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EXPERIMENTAL

DATA COLLECTION

A black plate-like crystal of $(Me_5Cp)Co(B_3H_7)Fe(CO)_3$ having approximate dimensions of 0.38 x 0.28 x 0.15 mm was mounted on a glass fiber in a random orientation. Preliminary examination and data collection were performed with MoKα radiation (λ = 0.71073 Å) on an Enraf-Nonius CAD4 computer controlled kappa axis diffractometer equipped with a graphite crystal, incident beam monochromator. The crystal was found to have weak sattelite diffraction. Since the settelite diffraction did not seem to affect seriously profiles of the principal diffraction and no crystals could be found with better quality, the crystal was chosen for the diffraction work.

Cell constants and an orientation matrix for data collection were obtained from least-squares refinement, using the setting angles of 25 reflections in the range $30^\circ < 2\theta < 32^\circ$, measured by the computer controlled diagonal slit method of centering. The monoclinic cell parameters and calculated volume are: a = 29.204(3), b = 8.5268(6), c = 15.905(3) Å, β = 120.803(13)°, V = 3401.9(8) $Å^3$. For Z = 8 and F.W. = 373.52 the calculated density is 1.459 g/cm^3. As a check on crystal quality, an omega/theta profile analysis of reflections was carried out, which showed that Δω was less than 0.60° and Δθ was less than 0.55°, indicating good crystal quality. From the following systematic absence conditions

hkl: h + k = 2n; h01: l = 2n

and the results of final structure refinement; the space group was determined to be C2/c (No. 15).

The data were collected at a temperature of 20°C using the ω/2θ scan technique. The scan rate varied from 1.37 to 8.24°/min (in ω). The variable scan rate allows rapid data collection for intense reflections where a fast scan rate is used and assures good counting statistics for weak reflections and reflections with even negative intensity counts, where a slow scan rate is used. Data were collected to a maximum 2θ of 50.0°. The scan range (in degrees) was determined as a function of θ to correct for the separation of the Kα doublet; the scan width was calculated as follows:

ω scan width = $0.70^{\circ} + 0.35^{\circ}\tan\theta$

Moving-crystal static-background counts were made by scanning an additional 25% nabove and below this range. Tus the ratio of peak counting time to background counting time was 2:1. The counter aperture was also adjusted as a function of θ. The horizontal aperture width ranged from 2.0 to 2.4 mm; the vertical aperture was set at 4.0 mm. The diameter of the incident beam collimator was 0.8 mm and the crystal to detector distance was 21 cm. For intense reflections an attenuator was automatically inserted in front of the detector; the attenuator factor was 19.455.

A total of 5949 reflections were collected. As a check on crystal and electronic stability 3 representative reflections were measured every 120 minutes of X-ray exposure. A total of intensity loss of 5.6% was found for the three standard reflections during 56.8 h of X-ray exposure for the data collection.

DATA REDUCTION

SDP software was used to precess intensity data on a VAXstation 3200 computer.[1] Lorentz and polarization corrections were applied to the data. An isotropic decay correction was made. The linear absorption coefficient is 18.30 cm^{-1} for MoKα radiation. An empirical absorption correction based on a series of psi-scans was applied to the data. Relative transmission coefficients ranged from 0.9994 to 0.8160.

STRUCTURE SOLUTION AND REFINEMENT

Structure solution and refinement were performed on a PC by using the SHELXTL package.[2] Most of the nonhydrogen atoms were located by the direct method, the remaining nonhydrogen atoms were found in succeeding difference Fourier synthesis. Least-squares refinement was carried out on F^2 for all reflections. After all nonhydrogen atoms were refined anisotropically, difference Fourier synthesis located all hydrogen atoms. In the final refinement hydrogen atoms were refined isotropically. All reflections,

including those with negative intensities, were included in the refinement and the $I > 2\sigma(I)$ criterion was used only for calculating R_1. The refinement converged to a final value of $R_1 = 0.0229$ and $wR_2 = 0.0625$ for observed unique reflections ($I > 2\sigma(I)$) and $R_1 = 0.0258$ and $wR_2 = 0.0681$ for all unique reflections including those with negative intensities. The weighted R-factors, wR, are based on F^2 and conventional R-factors, R, on F, with F set to zero for negative intensities. The maximum and minimum residual electron densities on the final difference Fourier map were 0.254 e/Å^3 and -0.202 e/Å^3, respectively. All e.s.d's were estimated by the use of the full covariance matrix. The cell e.s.d's were included in the estimation of e.s.d's of bond distances and angles.

REFERENCES

(1) B. A. Frenz, ''The Enraf-Nonius CAD4 SDP - A Real-time System for Concurent X-Ray Data Collection and Crystal Structure Determination,'' in Computing in Crystallography, H. Schenk, R. Olthof-Hazelkamp, H. vanKonigsveld, and G. C. Bassi, Eds, Delft University Press. Delft, Holland, 1978, pp 64-71.

(2) SHELXTL V.5, Siemens Industrial Automation, Inc. 1994.

Table S1. Crystal data and structure refinement for $(Me_5Cp)Co(B_3H_7)Fe(CO)_3$.

Molecule	$(Me_5Cp)Co(B_3H_7)Fe(CO)_3$
Empirical formula	$C_{13}\ H_{22}\ B_3\ Co\ Fe\ O_3$
Formula weight	373.52
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 29.204(3) Å b = 8.5268(6) Å c = 15.905(3) Å β = 120.803(13)°
Volume	3401.9(8) $Å^3$
Z	8
Density (calculated)	1.459 Mg/m^3
F(000)	1536
Wavelength	0.71073 Å
Absorption coefficient	1.830 mm^{-1}
Crystal size	0.38 x 0.28 x 0.15 mm
Temperature	293(2) K
Diffractometer	Enraf-Nonius CAD4
Theta range for data collection	2.52 to 24.98°
Index ranges	$-34 \le h \le 31$, $-9 \le k \le 10$, $-18 \le l \le 15$
Scan method	ω/2θ
Scan rate	1.34 - 8.24 °/min (in ω)
Scan width	0.70° + 0.35°tanθ (in ω)
Total data collected	5949
Unique data	2974 [R(int) = 0.0140]
Unique observed data [I>2σ(I)]	2750
Decay correction	Linear decay (-5.6%/56.8 h)
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.9994 and 0.8160
Refinement method	Full-matrix on F^2 (SHELXL-93)
Weighting scheme	sigma weight
Data / restraints / parameters	2974 / 0 / 279

Table S1. continued Page 2.

Goodness-of-fit on F^2	1.090
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0229, wR_2 = 0.0625
R indices (all data)	R_1 = 0.0258, wR_2 = 0.0651
Extinction coefficient	0.00036(8)
Largest diff. peak and hole	0.254 and -0.202 e·Å^{-3}

Table S2. Atomic coordinates and equivalent isotropic displacement parameters U_{eq} for $(Me_5Cp)Co(B_3H_7)Fe(CO)_3$.

	x	y	z	U_{eq}(Å^2)
Co	0.63861(1)	0.84975(3)	0.55585(2)	0.0366(1)
Fe	0.57381(1)	0.74318(3)	0.59446(2)	0.0476(1)
C(1)	0.68860(8)	0.7075(2)	0.53024(15)	0.0439(4)
C(2)	0.70930(8)	0.8613(2)	0.5575(2)	0.0452(5)
C(3)	0.67123(8)	0.9674(2)	0.4862(2)	0.0459(4)
C(4)	0.62712(8)	0.8794(3)	0.41571(14)	0.0458(4)
C(5)	0.63810(8)	0.7185(2)	0.44256(14)	0.0436(4)
C(6)	0.71790(12)	0.5603(3)	0.5808(2)	0.0661(7)
C(7)	0.76345(10)	0.9013(4)	0.6421(2)	0.0659(7)
C(8)	0.67822(14)	1.1412(3)	0.4832(3)	0.0690(7)
C(9)	0.57960(11)	0.9445(4)	0.3257(2)	0.0694(7)
C(10)	0.60520(11)	0.5825(4)	0.3817(2)	0.0656(7)
C(11)	0.52867(10)	0.7312(3)	0.4667(2)	0.0619(6)
O(11)	0.49825(9)	0.7230(3)	0.38562(15)	0.0888(6)
C(12)	0.52766(11)	0.6960(3)	0.6340(2)	0.0664(6)
O(12)	0.49745(10)	0.6651(3)	0.6553(2)	0.1044(8)
C(13)	0.59954(11)	0.5524(3)	0.5997(2)	0.0677(6)
O(13)	0.61510(10)	0.4298(2)	0.6030(2)	0.1040(7)
B(1)	0.58500(10)	0.9910(3)	0.5602(2)	0.0495(5)
B(2)	0.65304(10)	1.0123(3)	0.6550(2)	0.0515(6)
B(3)	0.65887(11)	0.8147(3)	0.6950(2)	0.0527(6)

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$.

Table S3. Bond lengths (Å) for $(Me_5Cp)Co(B_3H_7)Fe(CO)_3$.

Co-B(2)	1.975(2)	C(6)-H(6C)	0.93(4)
Co-B(3)	1.999(3)	C(7)-H(7A)	0.88(3)
Co-B(1)	2.005(2)	C(7)-H(7B)	0.91(4)
Co-C(2)	2.054(2)	C(7)-H(7C)	0.91(4)
Co-C(3)	2.054(2)	C(8)-H(8A)	0.92(3)
Co-C(1)	2.092(2)	C(8)-H(8B)	0.91(3)
Co-C(4)	2.093(2)	C(8)-H(8C)	0.92(4)
Co-C(5)	2.115(2)	C(9)-H(9A)	0.97(4)
Co-Fe	2.4443(4)	C(9)-H(9B)	0.98(4)
Fe-C(11)	1.770(3)	C(9)-H(9C)	0.86(4)
Fe-C(13)	1.776(3)	C(10)-H(10A)	0.93(4)
Fe-C(12)	1.800(3)	C(10)-H(10B)	0.90(3)
Fe-B(3)	2.243(3)	C(10)-H(10C)	1.01(3)
Fe-B(1)	2.248(3)	C(11)-O(11)	1.134(3)
Fe-H(1)	1.66(3)	C(12)-O(12)	1.127(3)
Fe-H(6)	1.67(3)	C(13)-O(13)	1.131(3)
C(1)-C(2)	1.416(3)	B(1)-B(2)	1.785(4)
C(1)-C(5)	1.422(3)	B(1)-H(1)	1.29(2)
C(1)-C(6)	1.500(3)	B(1)-H(2)	1.28(3)
C(2)-C(3)	1.431(3)	B(1)-H(3)	1.01(2)
C(2)-C(7)	1.499(3)	B(2)-B(3)	1.778(4)
C(3)-C(4)	1.414(3)	B(2)-H(2)	1.21(3)
C(3)-C(8)	1.500(3)	B(2)-H(4)	1.24(3)
C(4)-C(5)	1.424(3)	B(2)-H(5)	1.05(3)
C(4)-C(9)	1.500(3)	B(3)-H(4)	1.32(3)
C(5)-C(10)	1.500(3)	B(3)-H(6)	1.29(3)
C(6)-H(6A)	0.86(5)	B(3)-H(7)	1.07(3)
C(6)-H(6B)	0.97(4)		

Table S4. Bond angles (deg) for $(Me_5Cp)Co(B_3H_7)Fe(CO)_3$.

B(2)-Co-B(3)	53.13(11)	C(4)-Co-Fe	126.16(6)
B(2)-Co-B(1)	53.27(11)	C(5)-Co-Fe	110.41(6)
B(3)-Co-B(1)	81.07(11)	C(11)-Fe-C(13)	92.85(12)
B(2)-Co-C(2)	98.87(9)	C(11)-Fe-C(12)	97.88(12)
B(3)-Co-C(2)	105.53(10)	C(13)-Fe-C(12)	98.83(13)
B(1)-Co-C(2)	140.23(9)	C(11)-Fe-B(3)	137.40(11)
B(2)-Co-C(3)	96.85(10)	C(13)-Fe-B(3)	85.88(11)
B(3)-Co-C(3)	135.53(10)	C(12)-Fe-B(3)	124.44(11)
B(1)-Co-C(3)	108.14(9)	C(11)-Fe-B(1)	83.76(11)
C(2)-Co-C(3)	40.77(8)	C(13)-Fe-B(1)	139.64(11)
B(2)-Co-C(1)	132.61(9)	C(12)-Fe-B(1)	121.50(11)
B(3)-Co-C(1)	106.78(10)	B(3)-Fe-B(1)	70.83(10)
B(1)-Co-C(1)	172.03(9)	C(11)-Fe-Co	87.16(8)
C(2)-Co-C(1)	39.92(8)	C(13)-Fe-Co	89.35(9)
C(3)-Co-C(1)	67.40(8)	C(12)-Fe-Co	170.12(9)
B(2)-Co-C(4)	128.13(10)	B(3)-Fe-Co	50.27(7)
B(3)-Co-C(4)	172.96(9)	B(1)-Fe-Co	50.37(6)
B(1)-Co-C(4)	105.20(9)	C(11)-Fe-H(1)	88.7(8)
C(2)-Co-C(4)	67.62(8)	C(13)-Fe-H(1)	173.9(9)
C(3)-Co-C(4)	39.87(8)	C(12)-Fe-H(1)	86.8(9)
C(1)-Co-C(4)	67.04(8)	B(3)-Fe-H(1)	89.0(8)
B(2)-Co-C(5)	163.09(10)	B(1)-Fe-H(1)	34.7(8)
B(3)-Co-C(5)	137.16(10)	Co-Fe-H(1)	84.8(9)
B(1)-Co-C(5)	133.06(10)	C(11)-Fe-H(6)	172.0(9)
C(2)-Co-C(5)	66.70(8)	C(13)-Fe-H(6)	88.4(8)
C(3)-Co-C(5)	66.56(8)	C(12)-Fe-H(6)	89.7(9)
C(1)-Co-C(5)	39.51(8)	B(3)-Fe-H(6)	34.8(9)
C(4)-Co-C(5)	39.57(8)	B(1)-Fe-H(6)	90.2(9)
B(2)-Co-Fe	86.36(8)	Co-Fe-H(6)	85.0(9)
B(3)-Co-Fe	59.64(8)	H(1)-Fe-H(6)	89.2(12)
B(1)-Co-Fe	59.72(7)	C(2)-C(1)-C(5)	107.8(2)
C(2)-Co-Fe	156.54(6)	C(2)-C(1)-C(6)	125.0(2)
C(3)-Co-Fe	161.69(6)	C(5)-C(1)-C(6)	126.9(2)
C(1)-Co-Fe	122.73(6)	C(2)-C(1)-Co	68.59(11)

Table S4. continued Page 2.

C(5)-C(1)-Co	71.11(11)	C(2)-C(7)-H(7B)	111(2)
C(6)-C(1)-Co	130.1(2)	H(7A)-C(7)-H(7B)	109(3)
C(1)-C(2)-C(3)	107.8(2)	C(2)-C(7)-H(7C)	111(2)
C(1)-C(2)-C(7)	125.0(2)	H(7A)-C(7)-H(7C)	110(3)
C(3)-C(2)-C(7)	127.0(2)	H(7B)-C(7)-H(7C)	109(3)
C(1)-C(2)-Co	71.49(11)	C(3)-C(8)-H(8A)	115(2)
C(3)-C(2)-Co	69.63(11)	C(3)-C(8)-H(8B)	110(2)
C(7)-C(2)-Co	127.8(2)	H(8A)-C(8)-H(8B)	109(3)
C(4)-C(3)-C(2)	108.4(2)	C(3)-C(8)-H(8C)	112(2)
C(4)-C(3)-C(8)	125.6(2)	H(8A)-C(8)-H(8C)	107(3)
C(2)-C(3)-C(8)	125.9(2)	H(8B)-C(8)-H(8C)	103(3)
C(4)-C(3)-Co	71.53(11)	C(4)-C(9)-H(9A)	114(2)
C(2)-C(3)-Co	69.61(11)	C(4)-C(9)-H(9B)	110(2)
C(8)-C(3)-Co	127.5(2)	H(9A)-C(9)-H(9B)	101(3)
C(3)-C(4)-C(5)	107.4(2)	C(4)-C(9)-H(9C)	111(2)
C(3)-C(4)-C(9)	125.7(2)	H(9A)-C(9)-H(9C)	110(3)
C(5)-C(4)-C(9)	126.8(2)	H(9B)-C(9)-H(9C)	111(3)
C(3)-C(4)-Co	68.60(11)	C(5)-C(10)-H(10A)	112(2)
C(5)-C(4)-Co	71.05(11)	C(5)-C(10)-H(10B)	110(2)
C(9)-C(4)-Co	128.8(2)	H(10A)-C(10)-H(10B)	102(3)
C(1)-C(5)-C(4)	108.6(2)	C(5)-C(10)-H(10C)	113(2)
C(1)-C(5)-C(10)	125.6(2)	H(10A)-C(10)-H(10C)	105(3)
C(4)-C(5)-C(10)	125.4(2)	H(10B)-C(10)-H(10C)	115(3)
C(1)-C(5)-Co	69.38(11)	O(11)-C(11)-Fe	177.4(2)
C(4)-C(5)-Co	69.38(11)	O(12)-C(12)-Fe	177.5(3)
C(10)-C(5)-Co	132.3(2)	O(13)-C(13)-Fe	178.7(3)
C(1)-C(6)-H(6A)	111(3)	B(2)-B(1)-Co	62.53(11)
C(1)-C(6)-H(6B)	113(2)	B(2)-B(1)-Fe	97.36(14)
H(6A)-C(6)-H(6B)	107(3)	Co-B(1)-Fe	69.91(7)
C(1)-C(6)-H(6C)	112(2)	B(2)-B(1)-H(1)	112.9(11)
H(6A)-C(6)-H(6C)	115(4)	Co-B(1)-H(1)	116.4(11)
H(6B)-C(6)-H(6C)	99(3)	Fe-B(1)-H(1)	47.0(11)
C(2)-C(7)-H(7A)	108(2)	B(2)-B(1)-H(2)	42.6(13)

Table S4. continued Page 3.

Co-B(1)-H(2)	105.1(13)	B(1)-B(2)-H(5)	131.8(13)
Fe-B(1)-H(2)	113.4(13)	Co-B(2)-H(5)	121.2(13)
H(1)-B(1)-H(2)	95(2)	H(2)-B(2)-H(5)	107(2)
B(2)-B(1)-H(3)	131.3(14)	H(4)-B(2)-H(5)	108(2)
Co-B(1)-H(3)	124.1(13)	B(2)-B(3)-Co	62.74(11)
Fe-B(1)-H(3)	131.1(14)	B(2)-B(3)-Fe	97.72(14)
H(1)-B(1)-H(3)	105(2)	Co-B(3)-Fe	70.09(8)
H(2)-B(1)-H(3)	107(2)	B(2)-B(3)-H(4)	44.4(12)
B(3)-B(2)-B(1)	93.9(2)	Co-B(3)-H(4)	107.0(12)
B(3)-B(2)-Co	64.12(11)	Fe-B(3)-H(4)	111.3(12)
B(1)-B(2)-Co	64.20(11)	B(2)-B(3)-H(6)	114.9(11)
B(3)-B(2)-H(2)	114.5(14)	Co-B(3)-H(6)	117.3(12)
B(1)-B(2)-H(2)	45.9(13)	Fe-B(3)-H(6)	47.4(12)
Co-B(2)-H(2)	110.1(14)	H(4)-B(3)-H(6)	93(2)
B(3)-B(2)-H(4)	48.0(13)	B(2)-B(3)-H(7)	128(2)
B(1)-B(2)-H(4)	112.2(13)	Co-B(3)-H(7)	122(2)
Co-B(2)-H(4)	112.0(14)	Fe-B(3)-H(7)	134(2)
H(2)-B(2)-H(4)	95(2)	H(4)-B(3)-H(7)	107(2)
B(3)-B(2)-H(5)	133.2(13)	H(6)-B(3)-H(7)	106(2)

Table S5. Anisotropic displacement parameters ($Å^2$) for $(Me_5Cp)Co(B_3H_7)Fe(CO)_3$.

	U11	U22	U33	U23	U13	U12
Co	0.0338(2)	0.0348(2)	0.0382(2)	-0.0016(1)	0.0162(1)	0.0016(1)
Fe	0.0469(2)	0.0486(2)	0.0511(2)	0.0016(1)	0.0277(2)	-0.0013(1)
C(1)	0.0391(10)	0.0416(10)	0.0500(11)	-0.0061(9)	0.0222(9)	0.0036(8)
C(2)	0.0359(10)	0.0485(11)	0.0506(11)	-0.0090(9)	0.0218(9)	-0.0029(8)
C(3)	0.0476(11)	0.0411(10)	0.0556(12)	-0.0007(9)	0.0312(10)	-0.0018(8)
C(4)	0.0415(10)	0.0561(11)	0.0401(10)	0.0017(9)	0.0210(9)	0.0018(9)
C(5)	0.0402(10)	0.0466(10)	0.0448(10)	-0.0111(9)	0.0224(9)	-0.0046(8)
C(6)	0.060(2)	0.0513(14)	0.082(2)	0.0063(13)	0.0329(14)	0.0181(12)
C(7)	0.0389(12)	0.079(2)	0.068(2)	-0.0200(15)	0.0183(12)	-0.0104(12)
C(8)	0.083(2)	0.0441(13)	0.095(2)	0.0038(13)	0.056(2)	-0.0052(13)
C(9)	0.0562(15)	0.097(2)	0.0476(13)	0.0201(14)	0.0212(12)	0.0111(15)
C(10)	0.060(2)	0.067(2)	0.069(2)	-0.0291(14)	0.0332(14)	-0.0188(13)
C(11)	0.0612(14)	0.0635(14)	0.062(2)	0.0017(11)	0.0319(13)	0.0025(11)
O(11)	0.0780(13)	0.111(2)	0.0567(12)	-0.0030(11)	0.0197(10)	0.0022(12)
C(12)	0.069(2)	0.072(2)	0.068(2)	0.0031(13)	0.0429(14)	-0.0077(13)
O(12)	0.110(2)	0.125(2)	0.121(2)	0.0007(15)	0.089(2)	-0.0245(15)
C(13)	0.0625(15)	0.0578(15)	0.076(2)	0.0018(12)	0.0307(13)	-0.0004(12)
O(13)	0.111(2)	0.0544(12)	0.141(2)	0.0065(12)	0.060(2)	0.0166(12)
B(1)	0.0513(13)	0.0414(12)	0.0562(14)	0.0026(10)	0.0277(12)	0.0067(10)
B(2)	0.0535(14)	0.0474(13)	0.0533(14)	-0.0110(11)	0.0271(12)	-0.0036(11)
B(3)	0.0503(13)	0.0569(14)	0.0411(12)	0.0006(11)	0.0163(11)	0.0029(11)

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

Table S6. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for $(Me_5Cp)Co(B_3H_7)Fe(CO)_3$.

	x	y	z	$U_{iso}(Å^2)$
H(6A)	0.6965(17)	0.4814(54)	0.5617(30)	0.133(16)
H(6B)	0.7342(15)	0.5659(44)	0.6512(30)	0.114(12)
H(6C)	0.7487(16)	0.5462(44)	0.5779(26)	0.115(12)
H(7A)	0.7643(12)	1.0032(42)	0.6528(22)	0.089(10)
H(7B)	0.7892(15)	0.8768(40)	0.6283(25)	0.102(11)
H(7C)	0.7700(15)	0.8475(43)	0.6963(29)	0.109(13)
H(8A)	0.7022(13)	1.1869(39)	0.5423(24)	0.086(10)
H(8B)	0.6460(13)	1.1894(36)	0.4579(22)	0.081(9)
H(8C)	0.6888(13)	1.1673(40)	0.4395(26)	0.102(11)
H(9A)	0.5668(16)	1.0432(53)	0.3366(28)	0.131(15)
H(9B)	0.5487(15)	0.8771(44)	0.3063(26)	0.114(12)
H(9C)	0.5859(14)	0.9538(41)	0.2791(26)	0.105(11)
H(10A)	0.6077(13)	0.4969(43)	0.4200(24)	0.094(11)
H(10B)	0.6191(13)	0.5437(39)	0.3473(24)	0.098(11)
H(10C)	0.5661(13)	0.6073(35)	0.3422(21)	0.081(8)
H(1)	0.5557(10)	0.9288(30)	0.5907(17)	0.067(7)
H(2)	0.6120(11)	1.0761(34)	0.6367(20)	0.082(8)
H(3)	0.5603(9)	1.0637(28)	0.5052(17)	0.059(6)
H(4)	0.6619(11)	0.9543(34)	0.7337(20)	0.082(8)
H(5)	0.6810(9)	1.1019(30)	0.6704(17)	0.060(6)
H(6)	0.6217(10)	0.7687(28)	0.7108(19)	0.073(8)
H(7)	0.6941(12)	0.7523(32)	0.7456(21)	0.080(8)

Table S7. Selected torsion angles for $(Me_5Cp)Co(B_3H_7)Fe(CO)_3$.

133.20	(0.11)	B(2)-Co-Fe-C(11)	-165.57	(0.52)	C(5)-Co-Fe-C(12)
-178.06	(0.12)	B(3)-Co-Fe-C(11)	-48.74	(0.12)	B(2)-Co-Fe-B(3)
84.25	(0.12)	B(1)-Co-Fe-C(11)	0.00		B(3)-Co-Fe-B(3)
-122.84	(0.16)	C(2)-Co-Fe-C(11)	-97.69	(0.13)	B(1)-Co-Fe-B(3)
32.36	(0.20)	C(3)-Co-Fe-C(11)	55.22	(0.17)	C(2)-Co-Fe-B(3)
-86.85	(0.11)	C(1)-Co-Fe-C(11)	-149.57	(0.20)	C(3)-Co-Fe-B(3)
-2.84	(0.11)	C(4)-Co-Fe-C(11)	91.22	(0.11)	C(1)-Co-Fe-B(3)
-44.53	(0.10)	C(5)-Co-Fe-C(11)	175.22	(0.12)	C(4)-Co-Fe-B(3)
-133.92	(0.12)	B(2)-Co-Fe-C(13)	133.53	(0.11)	C(5)-Co-Fe-B(3)
-85.18	(0.13)	B(3)-Co-Fe-C(13)	48.95	(0.12)	B(2)-Co-Fe-B(1)
177.13	(0.13)	B(1)-Co-Fe-C(13)	97.69	(0.13)	B(3)-Co-Fe-B(1)
-29.96	(0.17)	C(2)-Co-Fe-C(13)	0.00		B(1)-Co-Fe-B(1)
125.24	(0.20)	C(3)-Co-Fe-C(13)	152.91	(0.17)	C(2)-Co-Fe-B(1)
6.03	(0.11)	C(1)-Co-Fe-C(13)	-51.88	(0.20)	C(3)-Co-Fe-B(1)
90.04	(0.11)	C(4)-Co-Fe-C(13)	-171.09	(0.11)	C(1)-Co-Fe-B(1)
48.35	(0.11)	C(5)-Co-Fe-C(13)	-87.09	(0.11)	C(4)-Co-Fe-B(1)
12.16	(0.53)	B(2)-Co-Fe-C(12)	-128.78	(0.11)	C(5)-Co-Fe-B(1)
60.90	(0.53)	B(3)-Co-Fe-C(12)	-39.37	(0.18)	B(2)-Co-C(1)-C(2)
-36.79	(0.53)	B(1)-Co-Fe-C(12)	-94.33	(0.14)	B(3)-Co-C(1)-C(2)
116.12	(0.54)	C(2)-Co-Fe-C(12)	95.87	(0.65)	B(1)-Co-C(1)-C(2)
-88.67	(0.55)	C(3)-Co-Fe-C(12)	0.00		C(2)-Co-C(1)-C(2)
152.12	(0.52)	C(1)-Co-Fe-C(12)	38.66	(0.12)	C(3)-Co-C(1)-C(2)
-123.88	(0.52)	C(4)-Co-Fe-C(12)	82.07	(0.13)	C(4)-Co-C(1)-C(2)

Table S7. continued Page 2.

118.73	(0.17)	C(5)-Co-C(1)-C(2)	123.72	(0.24)	Co-C(1)-C(2)-C(7)
-158.62	(0.10)	Fe-Co-C(1)-C(2)	60.60	(0.14)	C(5)-C(1)-C(2)-Co
-158.09	(0.14)	B(2)-Co-C(1)-C(5)	-124.73	(0.23)	C(6)-C(1)-C(2)-Co
146.94	(0.13)	B(3)-Co-C(1)-C(5)	0.00		Co-C(1)-C(2)-Co
-22.86	(0.70)	B(1)-Co-C(1)-C(5)	151.81	(0.13)	B(2)-Co-C(2)-C(1)
-118.73	(0.17)	C(2)-Co-C(1)-C(5)	97.75	(0.14)	B(3)-Co-C(2)-C(1)
-80.07	(0.13)	C(3)-Co-C(1)-C(5)	-167.54	(0.15)	B(1)-Co-C(2)-C(1)
-36.66	(0.12)	C(4)-Co-C(1)-C(5)	-117.97	(0.17)	C(3)-Co-C(2)-C(1)
0.00		C(5)-Co-C(1)-C(5)	0.00		C(1)-Co-C(2)-C(1)
82.65	(0.12)	Fe-Co-C(1)-C(5)	-80.49	(0.13)	C(4)-Co-C(2)-C(1)
79.06	(0.26)	B(2)-Co-C(1)-C(6)	-37.40	(0.12)	C(5)-Co-C(2)-C(1)
24.10	(0.25)	B(3)-Co-C(1)-C(6)	50.39	(0.20)	Fe-Co-C(2)-C(1)
-145.70	(0.62)	B(1)-Co-C(1)-C(6)	-90.22	(0.14)	B(2)-Co-C(2)-C(3)
118.43	(0.27)	C(2)-Co-C(1)-C(6)	-144.29	(0.13)	B(3)-Co-C(2)-C(3)
157.09	(0.25)	C(3)-Co-C(1)-C(6)	-49.57	(0.19)	B(1)-Co-C(2)-C(3)
-159.50	(0.25)	C(4)-Co-C(1)-C(6)	0.00		C(3)-Co-C(2)-C(3)
-122.84	(0.27)	C(5)-Co-C(1)-C(6)	117.97	(0.17)	C(1)-Co-C(2)-C(3)
-40.19	(0.25)	Fe-Co-C(1)-C(6)	37.48	(0.12)	C(4)-Co-C(2)-C(3)
0.17	(0.22)	C(5)-C(1)-C(2)-C(3)	80.57	(0.13)	C(5)-Co-C(2)-C(3)
174.83	(0.22)	C(6)-C(1)-C(2)-C(3)	168.36	(0.12)	Fe-Co-C(2)-C(3)
-60.43	(0.13)	Co-C(1)-C(2)-C(3)	31.40	(0.25)	B(2)-Co-C(2)-C(7)
-175.68	(0.22)	C(5)-C(1)-C(2)-C(7)	-22.66	(0.25)	B(3)-Co-C(2)-C(7)
-1.01	(0.36)	C(6)-C(1)-C(2)-C(7)	72.05	(0.28)	B(1)-Co-C(2)-C(7)

Table S7. continued Page 3.

121.62	(0.27)	C(3)-Co-C(2)-C(7)
-120.41	(0.28)	C(1)-Co-C(2)-C(7)
159.10	(0.25)	C(4)-Co-C(2)-C(7)
-157.81	(0.25)	C(5)-Co-C(2)-C(7)
-70.02	(0.28)	Fe-Co-C(2)-C(7)
0.30	(0.23)	C(1)-C(2)-C(3)-C(4)
176.04	(0.22)	C(7)-C(2)-C(3)-C(4)
-61.32	(0.14)	Co-C(2)-C(3)-C(4)
-176.22	(0.22)	C(1)-C(2)-C(3)-C(8)
-0.48	(0.38)	C(7)-C(2)-C(3)-C(8)
122.16	(0.24)	Co-C(2)-C(3)-C(8)
61.62	(0.14)	C(1)-C(2)-C(3)-Co
-122.64	(0.24)	C(7)-C(2)-C(3)-Co
0.00		Co-C(2)-C(3)-Co
-145.72	(0.13)	B(2)-Co-C(3)-C(4)
172.04	(0.14)	B(3)-Co-C(3)-C(4)
-92.19	(0.14)	B(1)-Co-C(3)-C(4)
118.63	(0.16)	C(2)-Co-C(3)-C(4)
80.76	(0.13)	C(1)-Co-C(3)-C(4)
0.00		C(4)-Co-C(3)-C(4)
37.68	(0.12)	C(5)-Co-C(3)-C(4)
-46.56	(0.24)	Fe-Co-C(3)-C(4)
95.65	(0.13)	B(2)-Co-C(3)-C(2)
53.40	(0.18)	B(3)-Co-C(3)-C(2)
149.18	(0.12)	B(1)-Co-C(3)-C(2)
0.00		C(2)-Co-C(3)-C(2)
-37.87	(0.11)	C(1)-Co-C(3)-C(2)
-118.63	(0.16)	C(4)-Co-C(3)-C(2)
-80.96	(0.12)	C(5)-Co-C(3)-C(2)
-165.19	(0.14)	Fe-Co-C(3)-C(2)
-24.61	(0.26)	B(2)-Co-C(3)-C(8)
-66.85	(0.28)	B(3)-Co-C(3)-C(8)
28.92	(0.27)	B(1)-Co-C(3)-C(8)
-120.26	(0.28)	C(2)-Co-C(3)-C(8)
-158.13	(0.27)	C(1)-Co-C(3)-C(8)
121.11	(0.28)	C(4)-Co-C(3)-C(8)
158.79	(0.27)	C(5)-Co-C(3)-C(8)
74.56	(0.32)	Fe-Co-C(3)-C(8)
-0.65	(0.22)	C(2)-C(3)-C(4)-C(5)
175.89	(0.22)	C(8)-C(3)-C(4)-C(5)
-60.76	(0.14)	Co-C(3)-C(4)-C(5)
-176.68	(0.22)	C(2)-C(3)-C(4)-C(9)
-0.14	(0.36)	C(8)-C(3)-C(4)-C(9)
123.21	(0.23)	Co-C(3)-C(4)-C(9)
60.11	(0.14)	C(2)-C(3)-C(4)-Co
-123.35	(0.23)	C(8)-C(3)-C(4)-Co

Table S7. continued Page 4.

0.00		Co-C(3)-C(4)-Co	122.44	(0.28)	C(5)-Co-C(4)-C(9)
45.31	(0.16)	B(2)-Co-C(4)-C(3)	44.35	(0.26)	Fe-Co-C(4)-C(9)
-52.33	(0.83)	B(3)-Co-C(4)-C(3)	-0.57	(0.22)	C(2)-C(1)-C(5)-C(4)
100.25	(0.13)	B(1)-Co-C(4)-C(3)	-175.10	(0.23)	C(6)-C(1)-C(5)-C(4)
-38.30	(0.12)	C(2)-Co-C(4)-C(3)	58.44	(0.14)	Co-C(1)-C(5)-C(4)
0.00		C(3)-Co-C(4)-C(3)	172.25	(0.21)	C(2)-C(1)-C(5)-C(10)
-81.72	(0.12)	C(1)-Co-C(4)-C(3)	-2.28	(0.36)	C(6)-C(1)-C(5)-C(10)
-118.33	(0.16)	C(5)-Co-C(4)-C(3)	-128.74	(0.22)	Co-C(1)-C(5)-C(10)
163.59	(0.09)	Fe-Co-C(4)-C(3)	-59.01	(0.13)	C(2)-C(1)-C(5)-Co
163.64	(0.13)	B(2)-Co-C(4)-C(5)	126.45	(0.24)	C(6)-C(1)-C(5)-Co
66.00	(0.81)	B(3)-Co-C(4)-C(5)	0.00		Co-C(1)-C(5)-Co
-141.43	(0.13)	B(1)-Co-C(4)-C(5)	0.75	(0.22)	C(3)-C(4)-C(5)-C(1)
80.02	(0.12)	C(2)-Co-C(4)-C(5)	176.72	(0.22)	C(9)-C(4)-C(5)-C(1)
118.33	(0.16)	C(3)-Co-C(4)-C(5)	-58.45	(0.14)	Co-C(4)-C(5)-C(1)
36.61	(0.11)	C(1)-Co-C(4)-C(5)	-172.08	(0.21)	C(3)-C(4)-C(5)-C(10)
0.00	(0.00)	C(5)-Co-C(4)-C(5)	3.89	(0.36)	C(9)-C(4)-C(5)-C(10)
-78.09	(0.12)	Fe-Co-C(4)-C(5)	128.72	(0.22)	Co-C(4)-C(5)-C(10)
-73.92	(0.27)	B(2)-Co-C(4)-C(9)	59.20	(0.13)	C(3)-C(4)-C(5)-Co
-171.56	(0.74)	B(3)-Co-C(4)-C(9)	-124.83	(0.23)	C(9)-C(4)-C(5)-Co
-18.99	(0.26)	B(1)-Co-C(4)-C(9)	0.00		Co-C(4)-C(5)-Co
-157.54	(0.26)	C(2)-Co-C(4)-C(9)	70.72	(0.36)	B(2)-Co-C(5)-C(1)
-119.23	(0.28)	C(3)-Co-C(4)-C(9)	-50.18	(0.18)	B(3)-Co-C(5)-C(1)
159.05	(0.26)	C(1)-Co-C(4)-C(9)	175.77	(0.13)	B(1)-Co-C(5)-C(1)

Table S7. continued Page 5.

37.78	(0.12)	C(2)-Co-C(5)-C(1)	-165.47	(5.47)	B(3)-Fe-C(11)-O(11)
82.38	(0.13)	C(3)-Co-C(5)-C(1)	-112.83	(5.54)	B(1)-Fe-C(11)-O(11)
0.00	(0.00)	C(1)-Co-C(5)-C(1)	-163.27	(5.54)	Co-Fe-C(11)-O(11)
120.34	(0.17)	C(4)-Co-C(5)-C(1)	9.14	(6.40)	C(11)-Fe-C(12)-O(12)
-117.10	(0.11)	Fe-Co-C(5)-C(1)	-85.00	(6.38)	C(13)-Fe-C(12)-O(12)
-49.62	(0.36)	B(2)-Co-C(5)-C(4)	-176.05	(6.33)	B(3)-Fe-C(12)-O(12)
-170.52	(0.14)	B(3)-Co-C(5)-C(4)	96.63	(6.38)	B(1)-Fe-C(12)-O(12)
55.43	(0.17)	B(1)-Co-C(5)-C(4)	129.38	(6.12)	Co-Fe-C(12)-O(12)
-82.55	(0.13)	C(2)-Co-C(5)-C(4)	-80.11	(12.47)	C(11)-Fe-C(13)-O(13)
-37.96	(0.12)	C(3)-Co-C(5)-C(4)	18.32	(12.49)	C(12)-Fe-C(13)-O(13)
-120.34	(0.17)	C(1)-Co-C(5)-C(4)	142.56	(12.48)	B(3)-Fe-C(13)-O(13)
0.00	(0.00)	C(4)-Co-C(5)-C(4)	-163.82	(12.38)	B(1)-Fe-C(13)-O(13)
122.56	(0.10)	Fe-Co-C(5)-C(4)	-167.24	(12.47)	Co-Fe-C(13)-O(13)
-169.35	(0.32)	B(2)-Co-C(5)-C(10)	0.00	(0.00)	B(2)-Co-B(1)-B(2)
69.75	(0.29)	B(3)-Co-C(5)-C(10)	50.17	(0.14)	B(3)-Co-B(1)-B(2)
-64.30	(0.28)	B(1)-Co-C(5)-C(10)	-53.43	(0.19)	C(2)-Co-B(1)-B(2)
157.71	(0.27)	C(2)-Co-C(5)-C(10)	-84.96	(0.13)	C(3)-Co-B(1)-B(2)
-157.69	(0.27)	C(3)-Co-C(5)-C(10)	-139.72	(0.63)	C(1)-Co-B(1)-B(2)
119.93	(0.29)	C(1)-Co-C(5)-C(10)	-126.56	(0.13)	C(4)-Co-B(1)-B(2)
-119.73	(0.29)	C(4)-Co-C(5)-C(10)	-159.48	(0.13)	C(5)-Co-B(1)-B(2)
2.82	(0.26)	Fe-Co-C(5)-C(10)	110.11	(0.13)	Fe-Co-B(1)-B(2)
107.52	(5.54)	C(13)-Fe-C(11)-O(11)	-110.11	(0.13)	B(2)-Co-B(1)-Fe
8.20	(5.55)	C(12)-Fe-C(11)-O(11)	-59.95	(0.09)	B(3)-Co-B(1)-Fe

-163.54	(0.11)	C(2)-Co-B(1)-Fe	-143.94	(0.13)	C(3)-Co-B(2)-B(3)
164.92	(0.07)	C(3)-Co-B(1)-Fe	-78.49	(0.16)	C(1)-Co-B(2)-B(3)
110.17	(0.64)	C(1)-Co-B(1)-Fe	-171.26	(0.12)	C(4)-Co-B(2)-B(3)
123.33	(0.07)	C(4)-Co-B(1)-Fe	-133.17	(0.31)	C(5)-Co-B(2)-B(3)
90.40	(0.11)	C(5)-Co-B(1)-Fe	54.17	(0.11)	Fe-Co-B(2)-B(3)
0.00		Fe-Co-B(1)-Fe	-108.51	(0.17)	B(3)-Co-B(2)-B(1)
-148.63	(0.15)	C(11)-Fe-B(1)-B(2)	0.00		B(1)-Co-B(2)-B(1)
-61.58	(0.22)	C(13)-Fe-B(1)-B(2)	148.67	(0.12)	C(2)-Co-B(2)-B(1)
115.93	(0.15)	C(12)-Fe-B(1)-B(2)	107.55	(0.12)	C(3)-Co-B(2)-B(1)
-3.35	(0.13)	B(3)-Fe-B(1)-B(2)	173.00	(0.12)	C(1)-Co-B(2)-B(1)
-57.14	(0.11)	Co-Fe-B(1)-B(2)	80.22	(0.15)	C(4)-Co-B(2)-B(1)
-91.48	(0.10)	C(11)-Fe-B(1)-Co	118.31	(0.31)	C(5)-Co-B(2)-B(1)
-4.44	(0.19)	C(13)-Fe-B(1)-Co	-54.34	(0.11)	Fe-Co-B(2)-B(1)
173.08	(0.10)	C(12)-Fe-B(1)-Co	58.83	(0.12)	B(1)-B(2)-B(3)-Co
53.80	(0.09)	B(3)-Fe-B(1)-Co	0.00	(0.00)	Co-B(2)-B(3)-Co
0.00		Co-Fe-B(1)-Co	-4.01	(0.15)	B(1)-B(2)-B(3)-Fe
-58.77	(0.12)	Co-B(1)-B(2)-B(3)	-62.85	(0.08)	Co-B(2)-B(3)-Fe
4.00	(0.15)	Fe-B(1)-B(2)-B(3)	0.00	(0.00)	B(2)-Co-B(3)-B(2)
0.00		Co-B(1)-B(2)-Co	-50.29	(0.13)	B(1)-Co-B(3)-B(2)
62.77	(0.08)	Fe-B(1)-B(2)-Co	89.52	(0.13)	C(2)-Co-B(3)-B(2)
0.00	(0.00)	B(3)-Co-B(2)-B(3)	56.55	(0.17)	C(3)-Co-B(3)-B(2)
108.51	(0.17)	B(1)-Co-B(2)-B(3)	131.13	(0.12)	C(1)-Co-B(3)-B(2)
-102.81	(0.13)	C(2)-Co-B(2)-B(3)	102.97	(0.79)	C(4)-Co-B(3)-B(2)

Table S7. continued Page 7.

161.82	(0.13)	C(5)-Co-B(3)-B(2)	60.13	(0.21)	C(11)-Fe-B(3)-B(2)
-110.32	(0.13)	Fe-Co-B(3)-B(2)	149.86	(0.15)	C(13)-Fe-B(3)-B(2)
110.32	(0.13)	B(2)-Co-B(3)-Fe	-112.25	(0.16)	C(12)-Fe-B(3)-B(2)
60.03	(0.08)	B(1)-Co-B(3)-Fe	3.36	(0.13)	B(1)-Fe-B(3)-B(2)
-160.16	(0.06)	C(2)-Co-B(3)-Fe	57.27	(0.11)	Co-Fe-B(3)-B(2)
166.87	(0.09)	C(3)-Co-B(3)-Fe	2.86	(0.18)	C(11)-Fe-B(3)-Co
-118.55	(0.07)	C(1)-Co-B(3)-Fe	92.59	(0.11)	C(13)-Fe-B(3)-Co
-146.71	(0.77)	C(4)-Co-B(3)-Fe	-169.53	(0.11)	C(12)-Fe-B(3)-Co
-87.86	(0.13)	C(5)-Co-B(3)-Fe	-53.91	(0.08)	B(1)-Fe-B(3)-Co
0.00		Fe-Co-B(3)-Fe	0.00		Co-Fe-B(3)-Co

Table S8. Least-squares planes for $(Me_5Cp)Co(B_3H_7)Fe(CO)_3$.

Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane)

```
 11.194 (0.013) x-4.919 (0.009) y + 6.732 (0.014) z = 6.736 (0.013)
*   -0.025 (0.001)  Co
*    0.034 (0.001)  Fe
*    0.004 (0.000)  B(2)
*    0.015 (0.002)  C(12)
*   -0.027 (0.002)  O(12)
    -1.291 (0.003)  B(1)
     1.311 (0.003)  B(3)
    -1.273 (0.003)  C(11)
     1.295 (0.003)  C(13)
     1.061 (0.003)  C(1)
     0.720 (0.003)  C(2)
    -0.707 (0.003)  C(3)
    -1.243 (0.003)  C(4)
    -0.148 (0.003)  C(5)
Rms deviation of fitted atoms =   0.023

 20.089 (0.022) x-2.694 (0.008) y-14.530 (0.009) z = 0.912 (0.015)
Angle to previous plane (with approximate esd) = 88.54 ( 0.07 )
*   -0.024 (0.001)  Fe
*    0.030 (0.001)  B(1)
*   -0.037 (0.001)  B(2)
*    0.031 (0.001)  B(3)
     1.551 (0.001)  Co
     0.957 (0.003)  C(11)
    -1.399 (0.003)  C(12)
     0.931 (0.004)  C(13)
Rms deviation of fitted atoms =   0.031

 24.464 (0.012) x-0.665 (0.005) y-14.207 (0.006) z = 8.905 (0.010)
Angle to previous plane (with approximate esd) = 17.43 ( 0.10 )
*   -0.063 (0.002)  C(1)
*   -0.045 (0.002)  C(2)
*   -0.035 (0.002)  C(3)
*   -0.054 (0.002)  C(4)
*   -0.060 (0.002)  C(5)
*    0.034 (0.002)  C(6)
*    0.051 (0.002)  C(7)
*    0.064 (0.002)  C(8)
*    0.019 (0.002)  C(9)
*    0.090 (0.002)  C(10)
    -1.744 (0.001)  Co
    -3.212 (0.003)  B(1)
    -2.907 (0.003)  B(2)
    -3.202 (0.003)  B(3)
    -3.807 (0.001)  Fe
Rms deviation of fitted atoms =   0.055
```

EXPERIMENTAL

DATA COLLECTION

A brown block-like crystal of $(Me_5Cp)Co(CO)(B_3H_7)$ having approximate dimensions of 0.38 x 0.35 x 0.30 mm was mounted on a glass fiber in a random orientation. Preliminary examination and data collection were performed with MoKα radiation (λ = 0.71073 Å) on an Enraf-Nonius CAD4 computer controlled kappa axis diffractometer equipped with a graphite crystal, incident beam monochromator.

Cell constants and an orientation matrix for data collection were obtained from least-squares refinement, using the setting angles of 25 reflections in the range $30^\circ < 2\theta < 32^\circ$, measured by the computer controlled diagonal slit method of centering. The monoclinic cell parameters and calculated volume are: a = 7.0216(11), b = 27.298(2), c = 8.0282(12) Å, β = 111.739(6)°, V = 1429.4(3) $Å^3$. For Z = 4 and F.W. = 261.65 the calculated density is 1.216 g/cm^3. As a check on crystal quality, an omega/theta profile analysis of reflections was carried out, which showed that Δω was less than 0.65° and Δθ was less than 0.60°, indicating good crystal quality. From the following systematic absence conditions

h0l: h + l = 2n; 0k0: k = 2n;

and the results of final structure refinement; the space group was determined to be $P2_1/n$ (No. 14).

The data were collected at a temperature of 20°C using the ω/2θ scan technique. The scan rate varied from 1.27 to 8.24°/min (in ω). The variable scan rate allows rapid data collection for intense reflections where a fast scan rate is used and assures good counting statistics for weak reflections and reflections with even negative intensity counts, where a slow scan rate is used. Data were collected to a maximum 2θ of 50.0°. The scan range (in degrees) was determined as a function of θ to correct for the separation of the Kα doublet; the scan width was calculated as follows:

$$\omega \text{ scan width} = 0.75^\circ + 0.35^\circ \tan\theta$$

Moving-crystal static-background counts were made by scanning an additional 25% nabove and below this range. Tus the ratio of peak counting time to

background counting time was 2:1. The counter aperture was also adjusted as a function of θ. The horizontal aperture width ranged from 2.0 to 2.4 mm; the vertical aperture was set at 4.0 mm. The diameter of the incident beam collimator was 0.8 mm and the crystal to detector distance was 21 cm. For intense reflections an attenuator was automatically inserted in front of the detector; the attenuator factor was 19.455.

A total of 2422 reflections were collected. As a check on crystal and electronic stability 3 representative reflections were measured every 120 minutes of X-ray exposure. A total intensity loss of -16.2% was found for the three standard reflections during 28.4 h of X-ray exposure for the data collection.

DATA REDUCTION

SDP software was used to precess intensity data on a VAXstation 3200 computer.[1] Lorentz and polarization corrections and a linear decay correction were applied to the data. The linear absorption coefficient is 11.76 cm^{-1} for MoKα radiation. An empirical absorption correction based on a series of psi-scans was applied to the data. Relative transmission coefficients ranged from 0.9983 to 0.8563.

STRUCTURE SOLUTION AND REFINEMENT

Structure solution and refinement were performed on a PC by using the SHELXTL package.[2] Most of the nonhydrogen atoms were located by the direct method, the remaining nonhydrogen atoms were found in succeeding difference Fourier synthesis. Least-squares refinement was carried out on F^2 for all reflections. After all nonhydrogen atoms were refined anisotropically, difference Fourier synthesis located all hydrogen atoms. In the final refinement methyl hydrogen atoms were refined with riding model, while the borane ones isotropically with bond length restraints. All reflections, including those with negative intensities, were included in the refinement and the $I > 2\sigma(I)$ criterion was used only for calculating R_1. The refinement

converged to a final value of R_1 = 0.0470 and wR_2 = 0.1168 for observed unique reflections ($I > 2\sigma(I)$) and R_1 = 0.0552 and wR_2 = 0.1505 for all unique reflections including those with negative intensities. The weighted R-factors, wR, are based on F^2 and conventional R-factors, R, on F, with F set to zero for negative intensities. The maximum and minimum residual electron densities on the final difference Fourier map were 0.424 e/Å^3 and -0.457 e/Å^3, respectively. All e.s.d's were estimated by the use of the full covariance matrix. The cell e.s.d's were included in the estimation of e.s.d's of bond distances and angles.

REFERENCES

(1) B. A. Frenz, ''The Enraf-Nonius CAD4 SDP - A Real-time System for Concurent X-Ray Data Collection and Crystal Structure Determination,'' in Computing in Crystallography, H. Schenk, R. Olthof-Hazelkamp, H. vanKonigsveld, and G. C. Bassi, Eds, Delft University Press. Delft, Holland, 1978, pp 64-71.

(2) SHELXTL V.5, Siemens Industrial Automation, Inc. 1994.

Table S1. Crystal data and structure refinement for $(Me_5Cp)Co(CO)(B_3H_7)$.

Molecule	$(Me_5Cp)Co(CO)(B_3H_7)$
Empirical formula	$C_{11}\ H_{22}\ B_3\ Co\ O$
Formula weight	261.65
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 7.0216(11) Å
	b = 27.298(2) Å
	c = 8.0282(12) Å
	β = 111.739(6)°
Volume	1429.4(3) $Å^3$
Z	4
Density (calculated)	1.216 Mg/m^3
F(000)	552
Wavelength	0.71073 Å
Absorption coefficient	1.176 mm^{-1}
Crystal size	0.38 x 0.35 x 0.30 mm
Temperature	293(2) K
Diffractometer	Enraf-Nonius CAD4
Theta range for data collection	2.83 to 25.00°
Index ranges	$0 \le h \le 8$, $0 \le k \le 32$, $-9 \le l \le 8$
Scan method	ω/2θ
Scan rate	1.27 - 8.24 °/min (in ω)
Scan width	0.75 + 0.35°tanθ (in ω)
Total data collected	2712
Unique data	2510 [R(int) = 0.0142]
Unique observed data [$I>2\sigma(I)$]	2240
Decay correction	Linear decay (16.2%/28.4h)
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.9983 and 0.8563
Refinement method	Full-matrix on F^2 (SHELXL-93)
Weighting scheme	sigma weight
Data / restraints / parameters	2485 / 9 / 175

Table S1. continued Page 2.

Goodness-of-fit on F^2	1.157
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0470, wR_2 = 0.1168
R indices (all data)	R_1 = 0.0552, wR_2 = 0.1505
Largest diff. peak and hole	0.424 and -0.457 $e \cdot Å^{-3}$

Table S2. Atomic coordinates and equivalent isotropic displacement parameters Ueq for $(Me_5Cp)Co(CO)(B_3H_7)$.

	x	y	z	$U_{eq}(Å^2)$
Co	0.94556(7)	0.12359(2)	0.88268(7)	0.0517(2)
C(1)	0.7584(6)	0.0850(2)	0.9875(6)	0.0618(10)
C(2)	0.7864(6)	0.1329(2)	1.0560(5)	0.0585(10)
C(3)	0.7090(5)	0.16640(14)	0.9108(5)	0.0515(8)
C(4)	0.6347(5)	0.1389(2)	0.7515(5)	0.0546(9)
C(5)	0.6648(6)	0.0888(2)	0.7979(6)	0.0633(10)
C(6)	0.8036(8)	0.0386(2)	1.0961(9)	0.105(2)
C(7)	0.8640(8)	0.1460(2)	1.2514(6)	0.097(2)
C(8)	0.6929(8)	0.2206(2)	0.9263(7)	0.0795(13)
C(9)	0.5315(7)	0.1595(2)	0.5659(6)	0.089(2)
C(10)	0.5894(8)	0.0467(2)	0.6691(9)	0.110(2)
C(11)	1.0230(7)	0.0888(2)	0.7379(6)	0.0738(12)
O	1.0647(6)	0.0644(2)	0.6396(5)	0.1147(14)
B(1)	1.2334(9)	0.1022(3)	1.0671(8)	0.087(2)
B(2)	1.1785(9)	0.1683(3)	1.0218(10)	0.088(2)
B(3)	1.0833(10)	0.1786(3)	0.7836(11)	0.094(2)

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$.

Table S3. Bond lengths (Å) for $(Me_5Cp)Co(CO)(B_3H_7)$.

Co-C(11)	1.736(5)	C(7)-H(7A)	0.96
Co-B(2)	2.014(6)	C(7)-H(7B)	0.96
Co-C(5)	2.063(4)	C(7)-H(7C)	0.96
Co-C(4)	2.085(3)	C(8)-H(8A)	0.96
Co-C(1)	2.088(4)	C(8)-H(8B)	0.96
Co-B(3)	2.096(6)	C(8)-H(8C)	0.96
Co-B(1)	2.098(6)	C(9)-H(9A)	0.96
Co-C(2)	2.098(4)	C(9)-H(9B)	0.96
Co-C(3)	2.110(4)	C(9)-H(9C)	0.96
C(1)-C(2)	1.403(6)	C(10)-H(10A)	0.96
C(1)-C(5)	1.420(6)	C(10)-H(10B)	0.96
C(1)-C(6)	1.505(6)	C(10)-H(10C)	0.96
C(2)-C(3)	1.422(5)	C(11)-O	1.151(5)
C(2)-C(7)	1.501(6)	B(1)-B(2)	1.853(11)
C(3)-C(4)	1.405(5)	B(1)-H(1)	1.09(2)
C(3)-C(8)	1.491(6)	B(1)-H(2)	1.10(3)
C(4)-C(5)	1.413(6)	B(1)-H(3)	1.27(4)
C(4)-C(9)	1.504(6)	B(2)-B(3)	1.798(10)
C(5)-C(10)	1.506(6)	B(2)-H(4)	1.10(3)
C(6)-H(6A)	0.96	B(2)-H(5)	1.25(4)
C(6)-H(6B)	0.96	B(3)-H(6)	1.11(3)
C(6)-H(6C)	0.96	B(3)-H(7)	1.11(3)

Table S4. Bond angles (deg) for $(Me_5Cp)Co(CO)(B_3H_7)$.

C(11)-Co-B(2)	108.1(3)	B(1)-Co-C(3)	132.0(2)
C(11)-Co-C(5)	91.5(2)	C(2)-Co-C(3)	39.5(2)
B(2)-Co-C(5)	160.4(2)	C(2)-C(1)-C(5)	107.1(3)
C(11)-Co-C(4)	107.5(2)	C(2)-C(1)-C(6)	126.0(4)
B(2)-Co-C(4)	129.9(2)	C(5)-C(1)-C(6)	126.6(5)
C(5)-Co-C(4)	39.8(2)	C(2)-C(1)-Co	70.8(2)
C(11)-Co-C(1)	113.2(2)	C(5)-C(1)-Co	69.1(2)
B(2)-Co-C(1)	125.8(2)	C(6)-C(1)-Co	129.0(3)
C(5)-Co-C(1)	40.0(2)	C(1)-C(2)-C(3)	108.7(3)
C(4)-Co-C(1)	66.9(2)	C(1)-C(2)-C(7)	125.2(4)
C(11)-Co-B(3)	80.5(3)	C(3)-C(2)-C(7)	125.8(4)
B(2)-Co-B(3)	51.9(3)	C(1)-C(2)-Co	70.0(2)
C(5)-Co-B(3)	136.3(2)	C(3)-C(2)-Co	70.7(2)
C(4)-Co-B(3)	102.0(2)	C(7)-C(2)-Co	130.2(3)
C(1)-Co-B(3)	164.1(2)	C(4)-C(3)-C(2)	107.7(3)
C(11)-Co-B(1)	82.0(2)	C(4)-C(3)-C(8)	126.2(4)
B(2)-Co-B(1)	53.5(3)	C(2)-C(3)-C(8)	125.9(4)
C(5)-Co-B(1)	131.1(2)	C(4)-C(3)-Co	69.4(2)
C(4)-Co-B(1)	165.3(2)	C(2)-C(3)-Co	69.8(2)
C(1)-Co-B(1)	99.3(2)	C(8)-C(3)-Co	130.1(3)
B(3)-Co-B(1)	90.5(3)	C(3)-C(4)-C(5)	107.9(3)
C(11)-Co-C(2)	152.4(2)	C(3)-C(4)-C(9)	125.6(4)
B(2)-Co-C(2)	94.7(2)	C(5)-C(4)-C(9)	126.4(4)
C(5)-Co-C(2)	66.2(2)	C(3)-C(4)-Co	71.4(2)
C(4)-Co-C(2)	66.14(14)	C(5)-C(4)-Co	69.3(2)
C(1)-Co-C(2)	39.2(2)	C(9)-C(4)-Co	127.3(3)
B(3)-Co-C(2)	126.8(3)	C(4)-C(5)-C(1)	108.5(3)
B(1)-Co-C(2)	100.2(2)	C(4)-C(5)-C(10)	125.3(4)
C(11)-Co-C(3)	145.9(2)	C(1)-C(5)-C(10)	125.9(5)
B(2)-Co-C(3)	96.6(2)	C(4)-C(5)-Co	70.9(2)
C(5)-Co-C(3)	66.2(2)	C(1)-C(5)-Co	70.9(2)
C(4)-Co-C(3)	39.14(14)	C(10)-C(5)-Co	128.9(3)
C(1)-Co-C(3)	66.3(2)	C(1)-C(6)-H(6A)	109.5(3)
B(3)-Co-C(3)	97.8(2)	C(1)-C(6)-H(6B)	109.5(3)

Table S4. continued Page 2.

H(6A)-C(6)-H(6B)	109.5	B(2)-B(1)-H(2)	116(3)
C(1)-C(6)-H(6C)	109.5(3)	Co-B(1)-H(2)	115(3)
H(6A)-C(6)-H(6C)	109.5	H(1)-B(1)-H(2)	102(3)
H(6B)-C(6)-H(6C)	109.5	B(2)-B(1)-H(3)	42(2)
C(2)-C(7)-H(7A)	109.5(3)	Co-B(1)-H(3)	102(2)
C(2)-C(7)-H(7B)	109.5(3)	H(1)-B(1)-H(3)	111(3)
H(7A)-C(7)-H(7B)	109.5	H(2)-B(1)-H(3)	92(4)
C(2)-C(7)-H(7C)	109.5(3)	B(3)-B(2)-B(1)	109.3(5)
H(7A)-C(7)-H(7C)	109.5	B(3)-B(2)-Co	66.4(3)
H(7B)-C(7)-H(7C)	109.5	B(1)-B(2)-Co	65.6(3)
C(3)-C(8)-H(8A)	109.5(3)	B(3)-B(2)-H(3)	121(3)
C(3)-C(8)-H(8B)	109.5(2)	B(1)-B(2)-H(3)	43(2)
H(8A)-C(8)-H(8B)	109.5	Co-B(2)-H(3)	108(2)
C(3)-C(8)-H(8C)	109.5(2)	B(3)-B(2)-H(4)	120(3)
H(8A)-C(8)-H(8C)	109.5	B(1)-B(2)-H(4)	127(3)
H(8B)-C(8)-H(8C)	109.5	Co-B(2)-H(4)	116(3)
C(4)-C(9)-H(9A)	109.5(3)	H(3)-B(2)-H(4)	115(4)
C(4)-C(9)-H(9B)	109.5(3)	B(3)-B(2)-H(5)	44(2)
H(9A)-C(9)-H(9B)	109.5	B(1)-B(2)-H(5)	130(3)
C(4)-C(9)-H(9C)	109.5(2)	Co-B(2)-H(5)	111(2)
H(9A)-C(9)-H(9C)	109.5	H(3)-B(2)-H(5)	106(4)
H(9B)-C(9)-H(9C)	109.5	H(4)-B(2)-H(5)	101(4)
C(5)-C(10)-H(10A)	109.5(3)	B(2)-B(3)-Co	61.7(3)
C(5)-C(10)-H(10B)	109.5(3)	B(2)-B(3)-H(5)	44(2)
H(10A)-C(10)-H(10B)	109.5	Co-B(3)-H(5)	106(2)
C(5)-C(10)-H(10C)	109.5(3)	B(2)-B(3)-H(6)	122(3)
H(10A)-C(10)-H(10C)	109.5	Co-B(3)-H(6)	115(3)
H(10B)-C(10)-H(10C)	109.5	H(5)-B(3)-H(6)	103(4)
O-C(11)-Co	176.3(5)	B(2)-B(3)-H(7)	123(3)
B(2)-B(1)-Co	60.9(3)	Co-B(3)-H(7)	121(3)
B(2)-B(1)-H(1)	130(2)	H(5)-B(3)-H(7)	101(4)
Co-B(1)-H(1)	129(2)	H(6)-B(3)-H(7)	108(4)

Table S5. Anisotropic displacement parameters ($Å^2$) for $(Me_5Cp)Co(CO)(B_3H_7)$.

	U11	U22	U33	U23	U13	U12
Co	0.0368(3)	0.0661(4)	0.0523(3)	0.0035(2)	0.0167(2)	-0.0016(2)
C(1)	0.044(2)	0.072(3)	0.073(3)	0.015(2)	0.027(2)	-0.003(2)
C(2)	0.045(2)	0.089(3)	0.044(2)	0.002(2)	0.020(2)	-0.006(2)
C(3)	0.043(2)	0.060(2)	0.055(2)	-0.001(2)	0.022(2)	-0.003(2)
C(4)	0.037(2)	0.079(3)	0.046(2)	-0.002(2)	0.0126(15)	0.003(2)
C(5)	0.039(2)	0.077(3)	0.073(3)	-0.018(2)	0.020(2)	-0.011(2)
C(6)	0.085(4)	0.096(4)	0.142(5)	0.051(4)	0.051(4)	0.010(3)
C(7)	0.088(3)	0.158(5)	0.048(2)	-0.005(3)	0.028(2)	-0.007(4)
C(8)	0.079(3)	0.063(3)	0.106(4)	-0.007(2)	0.045(3)	-0.001(2)
C(9)	0.063(3)	0.149(5)	0.049(2)	0.012(3)	0.014(2)	0.017(3)
C(10)	0.075(3)	0.108(4)	0.141(5)	-0.067(4)	0.034(3)	-0.018(3)
C(11)	0.065(3)	0.100(3)	0.062(3)	0.011(2)	0.030(2)	0.023(2)
O	0.119(3)	0.153(4)	0.087(3)	-0.002(2)	0.056(2)	0.041(3)
B(1)	0.052(3)	0.121(5)	0.071(4)	0.003(3)	0.004(3)	0.006(3)
B(2)	0.052(3)	0.109(5)	0.099(4)	-0.019(4)	0.023(3)	-0.020(3)
B(3)	0.070(4)	0.117(5)	0.112(5)	0.029(4)	0.053(4)	-0.007(4)

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

Table S6. Hydrogen coordinates and isotropic displacement parameters (Å^2) for $(Me_5Cp)Co(CO)(B_3H_7)$.

	x	y	z	U_{iso}(Å^2)
H(6A)	0.7711(8)	0.0109(2)	1.0170(9)	0.158
H(6B)	0.7222(8)	0.0376(2)	1.1693(9)	0.158
H(6C)	0.9464(8)	0.0377(2)	1.1714(9)	0.158
H(7A)	0.8696(8)	0.1810(2)	1.2641(6)	0.146
H(7B)	0.9988(8)	0.1326(2)	1.3102(6)	0.146
H(7C)	0.7733(8)	0.1329(2)	1.3049(6)	0.146
H(8A)	0.7559(8)	0.2300(2)	1.0499(7)	0.119
H(8B)	0.5511(8)	0.2299(2)	0.8813(7)	0.119
H(8C)	0.7614(8)	0.2365(2)	0.8577(7)	0.119
H(9A)	0.4952(7)	0.1332(2)	0.4803(6)	0.134
H(9B)	0.6234(7)	0.1815(2)	0.5399(6)	0.134
H(9C)	0.4099(7)	0.1769(2)	0.5590(6)	0.134
H(10A)	0.6292(8)	0.0163(2)	0.7330(9)	0.165
H(10B)	0.6484(8)	0.0487(2)	0.5788(9)	0.165
H(10C)	0.4427(8)	0.0481(2)	0.6132(9)	0.165
H(1)	1.2712(45)	0.0814(10)	1.1910(36)	0.033(7)
H(2)	1.3356(70)	0.0854(18)	1.0082(65)	0.103(17)
H(3)	1.3316(69)	0.1425(11)	1.0956(66)	0.104(17)
H(4)	1.1457(78)	0.1952(16)	1.1094(61)	0.104(17)
H(5)	1.2240(81)	0.1961(20)	0.9183(41)	0.137(22)
H(6)	1.1662(69)	0.1656(17)	0.6976(59)	0.095(15)
H(7)	0.9980(66)	0.2120(13)	0.7209(62)	0.092(15)