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Structures of Metallocarboranes. 8. Crystal and Molecular Structure of the 11-Vertex Heterobimetallocarborane 1,8-Di-η-cyclopentadienyl-1-ferra-8-cobalta-2,3-dicarbaundecaborane(9), $1,8\text{-}(\eta\text{-C}_5\text{H}_5)_2\text{-1-Fe-8-Co-2,3-C}_2\text{B}_7\text{H}_9$[1]

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Received October 26, 1977

The crystal and molecular structure of $1,8\text{-}(\eta\text{-C}_5\text{H}_5)_2\text{-1-Fe-8-Co-2,3-C}_2\text{B}_7\text{H}_9$ has been determined by three-dimensional x-ray diffraction techniques. The compound crystallizes in the monoclinic space group $P2_1/c$ with a = 7.923 (1) Å, b = 13.474 (3) Å, c = 14.707 (4) Å, β = 107.10 (3)°, and Z = 4. Observed and calculated densities are 1.58 (2) and 1.57 g cm^{-3}, respectively. Diffraction data to $2\theta_{\max}$ = 45° (Mo Kα radiation) were collected on a Syntex $P\bar{1}$ automated diffractometer, and the structure was solved by conventional Patterson, Fourier, and full-matrix least-squares techniques to a final discrepancy index of R = 0.04 for the 1346 independent nonzero reflections. All atoms, including hydrogens, were located, and the iron and cobalt atoms were unambiguously differentiated. Although it is one electron short of the ideal $2n + 2$ electrons for closo polyhedral bonding, the molecule has the closo 11-vertex octadecahedral geometry with the iron atom in the six-coordinate vertex, the two carbon atoms located at the four-coordinate vertices, and the cobalt atom situated in a five-coordinate position, adjacent to a carbon atom and nonadjacent to the iron vertex. The molecule exhibits some unusual bond length asymmetries.

Introduction

Polyhedral metallocarboranes containing two different transition-metal vertices can be prepared by use of either polyhedral expansion[2] or polyhedral subrogation[3] reactions on previously prepared metallocarboranes.[4] When the 10-vertex compound $2\text{-}(\eta\text{-C}_5\text{H}_5)\text{-2-Co-1,6-C}_2\text{B}_7\text{H}_9$[5] was subjected to polyhedral expansion conditions with FeCl_2 and C_5H_5^-, the 11-vertex complex $(\text{C}_5\text{H}_5)_2\text{CoFeC}_2\text{B}_7\text{H}_9$ was isolated.[4] According to commonly accepted electron-counting rules,[6,7] this complex has one electron less than required for idealized closo octadecahedral geometry. In $(\text{C}_5\text{H}_5)_2\text{Fe}_2\text{C}_2\text{B}_6\text{H}_8$, which is two electrons short of the required $2n + 2$ (where n is the number of vertices in the polyhedron), a large distortion from the usual 10-vertex bicapped square antiprism geometry was observed.[8] To assess the effect of a one-electron deficiency, the x-ray structural determination of $(\text{C}_5\text{H}_5)_2\text{FeCoC}_2\text{B}_7\text{H}_9$ was undertaken.

Experimental Section

Crystals of the title compound were kindly provided by Dr. W. J. Evans, who prepared them by the polyhedral expansion of $2\text{-}(\eta\text{-C}_5\text{H}_5)\text{-2-Co-1,6-C}_2\text{B}_7\text{H}_9$ with FeCl_2 and C_5H_5^-.[4] Spectroscopic studies (^{1}H and ^{11}B NMR) on this compound and on the reduced diamagnetic Fe(II) species were consistent with the proposed octadecahedral geometry, but the precise locations of the two metal atoms could not be determined by these methods.

A single crystal of dimensions 0.1 × 0.2 × 0.3 mm was selected for crystallographic investigation and mounted on a glass fiber enclosed in a thin-walled glass capillary. Preliminary oscillation and Weissenberg photographs indicated that the compound crystallized in space group $P2_1/c$ with systematic absences of the type $h0l$, $l \neq 2n$, and $0k0$, $k \neq 2n$.

The crystal was transferred to a Syntex $P\bar{1}$ automated diffractometer, and 12 automatically centered reflections were used to accurately determine the unit cell parameters as a = 7.923 (1) Å, b = 13.474 (3) Å, c = 14.707 (4) Å, and β = 107.10 (3)°. A graphite crystal was used to provide monochromatic Mo Kα radiation (0.71069 Å). The sample density was found to be 1.58 (2) g cm^{-3} by flotation, while the calculated density was 1.57 g cm^{-3} (Z = 4).

Intensity data were collected with a θ–2θ scan technique to a limit of 2θ = 45° and with a takeoff angle of 4°. Reflections were scanned at a constant rate of 2.4°/min from 1.0° below the Kα_1 reflection to 1.0° above the Kα_2 reflection. Backgrounds were measured at each end of the scan. The total time spent counting background radiation was equal to the scan time for each reflection. The intensities of three standard reflections were measured every 97 reflections to monitor the tube efficiency and possible crystal deterioration. No significant deviations were observed.

The data were corrected for Lorentz and polarization effects and for absorption (T = 0.76–0.85).[9] The intensity of a reflection, $I(hkl)$, and $\sigma[I(hkl)]$, its estimated standard deviation, were calculated according to the equations $I = \text{CT} - (t_c/t_b)(B_1 + B_2)/2$ and $\sigma(I) =$

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Table I. Final Atomic Parameters[a]

Atom	x	y	z
Fe1	0.25478 (11)	0.36406 (7)	0.33798 (6)
Co8	0.60558 (11)	0.19897 (7)	0.43194 (6)
Cp1	0.0005 (10)	0.4130 (7)	0.3300 (9)
Cp2	0.0646 (13)	0.4646 (7)	0.2682 (7)
Cp3	0.2142 (13)	0.5153 (6)	0.3185 (9)
Cp4	0.2402 (11)	0.4926 (7)	0.4135 (8)
Cp5	0.1088 (14)	0.4292 (7)	0.4200 (7)
Cp6	0.7433 (15)	0.1899 (11)	0.5744 (6)
Cp7	0.8497 (12)	0.2257 (7)	0.5261 (9)
Cp8	0.8648 (10)	0.1583 (10)	0.4607 (7)
Cp9	0.7634 (14)	0.0761 (7)	0.4677 (7)
Cp10	0.6892 (11)	0.0990 (10)	0.5408 (9)
C2	0.4500 (7)	0.3069 (5)	0.4389 (4)
C3	0.2335 (11)	0.2983 (6)	0.2173 (5)
B4	0.5429 (10)	0.3411 (6)	0.3640 (6)
B5	0.3272 (9)	0.2145 (6)	0.4090 (6)
B6	0.2013 (11)	0.2115 (6)	0.2826 (6)
B7	0.4224 (14)	0.3360 (7)	0.2409 (7)
B9	0.3577 (13)	0.2047 (7)	0.2114 (6)
B10	0.5613 (11)	0.2362 (7)	0.2900 (6)
B11	0.4157 (13)	0.1426 (6)	0.3187 (6)
CpH1	−0.1074	0.3702	0.3123
CpH2	0.0140	0.4692	0.1943
CpH3	0.2956	0.5627	0.2916
CpH4	0.3483	0.5215	0.4698
CpH5	0.0992	0.4025	0.4831
CpH6	0.7087	0.2245	0.6264
CpH7	0.9152	0.2942	0.5337
CpH8	0.9413	0.1616	0.4107
CpH9	0.7511	0.0099	0.4274
CpH10	0.6073	0.0487	0.5607
C2H	0.4678	0.3456	0.4870
C3H	0.1389	0.3229	0.1477
B4H	0.6420	0.4055	0.3770
B5H	0.2503	0.1755	0.4550
B6H	0.0664	0.1770	0.2591
B7H	0.4660	0.4004	0.1929
B9H	0.3255	0.1646	0.1354
B10H	0.6699	0.2233	0.2580
B11H	0.4113	0.0764	0.3139

[a] Values in parentheses are estimated standard deviations and refer to the last digit of the preceding number.

$\{\sigma_s^2 + (0.04I)^2\}^{1/2}$, where I is the net integrated intensity, CT is the total integrated count, t_c and t_b are the times employed for counting the scan and background, respectively, B_1 and B_2 are the background counts on the low and high sides of the reflection, and σ_s is the standard deviation in the intensity due to counting statistics. Reflections having intensities less than 3 times their standard deviations were defined as unobserved and not included in subsequent calculations.

Solution and Refinement of the Structure

The coordinates of the two metal atoms were determined by solution of a three-dimensional Patterson map, and a subsequent Fourier synthesis resulted in the location of all nonhydrogen atoms. After several cycles of full-matrix least-squares refinement, hydrogen atom positions were obtained from a Fourier difference map. Hydrogen atom positions were included but not refined in final least-squares cycles. Temperature factors of 6.0 and 7.0 Å^2 were assigned to the cage and cyclopentadienyl hydrogen atoms, respectively. The assignment of the iron atom to the high-coordinate site was conclusively established by least-squares calculations in which the positions of the two metals were deliberately interchanged. The elevated residual thereby obtained, $R_w = 0.048$ vs. 0.044, along with the alterations in the temperature factors, indicated that the iron atom was located at position 1. Similar evidence led to the location of the polyhedral carbon atoms at the low-coordinate positions 2 and 3. The final refinement of positional and anisotropic thermal parameters for all nonhydrogen atoms converged to $R = 0.040$ and $R_w = 0.044$. Scattering factors for neutral iron, cobalt, carbon, and boron were taken from Hanson et al.,[10] hydrogen scattering factors were obtained from Stewart, Davidson, and Simpson,[11] and the real and imaginary corrections for anomalous scattering by iron and cobalt were taken from Cromer.[12] The function $\sum w||F_o| - |F_c||^2$ was minimized in the refinement. The standard deviation of an observation of unit weight was 1.43. Because of an unexpected asymmetry in the observed molecular structure, a second series of refinements was carried out in which the cage atoms were constrained to have C_s symmetry.[13] In this refinement, all atoms were given isotropic temperature factors which were refined along with the positional parameters. This refinement converged to $R = 0.073$ and $R_w = 0.080$. The C_s constraint was then removed and the refinement converged to $R = 0.071$ and $R_w = 0.077$. In a final refinement anisotropic thermal parameters were refined for all nonhydrogen atoms. Structural parameters and R values obtained in this refinement did not differ significantly from those obtained originally.

The final observed and calculated structure factors are available.[14] Atomic fractional coordinates are collected in Table I. Anisotropic thermal parameters of the nonhydrogen atoms are listed in Table II.

Molecular Structure

Intramolecular distances and their estimated deviations (esd's) are listed in Table III. Average bond distances, with their root-mean-square deviations, are collected in Table IV. The individual bond angles and their associated esd's are presented in Table V. The structure of 1,8-(η-C_5H_5)$_2$-1-

Table II. Anisotropic Thermal Parameters (×10^4)[a]

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Fe1	108.2 (17)	37.2 (6)	48.4 (6)	−9.7 (9)	16.1 (7)	−1.4 (5)
Co8	138.9 (18)	59.6 (7)	40.9 (5)	13.5 (9)	35.7 (8)	8.1 (5)
Cp1	141 (16)	69 (6)	147 (10)	9 (8)	67 (11)	−20 (7)
Cp2	240 (21)	72 (7)	97 (7)	70 (10)	12 (10)	11 (6)
Cp3	289 (25)	38 (5)	163 (11)	4 (9)	108 (14)	3 (7)
Cp4	167 (17)	71 (7)	115 (8)	22 (9)	1 (10)	−55 (6)
Cp5	273 (22)	99 (8)	92 (7)	47 (12)	84 (11)	−9 (6)
Cp6	322 (28)	162 (12)	37 (5)	91 (16)	9 (9)	−9 (7)
Cp7	205 (20)	93 (8)	98 (8)	−18 (10)	−37 (10)	19 (7)
Cp8	146 (16)	147 (11)	77 (6)	54 (11)	48 (8)	28 (7)
Cp9	272 (23)	72 (7)	89 (7)	59 (11)	−25 (11)	−8 (6)
Cp10	144 (16)	140 (11)	98 (9)	13 (11)	14 (10)	80 (8)
C2	118 (12)	52 (4)	38 (4)	−3 (6)	25 (5)	−6 (4)
C3	320 (21)	70 (6)	54 (5)	9 (10)	25 (8)	−5 (5)
B4	161 (17)	46 (6)	61 (5)	−1 (7)	42 (8)	−2 (4)
B5	135 (15)	50 (6)	53 (5)	−12 (8)	22 (7)	11 (4)
B6	175 (17)	62 (6)	50 (5)	−31 (9)	−3 (8)	0 (5)
B7	310 (25)	76 (8)	53 (6)	41 (11)	43 (10)	2 (5)
B9	309 (24)	82 (8)	39 (5)	35 (11)	1 (9)	−17 (6)
B10	227 (19)	66 (7)	49 (5)	16 (9)	62 (8)	1 (5)
B11	327 (24)	42 (5)	51 (6)	6 (10)	−42 (9)	2 (5)

[a] See footnote a of Table I. The anisotropic temperature factor T is defined as $T = \exp[-(B_{11}h^2 + B_{22}k^2 + B_{33}l^2 + 2B_{12}hk + 2B_{13}hl + 2B_{23}kl)]$. Thermal ellipsoids are depicted in the figure.

Table III. Interatomic Distances[a]

Atoms	Distance, Å	Atoms	Distance, Å
Distances in the Cyclopentadienyl Rings			
Cp1-Cp2	1.357 (12)	Cp6-Cp7	1.342 (13)
Cp1-Cp5	1.366 (12)	Cp6-Cp10	1.342 (13)
Cp2-Cp3	1.379 (11)	Cp7-Cp8	1.352 (13)
Cp3-Cp4	1.385 (12)	Cp8-Cp9	1.389 (12)
Cp4-Cp5	1.372 (12)	Cp9-Cp10	1.404 (13)
Cp1-CpH1	1.000 (8)	Cp6-CpH6	1.000 (9)
Cp2-CpH2	1.044 (9)	Cp7-CpH7	1.049 (9)
Cp3-CpH3	1.064 (9)	Cp8-CpH8	1.083 (8)
Cp4-CpH4	1.074 (8)	Cp9-CpH9	1.059 (9)
Cp5-CpH5	1.020 (9)	Cp10-CpH10	1.038 (9)
Distances around Iron			
Fe-Cp1	2.091 (7)	Fe-C2	1.959 (6)
Fe-Cp2	2.062 (7)	Fe-C3	1.945 (8)
Fe-Cp3	2.070 (8)	Fe-B4	2.223 (7)
Fe-Cp4	2.078 (8)	Fe-B5	2.266 (8)
Fe-Cp5	2.093 (8)	Fe-B6	2.205 (9)
		Fe-B7	2.249 (10)
Distances around Cobalt			
Co-Cp6	2.062 (8)	Co-C2	1.928 (6)
Co-Cp7	2.052 (8)	Co-B4	2.150 (8)
Co-Cp8	2.046 (7)	Co-B5	2.142 (7)
Co-Cp9	2.049 (8)	Co-B10	2.074 (8)
Co-Cp10	2.049 (8)	Co-B11	2.034 (8)
Boron-Boron Distances			
B4-B7	1.783 (12)	B7-B9	1.858 (14)
B4-B10	1.814 (11)	B7-B10	1.755 (12)
B5-B6	1.833 (11)	B9-B10	1.738 (12)
B5-B11	1.933 (13)	B9-B11	1.726 (12)
B6-B9	1.846 (13)	B10-B11	1.839 (13)
B6-B11	1.871 (12)		
Carbon-Boron Distances			
C2-B4	1.564 (9)	C3-B7	1.521 (12)
C2-B5	1.561 (9)	C3-B9	1.618 (11)
C3-B6	1.581 (11)		
Carbon-Hydrogen Distances			
C2-CH2	0.857 (6)	C3-CH3	1.127 (8)
Boron-Hydrogen Distances			
B4-B4H	1.148 (8)	B9-B9H	1.199 (9)
B5-B5H	1.160 (7)	B10-B10H	1.110 (8)
B6-B6H	1.123 (8)	B11-B11H	0.895 (9)
B7-B7H	1.230 (10)		

[a] See footnote *a* of Table I.

Table IV. Average Bond Lengths[a]

Atoms	No.	Range, Å	Average,[b] Å
Fe-C	7	1.945 (8)-2.093 (8)	2.04 (6)
Co-C	6	1.928 (6)-2.062 (8)	2.03 (5)
Fe-B	4	2.205 (9)-2.249 (10)	2.24 (3)
Co-B	4	2.034 (8)-2.150 (8)	2.10 (6)
C-C	10	1.342 (13)-1.404 (13)	1.37 (2)
B-B	11	1.726 (12)-1.933 (13)	1.82 (6)
C-B	5	1.521 (12)-1.618 (11)	1.57 (4)
B-H	7	0.895 (9)-1.230 (10)	1.12 (11)
C-H	12	0.857 (6)-1.127 (8)	1.03 (6)

[a] See footnote *a* of Table I. [b] Esd's for average bond lengths were calculated using the internal routine of an HP-45 calculator.

Fe-8-Co-2,3-$C_2B_7H_9$ is shown in Figure 1, which also illustrates the numbering system employed.[15]

The complex exhibits an overall geometry based on the octadecahedron, a closed 11-vertex polyhedron. In this geometry, one vertex is high coordinate (position 1), having six adjacent polyhedral vertices, while two positions (vertices 2 and 3) are adjacent to only four other polyhedral sites. The remaining eight vertices are coordinated to five atoms in the polyhedron. In $(C_5H_5)_2CoFeC_2B_7H_9$, the iron atom occupies the high-coordinate position, while the cobalt is located in a five-coordinate position nonadjacent to the iron atom. The two low-coordinate positions are occupied by carbon atoms. A monometallocarborane fragment with similar geometry was recently reported.[16] In this structure, a cobalt atom occupied the high-coordinate position and two carbon atoms occupied the low-coordinate positions.

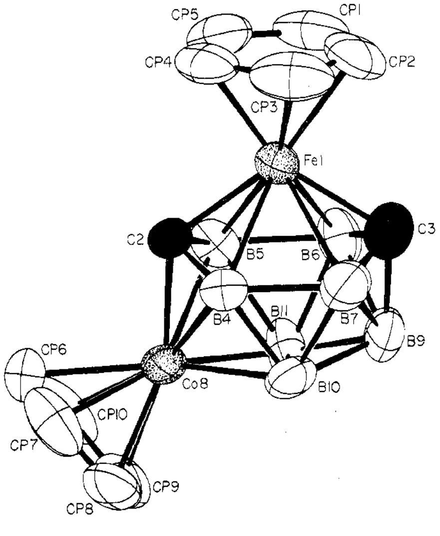

Figure 1.

Both metal vertices in $(C_5H_5)_2FeCoC_2B_7H_9$ are coordinated to π-bonded cyclopentadienyl rings, with metal-carbon distances equal within three standard deviations. The iron-boron bonds, however, are significantly longer than the cobalt-boron bonds. This probably reflects the greater coordination number at the iron atom; such an effect has been noted previously.[8]

Neglecting the cyclopentadienyl rings attached to the metal vertices, the molecule has potential mirror symmetry, the mirror passing through atoms Fe(1), C(2), C(3), Co(8), and B(9). Significant deviations from this potential symmetry are observed, however. Two bonds, related by this "pseudomirror", differ by large amounts: B(4)-B(10) = 1.814 (11) vs. B(5)-B(11) = 1.933 (13) Å, $\Delta = 0.119$ Å, and B(6)-B(11) = 1.871 (12) vs. B(7)-B(10) = 1.755 (12) Å, $\Delta = 0.116$ Å. These discrepancies from mirror symmetry are reminiscent of similar distortions noted by Churchill and DeBoer[17] in the structure of 2-(η-C_5H_5)-2-Co-1,6-$C_2B_{10}H_{12}$; the bond length differences noted by these authors were of the same magnitude as those observed in this work. Churchill and DeBoer suggested[17] that the distortions they observed were due to strains in the "awkward" 13-vertex polyhedron. The observation of considerably less distortion in another 13-vertex metallocarborane,[18] and the results reported here, seems to discount this interpretation. Distortions of this type are often attributed to "crystal packing forces", but no particularly short intermolecular distances are observed.

Since the formal two-electron deficiency of $(C_5H_5)_2Fe_2C_2B_6H_8$ is accompanied by a significant deviation from the usual 10-vertex geometry, but the one-electron-deficient $(C_5H_5)_2CoFeC_2B_7H_9$ has the usual 11-vertex octadecahedral geometry, it is clear that further structural data must be acquired before the effects of electron deficiency on the polyhedral geometries of metallocarboranes can be safely generalized. Our results reaffirm the structural sensitivity of metallocarboranes to the number of available bonding electrons but also indicate that these alterations are not necessarily related to the electron deficiency of the molecule. It appears that further work will be needed to clarify the electronic effects on the structures of metallocarboranes and related compounds.

Table V. Interatomic Angles[a]

Atoms 1,2,3	Angle, deg	Atoms 1,2,3	Angle, deg
I. Angles around Iron			
A. C_5H_5-Fe-C_5H_5			
Cp1-Fe-Cp2	38.1 (3)	Cp1-Fe-Cp3	64.8 (3)
Cp1-Fe-Cp5	38.1 (3)	Cp1-Fe-Cp4	64.1 (3)
Cp2-Fe-Cp3	39.0 (3)	Cp2-Fe-Cp4	64.6 (3)
Cp3-Fe-Cp4	39.0 (4)	Cp2-Fe-Cp5	64.2 (4)
Cp4-Fe-Cp5	38.4 (3)	Cp3-Fe-Cp5	65.1 (4)
B. $C_2B_7H_9$-Fe-$C_2B_7H_9$			
C2-Fe-B4	43.3 (3)	C3-Fe-B7	41.7 (3)
C2-Fe-B5	42.6 (2)	B4-Fe-B5	71.8 (3)
C2-Fe-B6	86.3 (3)	B4-Fe-B6	90.6 (3)
C2-Fe-B7	86.2 (3)	B4-Fe-B7	47.0 (3)
C2-Fe-C3	110.4 (3)	B5-Fe-B6	48.4 (3)
C3-Fe-B4	84.4 (3)	B5-Fe-B7	91.6 (3)
C3-Fe-B5	87.6 (3)	B6-Fe-B7	72.3 (3)
C3-Fe-B6	44.3 (3)		
C. C_5H_5-Fe-$C_2B_7H_9$			
Cp1-Fe-C2	134.4 (4)	Cp3-Fe-B5	161.4 (4)
Cp1-Fe-C3	105.6 (4)	Cp3-Fe-B6	149.4 (4)
Cp1-Fe-B4	167.9 (3)	Cp3-Fe-B7	100.0 (4)
Cp1-Fe-B5	114.6 (3)	Cp4-Fe-C2	94.5 (3)
Cp1-Fe-B6	101.3 (3)	Cp4-Fe-C3	149.6 (4)
Cp1-Fe-B7	139.2 (4)	Cp4-Fe-B4	103.9 (3)
Cp2-Fe-C2	159.1 (3)	Cp4-Fe-B5	122.8 (4)
Cp2-Fe-C3	89.5 (3)	Cp4-Fe-B6	159.8 (4)
Cp2-Fe-B4	137.8 (4)	Cp4-Fe-B7	127.9 (4)
Cp2-Fe-B5	149.7 (4)	Cp5-Fe-C2	100.1 (3)
Cp2-Fe-B6	113.3 (4)	Cp5-Fe-C3	143.3 (4)
Cp2-Fe-B7	106.0 (4)	Cp5-Fe-B4	132.3 (4)
Cp3-Fe-C2	123.3 (4)	Cp5-Fe-B5	102.4 (3)
Cp3-Fe-C3	110.7 (4)	Cp5-Fe-B6	121.6 (4)
Cp3-Fe-B4	105.7 (3)	Cp5-Fe-B7	164.9 (4)
II. Angles around Cobalt			
A. C_5H_5-Co-C_5H_5			
Cp6-Co-Cp7	38.1 (4)	Cp6-Co-Cp8	64.8 (4)
Cp6-Co-Cp10	38.1 (4)	Cp6-Co-Cp9	65.8 (4)
Cp7-Co-Cp8	38.5 (4)	Cp7-Co-Cp9	65.5 (4)
Cp8-Co-Cp9	39.7 (3)	Cp7-Co-Cp10	64.1 (4)
Cp9-Co-Cp10	40.1 (4)	Cp8-Co-Cp10	65.7 (3)
B. $C_2B_7H_9$-Co-$C_2B_7H_9$			
C2-Co-B4	44.7 (3)	B4-Co-B10	50.8 (3)
C2-Co-B5	44.7 (3)	B4-Co-B11	86.4 (3)
C2-Co-B10	87.0 (3)	B5-Co-B10	87.5 (3)
C2-Co-B11	89.6 (3)	B5-Co-B11	55.1 (4)
B4-Co-B5	75.7 (3)	B10-Co-B11	53.2 (4)
C. C_5H_5-Co-$C_2B_7H_9$			
Cp6-Co-C2	98.5 (3)	Cp8-Co-B10	97.8 (3)
Cp6-Co-B4	120.5 (5)	Cp8-Co-B11	121.7 (5)
Cp6-Co-B5	112.3 (4)	Cp9-Co-C2	161.4 (4)
Cp6-Co-B10	156.9 (5)	Cp9-Co-B4	151.6 (4)
Cp6-Co-B11	148.5 (5)	Cp9-Co-B5	130.0 (4)
Cp7-Co-C2	108.9 (4)	Cp9-Co-B10	111.4 (4)
Cp7-Co-B4	101.6 (3)	Cp9-Co-B11	99.1 (4)
Cp7-Co-B5	144.3 (5)	Cp10-Co-C2	121.3 (5)
Cp7-Co-B10	118.9 (4)	Cp10-Co-B4	158.0 (5)
Cp7-Co-B11	160.2 (5)	Cp10-Co-B5	105.6 (3)
Cp8-Co-C2	144.1 (4)	Cp10-Co-B10	150.0 (5)
Cp8-Co-B4	114.5 (4)	Cp10-Co-B11	112.7 (5)
Cp8-Co-B5	169.6 (4)		
III. Cyclopentadienyl Ring Angles			
Cp1-Cp2-Cp3	109.1 (9)	Cp6-Cp7-Cp8	109.6 (9)
Cp2-Cp3-Cp4	106.3 (8)	Cp7-Cp8-Cp9	107.9 (8)
Cp3-Cp4-Cp5	108.5 (8)	Cp8-Cp9-Cp10	105.3 (8)
Cp4-Cp5-Cp1	107.7 (9)	Cp9-Cp10-Cp6	108.7 (9)
Cp5-Cp1-Cp2	108.4 (8)	Cp10-Cp6-Cp7	108.4 (10)
IV. $C_2B_7H_9$ Cage Angles			
A. B-B-B Angles			
B7-B4-B10	58.4 (5)	B10-B9-B11	64.1 (5)
B6-B5-B11	59.5 (4)	B4-B10-B7	59.9 (5)
B5-B6-B9	108.7 (5)	B4-B10-B9	111.5 (6)
B5-B6-B11	62.9 (4)	B4-B10-B11	103.3 (5)
B9-B6-B11	55.3 (5)	B7-B10-B9	64.3 (5)
B4-B7-B9	107.5 (6)	B7-B10-B11	105.1 (6)
B4-B7-B10	61.7 (5)	B9-B10-B11	57.6 (5)
B9-B7-B10	57.4 (5)	B5-B11-B6	57.6 (4)
B6-B9-B7	90.3 (6)	B5-B11-B9	109.4 (6)
B6-B9-B10	104.9 (5)	B5-B11-B10	101.1 (5)
B6-B9-B11	63.1 (5)	B6-B11-B9	61.6 (5)
B7-B9-B10	58.3 (5)	B6-B11-B10	100.0 (5)
B7-B9-B11	105.5 (6)	B9-B11-B10	58.2 (5)
B. C-B-B Angles			
C2-B4-B7	118.8 (6)	C3-B7-B4	116.1 (7)
C2-B4-B10	109.3 (5)	C3-B7-B9	56.2 (5)
C2-B5-B6	114.2 (6)	C3-B7-B10	107.1 (7)
C2-B5-B11	105.6 (5)	C3-B9-B6	53.8 (5)
C3-B6-B5	117.6 (6)	C3-B9-B7	51.3 (5)
C3-B6-B9	55.7 (5)	C3-B9-B10	103.6 (6)
C3-B6-B11	104.2 (6)	C3-B9-B11	109.3 (7)
C. B-C-B Angles			
B4-C2-B5	114.9 (5)	B6-C3-B9	70.5 (6)
B6-C3-B7	115.6 (7)	B7-C3-B9	72.5 (6)

[a] See footnote *a* of Table I.

Acknowledgment. We are grateful to the Office of Naval Research for financial support and the UCLA Campus Computing Network for computer time.

Registry No. 1,8-(η-C_5H_5)$_2$-1-Fe-8-Co-2,3-$C_2B_7H_9$, 51746-29-3.

Supplementary Material Available: A listing of structure factor amplitudes (5 pages). Ordering information is given on any current masthead page.

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