300.1 MHz, $CDCl_3$) δ 1.39 (s, 3H, N*Me*$_2$), 1.75 (s, 3H, N*Me*$_2$), 2.70 (d, 1H, NC*H*$_2$, $^2J_{HH}$ = 14 Hz), 3.02 (d, 1H, NC*H*$_2$, $^2J_{HH}$ = 14 Hz), 3.71 (s, 1H, C_{cab}-*H*)

^{13}C NMR (75.4 MHz, $CDCl_3$) δ 55.04 (N*Me*$_2$), 56.33 (N*Me*$_2$), 72.88 (N*C*H$_2$)

^{11}B NMR (96.3 MHz, $CDCl_3$) δ -10.70 (1B), -7.59 (1B), -5.74 (1B), - 4.37 (1B), -2.03 (1B), 3.53 (1B), 6.24 (1B), 9.06 (1B), 28.47 (1B)

[Zr(η^5:η^1-$C_2B_9H_{10}$-CH_2NMe_2)$_2$] 8

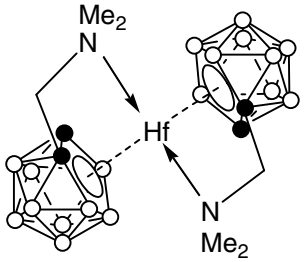


^{1}H NMR (300.1 MHz, $CDCl_3$) d 1.81 (s, 3H, N*Me*$_2$), 2.07 (s, 3H, N*Me*$_2$), 2.74 (d, 1H, NC*H*$_2$, $^2J_{HH}$ = 14 Hz), 2.89 (d, 1H, NC*H*$_2$, $^2J_{HH}$ = 14 Hz), 3.45 (s, 1H, C_{cab}-*H*)

^{13}C NMR (75.4 MHz, $CDCl_3$) d 52.65 (N*Me*$_2$), 56.01 (N*Me*$_2$), 72.99 (N*C*H$_2$)

^{11}B NMR (96.3 MHz, $CDCl_3$) d -13.23 (1B), -10.03 (1B), -7.84 (1B), -4.81 (1B), -3.35 (1B), -0.25 (2B), 2.84 (1B), 12.11 (1B)

[Hf(η^5:η^1-$C_2B_9H_{10}$-CH_2NMe_2)$_2$] 9

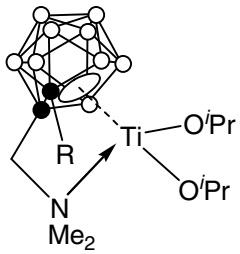


^{1}H NMR (300.1 MHz, $CDCl_3$) δ 1.79 (s, 3H, N*Me*$_2$), 2.19 (s, 3H, N*Me*$_2$), 2.68 (d, 1H, NC*H*$_2$, $^2J_{HH}$ = 14 Hz), 2.89 (d, 1H, NC*H*$_2$, $^2J_{HH}$ = 14 Hz), 3.33 (s, 1H, C_{cab}-*H*)

^{13}C NMR (75.4 MHz, $CDCl_3$) δ 54.86 (N*Me*$_2$), 57.07 (N*Me*$_2$), 74.10 (N*C*H$_2$)

^{11}B NMR (96.3 MHz, $CDCl_3$) δ -23.17 (1B), -15.51 (1B), -12.83 (1B), -11.13 (1B), -9.26 (1B), -4.50 (1B), -1.75 (1B) 1.87 (1B) 9.18 (1B)

[η^5:η^1-$C_2B_9H_9$-CH_2NMe_2]Ti(OPr^i)$_2$ 10

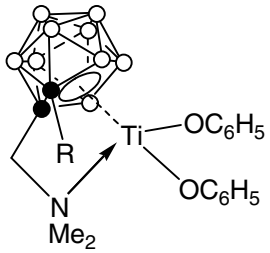


^{1}H NMR (300.1 MHz, $CDCl_3$) δ 1.25 (d, 12H, TiOCH*Me*$_2$), 1.35 (s, 6H, N*Me*$_2$), 3.05 (b, 1H, NC*H*$_2$), 3.15 (b, 1H, NC*H*$_2$), 4.49 (s, 1H, TiOC*H*Me$_2$)

^{13}C NMR (75.4 MHz, $CDCl_3$) δ 26.82 (TiOCH*Me*$_2$), 30.65 (N*Me*$_2$), 49.10 (N*C*H$_2$), 52.90 (N*C*H$_2$), 77.16 (TiO*C*HMe$_2$)

^{11}B NMR (96.3 MHz, $CDCl_3$) δ -43.48 (1B), -25.81 (2B), -17.06 (3B), -11.05 (2B), -0.835 (1B)

[η^5:η^1-$C_2B_9H_9$-CH_2NMe_2]Ti(OPh)$_2$ 11

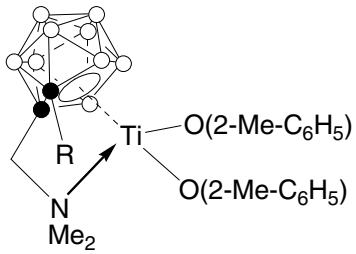


^{1}H NMR (300.1 MHz, CD_3COCD_3) δ 1.62 (s, 3H, N*Me*$_2$) 1.89 (s, 3H, N*Me*$_2$) 2.87 (d, 1H, NC*H*$_2$, $^2J_{HH}$ = 14 Hz) 3.10 (d, 1H, NC*H*$_2$, $^2J_{HH}$ = 14 Hz) 3.38 (br,1H, C_{cab}-*H*) 6.09-7.37 (m, 10H, TiO*Ph*)

^{13}C NMR (75.4 MHz, CD_3COCD_3) δ 21.27 (N*Me*$_2$) 37.55 (N*Me*$_2$) 55.82 (N*C*H$_2$) 62.55 (N*C*H$_2$) 120.19, 124.99, 126.40, 129.22, 130.02 (TiO*Ph*)

^{11}B NMR (96.3 MHz, $CDCl_3$) δ -2.74 (1B), -14.77 (2B), -8.30 (2B), -4.56 (3B), 9.14 (1B)

[η^5:η^1-$C_2B_9H_9$-CH_2NMe_2]Ti(OPh)$_2$ (Ph = 2-Me-C_6H_5) 12



^{1}H NMR (300.1 MHz, CD_3COCD_3) δ 2.16 (s, 3H, N*Me*$_2$), 2.33 (s, 3H, 2-*Me*Ph), 2.44 (s, 3H, 2-*Me*Ph), 3.70 (br,1H, C_{cab}-*H*), 3.87 (d, 1H, NC*H*$_2$, $^2J_{HH}$ = 14 Hz), 3.99 (d, 1H, NC*H*$_2$, $^2J_{HH}$ = 14 Hz), 6.80-7.74 (m, 10H, 2-Me*Ph*)

^{13}C NMR (75.4 MHz, CD_3COCD_3), δ 17.26 (N*Me*$_2$), 37.50 (2-*Me*Ph), 40.95 (2-*Me*Ph), 56.45 (N*C*H$_2$), 60.57 (N*C*H$_2$), 120.63, 121.79, 123.46, 124.99 (2-Me*Ph*)

^{11}B NMR (96.3 MHz, $CDCl_3$) δ -20.78 (2B), -14.37 (2B), -6.20 (3B), 9.50 (2B)

Table 1. Crystal data and structure refinement for **2a·NC$_4$H$_{12}$**.

Identification code	kor055
Empirical formula	$C_9H_{31}B_9N_2$
Formula weight	264.65
Temperature	293(2) K
Wavelength	0.71070 Å
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Unit cell dimensions	a = 10.5791(7) Å
	b = 11.3215(2) Å
	c = 14.9539(9) Å
Volume	1791.0(3) Å^3
Z, D_{calc}	4, 0.981 g/cm^3
μ	0.049 mm^{-1}
F(000)	576
Crystal size	0.5 x 0.5 x 0.4 mm
θ range for data collection	2.26 to 25.96 °
Limiting indices	$0 \le h \le 13$, $0 \le k \le 13$, $0 \le l \le 18$
Reflections collected / unique	2006 / 2006 [R(int) = 0.0000]
Completeness to θ = 25.96	100.0 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2006 / 0 / 201
Goodness-of-fit on F^2	1.059
Final R indices [I>2σ (I)]	[a]R_1 = 0.1164, [b]wR_2 = 0.2728
R indices (all data)	[a]R_1 = 0.2925, [b]wR_2 = 0.3492
Absolute structure parameter	9(10)
Largest diff. peak and hole	0.211 and -0.206 e.Å^{-3}

[a]$R_1 = \sum||F_o|-|F_c||$ (based on reflections with $F_o^2 > 2\sigma F^2$), [b]$wR_2 = [\sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2)+(0.095P)^2]$; , $P = [\max(F_o^2, 0)+2F_c^2]/3$(also with $F_o^2 > 2\sigma F^2$)

Table 2. Bond lengths [Å] for **2a** .

N(1)-C(5)	1.442(2)	C(1)-B(3)	1.740(2)
N(1)-C(4)	1.445(1)	B(1)-B(4)	1.73(3)
N(1)-C(3)	1.498(1)	B(1)-B(2)	1.73(3)
N(2)-C(7)	1.452(1)	B(1)-B(3)	1.75(2)
N(2)-C(8)	1.493(1)	B(1)-B(6)	1.76(2)
N(2)-C(9)	1.503(2)	B(1)-B(5)	1.77(2)
N(2)-C(6)	1.507(1)	B(2)-B(3)	1.70(2)
C(2)-C(1)	1.539(1)	B(2)-B(9)	1.71(3)
C(2)-B(3)	1.64(2)	B(2)-B(6)	1.73(2)
C(2)-B(9)	1.65(2)	B(3)-B(4)	1.73(2)
C(2)-B(2)	1.697(2)	B(4)-B(5)	1.75(2)
C(1)-C(3)	1.484(1)	B(4)-B(11)	1.75(2)
C(1)-B(11)	1.606(2)	B(5)-B(11)	1.69(2)
B(6)-B(10)	1.76(2)	B(5)-B(10)	1.74(2)
B(11)-B(10)	1.79(2)	B(5)-B(6)	1.79(2)
B(10)-B(9)	1.85(3)	B(6)-B(9)	1.73(2)
C(1)-B(4)	1.701(2)		

Table 3. Angles [deg] for **2a**.

C(5)-N(1)-C(4)	110.2(1)	B(2)-B(1)-B(6)	59.5(1)
C(5)-N(1)-C(3)	111.5(1)	B(3)-B(1)-B(6)	106.4(1)
C(4)-N(1)-C(3)	109.5(1)	B(4)-B(1)-B(5)	59.9(1)
C(7)-N(2)-C(8)	109.1(9)	B(2)-B(1)-B(5)	107.5(1)
C(7)-N(2)-C(9)	111.2(1)	B(3)-B(1)-B(5)	106.7(1)
C(8)-N(2)-C(9)	109.2(9)	B(6)-B(1)-B(5)	60.9(9)
C(7)-N(2)-C(6)	108.5(1)	B(4)-C(1)-B(3)	60.2(9)
C(8)-N(2)-C(6)	109.1(1)	C(1)-C(3)-N(1)	114.4(9)
C(9)-N(2)-C(6)	109.7(1)	C(2)-B(2)-B(3)	57.7(8)
C(1)-C(2)-B(3)	66.3(9)	C(2)-B(2)-B(9)	58.0(9)
C(1)-C(2)-B(9)	112.9(1)	B(3)-B(2)-B(9)	108.3(1)
B(3)-C(2)-B(9)	114.3(1)	C(2)-B(2)-B(1)	103.8(1)
C(1)-C(2)-B(2)	113.7(1)	B(3)-B(2)-B(1)	61.2(1)
B(3)-C(2)-B(2)	61.3(1)	B(9)-B(2)-B(1)	109.2(1)
B(9)-C(2)-B(2)	61.4(9)	C(2)-B(2)-B(6)	103.3(1)
C(3)-C(1)-C(2)	115.2(9)	B(3)-B(2)-B(6)	109.8(1)
C(3)-C(1)-B(11)	124.9(1)	B(9)-B(2)-B(6)	60.1(1)
C(2)-C(1)-B(11)	112.8(9)	B(1)-B(2)-B(6)	61.1(9)
C(3)-C(1)-B(4)	120.4(9)	C(2)-B(3)-B(2)	61.0(1)
C(2)-C(1)-B(4)	109.1(9)	C(2)-B(3)-B(4)	103.3(1)
B(11)-C(1)-B(4)	64.0(9)	B(2)-B(3)-B(4)	108.3(1)
C(3)-C(1)-B(3)	113.2(9)	C(2)-B(3)-C(1)	54.1(7)
C(2)-C(1)-B(3)	59.6(8)	B(2)-B(3)-C(1)	103.9(1)
B(11)-C(1)-B(3)	113.5(1)	B(4)-B(3)-C(1)	58.8(8)
B(4)-B(1)-B(2)	106.9(1)	C(2)-B(3)-B(1)	105.5(1)
B(4)-B(1)-B(3)	59.5(9)	B(2)-B(3)-B(1)	60.3(1)
B(2)-B(1)-B(3)	58.5(1)	B(4)-B(3)-B(1)	59.6(1)
B(4)-B(1)-B(6)	108.5(1)	C(1)-B(3)-B(1)	103.5(1)

C(1)-B(4)-B(3)	61.0(8)	B(2)-B(6)-B(1)	59.4(1)
C(1)-B(4)-B(1)	106.2(1)	B(10)-B(6)-B(1)	109.7(1)
B(3)-B(4)-B(1)	60.9(1)	B(9)-B(6)-B(5)	107.3(1)
C(1)-B(4)-B(5)	101.3(9)	B(2)-B(6)-B(5)	106.6(1)
B(3)-B(4)-B(5)	108.8(1)	B(10)-B(6)-B(5)	58.8(9)
B(1)-B(4)-B(5)	61.3(9)	B(1)-B(6)-B(5)	59.7(1)
C(1)-B(4)-B(11)	55.4(7)	C(1)-B(11)-B(5)	108.0(1)
B(3)-B(4)-B(11)	107.0(1)	C(1)-B(11)-B(4)	60.6(8)
B(1)-B(4)-B(11)	107.1(1)	B(5)-B(11)-B(4)	60.9(9)
B(5)-B(4)-B(11)	57.7(9)	C(1)-B(11)-B(10)	108.4(1)
B(11)-B(5)-B(10)	63.1(9)	B(5)-B(11)-B(10)	59.9(9)
B(11)-B(5)-B(4)	61.4(9)	B(4)-B(11)-B(10)	110.0(1)
B(10)-B(5)-B(4)	113.0(1)	B(5)-B(10)-B(6)	61.6(8)
B(11)-B(5)-B(1)	108.1(1)	B(5)-B(10)-B(11)	57.0(8)
B(10)-B(5)-B(1)	110.1(1)	B(6)-B(10)-B(11)	104.2(9)
B(4)-B(5)-B(1)	58.8(1)	B(5)-B(10)-B(9)	104.0(1)
B(11)-B(5)-B(6)	107.3(1)	B(6)-B(10)-B(9)	57.1(9)
B(10)-B(5)-B(6)	59.6(9)	B(11)-B(10)-B(9)	100.6(1)
B(4)-B(5)-B(6)	106.4(1)	C(2)-B(9)-B(2)	60.6(9)
B(1)-B(5)-B(6)	59.3(9)	C(2)-B(9)-B(6)	105.6(1)
B(9)-B(6)-B(2)	59.3(1)	B(2)-B(9)-B(6)	60.6(9)
B(9)-B(6)-B(10)	64.2(1)	C(2)-B(9)-B(10)	105.1(1)
B(2)-B(6)-B(10)	112.0(1)	B(2)-B(9)-B(10)	108.7(1)
B(9)-B(6)-B(1)	107.2(1)	B(6)-B(9)-B(10)	58.7(9)

Symmetry transformations used to generate equivalent atoms:

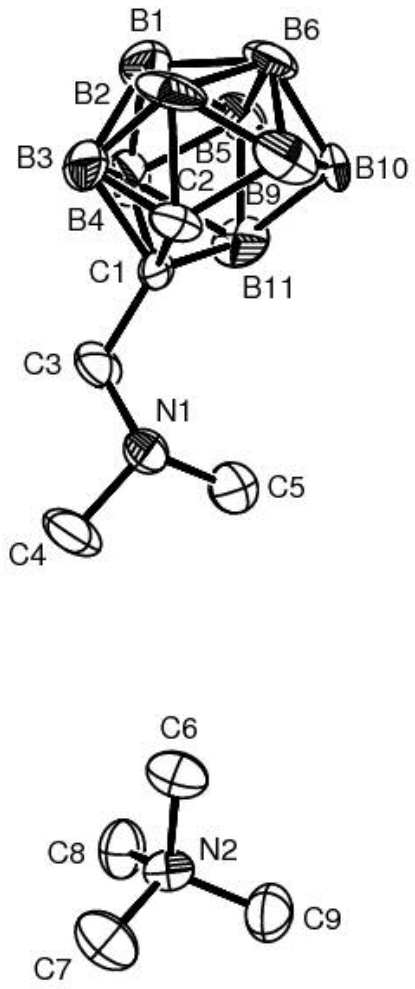


Figure 1. Molecular structure of **2a·NC$_4$H$_{12}$** with thermal ellipsoids drawn at the 30% level

Table 1. Crystal data and structure refinement for **5a**.

Identification code	kor113
Empirical formula	$C_9H_{30}B_9N_3Ti$
Formula weight	325.55
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, *Pnma*
Unit cell dimensions	a = 17.510(2) Å
	b = 13.151(2) Å
	c = 8.044(1)Å
Volume	1852.3(4) $Å^3$
Z, D_{calc}	4, 1.167 g/cm^3
μ	0.454 mm^{-1}
F(000)	688
Crystal size	0.25 x 0.15 x 0.10 mm
θ range for data collection	2.33 to 28.29 °
Limiting indices	$-22 \le h \le 23$, $-11 \le k \le 17$, $-10 \le l \le 10$
Reflections collected / unique	12979 / 2400 [R(int) = 0.1718]
Completeness to θ = 28.29	99.9 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2400 / 0 / 116
Goodness-of-fit on F^2	1.000
Final R indices [I>2σ(I)]	[a]R_1 = 0.0841, [b]wR_2 = 0.2149
R indices (all data)	[a]R_1 = 0.2187, [b]wR_2 = 0.3043
Extinction coefficient	0.0025(17)
Largest diff. peak and hole	0.808 and -0.828 e. $Å^{-3}$

[a]$R_1 = \sum||F_o|-|F_c||$ (based on reflections with $F_o^2>2\sigma F^2$), [b]$wR_2 = [\sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2)+(0.095P)^2]$; , $P = [\max(F_o^2, 0)+2F_c^2]/3$(also with $F_o^2>2\sigma F^2$)

Table 2. Bond lengths [Å] for **5a**.

Ti(1)-N(2)	1.891(5)	C(1)-B(2)*	1.717(9)
Ti(1)-N(2)*	1.891(5)	C(1)-B(2)	1.717(9)
Ti(1)-N(1)	2.220(7)	C(2)-B(5)	1.699(1)
Ti(1)-C(1)	2.351(7)	C(2)-B(2)	1.736(9)
Ti(1)-B(6)*	2.384(7)	C(2)-B(3)	1.739(1)
Ti(1)-C(2)*	2.384(7)	B(1)-B(3)	1.762(1)
Ti(1)-C(2)	2.384(7)	B(1)-B(3)*	1.762(1)
Ti(1)-B(5)	2.433(8)	B(1)-B(2)*	1.778(1)
Ti(1)-B(5)*	2.433(8)	B(1)-B(2)	1.778(1)
N(1)-C(4)	1.487(7)	B(1)-B(4)	1.781(2)
N(1)-C(4)*	1.487(7)	B(2)-B(2)*	1.776(2)
N(1)-C(3)	1.490(1)	B(2)-B(3)	1.777(1)
N(2)-C(6)	1.276(1)	B(3)-B(4)	1.758(1)
N(2)-C(5)	1.423(1)	B(3)-B(5)	1.796(1)
C(1)-C(3)	1.504(1)	B(4)-B(3)*	1.758(1)
C(1)-C(2)	1.602(8)	B(4)-B(5)	1.774(1)
C(1)-B(6)*	1.602(8)	B(4)-B(5) *	1.774(1)
C(1)-C(2)*	1.602(8)	B(5)-B(5)*	1.75(2)

Symmetry transformations used to generate equivalent atoms:

* x , -y+1/2 , z

Table 3. Angles [deg] for **5a**.

N(2)-Ti(1)-N(2)*	102.7(3)	N(2)-Ti(1)-B(5)*	123.6(3)
N(2)-Ti(1)-N(1)	103.4(2)	N(2)*-Ti(1)-B(5)*	89.6(3)
N(2)*-Ti(1)-N(1)	103.4(2)	N(1)-Ti(1)-B(5)*	127.1(3)
N(2)-Ti(1)-C(1)	128.5(2)	C(1)-Ti(1)-B(5)*	68.5(3)
N(2)*-Ti(1)-C(1)	128.5(2)	B(6)*-Ti(1)-B(5)*	41.3(3)
N(1)-Ti(1)-C(1)	63.4(3)	C(2)*-Ti(1)-B(5)*	41.3(3)
N(2)-Ti(1)-B(6)*	158.3(2)	C(2)-Ti(1)-B(5)*	69.3(3)
N(2)*-Ti(1)-B(6)*	93.7(2)	B(5)-Ti(1)-B(5)*	42.1(5)
N(1)-Ti(1)-B(6)*	86.3(2)	C(4)-N(1)-C(4)*	107.8(8)
C(1)-Ti(1)-B(6)*	39.6(2)	C(4)-N(1)-C(3)	110.7(5)
N(2)-Ti(1)-C(2) *	158.3(2)	C(4)*-N(1)-C(3)	110.7(5)
N(2)*-Ti(1)-C(2)*	93.7(2)	C(4)-N(1)-Ti(1)	114.8(4)
N(1)-Ti(1)-C(2)*	86.3(2)	C(4)*-N(1)-Ti(1)	114.8(4)
C(1)-Ti(1)-C(2)*	39.6(2)	C(3)-N(1)-Ti(1)	97.7(5)
N(2)-Ti(1)-C(2)	93.7(2)	C(6)-N(2)-C(5)	102.3(8)
N(2)*-Ti(1)-C(2)	158.3(2)	C(6)-N(2)-Ti(1)	123.5(7)
N(1)-Ti(1)-C(2)	86.3(2)	C(5)-N(2)-Ti(1)	134.2(5)
C(1)-Ti(1)-C(2)	39.6(2)	C(3)-C(1)-C(2)	118.6(4)
B(6)*-Ti(1)-C(2)	67.2(3)	C(3)-C(1)-B(6)*	118.6(4)
C(2)*-Ti(1)-C(2)	67.2(3)	C(2)-C(1)-B(6)*	110.9(7)
N(2)-Ti(1)-B(5)	89.6(3)	C(3)-C(1)-C(2)*	118.6(4)
N(2)*-Ti(1)-B(5)	123.6(3)	C(2)-C(1)-C(2)*	110.9(7)
N(1)-Ti(1)-B(5)	127.1(3)	C(3)-C(1)-B(2)*	119.9(6)
C(1)-Ti(1)-B(5)	68.5(3)	C(2)-C(1)-B(2)*	113.4(6)
B(6)*-Ti(1)-B(5)	69.3(3)	B(6)*-C(1)-B(2)*	63.0(4)
C(2)*-Ti(1)-B(5)	69.3(3)	C(2)*-C(1)-B(2)*	63.0(4)
C(2)-Ti(1)-B(5)	41.3(3)	C(3)-C(1)-B(2)	119.9(6)
C(2)-C(1)-B(2)	63.0(4)	B(3)-B(1)-B(3)*	107.6(8)

B(6)*-C(1)-B(2)	113.4(6)	B(3)-B(1)-B(2)*	108.0(6)
C(2)*-C(1)-B(2)	113.4(6)	B(3)*-B(1)-B(2)*	60.3(5)
B(2)*-C(1)-B(2)	62.3(6)	B(3)-B(1)-B(2)	60.3(5)
C(3)-C(1)-Ti(1)	92.0(5)	B(3)*-B(1)-B(2)	108.0(6)
C(2)-C(1)-Ti(1)	71.4(3)	B(2)*-B(1)-B(2)	59.9(6)
B(6)*-C(1)-Ti(1)	71.4(3)	B(3)-B(1)-B(4)	59.5(4)
C(2)*-C(1)-Ti(1)	71.4(3)	B(3)*-B(1)-B(4)	59.5(4)
B(2)*-C(1)-Ti(1)	132.6(4)	B(2)*-B(1)-B(4)	107.5(6)
B(2)-C(1)-Ti(1)	132.6(4)	B(2)-B(3)-B(5)	107.4(5)
C(1)-C(2)-B(5)	109.3(6)	B(3)*-B(4)-B(3)	107.9(8)
C(1)-C(2)-B(2)	61.8(4)	B(3)*-B(4)-B(5)	108.3(7)
B(5)-C(2)-B(2)	113.9(5)	B(3)-B(4)-B(5)	61.1(5)
C(1)-C(2)-B(3)	109.4(5)	B(3)*-B(4)-B(5)*	61.1(5)
B(5)-C(2)-B(3)	62.9(5)	B(3)-B(4)-B(5)*	108.3(7)
B(2)-C(2)-B(3)	61.5(4)	B(5)-B(4)-B(5)*	59.0(7)
C(1)-C(2)-Ti(1)	69.1(3)	B(3)*-B(4)-B(1)	59.7(4)
B(5)-C(2)-Ti(1)	70.9(3)	B(3)-B(4)-B(1)	59.7(4)
B(2)-C(2)-Ti(1)	129.3(4)	B(5)-B(4)-B(1)	108.6(7)
B(3)-C(2)-Ti(1)	130.3(5)	B(5)*-B(4)-B(1)	108.6(7)
N(1)-C(3)-C(1)	106.8(6)	C(2)-B(5)-B(5)*	105.2(4)
C(1)-B(2)-C(2)	55.3(3)	C(2)-B(5)-B(4)	105.1(6)
C(1)-B(2)-B(2)*	58.9(3)	B(5)*-B(5)-B(4)	60.5(3)
C(2)-B(2)-B(2)*	104.4(3)	C(2)-B(5)-B(3)	59.6(4)
C(1)-B(2)-B(3)	102.7(5)	B(5)*-B(5)-B(3)	107.8(4)
C(2)-B(2)-B(3)	59.3(4)	B(4)-B(5)-B(3)	59.0(5)
B(2)*-B(2)-B(3)	107.5(4)	C(2)-B(5)-Ti(1)	67.8(3)
C(1)-B(2)-B(1)	103.6(5)	B(5)*-B(5)-Ti(1)	69.0(2)
C(2)-B(2)-B(1)	104.8(6)	B(2)*-B(2)-B(1)	60.0(3)
B(3)-B(2)-B(1)	59.4(5)	B(1)-B(3)-B(2)	60.3(5)

C(2)-B(3)-B(4)	104.1(6)	C(2)-B(3)-B(5)	57.4(4)
C(2)-B(3)-B(1)	105.4(6)	B(4)-B(3)-B(5)	59.9(5)
B(4)-B(3)-B(1)	60.8(6)	B(1)-B(3)-B(5)	108.4(6)
C(2)-B(3)-B(2)	59.2(4)	B(4)-B(5)-Ti(1)	125.0(5)
B(4)-B(3)-B(2)	108.6(6)	B(3)-B(5)-Ti(1)	124.4(5)

Symmetry transformations used to generate equivalent atoms:

* x , -y+1/2 , z

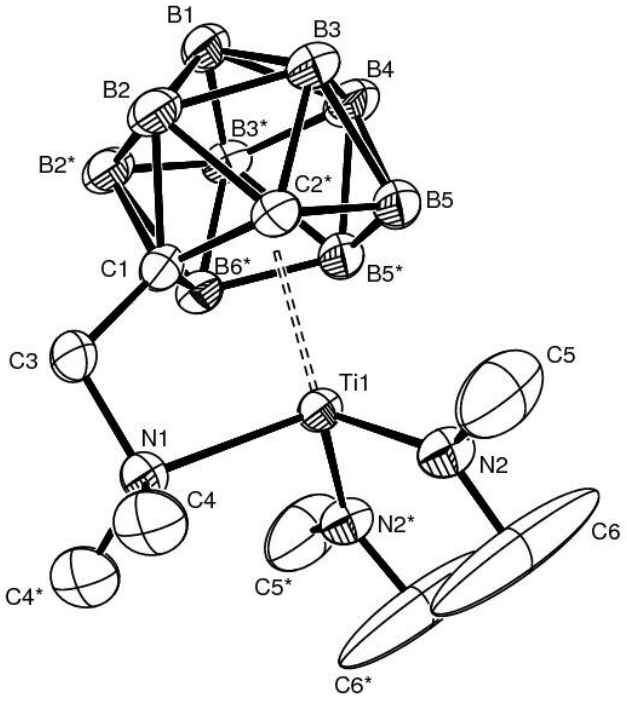


Figure 2. Molecular structure of **5a** with thermal ellipsoids drawn at the 30% level.

Table 1. Crystal data and structure refinement for **5b**.

Identification code	kor074m
Empirical formula	$C_{10}H_{32}B_9N_3Ti$
Formula weight	339.58
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, $P2_1/n$
Unit cell dimensions	a = 9.429(1) Å.
	b = 14.827(1) Å β = 91.795(2) º
	c = 13.606(1) Å
Volume	1901.2(3) $Å^3$
Z, D_{calc}	4, 1.186 g/cm^3
μ	0.445 mm^{-1}
F(000)	720
Crystal size	0.25 x 0.15 x 0.10 mm
θ range for data collection	2.03 to 28.32 º
Limiting indices	$-12 \le h \le 7$, $-19 \le k \le 17$, $-18 \le l \le 18$
Reflections collected / unique	13684 / 4727 [R(int) = 0.0643]
Completeness to θ = 28.32	99.7 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4727 / 0 / 224
Goodness-of-fit on F^2	0.997
Final R indices [I>2σ(I)]	[a]R_1 = 0.0495, [b]wR_2 = 0.1065
R indices (all data)	[a]R_1 = 0.1013, [b]wR_2 = 0.1248
Largest diff. peak and hole	0.402 and -0.327 e.$Å^{-3}$

[a]$R_1 = \sum||F_o|-|F_c||$ (based on reflections with $F_o^2>2\sigma F^2$), [b]$wR_2 = [\sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2)+(0.095P)^2]$; , $P = [\max(F_o^2, 0)+2F_c^2]/3$(also with $F_o^2>2\sigma F^2$)

Table 2. Bond lengths [Å] for **5b**.

Ti(1)-N(2)	1.900(2)	C(2)- B(9)	1.682(4)
Ti(1)-N(3)	1.901(2)	C(2)- B(4)	1.702(4)
Ti(1)-N(1)	2.255(2)	C(2)- B(3)	1.732(4)
Ti(1)-B(11)	2.359(3)	B(1)-B(3)	1.757(4)
Ti(1)-C(1)	2.385(2)	B(1)-B(4)	1.767(4)
Ti(1)-B(10)	2.426(3)	B(1)-B(2)	1.772(5)
Ti(1)-B(9)	2.456(3)	B(1)-B(6)	1.782(5)
Ti(1)-C(2)	2.484(2)	B(1)-B(5)	1.797(5)
N(1)-C(4)	1.485(3)	B(2)-B(11)	1.763(4)
N(1)-C(5)	1.494(3)	B(2)-B(3)	1.768(4)
N(1)-C(3)	1.503(3)	B(2)-B(6)	1.773(5)
N(2)-C(7)	1.461(3)	B(3)-B(4)	1.756(4)
N(2)-C(8)	1.483(3)	B(4)-B(5)	1.764(4)
N(3)-C(10)	1.462(4)	B(4)-B(9)	1.780(4)
N(3)-C(9)	1.473(3)	B(5)-B(6)	1.770(4)
C(1)- C(3)	1.514(3)	B(5)-B(10)	1.776(4)
C(1)- C(2)	1.593(3)	B(5)-B(9)	1.780(4)
C(1)- B(11)	1.663(4)	B(6)-B(11)	1.764(4)
C(1)- B(3)	1.725(4)	B(6)-B(10)	1.797(4)
C(1)- B(2)	1.726(4)	B(9)-B(10)	1.760(4)
C(2)- C(6)	1.531(3)	B(10)-B(11)	1.752(4)

Table 3. Angles [deg] for **5b**.

N(2)-Ti(1)-N(3)	99.8(9)	C(4)-N(1)-C(5)	106.6(2)
N(2)-Ti(1)-N(1)	104.4(9)	C(4)-N(1)-C(3)	110.4(2)
N(3)-Ti(1)-N(1)	108.7(9)	C(5)-N(1)-C(3)	110.3(2)
N(2)-Ti(1)-B(11)	157.5(1)	C(4)-N(1)-Ti(1)	114.0(2)
N(3)-Ti(1)-B(11)	97.2(1)	C(5)-N(1)-Ti(1)	117.4(2)
N(1)-Ti(1)-B(11)	83.9(9)	C(3)-N(1)-Ti(1)	97.8(1)
N(2)-Ti(1)-C(1)	124.4(9)	C(7)-N(2)-C(8)	107.7(2)
N(3)-Ti(1)-C(1)	135.8(9)	C(7)-N(2)-Ti(1)	141.8(2)
N(1)-Ti(1)-C(1)	62.8(8)	C(8)-N(2)-Ti(1)	110.5(2)
B(11)-Ti(1)-C(1)	41.1(9)	C(10)-N(3)-C(9)	108.2(2)
N(2)-Ti(1)-B(10)	122.6(1)	C(10)-N(3)-Ti(1)	122.8(2)
N(3)-Ti(1)-B(10)	88.8(1)	C(9)-N(3)-Ti(1)	126.9(2)
N(1)-Ti(1)-B(10)	126.3(9)	C(3)-C(1)-C(2)	117.8(2)
B(11)-Ti(1)-B(10)	42.9(1)	C(3)-C(1)-B(11)	118.2(2)
C(1)-Ti(1)-B(10)	69.5(9)	C(2)-C(1)-B(11)	112.3(2)
N(2)-Ti(1)-B(9)	88.3(9)	C(3)-C(1)-B(3)	120.0(2)
N(3)-Ti(1)-B(9)	120.8(9)	C(2)-C(1)-B(3)	62.8(2)
N(1)-Ti(1)-B(9)	125.9(9)	B(11)-C(1)-B(3)	113.7(2)
B(11)-Ti(1)-B(9)	70.2(1)	C(3)-C(1)-B(2)	121.5(2)
C(1)-Ti(1)-B(9)	66.8(9)	C(2)-C(1)-B(2)	112.6(2)
B(10)-Ti(1)-B(9)	42.3(9)	B(11)-C(1)-B(2)	62.6(2)
N(2)-Ti(1)-C(2)	91.4(8)	B(3)-C(1)-B(2)	61.7(2)
N(3)-Ti(1)-C(2)	157.8(9)	C(3)-C(1)-Ti(1)	92.2(2)
N(1)-Ti(1)-C(2)	86.8(8)	C(2)-C(1)-Ti(1)	74.3(1)
B(11)-Ti(1)-C(2)	67.9(9)	B(11)-C(1)-Ti(1)	68.6(1)
C(1)-Ti(1)-C(2)	38.1(8)	B(3)-C(1)-Ti(1)	134.6(2)
B(10)-Ti(1)-C(2)	69.0(9)	B(2)-C(1)-Ti(1)	129.5(2)
B(9)-Ti(1)-C(2)	39.8(9)	C(6)-C(2)-C(1)	120.3(2)

C(6)-C(2)-B(9)	125.0(2)	C(1)-B(3)-C(2)	54.9(1)
C(1)-C(2)-B(9)	108.9(2)	C(1)-B(3)-B(4)	101.9(2)
C(6)-C(2)-B(4)	115.3(2)	C(2)-B(3)-B(4)	58.4(2)
C(1)-C(2)-B(4)	110.2(2)	C(1)-B(3)-B(1)	104.6(2)
B(9)-C(2)-B(4)	63.5(2)	C(2)-B(3)-B(1)	105.4(2)
C(6)-C(2)-B(3)	109.9(2)	B(4)-B(3)-B(1)	60.4(2)
C(1)-C(2)-B(3)	62.3(2)	C(1)-B(3)-B(2)	59.2(2)
B(9)-C(2)-B(3)	113.9(2)	C(2)-B(3)-B(2)	104.2(2)
B(4)-C(2)-B(3)	61.5(2)	B(4)-B(3)-B(2)	107.6(2)
C(6)-C(2)-Ti(1)	107.3(2)	B(1)-B(3)-B(2)	60.3(2)
C(1)-C(2)-Ti(1)	67.6(1)	C(2)-B(4)-B(3)	60.1(2)
B(9)-C(2)-Ti(1)	69.2(1)	C(2)-B(4)-B(5)	105.4(2)
B(4)-C(2)-Ti(1)	128.6(2)	B(3)-B(4)-B(5)	109.0(2)
B(3)-C(2)-Ti(1)	127.7(2)	C(2)-B(4)-B(1)	106.3(2)
N(1)-C(3)-C(1)	106.6(2)	B(3)-B(4)-B(1)	59.8(2)
B(3)-B(1)-B(4)	59.8(2)	B(5)-B(4)-B(1)	61.2(2)
B(3)-B(1)-B(2)	60.1(2)	C(2)-B(4)-B(9)	57.7(2)
B(4)-B(1)-B(2)	107.0(2)	B(3)-B(4)-B(9)	108.1(2)
B(3)-B(1)-B(6)	108.1(2)	B(5)-B(4)-B(9)	60.3(2)
B(4)-B(1)-B(6)	106.7(2)	B(1)-B(4)-B(9)	108.9(2)
B(2)-B(1)-B(6)	59.9(2)	B(4)-B(5)-B(6)	107.4(2)
B(3)-B(1)-B(5)	107.5(2)	B(4)-B(5)-B(10)	108.5(2)
B(4)-B(1)-B(5)	59.3(2)	B(6)-B(5)-B(10)	60.9(2)
B(2)-B(1)-B(5)	106.8(2)	B(4)-B(5)-B(9)	60.3(2)
B(6)-B(1)-B(5)	59.3(2)	B(6)-B(5)-B(9)	107.2(2)
C(1)-B(2)-B(11)	56.9(2)	B(10)-B(5)-B(9)	59.3(2)
C(1)-B(2)-B(3)	59.1(2)	B(4)-B(5)-B(1)	59.5(2)
B(11)-B(2)-B(3)	106.9(2)	B(6)-B(5)-B(1)	59.9(2)
C(1)-B(2)-B(1)	103.9(2)	B(10)-B(5)-B(1)	109.2(2)

B(11)-B(2)-B(1)	107.3(2)	B(10)-B(9)-Ti(1)	68.0(1)
B(3)-B(2)-B(1)	59.5(2)	B(4)-B(9)-Ti(1)	126.1(2)
C(1)-B(2)-B(6)	103.5(2)	B(5)-B(9)-Ti(1)	124.2(2)
B(11)-B(2)-B(6)	59.9(2)	B(11)-B(10)-B(9)	104.2(2)
B(3)-B(2)-B(6)	108.0(2)	B(11)-B(10)-B(5)	105.9(2)
B(1)-B(2)-B(6)	60.4(2)	B(9)-B(10)-B(5)	60.4(2)
B(9)-B(5)-B(1)	107.6(2)	B(11)-B(10)-B(6)	59.6(2)
B(11)-B(6)-B(5)	105.6(2)	B(9)-B(10)-B(6)	106.9(2)
B(11)-B(6)-B(2)	59.8(2)	B(5)-B(10)-B(6)	59.4(2)
B(5)-B(6)-B(2)	107.9(2)	B(11)-B(10)-Ti(1)	66.5(1)
B(11)-B(6)-B(1)	106.8(2)	B(9)-B(10)-Ti(1)	69.8(1)
B(5)-B(6)-B(1)	60.8(2)	B(5)-B(10)-Ti(1)	126.0(2)
B(2)-B(6)-B(1)	59.8(2)	B(6)-B(10)-Ti(1)	123.2(2)
B(11)-B(6)-B(10)	58.9(2)	C(1)-B(11)-B(10)	106.7(2)
B(5)-B(6)-B(10)	59.7(2)	C(1)-B(11)-B(2)	60.4(2)
B(2)-B(6)-B(10)	108.3(2)	B(10)-B(11)-B(2)	110.8(2)
B(1)-B(6)-B(10)	108.9(2)	C(1)-B(11)-B(6)	106.6(2)
C(2)-B(9)-B(10)	107.8(2)	B(10)-B(11)-B(6)	61.5(2)
C(2)-B(9)-B(4)	58.8(2)	B(2)-B(11)-B(6)	60.4(2)
B(10)-B(9)-B(4)	108.5(2)	C(1)-B(11)-Ti(1)	70.3(1)
C(2)-B(9)-B(5)	105.6(2)	B(10)-B(11)-Ti(1)	70.6(1)
B(10)-B(9)-B(5)	60.2(2)	B(2)-B(11)-Ti(1)	129.0(2)
B(4)-B(9)-B(5)	59.4(2)	B(6)-B(11)-Ti(1)	128.9(3)
C(2)-B(9)-Ti(1)	71.0(1)		

Symmetry transformations used to generate equivalent atoms:

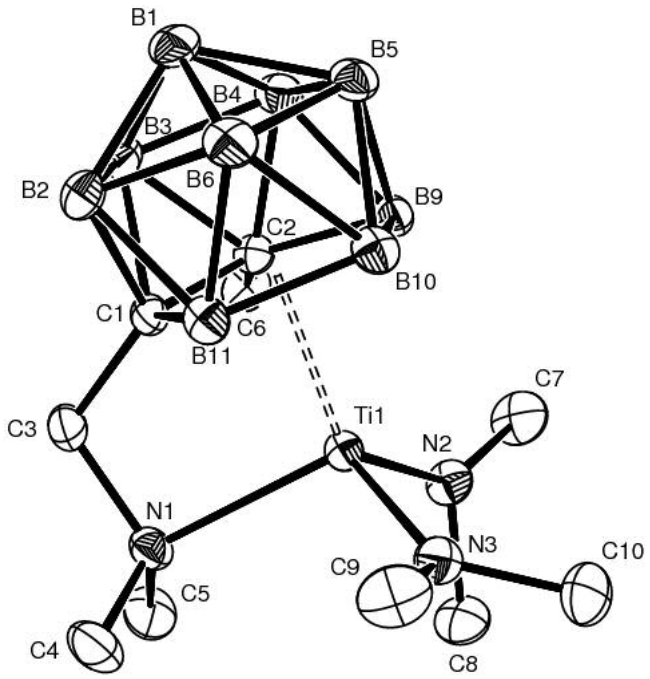


Figure 3. Molecular structure of **5b** with thermal ellipsoids drawn at the 30% level.

Table 1. Crystal data and structure refinement for **6a**.

Identification code	kor017m	
Empirical formula	$C_{11}H_{37}B_9N_4Zr$	
Formula weight	413.96	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Triclinic, $P\bar{1}$	
Unit cell dimensions	a = 9.2199(8) Å	α = 90.037(2) °
	b = 9.2777(8) Å	β = 96.908(2) °
	c = 13.842(1) Å	γ = 113.269(2) °
Volume	1078.3(2) $Å^3$	
Z, D_{calc}	2, 1.275 g/cm^3	
μ	0.511 mm^{-1}	
F(000)	432	
Crystal size	0.30 x 0.15 x 0.15 mm	
θ range for data collection	2.39 to 28.35 °	
Limiting indices	$-12 \le h \le 11$, $-12 \le k \le 12$, $-18 \le l \le 13$	
Reflections collected / unique	8012 / 5315 [R(int) = 0.0800]	
Completeness to θ = 28.35	98.4 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5315 / 0 / 244	
Goodness-of-fit on F^2	0.923	
Final R indices [I>2σ(I)]	[a]R_1 = 0.0388, [b]wR_2 = 0.0855	
R indices (all data)	[a]R_1 = 0.0556, [b]wR_2 = 0.0894	
Largest diff. peak and hole	0.963 and -0.760 e.$Å^{-3}$	

[a]$R_1 = \sum||F_o|-|F_c|| / \sum|F_o|$ (based on reflections with $F_o^2 > 2\sigma F^2$), [b]$wR_2 = [\sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2)+(0.095P)^2]$; , $P = [\max(F_o^2, 0)+2F_c^2]/3$(also with $F_o^2 > 2\sigma F^2$)

Table 2. Bond lengths [Å] for **6a**.

Zr(1)-N(3)	2.033(2)	C(1)- B(3)	1.721(4)
Zr(1)-N(2)	2.054(2)	C(2)- B(9)	1.642(4)
Zr(1)-N(4)	2.450(2)	C(2)- B(3)	1.723(4)
Zr(1)-B(11)	2.567(3)	C(2)- B(4)	1.725(4)
Zr(1)-B(10)	2.577(3)	B(1)-B(2)	1.761(5)
Zr(1)-N(1)	2.579(2)	B(1)-B(3)	1.762(5)
Zr(1)-B(9)	2.609(3)	B(1)-B(4)	1.774(5)
Zr(1)-C(1)	2.617(2)	B(1)-B(6)	1.776(5)
Zr(1)-C(2)	2.655(3)	B(1)-B(5)	1.792(5)
N(1)-C(4)	1.461(4)	B(2)-B(3)	1.757(5)
N(1)-C(5)	1.476(4)	B(2)-B(6)	1.764(5)
N(1)-C(3)	1.486(4)	B(2)-B(11)	1.769(4)
N(2)-C(6)	1.458(4)	B(3)-B(4)	1.780(5)
N(2)-C(7)	1.462(4)	B(4)-B(5)	1.764(5)
N(3)-C(8)	1.454(4)	B(4)-B(9)	1.786(4)
N(3)-C(9)	1.467(4)	B(5)-B(6)	1.773(5)
N(4)-C(10)	1.465(4)	B(5)-B(10)	1.781(5)
N(4)-C(11)	1.484(3)	B(5)-B(9)	1.784(4)
C(1)- C(3)	1.502(4)	B(6)-B(11)	1.773(4)
C(1)- C(2)	1.573(4)	B(6)-B(10)	1.777(4)
C(1)- B(11)	1.656(4)	B(9)-B(10)	1.763(4)
C(1)- B(2)	1.714(4)	B(10)-B(11)	1.754(4)

Table 3. Angles [deg] for **6a**.

N(3)-Zr(1)-N(2)	116.4(9)	N(3)-Zr(1)-C(2)	83.5(9)
N(3)-Zr(1)-N(4)	89.0(9)	N(2)-Zr(1)-C(2)	153.9(9)
N(2)-Zr(1)-N(4)	80.6(8)	N(4)-Zr(1)-C(2)	118.5(8)
N(3)-Zr(1)-B(11)	144.0(1)	B(11)-Zr(1)-C(2)	61.5(9)
N(2)-Zr(1)-B(11)	95.3(1)	B(10)-Zr(1)-C(2)	62.6(9)
N(4)-Zr(1)-B(11)	114.0(9)	N(1)-Zr(1)-C(2)	78.3(8)
N(3)-Zr(1)-B(10)	130.9(1)	B(9)-Zr(1)-C(2)	36.3(9)
N(2)-Zr(1)-B(10)	108.2(1)	C(1)- Zr(1)-C(2)	34.7(8)
N(4)-Zr(1)-B(10)	78.8(8)	C(4)- N(1)-C(5)	108.6(3)
B(11)-Zr(1)-B(10)	39.9(9)	C(4)- N(1)-C(3)	109.5(3)
N(3)-Zr(1)-N(1)	88.4(9)	C(5)- N(1)-C(3)	107.9(3)
N(2)-Zr(1)-N(1)	85.2(8)	C(4)- N(1)-Zr(1)	117.9(2)
N(4)-Zr(1)-N(1)	162.6(8)	C(5)- N(1)-Zr(1)	114.7(2)
B(11)-Zr(1)-N(1)	77.2(9)	C(3)- N(1)-Zr(1)	97.2(2)
B(10)-Zr(1)-N(1)	115.5(8)	C(6)- N(2)-C(7)	109.2(3)
N(3)-Zr(1)-B(9)	92.0(1)	C(6)- N(2)-Zr(1)	119.4(2)
N(2)-Zr(1)-B(9)	146.9(1)	C(7)- N(2)-Zr(1)	131.0(2)
N(4)-Zr(1)-B(9)	83.5(9)	C(8)- N(3)-C(9)	108.4(2)
B(11)-Zr(1)-B(9)	65.3(1)	C(8)- N(3)-Zr(1)	135.4(2)
B(10)-Zr(1)-B(9)	39.8(1)	C(9)- N(3)-Zr(1)	116.3(2)
N(1)-Zr(1)-B(9)	113.8(9)	C(10)- N(4)-C(11)	109.1(2)
N(3)-Zr(1)-C(1)	108.0(9)	C(10)- N(4)-Zr(1)	123.9(2)
N(2)-Zr(1)-C(1)	119.3(9)	C(11)-N(4)-Zr(1)	110.6(2)
N(4)-Zr(1)-C(1)	140.6(8)	C(3)- C(1)- C(2)	115.7(2)
B(11)-Zr(1)-C(1)	37.2(9)	C(3)- C(1)- B(11)	123.4(2)
B(10)-Zr(1)-C(1)	63.1(9)	C(2)- C(1)- B(11)	111.7(2)
N(1)-Zr(1)-C(1)	56.1(8)	C(3)- C(1)- B(2)	120.8(2)
B(9)-Zr(1)-C(1)	61.2(9)	C(2)- C(1)- B(2)	111.6(2)

B(11)-C(1)- B(2)	63.3(2)	B(4)-B(1)-B(5)	59.3(2)
C(8)- C(1)- B(3)	113.4(2)	B(6)-B(1)-B(5)	59.6(2)
C(2)- C(1)- B(3)	62.9(2)	C(1)- B(2)-B(3)	59.4(2)
B(11)-C(1)- B(3)	114.8(2)	C(1)- B(2)-B(1)	104.7(2)
B(2)-C(1)- B(3)	61.5(2)	B(3)-B(2)-B(1)	60.1(2)
C(8)- C(1)- Zr(1)	95.2(2)	C(1)- B(2)-B(6)	103.4(2)
C(2)- C(1)- Zr(1)	74.0(1)	B(3)-B(2)-B(6)	108.5(3)
B(11)-C(1)- Zr(1)	69.7(1)	B(1)-B(2)-B(6)	60.5(2)
B(2)-C(1)- Zr(1)	131.3(2)	C(1)- B(2)-B(11)	56.8(2)
B(3)-C(1)- Zr(1)	135.2(2)	B(3)-B(2)-B(11)	107.6(2)
C(1)- C(2)- B(9)	111.7(2)	B(1)-B(2)-B(11)	108.3(2)
C(1)- C(2)- B(3)	62.8(2)	B(6)-B(2)-B(11)	60.2(2)
B(9)-C(2)- B(3)	115.6(2)	C(1)- B(3)-C(2)	54.3(2)
C(1)- C(2)- B(4)	112.3(2)	C(1)- B(3)-B(2)	59.0(2)
B(9)-C(2)- B(4)	64.0(2)	C(2)- B(3)-B(2)	102.8(2)
B(3)-C(2)- B(4)	62.2(2)	C(1)- B(3)-B(1)	104.3(2)
C(1)- C(2)- Zr(1)	71.4(1)	C(2)- B(3)-B(1)	104.1(2)
B(9)-C(2)- Zr(1)	70.3(1)	B(2)-B(3)-B(1)	60.1(2)
B(3)-C(2)- Zr(1)	132.5(2)	C(1)- B(3)-B(4)	103.0(2)
B(4)-C(2)- Zr(1)	131.9(2)	C(2)- B(3)-B(4)	59.0(2)
N(1)-C(8)- C(1)	109.9(2)	B(2)-B(3)-B(4)	107.8(2)
B(2)-B(1)-B(3)	59.8(2)	B(1)-B(3)-B(4)	60.1(2)
B(2)-B(1)-B(4)	107.9(2)	C(2)- B(4)-B(5)	102.7(2)
B(3)-B(1)-B(4)	60.5(2)	C(2)- B(4)-B(1)	103.6(2)
B(2)-B(1)-B(6)	59.8(2)	B(5)-B(4)-B(1)	60.8(2)
B(3)-B(1)-B(6)	107.7(2)	C(2)- B(4)-B(3)	58.9(2)
B(4)-B(1)-B(6)	107.3(2)	B(5)-B(4)-B(3)	107.9(3)
B(2)-B(1)-B(5)	107.2(2)	B(1)-B(4)-B(3)	59.4(2)
B(3)-B(1)-B(5)	107.5(2)	C(2)- B(4)-B(9)	55.7(2)

B(5)-B(4)-B(9)	60.3(2)	B(10)-B(9)-B(4)	108.6(2)
B(1)-B(4)-B(9)	107.8(2)	B(5)-B(9)-B(4)	59.2(2)
B(3)-B(4)-B(9)	106.0(2)	C(2)- B(9)-Zr(1)	73.4(1)
B(4)-B(5)-B(6)	107.9(2)	B(10)-B(9)-Zr(1)	69.2(1)
B(4)-B(5)-B(10)	108.9(2)	B(5)-B(9)-Zr(1)	127.0(2)
B(6)-B(5)-B(10)	60.0(2)	B(4)-B(9)-Zr(1)	131.3(2)
B(4)-B(5)-B(9)	60.5(2)	B(11)-B(10)-B(9)	105.0(2)
B(6)-B(5)-B(9)	106.5(2)	B(11)-B(10)-B(6)	60.3(2)
B(10)-B(5)-B(9)	59.3(2)	B(9)-B(10)-B(6)	107.1(2)
B(4)-B(5)-B(1)	59.9(2)	B(11)-B(10)-B(5)	107.3(2)
B(6)-B(5)-B(1)	59.8(2)	B(9)-B(10)-B(5)	60.4(2)
B(10)-B(5)-B(1)	108.2(2)	B(6)-B(10)-B(5)	59.8(2)
B(9)-B(5)-B(1)	107.2(2)	B(11)-B(10)-Zr(1)	69.8(1)
B(2)-B(6)-B(5)	107.9(3)	B(9)-B(10)-Zr(1)	71.1(1)
B(2)-B(6)-B(11)	60.0(2)	B(6)-B(10)-Zr(1)	127.8(2)
B(5)-B(6)-B(11)	106.8(2)	B(5)-B(10)-Zr(1)	129.0(2)
B(2)-B(6)-B(1)	59.7(2)	C(1)- B(11)-B(10)	105.6(2)
B(5)-B(6)-B(1)	60.7(2)	C(1)- B(11)-B(2)	59.9(2)
B(11)-B(6)-B(1)	107.5(2)	B(10)-B(11)-B(2)	109.0(2)
B(2)-B(6)-B(10)	108.2(2)	C(1)- B(11)-B(6)	105.4(2)
B(5)-B(6)-B(10)	60.2(2)	B(10)-B(11)-B(6)	60.5(2)
B(11)-B(6)-B(10)	59.2(2)	B(2)-B(11)-B(6)	59.7(2)
B(1)-B(6)-B(10)	109.1(2)	C(1)- B(11)-Zr(1)	73.0(1)
C(2)- B(9)-B(10)	105.9(2)	B(10)-B(11)-Zr(1)	70.4(1)
C(2)- B(9)-B(5)	105.3(2)	B(2)-B(11)-Zr(1)	131.2(2)
B(10)-B(9)-B(5)	60.3(2)	B(6)-B(11)-Zr(1)	128.6(2)
C(2)- B(9)-B(4)	60.2(2)		

Symmetry transformations used to generate equivalent atoms:

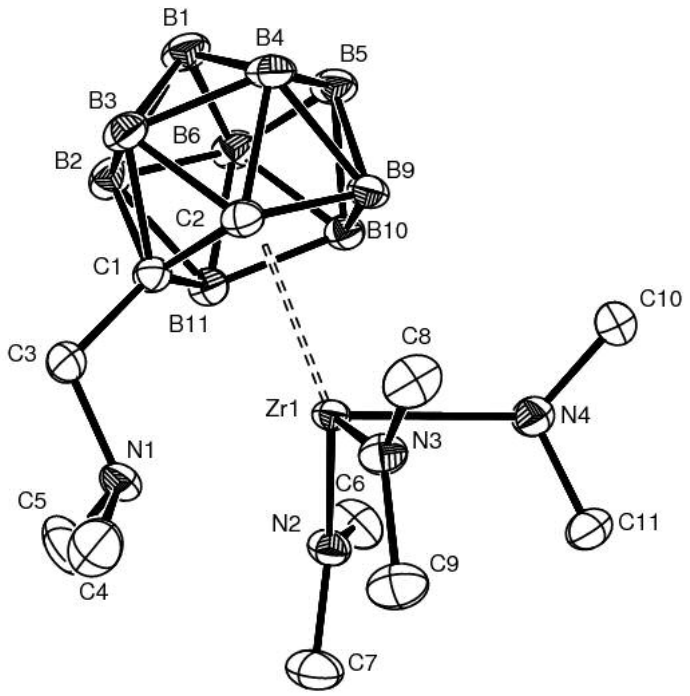


Figure 4. Molecular structure of **6a** with thermal ellipsoids drawn at the 30% level.

Table 1. Crystal data and structure refinement for **8·C_7H_8**.

Identification code	kor173
Empirical formula	$C_{17}B_{18}H_{44}N_2Zr$
Formula weight	562.34
Temperature	293(2) K
Wavelength	0.71070 Å
Crystal system, space group	Monoclinic, $P2_1/c$
Unit cell dimensions	a = 18.0299(1) Å
	b = 10.4035(6) Å β = 96.555(9) °
	c = 16.090(2) Å
Volume	2998.3(5) Å^3
Z, D_{calc}	4, 1.246 g/cm^3
μ	0.380 mm^{-1}
F(000)	1160
Crystal size	0.50 x 0.40 x 0.4 mm
θ range for data collection	1.14 to 25.97 °
Limiting indices	$-22 \le h \le 22$, $0 \le k \le 12$, $0 \le l \le 19$
Reflections collected / unique	6093 / 5868 [R(int) = 0.0336]
Completeness to θ = 25.97	100.0 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5868 / 0 / 368
Goodness-of-fit on F^2	0.589
Final R indices [I>2σ (I)]	[a]R_1 = 0.0356, [b]wR_2 = 0.0913
R indices (all data)	[a]R_1 = 0.0699, [b]wR_2 = 0.1180
Largest diff. peak and hole	0.941 and -0.577 e.Å^{-3}

[a]$R_1 = \sum||F_o|-|F_c|| / \sum|F_o|$ (based on reflections with $F_o^2 > 2\sigma F^2$), [b]$wR_2 = [\sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2)+(0.095P)^2]$; , $P = [\max(F_o^2, 0)+2F_c^2]/3$(also with $F_o^2 > 2\sigma F^2$)

Table 2. Bond lengths [Å] for **8·C_7H_8**.

Zr(1)-N(2)	2.461(3)	B(1)-B(2)	1.752(6)
Zr(1)-C(1)	2.466(3)	B(1)-B(3)	1.765(6)
Zr(1)-C(6)	2.470(3)	B(1)-B(6)	1.781(6)
Zr(1)-B(11)	2.474(4)	B(1)-B(4)	1.783(6)
Zr(1)-N(1)	2.486(3)	B(1)-B(5)	1.786(6)
Zr(1)-C(7)	2.488(3)	B(2)-B(6)	1.762(6)
Zr(1)-B(22)	2.496(4)	B(2)-B(3)	1.770(6)
Zr(1)-C(2)	2.507(3)	B(3)-B(11)	1.771(5)
Zr(1)-B(20)	2.577(4)	B(3)-B(4)	1.773(6)
Zr(1)-B(10)	2.577(4)	B(4)-B(11)	1.764(6)
Zr(1)-B(21)	2.591(4)	B(4)-B(5)	1.766(6)
Zr(1)-B(9)	2.595(4)	B(4)-B(10)	1.784(6)
N(1)-C(5)	1.485(5)	B(5)-B(6)	1.764(6)
N(1)-C(3)	1.487(5)	B(5)-B(10)	1.769(5)
N(1)-C(4)	1.489(5)	B(5)-B(9)	1.769(6)
N(2)-C(10)	1.484(4)	B(6)-B(9)	1.772(6)
N(2)-C(9)	1.487(4)	B(13)-B(22)	1.766(6)
N(2)-C(8)	1.499(4)	B(13)-B(14)	1.768(6)
C(1)-C(3)	1.511(5)	B(13)-B(17)	1.771(7)
C(1)-C(2)	1.597(4)	B(14)-B(15)	1.768(7)
C(1)-B(11)	1.662(5)	B(15)-B(16)	1.763(7)
C(1)-B(3)	1.708(5)	B(15)-B(20)	1.772(6)
C(1)-B(2)	1.714(5)	B(16)-B(17)	1.756(7)
C(2)-B(9)	1.679(5)	B(16)-B(21)	1.763(6)
C(2)-B(6)	1.709(6)	B(16)-B(20)	1.769(7)
C(2)-B(2)	1.731(5)	B(17)-B(22)	1.762(6)
B(9)-B(10)	1.730(6)	B(17)-B(21)	1.775(7)
B(10)-B(11)	1.758(5)	B(20)-B(21)	1.747(7)

C(6)-C(8)	1.494(5)	B(12)-B(16)	1.784(7)
C(6)-C(7)	1.592(5)	B(12)-B(17)	1.784(7)
C(6)-B(22)	1.665(5)	B(21)-B(22)	1.740(6)
C(6)-B(14)	1.706(5)	C(100)-C(105)	1.357(8)
C(6)-B(13)	1.708(5)	C(100)-C(101)	1.412(9)
C(7)-B(20)	1.675(6)	C(100)-C(106)	1.492(9)
C(7)-B(15)	1.711(5)	C(101)-C(102)	1.415(10)
C(7)-B(14)	1.733(5)	C(102)-C(103)	1.288(9)
B(12)-B(14)	1.750(6)	C(103)-C(104)	1.331(8)
B(12)-B(13)	1.760(7)	C(104)-C(105)	1.366(8)
B(12)-B(15)	1.773(7)		

Table 3. Angles [deg] for **8·C$_7$H$_8$**.

N(2)-Zr(1)-C(1)	119.8(9)	B(5)-B(6)-B(9)	60.0(2)
N(2)-Zr(1)-C(6)	59.0(1)	C(2)-B(6)-B(1)	104.6(3)
C(1)-Zr(1)-C(6)	178.8(1)	B(2)-B(6)-B(1)	59.3(2)
N(2)-Zr(1)-B(11)	83.4(1)	B(5)-B(6)-B(1)	60.5(3)
C(1)-Zr(1)-B(11)	39.3(1)	B(9)-B(6)-B(1)	108.2(3)
C(6)-Zr(1)-B(11)	139.5(1)	C(2)-B(9)-B(10)	105.5(3)
N(2)-Zr(1)-N(1)	103.4(1)	C(2)-B(9)-B(5)	105.1(3)
C(1)-Zr(1)-N(1)	58.8(1)	B(10)-B(9)-B(5)	60.7(2)
C(6)-Zr(1)-N(1)	121.2(1)	C(2)-B(9)-B(6)	59.3(2)
B(11)-Zr(1)-N(1)	78.9(1)	B(10)-B(9)-B(6)	108.9(3)
N(2)-Zr(1)-C(7)	84.4(1)	B(5)-B(9)-B(6)	59.7(2)
C(1)-Zr(1)-C(7)	143.2(1)	C(2)-B(9)-Zr(1)	68.0(2)
C(6)-Zr(1)-C(7)	37.5(1)	B(10)-B(9)-Zr(1)	70.0(2)
B(11)-Zr(1)-C(7)	133.7(1)	B(5)-B(9)-Zr(1)	126.2(2)
N(1)-Zr(1)-C(7)	147.4(1)	B(6)-B(9)-Zr(1)	124.9(2)
N(2)-Zr(1)-B(22)	79.6(1)	B(9)-B(10)-B(11)	106.3(3)
C(1)-Zr(1)-B(22)	141.4(1)	B(9)-B(10)-B(5)	60.7(2)
C(6)-Zr(1)-B(22)	39.2(1)	B(11)-B(10)-B(5)	106.7(3)
B(11)-Zr(1)-B(22)	153.4(1)	B(9)-B(10)-B(4)	108.0(3)
N(1)-Zr(1)-B(22)	85.4(1)	B(11)-B(10)-B(4)	59.7(2)
C(7)-Zr(1)-B(22)	64.7(1)	B(5)-B(10)-B(4)	59.6(2)
N(2)-Zr(1)-C(2)	145.3(1)	B(9)-B(10)-Zr(1)	71.0(2)
C(1)-Zr(1)-C(2)	37.5(1)	B(11)-B(10)-Zr(1)	66.5(2)
C(6)-Zr(1)-C(2)	143.5(1)	B(5)-B(10)-Zr(1)	127.2(3)
B(11)-Zr(1)-C(2)	64.9(1)	B(4)-B(10)-Zr(1)	123.5(2)
N(1)-Zr(1)-C(2)	84.8(1)	C(1)-B(11)-B(10)	106.3(3)
C(7)-Zr(1)-C(2)	106.9(1)	C(1)-B(11)-B(4)	106.0(3)
B(22)-Zr(1)-C(2)	135.1(1)	B(10)-B(11)-B(4)	60.9(2)

N(2)-Zr(1)-B(20)	121.5(1)	C(1)-B(11)-B(3)	59.6(2)
C(1)-Zr(1)-B(20)	116.4(1)	B(10)-B(11)-B(3)	109.6(3)
C(6)-Zr(1)-B(20)	64.8(1)	B(4)-B(11)-B(3)	60.2(2)
B(11)-Zr(1)-B(20)	140.1(1)	C(1)-B(11)-Zr(1)	70.1(2)
N(1)-Zr(1)-B(20)	118.8(1)	B(10)-B(11)-Zr(1)	72.8(2)
C(7)-Zr(1)-B(20)	38.6(1)	B(4)-B(11)-Zr(1)	130.5(2)
B(22)-Zr(1)-B(20)	66.5(2)	B(3)-B(11)-Zr(1)	128.3(2)
C(2)-Zr(1)-B(20)	80.6(1)	C(8)-C(6)-C(7)	116.6(3)
N(2)-Zr(1)-B(10)	82.4(1)	C(8)-C(6)-B(22)	123.9(3)
C(1)-Zr(1)-B(10)	65.7(1)	C(7)-C(6)-B(22)	110.0(3)
C(6)-Zr(1)-B(10)	113.7(1)	C(8)-C(6)-B(14)	113.6(3)
B(11)-Zr(1)-B(10)	40.7(1)	C(7)-C(6)-B(14)	63.3(2)
N(1)-Zr(1)-B(10)	118.7(1)	B(22)-C(6)-B(14)	114.3(3)
C(7)-Zr(1)-B(10)	93.5(1)	C(8)-C(6)-B(13)	119.9(3)
B(22)-Zr(1)-B(10)	152.8(1)	C(7)-C(6)-B(13)	112.4(3)
C(2)-Zr(1)-B(10)	64.5(1)	B(22)-C(6)-B(13)	63.1(2)
B(20)-Zr(1)-B(10)	107.2(1)	B(14)-C(6)-B(13)	62.3(2)
N(2)-Zr(1)-B(21)	118.7(1)	C(8)-C(6)-Zr(1)	94.8(2)
C(1)-Zr(1)-B(21)	115.7(1)	C(7)-C(6)-Zr(1)	71.9(2)
C(6)-Zr(1)-B(21)	65.4(1)	B(22)-C(6)-Zr(1)	71.3(2)
B(11)-Zr(1)-B(21)	155.0(1)	B(14)-C(6)-Zr(1)	134.0(2)
N(1)-Zr(1)-B(21)	84.2(1)	B(13)-C(6)-Zr(1)	132.8(2)
C(7)-Zr(1)-B(21)	64.8(1)	C(6)-C(7)-B(20)	111.8(3)
B(22)-Zr(1)-B(21)	40.0(1)	C(6)-C(7)-B(15)	110.9(3)
C(2)-Zr(1)-B(21)	95.5(1)	B(20)-C(7)-B(15)	63.1(2)
B(20)-Zr(1)-B(21)	39.5(2)	C(6)-C(7)-B(14)	61.6(2)
B(10)-Zr(1)-B(21)	145.8(1)	B(20)-C(7)-B(14)	114.4(3)
N(2)-Zr(1)-B(9)	117.1(1)	B(15)-C(7)-B(14)	61.8(2)
C(1)-Zr(1)-B(9)	64.7(1)	C(6)-C(7)-Zr(1)	70.7(2)

C(6)-Zr(1)-B(9)	115.6(1)	B(20)-C(7)-Zr(1)	73.6(2)
B(11)-Zr(1)-B(9)	66.8(1)	B(15)-C(7)-Zr(1)	134.0(2)
N(1)-Zr(1)-B(9)	121.5(1)	B(14)-C(7)-Zr(1)	131.1(2)
C(7)-Zr(1)-B(9)	79.9(1)	C(6)-C(8)-N(2)	108.3(3)
B(22)-Zr(1)-B(9)	139.7(1)	B(14)-B(12)-B(13)	60.5(3)
C(2)-Zr(1)-B(9)	38.4(1)	B(14)-B(12)-B(15)	60.3(3)
B(20)-Zr(1)-B(9)	73.9(1)	B(13)-B(12)-B(15)	107.9(3)
B(10)-Zr(1)-B(9)	39.1(1)	B(14)-B(12)-B(16)	107.8(3)
B(21)-Zr(1)-B(9)	108.2(2)	B(13)-B(12)-B(16)	107.0(3)
C(5)-N(1)-C(3)	109.3(3)	B(15)-B(12)-B(16)	59.4(3)
C(5)-N(1)-C(4)	105.4(3)	B(14)-B(12)-B(17)	108.3(3)
C(3)-N(1)-C(4)	107.7(3)	B(13)-B(12)-B(17)	60.0(3)
C(5)-N(1)-Zr(1)	122.6(2)	B(15)-B(12)-B(17)	106.9(3)
C(3)-N(1)-Zr(1)	94.4(2)	B(16)-B(12)-B(17)	59.0(3)
C(4)-N(1)-Zr(1)	116.1(2)	C(6)-B(13)-B(12)	104.1(3)
C(10)-N(2)-C(9)	105.3(3)	C(6)-B(13)-B(22)	57.2(2)
C(10)-N(2)-C(8)	109.0(3)	B(12)-B(13)-B(22)	107.4(3)
C(9)-N(2)-C(8)	109.8(3)	C(6)-B(13) -B(14)	58.8(2)
C(10)-N(2)-Zr(1)	125.6(2)	B(12)-B(13)-B(14)	59.5(3)
C(9)-N(2)-Zr(1)	111.3(2)	B(22)-B(13)-B(14)	106.6(3)
C(8)-N(2)-Zr(1)	95.1(2)	C(6)-B(13)-B(17)	104.0(3)
C(3)-C(1)-C(2)	116.0(3)	B(12)-B(13)-B(17)	60.7(3)
C(3)-C(1)-B(11)	124.1(3)	B(22)-B(13)-B(17)	59.8(2)
C(2)-C(1)-B(11)	110.2(3)	B(14)-B(13)-B(17)	108.1(3)
C(3)-C(1)-B(3)	120.4(3)	C(6)-B(14)-C(7)	55.1(2)
C(2)-C(1)-B(3)	112.3(3)	C(6)-B(14)-B(12)	104.6(3)
B(11)-C(1)-B(3)	63.4(2)	C(7)-B(14)-B(12)	104.6(3)
C(3)-C(1)-B(2)	113.7(3)	C(6)-B(14)-B(13)	58.9(2)
C(2)-C(1)-B(2)	62.9(2)	C(7)-B(14)-B(13)	103.2(3)

B(11)-C(1)-B(2)	114.3(3)	B(12)-B(14)-B(13)	60.0(3)
B(3)-C(1)-B(2)	62.3(2)	C(6)-B(14)-B(15)	103.1(3)
C(3)-C(1)-Zr(1)	94.5(2)	C(7)-B(14)-B(15)	58.5(2)
C(2)-C(1)-Zr(1)	72.7(2)	B(12)-B(14)-B(15)	60.5(3)
B(11)-C(1)-Zr(1)	70.6(2)	B(13)-B(14)-B(15)	107.8(3)
B(3)-C(1)-Zr(1)	132.5(2)	C(7)-B(15)-B(16)	103.7(3)
B(2)-C(1)-Zr(1)	134.2(2)	C(7)-B(15)-B(14)	59.7(2)
C(1)-C(2)-B(9)	111.7(3)	B(16)-B(15)-B(14)	107.9(3)
C(1)-C(2)-B(6)	111.1(3)	C(7)-B(15)-B(20)	57.4(2)
B(9)-C(2)-B(6)	63.1(2)	B(16)-B(15)-B(20)	60.1(3)
C(1)-C(2)-B(2)	61.9(2)	B(14)-B(15)-B(20)	108.0(3)
B(9)-C(2)-B(2)	114.2(3)	C(7)-B(15)-B(12)	104.5(3)
B(6)-C(2)-B(2)	61.6(2)	B(16)-B(15)-B(12)	60.6(3)
C(1)-C(2)-Zr(1)	69.9(2)	B(14)-B(15)-B(12)	59.2(3)
B(9)-C(2)-Zr(1)	73.6(2)	B(20)-B(15)-B(12)	108.3(3)
B(6)-C(2)-Zr(1)	133.8(2)	B(17)-B(16)-B(15)	108.5(3)
B(2)-C(2)-Zr(1)	130.5(2)	B(17)-B(16)-B(21)	60.6(3)
N(1)-C(3)-C(1)	108.3(3)	B(15)-B(16)-B(21)	108.2(3)
B(2)-B(1)-B(3)	60.4(2)	B(17)-B(16)-B(20)	107.8(3)
B(2)-B(1)-B(6)	59.8(2)	B(15)-B(16)-B(20)	60.2(3)
B(3)-B(1)-B(6)	107.6(3)	B(21)-B(16)-B(20)	59.3(3)
B(2)-B(1)-B(4)	108.0(3)	B(17)-B(16)-B(12)	60.5(3)
B(3)-B(1)-B(4)	60.0(2)	B(15)-B(16)-B(12)	60.0(3)
B(6)-B(1)-B(4)	106.6(3)	B(21)-B(16)-B(12)	108.9(3)
B(2)-B(1)-B(5)	107.5(3)	B(20)-B(16)-B(12)	108.0(3)
B(3)-B(1)-B(5)	107.4(3)	B(16)-B(17)-B(22)	106.0(3)
B(6)-B(1)-B(5)	59.3(3)	B(16)-B(17)-B(13)	107.8(3)
B(4)-B(1)-B(5)	59.3(2)	B(22)-B(17)-B(13)	60.0(2)
C(1)-B(2)-C(2)	55.3(2)	B(16)-B(17)-B(21)	59.9(3)

C(1)-B(2)-B(1)	104.7(3)	B(22)-B(17)-B(21)	58.9(2)
C(2)-B(2)-B(1)	104.9(3)	B(13)-B(17)-B(21)	108.1(3)
C(1)-B(2)-B(6)	103.4(3)	B(16)-B(17)-B(12)	60.5(3)
C(2)-B(2)-B(6)	58.6(2)	B(22)-B(17)-B(12)	106.5(3)
B(1)-B(2)-B(6)	60.9(3)	B(13)-B(17)-B(12)	59.3(3)
C(1)-B(2)-B(3)	58.7(2)	B(21)-B(17)-B(12)	108.3(4)
C(2)-B(2)-B(3)	103.3(2)	C(7)-B(20)-B(21)	105.4(3)
B(1)-B(2)-B(3)	60.1(3)	C(7)-B(20)-B(16)	105.0(3)
B(6)-B(2)-B(3)	108.2(3)	B(21)-B(20)-B(16)	60.2(3)
C(1)-B(3)-B(1)	104.4(3)	C(7)-B(20)-B(15)	59.5(2)
C(1)-B(3)-B(2)	59.0(2)	B(21)-B(20)-B(15)	108.6(3)
B(1)-B(3)-B(2)	59.4(2)	B(16)-B(20)-B(15)	59.7(3)
C(1)-B(3)-B(11)	57.0(2)	C(7)-B(20)-Zr(1)	67.8(2)
B(1)-B(3)-B(11)	107.4(3)	B(21)-B(20)-Zr(1)	70.7(2)
B(2)-B(3)-B(11)	106.5(3)	B(16)-B(20)-Zr(1)	126.5(3)
C(1)-B(3)-B(4)	103.6(3)	B(15)-B(20)-Zr(1)	125.1(3)
B(1)-B(3)-B(4)	60.5(2)	B(22)-B(21)-B(20)	105.9(3)
B(2)-B(3)-B(4)	107.6(3)	B(22)-B(21)-B(16)	106.7(3)
B(11)-B(3)-B(4)	59.7(2)	B(20)-B(21)-B(16)	60.5(3)
B(11)-B(4)-B(5)	106.6(3)	B(22)-B(21)-B(17)	60.2(3)
B(11)-B(4)-B(3)	60.1(2)	B(20)-B(21)-B(17)	107.9(3)
B(5)-B(4)-B(3)	107.9(3)	B(16)-B(21)-B(17)	59.5(3)
B(11)-B(4)-B(1)	106.9(3)	B(22)-B(21)-Zr(1)	67.1(2)
B(5)-B(4)-B(1)	60.4(2)	B(20)-B(21)-Zr(1)	69.8(2)
B(3)-B(4)-B(1)	59.5(2)	B(16)-B(21)-Zr(1)	126.0(3)
B(11)-B(4)-B(10)	59.4(2)	B(17)-B(21)-Zr(1)	124.2(3)
B(5)-B(4)-B(10)	59.8(2)	C(6)-B(22)-B(21)	106.9(3)
B(3)-B(4)-B(10)	108.4(3)	C(6)-B(22)-B(17)	106.2(3)
B(1)-B(4)-B(10)	108.2(3)	B(21)-B(22)-B(17)	60.9(3)

B(6)-B(5)-B(4)	108.1(3)	C(6)-B(22)-B(13)	59.7(2)
B(6)-B(5)-B(10)	107.6(3)	B(21)-B(22)-B(13)	109.9(3)
B(4)-B(5)-B(10)	60.6(2)	B(17)-B(22)-B(13)	60.3(3)
B(6)-B(5)-B(9)	60.2(2)	C(6)-B(22)-Zr(1)	69.6(2)
B(4)-B(5)-B(9)	107.1(3)	B(21)-B(22)-Zr(1)	73.0(2)
B(10)-B(5)-B(9)	58.5(2)	B(17)-B(22)-Zr(1)	130.4(3)
B(6)-B(5)-B(1)	60.2(2)	B(13)-B(22)-Zr(1)	127.8(2)
B(4)-B(5)-B(1)	60.2(3)	C(105)-C(100)-C(101)	117.1(6)
B(10)-B(5) -B(1)	108.8(3)	C(105)-C(100)-C(106)	120.6(8)
B(9)-B(5)-B(1)	108.1(3)	C(101)-C(100)-C(106)	122.3(8)
C(2)-B(6)-B(2)	59.8(2)	C(100)-C(101)-C(102)	118.2(6)
C(2)-B(6)-B(5)	104.0(3)	C(103)-C(102)-C(101)	121.8(7)
B(2)-B(6)-B(5)	108.1(3)	C(102)-C(103)-C(104)	120.1(7)
C(2)-B(6)-B(9)	57.6(2)	C(103)-C(104)-C(105)	121.9(7)
B(2)-B(6)-B(9)	108.2(3)	C(100)-C(105)-C(104)	120.9(6)

Symmetry transformations used to generate equivalent atoms:

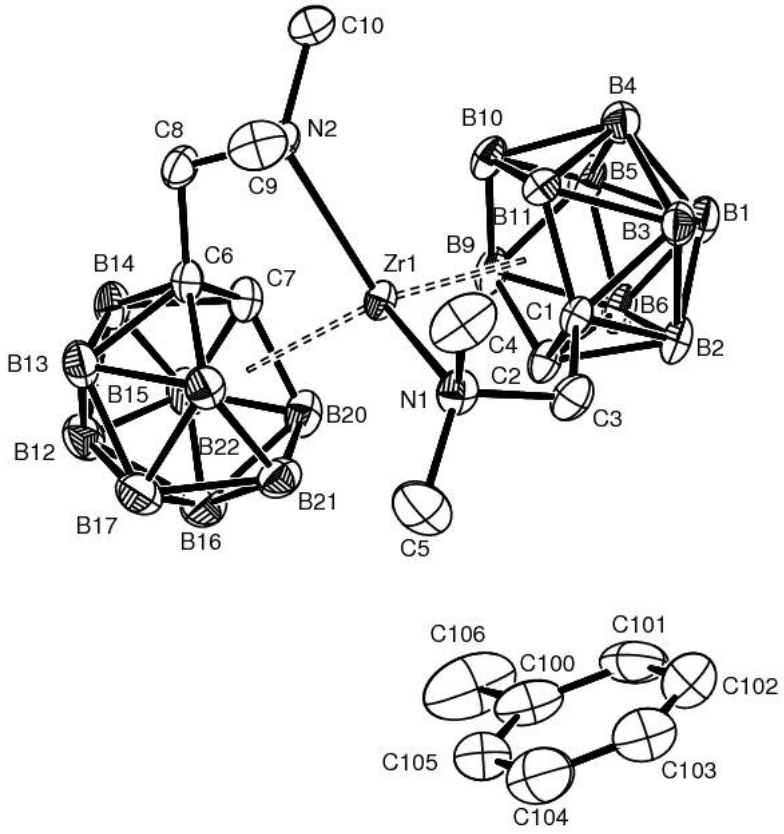


Figure 5. Molecular structure of **8·C_7H_8** with thermal ellipsoids drawn at the 30% level.

Table 1. Crystal data and structure refinement for **11·C_6H_6**.

Identification code	kor520
Empirical formula	C_{23} H_{34} B_9 N O_2 Ti
Formula weight	501.70
Temperature	233(2)K
Wavelength	0.71073Å
Crystal system, space group	Monoclinic, P $2_1/m$
Unit cell dimensions	a = 7.6576(3) Å
	b = 20.2081(9) Å β = 111.729 (1) °
	c = 9.4735(4) Å
Volume	1361.8(1) Å^3
Z, D_{calc}	2, 1.224 g/cm^3
μ	0.336 mm^{-1}
F(000)	524
Crystal size	0.18 x 0.16 x 0.14 mm
θ range for data collection	2.02 to 28.34 °
Limiting indices	$-10 \leq h \leq 10$, $-26 \leq k \leq 26$, $-12 \leq l \leq 12$
Reflections collected / unique	18785 / 3476 [R(int) = 0.0573]
Completeness to θ = 25.96	99.8 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3476 / 0 / 185
Goodness-of-fit on F^2	1.027
Final R indices [I>2σ (I)]	[a]R_1 = 0.0459, [b]wR_2 = 0.0964
R indices (all data)	[a]R_1 = 0.0996, [b]wR_2 = 0.1247
Largest diff. peak and hole	0.321 and -0.316 e.Å^{-3}

[a]$R_1 = \sum||F_o|-|F_c||$ (based on reflections with $F_o^2>2\sigma F^2$), [b]$wR_2 = [\sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2)+(0.095P)^2]$; , $P = [\max(F_o^2, 0)+2F_c^2]/3$(also with $F_o^2>2\sigma F^2$)

Table 2. Bond lengths [Å] for **11·C_6H_6**.

Ti(1)-O(1)	1.7789(2)	B(3)-C(2)	1.734(4)
Ti(1)-O(1)*	1.7789(2)	B(3)-B(3)*	1.770(8)
Ti(1)-N(1)	2.177(3)	B(4)-B(2)*	1.755(4)
Ti(1)-C(1)	2.332(3)	B(4)-B(5)*	1.776(4)
Ti(1)-C(2)	2.352(2)	B(4)-B(5)	1.776(4)
Ti(1)-B(6)*	2.352(2)	B(5)-C(2)	1.704(4)
Ti(1)-C(2)*	2.352(2)	B(5)-B(5)*	1.757(6)
Ti(1)-B(5)	2.387(3)	C(2)-C(1)	1.619(3)
Ti(1)-B(5)*	2.387(3)	C(1)-C(3)	1.508(5)
O(1)-C(5)	1.353(3)	C(1)-B(6)*	1.619(3)
N(1)-C(4)	1.489(3)	C(1)-C(2)*	1.619(3)
N(1)-C(4)*	1.489(3)	C(1)-B(3)*	1.707(4)
N(1)-C(3)	1.491(4)	C(5)-C(6)	1.372(3)
B(1)-B(3)*	1.757(5)	C(5)-C(10)	1.379(3)
B(1)-B(3)	1.757(5)	C(6)-C(7)	1.364(4)
B(1)-B(4)	1.763(7)	C(7)-C(8)	1.357(4)
B(1)-B(2)*	1.771(5)	C(8)-C(9)	1.382(4)
B(1)-B(2)	1.771(5)	C(9)-C(10)	1.386(4)
B(2)-C(2)	1.722(4)	C(101)-C(103)	1.360(4)
B(2)-B(4)	1.755(4)	C(101)-C(102)	1.365(4)
B(2)-B(3)	1.766(5)	C(102)-C(103)*	1.358(4)
B(2)-B(5)	1.775(4)	C(103)-C(102)*	1.358(4)
B(3)-C(1)	1.707(4)		

Symmetry transformations used to generate equivalent atoms:

* x, -y+1/2, z ** -x+1, -y+1, -z+1

Table 3. Angles [deg] for **11·C_6H_6**.

O(1)-Ti(1)-O(1)*	102.3(1)	O(1)-Ti(1)-B(5)*	92.7(9)
O(1)-Ti(1)-N(1)	98.3(7)	O(1)*-Ti(1)-B(5)*	128.3(9)
O(1)*-Ti(1)-N(1)	98.3(7)	N(1)-Ti(1)-B(5)*	128.3(1)
O(1)-Ti(1)-C(1)	127.6(6)	C(1)-Ti(1)-B(5)*	69.9(1)
O(1)*-Ti(1)-C(1)	127.6(6)	C(2)-Ti(1)-B(5)*	71.1(1)
N(1)-Ti(1)-C(1)	63.5(1)	B(6)*-Ti(1)-B(5)*	42.1(1)
O(1)-Ti(1)-C(2)	162.1(9)	C(2)*-Ti(1)-B(5)*	42.1(1)
O(1)*-Ti(1)-C(2)	93.9(9)	B(5)-Ti(1)-B(5)*	43.2(1)
N(1)-Ti(1)-C(2)	86.7(9)	C(5)-O(1)-Ti(1)	172.4(2)
C(1)-Ti(1)-C(2)	40.5(8)	C(4)-N(1)-C(4)*	108.5(3)
O(1)-Ti(1)-B(6)*	93.9(9)	C(4)-N(1)-C(3)	111.8(2)
O(1)*-Ti(1)-B(6)*	162.1(9)	C(4)*-N(1)-C(3)	111.8(2)
N(1)-Ti(1)-B(6)*	86.7(9)	C(4)-N(1)-Ti(1)	112.7(2)
C(1)-Ti(1)-B(6)*	40.5(8)	C(4)*-N(1)-Ti(1)	112.7(2)
C(2)-Ti(1)-B(6)*	69.2(1)	C(3)-N(1)-Ti(1)	99.3(2)
O(1)-Ti(1)-C(2)*	93.9(9)	B(3)*-B(1)-B(3)	60.5(3)
O(1)*-Ti(1)-C(2)*	162.1(9)	B(3)*-B(1)-B(4)	107.8(3)
N(1)-Ti(1)-C(2)*	86.7(9)	B(3)-B(1)-B(4)	107.8(3)
C(1)-Ti(1)-C(2)*	40.5(8)	B(3)*-B(1)-B(2)*	60.1(2)
C(2)-Ti(1)-C(2)*	69.2(1)	B(3)-B(1)-B(2)*	108.2(3)
O(1)-Ti(1)-B(5)	128.3(9)	B(4)-B(1)-B(2)*	59.6(2)
O(1)*-Ti(1)-B(5)	92.7(9)	B(3)*-B(1)-B(2)	108.2(3)
N(1)-Ti(1)-B(5)	128.3(1)	B(3)-B(1)-B(2)	60.1(2)
C(1)-Ti(1)-B(5)	69.9(1)	B(4)-B(1)-B(2)	59.6(2)
C(2)-Ti(1)-B(5)	42.1(1)	B(2)*-B(1)-B(2)	107.4(3)
B(6)*-Ti(1)-B(5)	71.1(1)	B(2)*-B(4)-B(2)	108.8(3)
C(2)*-Ti(1)-B(5)	71.1(1)	B(2)*-B(4)-B(1)	60.5(2)
C(2)-B(2)-B(4)	105.1(2)	B(2)-B(4)-B(1)	60.5(2)

C(2)-B(2)-B(3)	59.6(2)	B(2)*-B(4)-B(5)*	60.4(2)
B(4)-B(2)-B(3)	107.7(3)	B(2)-B(4)-B(5)*	108.0(2)
C(2)-B(2)-B(1)	105.5(2)	B(1)-B(4)-B(5)*	108.6(3)
B(4)-B(2)-B(1)	60.0(2)	B(2)*-B(4)-B(5)	108.0(2)
B(3)-B(2)-B(1)	59.6(2)	B(2)-B(4)-B(5)	60.4(2)
C(2)-B(2)-B(5)	58.3(2)	B(1)-B(4)-B(5)	108.6(3)
B(4)-B(2)-B(5)	60.4(2)	B(5)*-B(4)-B(5)	59.3(2)
B(3)-B(2)-B(5)	108.1(2)	C(2)-B(5)-B(5)*	105.6(1)
B(1)-B(2)-B(5)	108.3(2)	C(2)-B(5)-B(2)	59.3(2)
C(1)-B(3)-C(2)	56.1(2)	B(5)*-B(5)-B(2)	108.0(2)
C(1)-B(3)-B(1)	103.8(2)	C(2)-B(5)-B(4)	105.0(2)
C(2)-B(3)-B(1)	105.6(3)	B(5)*-B(5)-B(4)	60.4(1)
C(1)-B(3)-B(2)	103.1(2)	B(2)-B(5)-B(4)	59.3(2)
C(2)-B(3)-B(2)	58.9(2)	C(2)-B(5)-Ti(1)	67.8(1)
B(1)-B(3)-B(2)	60.4(2)	B(5)*-B(5)-Ti(1)	68.4(7)
C(1)-B(3)-B(3)*	58.8(1)	B(2)-B(5)-Ti(1)	123.9(2)
C(2)-B(3)-B(3)*	105.0(2)	B(4)-B(5)-Ti(1)	124.0(2)
B(1)-B(3)-B(3)*	59.8(2)	C(3)-C(1)-B(3)*	121.3(2)
B(2)-B(3)-B(3)*	107.9(2)	B(6)*-C(1)-B(3)*	62.8(2)
C(1)-C(2)-B(5)	108.9(2)	C(2)*-C(1)-B(3)*	62.8(2)
C(1)-C(2)-B(2)	109.0(2)	C(2)-C(1)-B(3)*	113.4(2)
B(5)-C(2)-B(2)	62.4(2)	B(3)-C(1)-B(3)*	62.4(3)
C(1)-C(2)-B(3)	61.1(2)	C(3)-C(1)-Ti(1)	92.4(2)
B(5)-C(2)-B(3)	112.9(2)	B(6)*-C(1)-Ti(1)	70.4(1)
B(2)-C(2)-B(3)	61.4(2)	C(2)*-C(1)-Ti(1)	70.4(1)
C(1)-C(2)-Ti(1)	69.1(1)	C(2)-C(1)-Ti(1)	70.4(1)
B(5)-C(2)-Ti(1)	70.0(1)	B(3)-C(1)-Ti(1)	131.1(2)
B(2)-C(2)-Ti(1)	128.8(2)	B(3)*-C(1)-Ti(1)	131.1(2)
B(3)-C(2)-Ti(1)	128.2(2)	N(1)-C(3)-C(1)	104.8(3)

C(3)-C(1)-B(6)*	118.1(2)	O(1)-C(5)-C(10)	118.7(2)
C(3)-C(1)-C(2)*	118.1(2)	C(6)-C(5)-C(10)	120.5(2)
C(3)-C(1)-C(2)	118.1(2)	C(7)-C(6)-C(5)	120.3(3)
B(6)*-C(1)-C(2)	111.0(3)	C(8)-C(7)-C(6)	120.3(3)
C(2)*-C(1)-C(2)	111.0(3)	C(7)-C(8)-C(9)	120.1(3)
C(3)-C(1)-B(3)	121.3(2)	C(8)-C(9)-C(10)	120.2(3)
B(6)*-C(1)-B(3)	113.4(2)	C(5)-C(10)-C(9)	118.6(3)
C(2)*-C(1)-B(3)	113.4(2)	C(103)-C(101)-C(102)	120.1(3)
C(2)-C(1)-B(3)	62.8(2)	C(103)*-C(102)-C(101)	120.2(3)
O(1)-C(5)-C(6)	120.8(2)	C(102)*-C(103)-C(101)	119.7(3)

Symmetry transformations used to generate equivalent atoms:

* x, -y+1/2, z ** -x+1, -y+1, -z+1

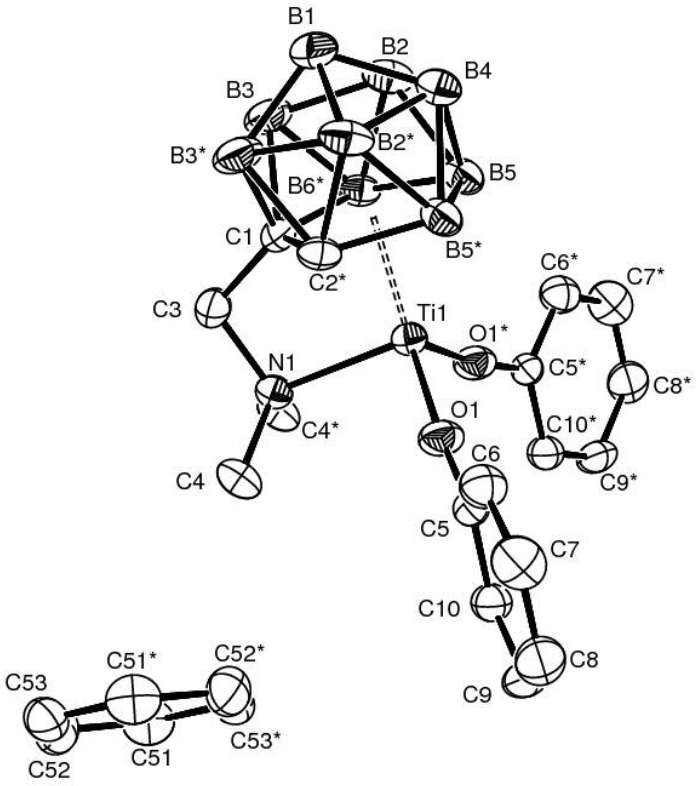


Figure 6. Molecular structure of **11·C_6H_6** with thermal ellipsoids drawn at the 30% level.

Table 1. Crystal data and structure refinement for **12·C_6H_6**.

Identification code	kor506
Empirical formula	C_{25} H_{38} B_9 N O_2 Ti
Formula weight	529.75
Temperature	233(2)K
Wavelength	0.71073Å
Crystal system, space group	Monoclinic, $P2_1/c$
Unit cell dimensions	a = 11.7288(7) Å
	b = 11.7786(7) Å β = 91.940(2) °
	c = 22.3691(1) Å
Volume	3088.5(3) Å^3
Z, D_{calc}	4, 1.139 g/cm^3
μ	0.300 mm^{-1}
F(000)	1112
Crystal size	0.2 x 0.17 x 0.09 mm
θ range for data collection	1.74 to 28.31 °
Limiting indices	$-15 \leq h \leq 15$, $-15 \leq k \leq 15$, $-28 \leq l \leq 29$
Reflections collected / unique	31249 / 7664 [R(int) = 0.1214]
Completeness to θ = 25.96	99.7 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7664 / 9 / 356
Goodness-of-fit on F^2	0.995
Final R indices [I>2σ (I)]	[a]R_1 = 0.0811, [b]wR_2 = 0.2134
R indices (all data)	[a]R_1 = 0.2357, [b]wR_2 = 0.3167
Largest diff. peak and hole	0.559 and -0.339 e.Å^{-3}

[a]$R_1 = \sum||F_o|-|F_c||$ (based on reflections with $F_o^2>2\sigma F^2$), [b]$wR_2 = [\sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2)+(0.095P)^2]$; , $P = [\max(F_o^2, 0)+2F_c^2]/3$(also with $F_o^2>2\sigma F^2$)

Table 3. Bond lengths [Å] for **12**·C_6H_6.

Ti(1)-O(1)	1.782(3)	B(8)-B(9)	1.800(1)
Ti(1)-O(2)	1.783(4)	B(9)-C(2)	1.695(9)
Ti(1)-N(1)	2.190(4)	B(9)-B(10)	1.759(9)
Ti(1)-C(1)	2.327(5)	B(10)-B(11)	1.718(8)
Ti(1)-C(2)	2.343(6)	B(11)-C(1)	1.640(8)
Ti(1)-B(11)	2.344(6)	C(1)-C(3)	1.503(7)
Ti(1)-B(9)	2.362(6)	C(1)-C(2)	1.594(8)
Ti(1)-B(10)	2.395(6)	C(13)-C(18)	1.378(7)
O(2)-C(13)	1.360(6)	C(13)-C(14)	1.387(7)
O(1)-C(6)	1.353(6)	C(14)-C(15)	1.409(8)
N(1)-C(5)	1.475(7)	C(14)-C(19)	1.505(8)
N(1)-C(3)	1.476(7)	C(15)-C(16)	1.368(8)
N(1)-C(4)	1.484(7)	C(16)-C(17)	1.356(9)
B(3)-B(5)	1.745(1)	C(17)-C(18)	1.386(8)
B(3)-B(4)	1.754(1)	C(6)-C(11')	1.288(1)
B(3)-B(8)	1.772(1)	C(6)-C(7)	1.431(9)
B(3)-B(6)	1.773(9)	C(6)-C(11)	1.720(3)
B(3)-B(7)	1.780(1)	C(7)-C(8')	1.355(1)
B(4)-C(2)	1.713(1)	C(7)-C(12)	1.486(1)
B(4)-C(1)	1.717(9)	C(7)-C(8)	1.660(4)
B(4)-B(8)	1.748(1)	C(8)-C(9)	1.370(5)
B(4)-B(5)	1.782(1)	C(9)-C(10)	1.380(5)
B(5)-C(1)	1.709(8)	C(10)-C(11)	1.400(4)
B(5)-B(11)	1.751(8)	C(8')-C(9')	1.398(2)
B(5)-B(6)	1.753(1)	C(9')-C(10')	1.342(2)
B(6)-B(11)	1.740(9)	C(10')-C(11')	1.422(2)
B(6)-B(7)	1.758(9)	C(105)-C(104)	1.330(2)
B(6)-B(10)	1.780(8)	C(105)-C(106)	1.394(2)

B(7)-B(10)	1.767(9)	C(104)-C(103)	1.407(2)
B(7)-B(8)	1.772(1)	C(103)-C(102)	1.422(1)
B(7)-B(9)	1.782(9)	C(102)-C(101)	1.500(2)
B(8)-C(2)	1.719(9)	C(101)-C(106)	1.374(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Angles [deg] for **12·C_6H_6**.

O(1)-Ti(1)-O(2)	103.3(2)	B(3)-B(8)-B(9)	107.8(5)
O(1)-Ti(1)-N(1)	98.3(2)	B(7)-B(8)-B(9)	59.8(4)
O(2)-Ti(1)-N(1)	102.0(2)	C(2)-B(9)-B(10)	105.7(4)
O(1)-Ti(1)-C(1)	126.7(2)	C(2)-B(9)-B(7)	104.4(5)
O(2)-Ti(1)-C(1)	128.5(2)	B(10)-B(9)-B(7)	59.9(4)
N(1)-Ti(1)-C(1)	63.1(2)	C(2)-B(9)-B(8)	58.9(4)
O(1)-Ti(1)-C(2)	93.6(2)	B(10)-B(9)-B(8)	108.0(4)
O(2)-Ti(1)-C(2)	159.7(2)	B(7)-B(9)-B(8)	59.3(4)
N(1)-Ti(1)-C(2)	86.3(2)	C(2)-B(9)-Ti(1)	68.3(3)
C(1)-Ti(1)-C(2)	39.9(2)	B(10)-B(9)-Ti(1)	69.3(3)
O(1)-Ti(1)-B(11)	162.1(2)	B(7)-B(9)-Ti(1)	124.4(4)
O(2)-Ti(1)-B(11)	92.5(2)	B(8)-B(9)-Ti(1)	124.2(4)
N(1)-Ti(1)-B(11)	86.4(2)	B(11)-B(10)-B(9)	105.0(4)
C(1)-Ti(1)-B(11)	41.1(2)	B(11)-B(10)-B(7)	105.7(4)
C(2)-Ti(1)-B(11)	69.3(2)	B(9)-B(10)-B(7)	60.7(4)
O(1)-Ti(1)-B(9)	92.0(2)	B(11)-B(10)-B(6)	59.6(3)
O(2)-Ti(1)-B(9)	124.7(2)	B(9)-B(10)-B(6)	107.9(4)
N(1)-Ti(1)-B(9)	128.2(2)	B(7)-B(10)-B(6)	59.4(4)
C(1)-Ti(1)-B(9)	70.1(2)	B(11)-B(10)-Ti(1)	67.2(3)
C(2)-Ti(1)-B(9)	42.2(2)	B(9)-B(10)-Ti(1)	67.3(3)
B(11)-Ti(1)-B(9)	71.8(2)	B(7)-B(10)-Ti(1)	123.3(4)
O(1)-Ti(1)-B(10)	128.0(2)	B(6)-B(10)-Ti(1)	123.1(4)
O(2)-Ti(1)-B(10)	89.5(2)	C(1)-B(11)-B(10)	108.3(4)
N(1)-Ti(1)-B(10)	128.4(2)	C(1)-B(11)-B(6)	107.4(4)
C(1)-Ti(1)-B(10)	70.4(2)	B(10)-B(11)-B(6)	62.0(4)
C(2)-Ti(1)-B(10)	71.1(2)	C(1)-B(11)-B(5)	60.4(3)
B(11)-Ti(1)-B(10)	42.5(2)	B(10)-B(11)-B(5)	111.3(5)
B(9)-Ti(1)-B(10)	43.4(2)	B(6)-B(11)-B(5)	60.3(4)

C(13)-O(2)-Ti(1)	158.5(3)	C(1)-B(11)-Ti(1)	68.9(3)
C(6)-O(1)-Ti(1)	172.2(4)	B(10)-B(11)-Ti(1)	70.3(3)
C(5)-N(1)-C(3)	113.0(5)	B(6)-B(11)-Ti(1)	128.2(4)
C(5)-N(1)-C(4)	106.8(5)	B(5)-B(11)-Ti(1)	127.1(4)
C(3)-N(1)-C(4)	111.7(5)	C(3)-C(1)-C(2)	116.7(5)
C(5)-N(1)-Ti(1)	112.7(3)	C(3)-C(1)-B(11)	119.3(5)
C(3)-N(1)-Ti(1)	99.0(3)	C(2)-C(1)-B(11)	111.0(4)
C(4)-N(1)-Ti(1)	113.8(4)	C(3)-C(1)-B(5)	123.0(5)
B(5)-B(3)-B(4)	61.2(4)	C(2)-C(1)-B(5)	112.6(5)
B(5)-B(3)-B(8)	108.2(5)	B(11)-C(1)-B(5)	63.0(3)
B(4)-B(3)-B(8)	59.4(4)	C(3)-C(1)-B(4)	120.1(5)
B(5)-B(3)-B(6)	59.8(4)	C(2)-C(1)-B(4)	62.2(4)
B(4)-B(3)-B(6)	108.7(5)	B(11)-C(1)-B(4)	114.2(5)
B(8)-B(3)-B(6)	107.7(5)	B(5)-C(1)-B(4)	62.7(4)
B(5)-B(3)-B(7)	107.1(5)	C(3)-C(1)-Ti(1)	92.5(3)
B(4)-B(3)-B(7)	107.4(5)	C(2)-C(1)-Ti(1)	70.6(3)
B(8)-B(3)-B(7)	59.9(4)	B(11)-C(1)-Ti(1)	70.0(3)
B(6)-B(3)-B(7)	59.3(4)	B(5)-C(1)-Ti(1)	130.5(4)
C(2)-B(4)-C(1)	55.4(3)	B(4)-C(1)-Ti(1)	130.7(4)
C(2)-B(4)-B(8)	59.6(4)	C(1)-C(2)-B(9)	109.9(4)
C(1)-B(4)-B(8)	103.5(5)	C(1)-C(2)-B(4)	62.4(4)
C(2)-B(4)-B(3)	105.5(5)	B(9)-C(2)-B(4)	114.2(5)
C(1)-B(4)-B(3)	103.6(5)	C(1)-C(2)-B(8)	110.4(5)
B(8)-B(4)-B(3)	60.8(4)	B(9)-C(2)-B(8)	63.6(4)
C(2)-B(4)-B(5)	103.7(5)	B(4)-C(2)-B(8)	61.2(4)
C(1)-B(4)-B(5)	58.4(4)	C(1)-C(2)-Ti(1)	69.5(3)
B(8)-B(4)-B(5)	107.6(5)	B(9)-C(2)-Ti(1)	69.5(3)
B(3)-B(4)-B(5)	59.1(4)	B(4)-C(2)-Ti(1)	129.9(4)
C(1)-B(5)-B(3)	104.3(5)	B(8)-C(2)-Ti(1)	129.7(4)

C(1)-B(5)-B(11)	56.6(3)	N(1)-C(3)-C(1)	105.2(4)
B(3)-B(5)-B(11)	106.9(5)	O(2)-C(13)-C(18)	119.0(5)
C(1)-B(5)-B(6)	103.8(4)	O(2)-C(13)-C(14)	119.5(5)
B(3)-B(5)-B(6)	60.9(4)	C(18)-C(13)-C(14)	121.5(5)
B(11)-B(5)-B(6)	59.6(3)	C(13)-C(14)-C(15)	117.1(5)
C(1)-B(5)-B(4)	58.9(4)	C(13)-C(14)-C(19)	121.0(5)
B(3)-B(5)-B(4)	59.6(4)	C(15)-C(14)-C(19)	121.8(6)
B(11)-B(5)-B(4)	105.9(5)	C(16)-C(15)-C(14)	120.9(6)
B(6)-B(5)-B(4)	108.3(5)	C(17)-C(16)-C(15)	120.8(6)
B(11)-B(6)-B(5)	60.2(4)	C(16)-C(17)-C(18)	120.1(6)
B(11)-B(6)-B(7)	105.2(4)	C(13)-C(18)-C(17)	119.5(6)
B(5)-B(6)-B(7)	107.7(5)	C(11')-C(6)-O(1)	122.8(7)
B(11)-B(6)-B(3)	106.2(5)	C(11')-C(6)-C(7)	120.0(8)
B(5)-B(6)-B(3)	59.3(4)	O(1)-C(6)-C(7)	117.2(6)
B(7)-B(6)-B(3)	60.5(4)	C(11')-C(6)-C(11)	24.4(9)
B(11)-B(6)-B(10)	58.4(3)	O(1)-C(6)-C(11)	104.3(1)
B(5)-B(6)-B(10)	108.3(4)	C(7)-C(6)-C(11)	136.2(1)
B(7)-B(6)-B(10)	59.9(4)	C(8')-C(7)-C(6)	121.5(9)
B(3)-B(6)-B(10)	108.6(5)	C(8')-C(7)-C(12)	117.2(9)
B(6)-B(7)-B(10)	60.7(4)	C(6)-C(7)-C(12)	121.2(6)
B(6)-B(7)-B(8)	108.4(5)	C(8')-C(7)-C(8)	28.4(1)
B(10)-B(7)-B(8)	108.9(5)	C(6)-C(7)-C(8)	93.2(1)
B(6)-B(7)-B(3)	60.2(4)	C(12)-C(7)-C(8)	145.2(2)
B(10)-B(7)-B(3)	108.9(5)	C(9)-C(8)-C(7)	136.0(3)
B(8)-B(7)-B(3)	59.9(4)	C(8)-C(9)-C(10)	120.0(4)
B(6)-B(7)-B(9)	107.9(5)	C(9)-C(10)-C(11)	124.0(3)
B(10)-B(7)-B(9)	59.4(4)	C(10)-C(11)-C(6)	109.0(2)
B(8)-B(7)-B(9)	60.8(4)	C(7)-C(8')-C(9')	116.0(1)
B(3)-B(7)-B(9)	108.2(5)	C(10')-C(9')-C(8')	123.4(1)

C(2)-B(8)-B(4)	59.2(4)	C(9')-C(10')-C(11')	118.1(1)
C(2)-B(8)-B(3)	104.5(5)	C(6)-C(11')-C(10')	120.9(1)
B(4)-B(8)-B(3)	59.8(4)	C(104)-C(105)-C(106)	113.0(3)
C(2)-B(8)-B(7)	103.8(5)	C(105)-C(104)-C(103)	120.0(2)
B(4)-B(8)-B(7)	108.0(5)	C(104)-C(103)-C(102)	124.8(2)
B(3)-B(8)-B(7)	60.3(4)	C(103)-C(102)-C(101)	118.7(2)
C(2)-B(8)-B(9)	57.5(3)	C(106)-C(101)-C(102)	106.0(2)
B(4)-B(8)-B(9)	107.5(5)	C(101)-C(106)-C(105)	138.0(3)

Symmetry transformations used to generate equivalent atoms:

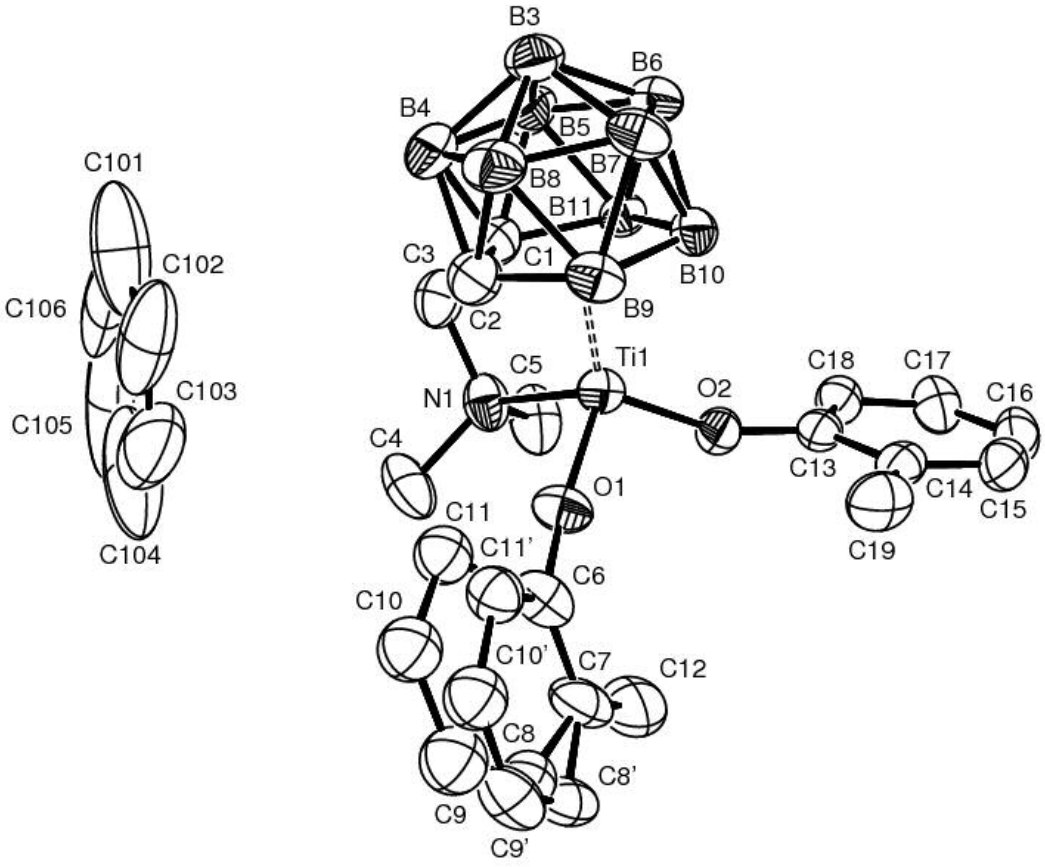


Figure 7. Molecular structure of **12·C_6H_6** with thermal ellipsoids drawn at the 30% level.