The One-Electron Oxidation of an Azazirconacyclobutene in the Presence of $B(C_6F_5)_3$

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SUPPORTING INFORMATION

Table of Contents

Experimental

All manipulations were carried out, and solvents dried, under an Ar or N_2 atmosphere using standard techniques. $B(C_6F_5)_3$ was used as received (Boulder Scientific) or purified via sublimation (10^{-5} torr, 50 °C or 10^{-2} torr, 90 °C), crystallization (hexanes) or a combination of both. The azazirconacycle **2**[i], Cp_2Co[ii] and $[C_5H_4Me)_2Fe][B(C_6F_5)_4]$[iii] were made according to literature procedures.

^1H NMR spectra were obtained on a Bruker Avance 300 DPX, Bruker Avance 300 DRX, Bruker Avance 400 DRX or a Bruker Avance 500 DMX referenced to TMS using residual protio solvent signals as an internal calibrant. ^{19}F NMR spectra were obtained on the Bruker Avance 300 DPX (282.4 MHz).

Assignment of the phenyl protons H_a–H_f of **2** was made using gradient COSY and 1-D selective NOESY. ^1H NMR (CD_2Cl_2): δ 6.35 (m, H_a); 6.89 (m, H_b); 6.69 (m, H_c); 7.12 (m, H_d); 7.32- 7.21(m, H_e and H_f); 6.26 (s, C_5H_5); 1.06 (s, $C(CH_3)_3$). The effect of $\mathbf{2}^{+\bullet}$ on the ^1H NMR resonances of **2** at various temperatures is given in Tables S-1 and S-2.

EPR spectra (Figure 2) were taken in NMR tubes on a Bruker 300 EMX using the following parameters: frequency = 9.775 GHz; power = 2.007 mW; modulation frequency = 100 kHz; modulation amplitude = 0.1 G; conversion = 81.92 ms; time

constant = 20.480 ms; sweep time = 83.886 s; receiver gain = 1.59×10^4 (Figures 2b and 2c), 1.59×10^5 (Figure 2a); sweep width = 60 G; resolution = 1024 points; number of scans = 2 (Figures 2b and 2c), 18 (Figure 2a). Simulated spectra were calculated with Win EPR using experimental parameters, with Gaussian line shapes.

The solutions used in Figure 2 were prepared as follows: solutions of **2** (4 mg, 8.5 mmol) and $[(C_5H_4CH_3)_2Fe][B(C_6F_5)_4]$ (8 mg, 8.9 mmol) in 0.4 mL CD_2Cl_2 apiece were mixed together rapidly, forming a red solution, and the volume increased to 1 mL. Some (0.05 mL) of the solution was added to 1 mL $CD_3C_6D_5$ (Figure 2c); another 0.05 mL of the solution was added to **2** (22 mg, 47 mM) in 1 mL $CD_3C_6D_5$ (Figure 2b). For Figure 2a, $B(C_6F_5)_3$ (6 mg, 12 mmol) was added to a solution of **2** (23 mg, 49 mmol) in 1 mL $CD_3C_6D_5$. Solutions used for NMR experiments were prepared similarly.

Preparation of 3 and 4 from Cp_2Co and $B(C_6F_5)_3$. Cp_2Co, (0.096 g, 0.51 mmol) and $B(C_6F_5)_3$ (0.54 g, 1.04 mmol) were each dissolved in toluene (20 mL), and the cobaltocene solution was added to the $B(C_6F_5)_3$ solution over several min with swirling. A small amount of oil and yellow crystals formed; the solution was cooled to –20 °C overnight and the liquid decanted. The solid material (160 mg) consisted primarily of **3**, $[(\eta^5\text{–}C_5H_5)_2Co][HB(C_6F_5)_3]$. (The ^{1}H NMR spectrum of **3** is given in ref 11e in the printed text; the ^{1}H chemical shift and J_{HB} of the anion matched those reported in refs 11a–d.)

The liquid was concentrated (ca. 7 mL) and hexanes (5 mL) were added, causing some brown oil and yellow crystals to precipitate. After the solution was decanted the

solid material (130 mg) was primarily $(\eta^5\text{–}C_5H_5)(\eta^5\text{–}C_5H_4B(C_6F_5)_3)Co$ (**4**) with some **3**. Compound **4** was extracted by toluene and crystallized by the addition of hexanes, while **3** was recrystallized from CH_2Cl_2/hexanes. After the decanted liquid sat at room temperature an additional 15 mg of yellow crystalline product **4** separated; $B(C_6F_5)_3$ (0.21 g; 0.41 mmol) was recovered from the solution.

Separate NMR tube experiments established (^1H) that the reaction between Cp_2Co and $B(C_6F_5)_3$ to form **3** and **4** occurs rapidly and quantitatively with a one-to-one **3/4** stoichiometry.

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[i] Walsh, P. J.; Hollander, F. J.; Bergman, R. G. *Organometallics* **1993**, *12*, 3705.

[ii] King, R. B.; Stone, F. G. A. *Inorg. Synth.* **1963**, *7*, 113.

[iii] The tetra(perfluorophenyl)borate salt was prepared by a modification of the method reported for the tetraphenyl salt of the same cation: Jordan, R. F.; LaPointe, R. E.; Bradley, P. K.; Baenziger, N. *Organometallics* **1989**, *8*, 2892. The tetra(perfluorophenyl)borate salt of another ferricinium cation has been reported: Antonelli, D. M.; Leins, A.; Stryker, J. M. *Organometallics* **1997**, *16*, 2500.

Table S1. $\Delta(T_{2e}^{-1})$ vs. Temperature for Cp ^{1}H NMR Resonance of **2** (300 MHz; CD_2Cl_2; [**2**] = 51 mM; [$\mathbf{2}^{+\bullet}$] = 1.5 mM)

T (K)	$\Delta(T_{2e}^{-1})$ (Hz)
243	10.97
253	7.79
263	5.61
273	4.35
283	3.29
293	2.52

Table S2. $\Delta(T_{2e}^{-1})$ vs. Temperature for ^{t}Bu ^{1}H NMR Resonance of **2** (300 MHz; CD_2Cl_2; [**2**] = 51 mM; [$\mathbf{2}^{+\bullet}$] = 15 μM)

T (K)	$\Delta(T_{2e}^{-1})$ (Hz)
243	3.21
253	2.29
263	1.60
273	1.09
283	0.69
293	0.40

Table S-3. Crystal data and structure refinement for Compound 4([C5H4B(C6F5)3]CoCp)

Identification code	cobs10
Empirical formula	$C_{28}H_9BCoF_{15}$
Formula weight	700.09
Temperature	203(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 15.9979(16) Å alpha = 90° b = 10.1159(10) Å beta = 110.918(2)° c = 16.4014(18) Å gamma = 90°
Volume, Z	2479.4(4) $Å^3$, 4
Density (calculated)	1.876 Mg/m^3
Absorption coefficient	0.825 mm^{-1}
F(000)	1376
Crystal size	0.20 x 0.20 x 0.10 mm
θ range for data collection	1.53 to 28.26°
Limiting indices	$-21 \le h \le 21$, $-13 \le k \le 9$, $-21 \le l \le 21$
Reflections collected	17962
Independent reflections	5696 (R_{int} = 0.4907)
Completeness to θ = 28.26°	92.6 %
Absorption correction	SADABS
Max. and min. transmission	0.9220 and 0.8523
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5696 / 0 / 407
Goodness-of-fit on F^2	1.023
Final R indices [I>2σ(I)]	R1 = 0.0666, wR2 = 0.1135
R indices (all data)	R1 = 0.1392, wR2 = 0.1478
Extinction coefficient	0.0000(7)
Largest diff. peak and hole	0.953 and -2.079 $eÅ^{-3}$

Table S-4. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for Compound 4. U(eq) is defined a one third of the trace of the orthogonalized U_{ij} tensor.

[C5H4B(C6F5)3]CoCp

	x	y	z	U(eq)
Co	5242(1)	8975(1)	8029(1)	27(1)
F(32)	4122(2)	12576(3)	4741(1)	47(1)
F(33)	5423(3)	13953(3)	4519(2)	59(1)
F(34)	6947(3)	14522(4)	5888(2)	65(1)
F(35)	7136(2)	13643(3)	7516(2)	55(1)
F(36)	5836(2)	12255(3)	7776(1)	36(1)
F(42)	4420(2)	14235(2)	7169(2)	41(1)
F(43)	4020(2)	15143(3)	8493(2)	53(1)
F(44)	3114(2)	13631(3)	9269(1)	48(1)
F(45)	2581(2)	11154(3)	8643(2)	47(1)
F(46)	3008(2)	10184(3)	7347(1)	40(1)
F(52)	4102(2)	9628(3)	5046(1)	37(1)
F(53)	2681(2)	8893(3)	3688(1)	42(1)
F(54)	1040(2)	9912(3)	3444(1)	45(1)
F(55)	869(2)	11759(3)	4591(1)	46(1)
F(56)	2263(2)	12551(3)	5925(1)	46(1)
C(11)	4648(3)	9907(4)	6822(2)	25(1)
C(12)	5562(3)	9558(4)	6986(2)	28(1)
C(13)	5688(3)	8177(4)	7128(2)	34(1)
C(14)	4852(3)	7621(4)	7052(2)	34(1)
C(15)	4230(3)	8671(4)	6868(2)	30(1)
C(21)	5214(3)	10239(5)	8997(2)	33(1)
C(22)	6101(3)	9862(5)	9125(2)	36(1)
C(23)	6162(4)	8463(5)	9211(2)	40(1)
C(24)	5312(4)	7975(5)	9133(2)	44(1)
C(25)	4721(4)	9072(5)	8994(2)	39(1)
C(31)	4901(3)	12294(4)	6273(2)	28(1)
C(32)	4865(4)	12785(4)	5463(2)	34(1)
C(33)	5518(4)	13512(5)	5326(3)	43(1)
C(34)	6286(4)	13825(5)	6011(3)	44(1)
C(35)	6376(4)	13378(5)	6829(3)	39(1)
C(36)	5699(3)	12653(4)	6932(2)	32(1)
C(41)	3830(3)	12081(4)	7242(2)	27(1)
C(42)	4018(3)	13375(4)	7544(2)	27(1)
C(43)	3798(3)	13896(4)	8223(2)	33(1)
C(44)	3335(3)	13134(5)	8611(2)	34(1)
C(45)	3075(3)	11898(5)	8301(2)	31(1)
C(46)	3323(3)	11409(4)	7631(2)	28(1)
C(51)	3262(3)	11068(4)	5600(2)	25(1)
C(52)	3307(3)	10155(4)	4973(2)	28(1)
C(53)	2588(3)	9789(4)	4259(2)	31(1)
C(54)	1758(3)	10304(4)	4124(2)	29(1)
C(55)	1669(3)	11240(4)	4704(2)	31(1)
C(56)	2427(3)	11603(4)	5409(2)	29(1)
B	4169(3)	11371(4)	6487(2)	24(1)

Table S-5. Bond lengths [Å] and angles [°] for Compound 4([C5H4B(C6F5)3]CoCp)

Co-C(13)	2.023(4)	Co-C(14)	2.030(4)
Co-C(15)	2.035(4)	Co-C(25)	2.038(4)
Co-C(23)	2.039(4)	Co-C(12)	2.039(4)
Co-C(22)	2.040(4)	Co-C(24)	2.043(4)
Co-C(21)	2.051(4)	Co-C(11)	2.089(3)
F(32)-C(32)	1.362(5)	F(33)-C(33)	1.354(5)
F(34)-C(34)	1.345(6)	F(35)-C(35)	1.356(6)
F(36)-C(36)	1.381(4)	F(42)-C(42)	1.353(5)
F(43)-C(43)	1.342(5)	F(44)-C(44)	1.347(4)
F(45)-C(45)	1.350(5)	F(46)-C(46)	1.356(5)
F(52)-C(52)	1.344(5)	F(53)-C(53)	1.350(4)
F(54)-C(54)	1.344(5)	F(55)-C(55)	1.334(5)
F(56)-C(56)	1.365(4)	C(11)-C(15)	1.432(6)
C(11)-C(12)	1.433(6)	C(11)-B	1.668(6)
C(12)-C(13)	1.419(6)	C(13)-C(14)	1.414(7)
C(14)-C(15)	1.412(6)	C(21)-C(22)	1.412(7)
C(21)-C(25)	1.419(7)	C(22)-C(23)	1.422(7)
C(23)-C(24)	1.410(8)	C(24)-C(25)	1.423(7)
C(31)-C(36)	1.393(6)	C(31)-C(32)	1.401(5)
C(31)-B	1.631(6)	C(32)-C(33)	1.360(7)
C(33)-C(34)	1.374(8)	C(34)-C(35)	1.374(6)
C(35)-C(36)	1.368(7)	C(41)-C(46)	1.377(6)
C(41)-C(42)	1.394(6)	C(41)-B	1.679(5)
C(42)-C(43)	1.387(6)	C(43)-C(44)	1.373(7)
C(44)-C(45)	1.358(7)	C(45)-C(46)	1.386(5)
C(51)-C(56)	1.369(6)	C(51)-C(52)	1.403(5)
C(51)-B	1.676(5)	C(52)-C(53)	1.368(6)
C(53)-C(54)	1.368(7)	C(54)-C(55)	1.385(6)
C(55)-C(56)	1.394(6)		

C(13)-Co-C(14)	40.85(19)	C(13)-Co-C(15)	68.08(19)
C(14)-Co-C(15)	40.66(17)	C(13)-Co-C(25)	159.2(2)
C(14)-Co-C(25)	123.4(2)	C(15)-Co-C(25)	108.97(19)
C(13)-Co-C(23)	105.64(19)	C(14)-Co-C(23)	119.56(18)
C(15)-Co-C(23)	156.15(18)	C(25)-Co-C(23)	68.3(2)
C(13)-Co-C(12)	40.87(17)	C(14)-Co-C(12)	68.38(18)
C(15)-Co-C(12)	67.24(18)	C(25)-Co-C(12)	158.79(19)
C(23)-Co-C(12)	124.0(2)	C(13)-Co-C(22)	121.1(2)
C(14)-Co-C(22)	155.9(2)	C(15)-Co-C(22)	162.16(18)
C(25)-Co-C(22)	68.19(19)	C(23)-Co-C(22)	40.81(18)
C(12)-Co-C(22)	108.63(18)	C(13)-Co-C(24)	121.8(2)
C(14)-Co-C(24)	105.65(19)	C(15)-Co-C(24)	121.9(2)
C(25)-Co-C(24)	40.8(2)	C(23)-Co-C(24)	40.4(2)
C(12)-Co-C(24)	159.4(2)	C(22)-Co-C(24)	68.31(19)
C(13)-Co-C(21)	157.6(2)	C(14)-Co-C(21)	161.1(2)
C(15)-Co-C(21)	126.06(18)	C(25)-Co-C(21)	40.60(18)
C(23)-Co-C(21)	68.30(18)	C(12)-Co-C(21)	123.37(18)
C(22)-Co-C(21)	40.39(19)	C(24)-Co-C(21)	68.41(19)
C(13)-Co-C(11)	69.40(16)	C(14)-Co-C(11)	69.43(16)
C(15)-Co-C(11)	40.61(16)	C(25)-Co-C(11)	122.71(18)
C(23)-Co-C(11)	161.0(2)	C(12)-Co-C(11)	40.61(16)
C(22)-Co-C(11)	124.89(17)	C(24)-Co-C(11)	157.8(2)
C(21)-Co-C(11)	108.89(16)	C(15)-C(11)-C(12)	103.9(4)
C(15)-C(11)-B	128.6(4)	C(12)-C(11)-B	126.7(4)
C(15)-C(11)-Co	67.7(2)	C(12)-C(11)-Co	67.8(2)

B-C(11)-Co	135.4(2)	C(13)-C(12)-C(11)	110.4(4)
C(13)-C(12)-Co	69.0(2)	C(11)-C(12)-Co	71.6(2)
C(14)-C(13)-C(12)	107.6(4)	C(14)-C(13)-Co	69.8(2)
C(12)-C(13)-Co	70.2(2)	C(15)-C(14)-C(13)	107.0(4)
C(15)-C(14)-Co	69.9(2)	C(13)-C(14)-Co	69.3(2)
C(14)-C(15)-C(11)	111.2(4)	C(14)-C(15)-Co	69.5(2)
C(11)-C(15)-Co	71.7(2)	C(22)-C(21)-C(25)	107.7(4)
C(22)-C(21)-Co	69.4(2)	C(25)-C(21)-Co	69.2(2)
C(21)-C(22)-C(23)	108.2(5)	C(21)-C(22)-Co	70.2(2)
C(23)-C(22)-Co	69.6(2)	C(24)-C(23)-C(22)	108.1(5)
C(24)-C(23)-Co	70.0(2)	C(22)-C(23)-Co	69.6(2)
C(23)-C(24)-C(25)	107.8(4)	C(23)-C(24)-Co	69.6(2)
C(25)-C(24)-Co	69.4(2)	C(21)-C(25)-C(24)	108.2(5)
C(21)-C(25)-Co	70.2(2)	C(24)-C(25)-Co	69.8(2)
C(36)-C(31)-C(32)	111.0(4)	C(36)-C(31)-B	120.8(3)
C(32)-C(31)-B	128.2(4)	C(33)-C(32)-F(32)	115.1(3)
C(33)-C(32)-C(31)	125.1(4)	F(32)-C(32)-C(31)	119.8(4)
F(33)-C(33)-C(32)	121.0(5)	F(33)-C(33)-C(34)	118.7(5)
C(32)-C(33)-C(34)	120.3(4)	F(34)-C(34)-C(35)	120.4(5)
F(34)-C(34)-C(33)	121.3(4)	C(35)-C(34)-C(33)	118.3(5)
F(35)-C(35)-C(36)	121.3(4)	F(35)-C(35)-C(34)	119.7(5)
C(36)-C(35)-C(34)	119.0(4)	C(35)-C(36)-F(36)	115.4(4)
C(35)-C(36)-C(31)	126.2(4)	F(36)-C(36)-C(31)	118.3(4)
C(46)-C(41)-C(42)	112.8(3)	C(46)-C(41)-B	121.9(4)
C(42)-C(41)-B	125.3(4)	F(42)-C(42)-C(43)	114.8(4)
F(42)-C(42)-C(41)	121.3(3)	C(43)-C(42)-C(41)	123.9(4)
F(43)-C(43)-C(44)	119.8(4)	F(43)-C(43)-C(42)	120.6(4)
C(44)-C(43)-C(42)	119.6(4)	F(44)-C(44)-C(45)	120.8(4)
F(44)-C(44)-C(43)	120.1(4)	C(45)-C(44)-C(43)	119.1(4)
F(45)-C(45)-C(44)	120.2(4)	F(45)-C(45)-C(46)	120.4(4)
C(44)-C(45)-C(46)	119.3(4)	F(46)-C(46)-C(41)	120.0(3)
F(46)-C(46)-C(45)	115.0(4)	C(41)-C(46)-C(45)	125.0(4)
C(56)-C(51)-C(52)	113.2(3)	C(56)-C(51)-B	126.7(3)
C(52)-C(51)-B	120.1(4)	F(52)-C(52)-C(53)	116.6(3)
F(52)-C(52)-C(51)	119.4(3)	C(53)-C(52)-C(51)	123.9(4)
F(53)-C(53)-C(52)	120.6(4)	F(53)-C(53)-C(54)	119.0(3)
C(52)-C(53)-C(54)	120.5(3)	F(54)-C(54)-C(53)	121.0(3)
F(54)-C(54)-C(55)	120.3(4)	C(53)-C(54)-C(55)	118.7(4)
F(55)-C(55)-C(54)	120.1(4)	F(55)-C(55)-C(56)	121.3(4)
C(54)-C(55)-C(56)	118.5(4)	F(56)-C(56)-C(51)	121.6(3)
F(56)-C(56)-C(55)	113.3(4)	C(51)-C(56)-C(55)	125.1(3)
C(31)-B-C(11)	107.4(3)	C(31)-B-C(51)	112.5(3)
C(11)-B-C(51)	106.1(3)	C(31)-B-C(41)	111.1(3)
C(11)-B-C(41)	111.6(3)	C(51)-B-C(41)	108.1(3)

Symmetry transformations used to generate equivalent atoms:

Table S-6. Anisotropic displacement parameters [$Å^2 \times 10^3$] for Compound 4([C5H4B(C6F5)3]CoCp)

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Co	32(1)	20(1)	30(1)	0(1)	12(1)	1(1)
F(32)	61(2)	45(2)	34(1)	3(1)	15(1)	-11(2)
F(33)	97(3)	37(2)	60(1)	4(1)	51(2)	-7(2)
F(34)	57(2)	55(2)	104(2)	-7(2)	55(2)	-17(2)
F(35)	34(2)	58(2)	74(2)	-19(1)	19(1)	-14(2)
F(36)	35(2)	34(2)	38(1)	-4(1)	11(1)	-4(1)
F(42)	47(2)	20(1)	64(1)	-8(1)	29(1)	-5(1)
F(43)	56(2)	28(2)	74(2)	-27(1)	23(1)	-2(2)
F(44)	57(2)	49(2)	41(1)	-8(1)	23(1)	19(2)
F(45)	54(2)	45(2)	58(1)	4(1)	39(1)	2(2)
F(46)	49(2)	24(1)	55(1)	-11(1)	29(1)	-10(1)
F(52)	33(2)	40(2)	38(1)	-9(1)	13(1)	10(1)
F(53)	53(2)	32(2)	38(1)	-14(1)	11(1)	2(2)
F(54)	39(2)	41(2)	40(1)	-2(1)	-5(1)	-4(2)
F(55)	31(2)	52(2)	51(1)	3(1)	10(1)	14(2)
F(56)	46(2)	44(2)	43(1)	-13(1)	8(1)	19(2)
C(11)	28(2)	23(2)	26(2)	-6(1)	11(2)	-2(2)
C(12)	29(2)	26(2)	34(2)	2(2)	18(2)	5(2)
C(13)	40(3)	28(2)	37(2)	-3(2)	16(2)	7(2)
C(14)	47(3)	17(2)	37(2)	-7(2)	12(2)	0(2)
C(15)	35(3)	22(2)	29(2)	-7(1)	6(2)	-3(2)
C(21)	34(3)	36(3)	28(2)	-3(2)	9(2)	3(2)
C(22)	37(3)	34(3)	33(2)	-1(2)	8(2)	-6(2)
C(23)	45(3)	32(2)	34(2)	6(2)	3(2)	8(3)
C(24)	57(3)	38(3)	36(2)	6(2)	16(2)	-3(3)
C(25)	40(3)	48(3)	34(2)	0(2)	20(2)	-3(3)
C(31)	36(3)	15(2)	37(2)	-4(1)	18(2)	1(2)
C(32)	48(3)	19(2)	42(2)	-6(2)	23(2)	-3(2)
C(33)	67(4)	27(2)	48(2)	-3(2)	37(2)	2(3)
C(34)	43(3)	27(3)	78(3)	-7(2)	43(2)	-10(3)
C(35)	36(3)	29(3)	56(2)	-12(2)	21(2)	-2(2)
C(36)	35(3)	26(2)	41(2)	-5(2)	21(2)	2(2)
C(41)	26(2)	25(2)	29(2)	-4(1)	9(1)	6(2)
C(42)	22(2)	23(2)	39(2)	-2(2)	13(2)	0(2)
C(43)	27(2)	20(2)	45(2)	-15(2)	7(2)	5(2)
C(44)	35(3)	35(3)	31(2)	-6(2)	12(2)	11(2)
C(45)	27(2)	31(2)	40(2)	2(2)	20(2)	6(2)
C(46)	28(2)	22(2)	35(2)	-5(1)	11(2)	-1(2)
C(51)	27(2)	18(2)	29(2)	-3(1)	11(1)	1(2)
C(52)	30(2)	25(2)	32(2)	3(1)	14(2)	7(2)
C(53)	48(3)	19(2)	28(2)	-1(1)	15(2)	0(2)
C(54)	29(2)	24(2)	28(2)	2(1)	4(2)	1(2)
C(55)	29(2)	29(2)	38(2)	12(2)	13(2)	8(2)
C(56)	36(3)	23(2)	31(2)	-2(1)	15(2)	7(2)
B	24(2)	19(2)	30(2)	-6(1)	12(2)	-3(2)

Table S-7. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for Compound 4([C5H4B(C6F5)3]CoCp)

	x	y	z	U(eq)
H(12A)	6042	10195	7015	33
H(13A)	6256	7689	7249	41
H(14A)	4725	6675	7108	41
H(15A)	3593	8570	6799	36
H(21A)	4976	11152	8914	40
H(22A)	6596	10467	9150	43
H(23A)	6706	7926	9308	48
H(24A)	5153	7035	9166	52
H(25A)	4078	9029	8913	47

Figure S-1. Thermal Ellipsoid Plot of $(\eta^{-5}\text{-}C_5H_5)(\eta^{-5}\text{-}C_5H_4B(C_6F_5)_3)Co$ (4)

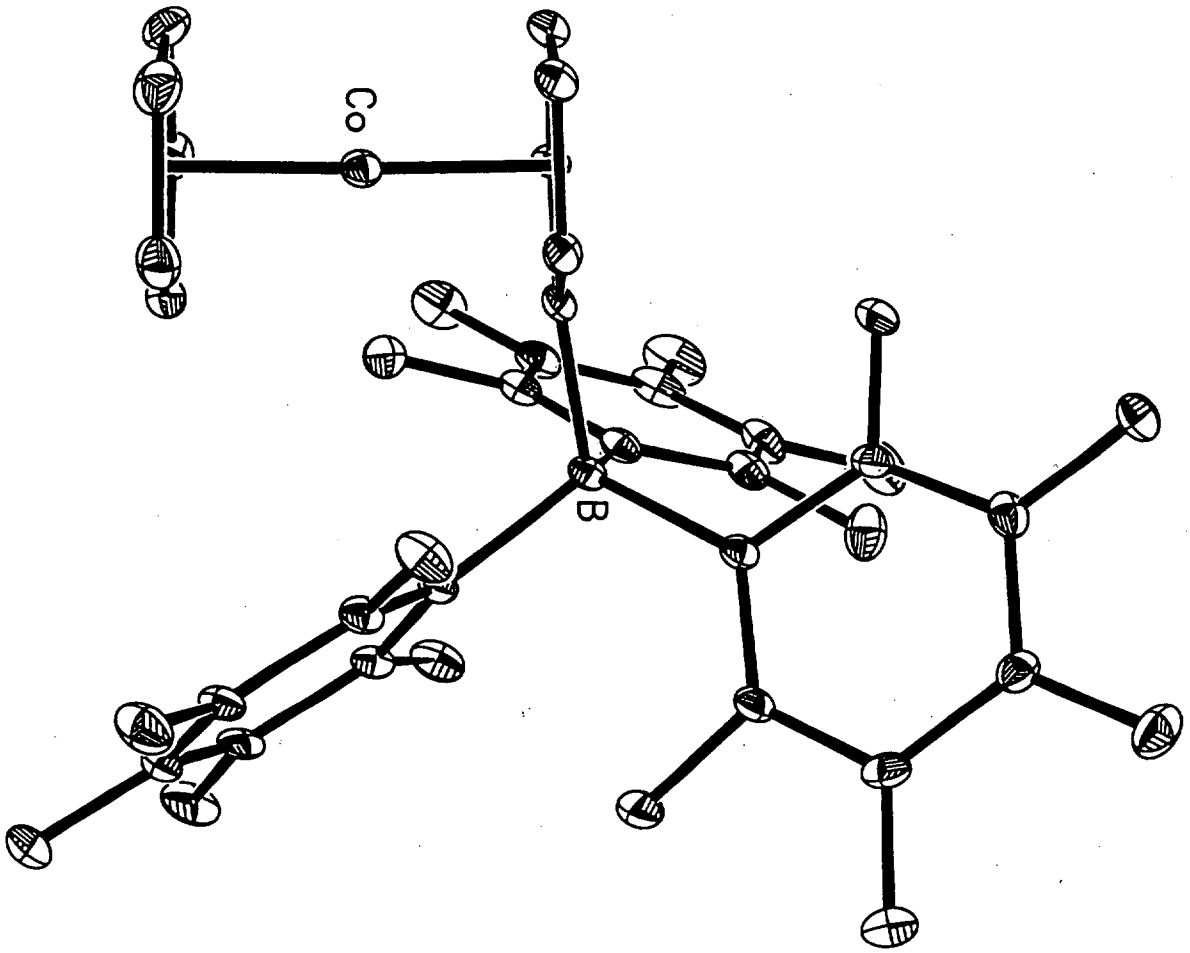

Figure S-2. Numbered Thermal Ellipsoid Plot of
$(\eta^{-5}\text{-}C_5H_5)(\eta^{-5}\text{-}C_5H_4B(C_6F_5)_3)Co$ (4)