from the idealized geometry than observed in $B_9H_9^{2-}$ or $(CH_3)_2C_2B_7H_7$. The extent of this distortion is evidenced by the dihedral angle between the two triangular faces of 11.2° and is due to the longer bonds to the cobalt atom.

The cesium cations reside in general positions in the unit cell. The closest contact between cation and anion is Cs–Cp3H at 3.807 (1) Å; all other contacts are greater than 4 Å. The eight molecules in the unit cell are arranged as shown in Figure 2.

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Registry No. $Cs^+[(C_5H_5)Co(CB_7H_8)]^-$, 51248-07-8; $Cs^+[(C_5H_5)Co(CB_7H_8)]^-$ (ref 8), 38882-83-6.

Supplementary Material Available. A listing of structure factor amplitudes will appear following these pages in the microfilm edition of this volume of the journal. Photocopies of the supplementary material from this paper only or microfiche (105 × 148 mm, 24× reduction, negatives) containing all of the supplementary material for the papers in this issue may be obtained from the Journals Department, American Chemical Society, 1155 16th St., N.W., Washington, D. C. 20036. Remit check or money order for \$3.00 for photocopy or \$2.00 for microfiche, referring to code number INORG-74-1393.

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Structures of Metallocarboranes. III. Crystal and Molecular Structure of the Bimetallocarborane Complex 2,3-Di-η-cyclopentadienyl-1,7-dicarba-2,3-dicobaltadodecaborane(10), $(\eta\text{-}C_5H_5)_2Co_2C_2B_8H_{10}$

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The crystal and molecular structure of $2,3\text{-}(\eta\text{-}C_5H_5)_2\text{-}2,3\text{-}Co_2\text{-}1,7\text{-}C_2B_8H_{10}$ has been determined by a complete three-dimensional X-ray diffraction study. The compound crystallizes in the monoclinic centrosymmetric space group $P2_1/n$ with a = 14.940 (4) Å, b = 9.006 (2) Å, c = 11.503 (3) Å, β = 93.08 (2)°, and Z = 4. Observed and calculated densities are 1.56 (2) and 1.585 g cm^{-3}, respectively. Diffraction data to $2\theta_{max}$ = 50° (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 refinement techniques. The final discrepancy index is R = 6.7% for 1435 independent nonzero reflections. The molecule can be described as a distorted icosahedron comprised of two cobalt, two carbon, and eight boron vertices. The cobalt atoms occupy adjacent vertices with a metal–metal distance of 2.387 (2) Å and are further coordinated to π-bonded cyclopentadienyl rings with an average bond distance of 2.05 (2) Å.

Introduction

The "polyhedral expansion reaction" of carboranes and metallocarboranes[1] has proven to be an important new synthetic route to mono- and polymetallocarboranes. The treatment of $1,6\text{-}C_2B_8H_{10}$ with sodium naphthalide, sodium cyclopentadienide, and cobalt(II) chloride afforded the eleven-vertex polyhedral complex $1\text{-}(\eta\text{-}C_5H_5)\text{-}1\text{-}Co\text{-}2,3\text{-}C_2B_8H_{10}$.[2] Further polyhedral expansion of this metallocarborane afforded the bimetallic complex $(C_5H_5)_2Co_2C_2B_8H_{10}$,[3] which was also formed in the direct expansion of $1,6\text{-}C_2B_8H_{10}$ but in much lower yield.

The nmr spectral properties of this bimetallocarborane were consistent with an icosahedral arrangement of the $Co_2C_2B_8$ framework, but the relative positions of the cobalt atoms and carbon atoms could not be uniquely defined.[3] When it was established[4] that adjacent cobalt atoms were present in $(C_5H_5)_2Co_2C_2B_6H_8$, a product from the polyhedral expansion of $1,7\text{-}C_2B_6H_8$,[5] a structure for $(C_5H_5)_2Co_2C_2B_8H_{10}$ involving a similar metal-metal interaction was suggested.[6] This work reports an X-ray crystallographic investigation which provides detailed molecular parameters for this compound.

Unit Cell and Space Group

A sample of the compound was furnished by Dr. W. J. Evans. It is air stable and does not decompose upon exposure to X-rays.

Preliminary X-ray diffraction photographs of the green needle-shaped crystals indicated monoclinic symmetry with systematic absences $h0l$, $h + l = 2n + 1$, and $0k0$, $k = 2n + 1$, indicative of space group $P2_1/n$, an alternate setting of $P2_1/c$ (C_{2h}^5, No. 14).[7] The density, measured by flotation in aqueous potassium iodide solution, was 1.56 (2) g cm^{-3}, in reasonable agreement with the calculated density of 1.585 g cm^{-3} for Z = 4.

Collection and Reduction of X-Ray Data

Intensity data were collected on a Syntex $P\bar{1}$ automated diffractometer equipped with scintillation counter and pulse height analyzer. A graphite crystal was employed to produce monochromatic Mo Kα

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radiation (λ 0.71069 Å). The crystal used for data collection was a parallelepiped bounded by {100}, {001}, {120}, and centrosymmetrically related faces. Crystal dimensions normal to these faces were 0.048 × 0.095 × 0.286 mm. The crystal was glued to a glass fiber parallel to the long axis. Lattice parameters, determined by a least-squares fit of 15 accurately centered, high-angle reflections, were found to be $a = 14.940$ (4) Å, $b = 9.006$ (2) Å, $c = 11.503$ (3) Å, and $\beta = 93.08$ (2)°.

Intensity data were collected at room temperature with the θ-2θ scan technique to a limit of $2\theta = 50°$ and with a takeoff angle of 4°. The scintillation counter was 18.5 cm from the crystal and equipped with a 1-mm collimator. Reflections were scanned at a rate of 2°/min from 1.0° below the $K\alpha_1$ reflection to 1.25° above the $K\alpha_2$ reflection. Background was measured at each end of the scan. The total time spent counting background was equal to the scan time for each reflection.

The intensities of three reflections were remeasured every 97 reflections to monitor the tube efficiency and possible crystal deterioration. No significant deviations were observed. The intensities of 3057 reflections were thus determined.

The intensity of a reflection, $I(hkl)$, and $\sigma[I(hkl)]$, its estimated standard deviation, were calculated according to the equations $I = \mathrm{CT} - (t_c/t_b)(B_1 + B_2)/2$ and $\sigma(I) = [\sigma_s^2 + (0.04I)^2]^{1/2}$, 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. The remaining 1452 reflections were corrected for Lorentz and polarization effects.

Solution and Refinement of the Structure

The coordinates of the two cobalt atoms were determined by solution of a three-dimensional Patterson map,[8] and a Fourier synthesis based on these input parameters ($R = 57.9\%$, $R_w = 56.7\%$)[9] showed six additional peaks which were in reasonable positions for cage atoms. Full-matrix least-squares refinement of the scale factor and positional parameters of these eight atoms resulted in $R = 29.3\%$ and $R_w = 34.7\%$. A Fourier map based on the refined atomic positions indicated the positions of the 14 remaining nonhydrogen atoms.

An absorption correction was applied to the data,[10] and the locations of the polyhedral carbon atoms were determined by their shorter bond distances and lower temperature factors. Nonhydrogen atoms were assigned anisotropic temperature factors, the cobalt scattering factors were corrected for anomalous dispersion, and the data were refined by full-matrix least squares.

A difference Fourier map showed peaks in reasonable positions for all cage hydrogen atoms except the one bonded to B12. Several peaks at reasonable distances from cyclopentadienyl carbon atoms were also located, but their associated bond angles were unreasonable. Accordingly all hydrogen atom positions were calculated, assuming B-H and C-H distances of 1.0 Å, and included but not refined in the final least-squares cycles. Isotropic temperature factors assigned to the hydrogens were based on the magnitudes of the temperature factors of the atoms to which they were bonded and were 4.0 Å^2 for cage hydrogens, 7.0 Å^2 for Cp1H-Cp5H, and 4.2 Å^2 for Cp6H-Cp10H. Convergence was reached at $R = 6.7\%$ and $R_w = 6.0\%$. The standard deviation of an observation of unit weight was 1.26.

Scattering factors for neutral cobalt, carbon, and boron were taken from ref 11; hydrogen scattering factors were obtained from Stewart, Davidson, and Simpson,[12] and the real and imaginary corrections for anomalous scattering of cobalt were taken from Cromer.[13] The function $\Sigma w||F_o| - |F_c||^2$ was minimized in least-squares refinement.

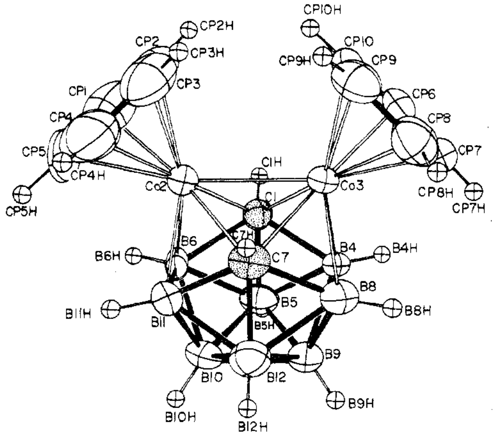

Figure 1. Structure and numbering system of 2,3-(η-C_5H_5)$_2$-2,3-Co_2-1,7-$C_2B_8H_{10}$. The hydrogens have been given arbitrary radii of 0.1 Å.

The final observed atomic fractional coordinates are collected in Table I. Anisotropic thermal parameters are listed in Table II.

The Molecular Structure

Intramolecular distances and their estimated standard deviations (esd's) are listed in Table IIIa. Average bond distances, with their root-mean-square deviations, are collected in Table IIIb. The individual bond angles and their associated esd's are presented in Table IV. The structure of $(C_5H_5)_2$-$Co_2C_2B_8H_{10}$ is shown in Figure 1, which also illustrates the numbering system employed.[14]

The structure of the complex can be described as a distorted icosahedron comprised of two cobalt, two carbon, and eight boron atom vertices. The boron and carbon atoms are further bonded to terminal hydrogen atoms, and the cobalt vertices are attached to η-cyclopentadienyl rings. The metals occupy adjacent vertices of the icosahedron at a distance of 2.387 (2) Å; the carbon atoms are nonadjacent but are in symmetry-related positions. Bond distances and angles indicate the molecule has C_{2v} symmetry within 3 standard deviations.

The two cobalt atoms in 2,3-(η-C_5H_5)-2,3-Co_2-1,7-$C_2B_8H_{10}$ are bonded to two equivalent boron atoms and to two equivalent carbon atoms, to planar (Table V) cyclopentadienyl rings, and to each other.

The ionic species $[(C_2B_9H_{11})_2Co_2(C_2B_8H_{10})]^{2-}$ is a close structural analog of $(C_5H_5)_2Co_2C_2B_8H_{10}$.[15] The C_5H_5Co groups of the neutral compound are replaced by $C_2B_9H_{11}Co$ groups in the ion, however, and the positions of the cobalt atoms and carbon atoms in the central $Co_2C_2B_8H_{10}$ group of the ion are interchanged from the positions observed in $(C_5H_5)_2Co_2C_2B_8H_{10}$. The trimetallic complex $[(C_2B_9H_{11})_2$-$Co_3(C_2B_8H_{10})_2]^{3-}$ has two of these $Co_2C_2B_8H_{10}$ subunits, which possess adjacent carbon atoms and separated metal atoms.[16] The comparable bond distances and angles in the isomeric cages are identical within experimental error. The average bond lengths observed in this study (Table IIIb) may be compared with those found[15] for the $Co_2C_2B_8H_{10}$ portion of the $[(C_2B_9H_{11})_2Co_2(C_2B_8H_{10})]^{2-}$ ion, which are Co-C = 2.065 (4) Å, Co-B = 2.078 (19) Å, B-B = 1.792 (15) Å, and C-B = 1.712 (12) Å.

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(8) The programs used in this work included locally written data reduction programs; JBPATT, JBFOUR, and PEAKLIST, modified versions of Fourier programs written by J. Blount; local versions of ORFLS (Busing, Martin, and Levy), structure factor calculations and full-matrix least-squares refinement; ORTEP (Johnson), figure plotting; ABSN (Coppens), absorption correction; MGTL (Gantzel and Trueblood), least-squares planes; and ORFFE (Busing, Martin, and Levy), distance, angle, and error computations. All calculations were performed on the IBM 360-91 KK computer operated by the UCLA Campus Computing Network.

(9) $R = [\Sigma||F_o| - |F_c||/\Sigma|F_o|]$; $R_w = [\Sigma w||F_o| - |F_c||^2/\Sigma w|F_o|^2]^{1/2}$; $w = 1/(\sigma_F)^2$.

(10) Maximum and minimum transmission factors were 0.9499 and 0.9019.

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Table I. Final Atomic Positions[a]

Atom	x	y	z	Atom	x	y	z
I. Heavy Atoms							
C1	0.7494 (8)	0.3260 (12)	0.6294 (9)	B12	0.7613 (11)	0.6022 (17)	0.4427 (12)
Co2	0.66926 (11)	0.27287 (18)	0.48153 (12)	Cp1	0.5689 (18)	0.1469 (34)	0.5350 (19)
Co3	0.82899 (10)	0.25704 (18)	0.49518 (11)	Cp2	0.6294 (14)	0.0517 (19)	0.4899 (24)
B4	0.8490 (10)	0.4181 (14)	0.6202 (12)	Cp3	0.6329 (14)	0.0968 (26)	0.3756 (19)
B5	0.7571 (11)	0.5020 (15)	0.6781 (11)	Cp4	0.5750 (18)	0.2090 (26)	0.3583 (20)
B6	0.6586 (9)	0.4385 (15)	0.6023 (11)	Cp5	0.5348 (14)	0.2401 (29)	0.4523 (41)
C7	0.7554 (9)	0.4202 (13)	0.4018 (9)	Cp6	0.9101 (10)	0.0972 (16)	0.5711 (12)
B8	0.8553 (13)	0.4792 (16)	0.4680 (15)	Cp7	0.9605 (10)	0.1953 (16)	0.5074 (14)
B9	0.8200 (10)	0.6044 (15)	0.5799 (11)	Cp8	0.9266 (11)	0.1841 (18)	0.3899 (12)
B10	0.7018 (11)	0.6140 (16)	0.5692 (13)	Cp9	0.8591 (12)	0.0803 (17)	0.3861 (13)
B11	0.6621 (11)	0.5000 (17)	0.4534 (14)	Cp10	0.8484 (11)	0.0314 (15)	0.4966 (16)
II. Hydrogen Atoms[b]							
C1H	0.7461	0.2414	0.6865	Cp1H	0.5525	0.1399	0.6132
B4H	0.9050	0.3934	0.6703	Cp2H	0.6601	−0.0289	0.5296
B5H	0.7577	0.5263	0.7622	Cp3H	0.6707	0.0522	0.3170
B6H	0.6007	0.4267	0.6422	Cp4H	0.5616	0.2642	0.2822
C7H	0.7550	0.3961	0.3175	Cp5H	0.4888	0.3197	0.4633
B8H	0.9149	0.4909	0.4294	Cp6H	0.9162	0.0810	0.6567
B9H	0.8595	0.6906	0.6053	Cp7H	1.0030	0.2597	0.5383
B10H	0.6697	0.7072	0.5919	Cp8H	0.9487	0.2420	0.3240
B11H	0.6067	0.5245	0.4037	Cp9H	0.8225	0.0488	0.3153
B12H	0.7647	0.6863	0.3865	Cp10H	0.8029	−0.0427	0.5191

[a] Estimated standard deviations, shown in parentheses, refer to the last digit of the preceding number. [b] Calculated positions, assuming B–H and C–H distances of 1.0 Å. Included but not refined in final least-squares cycles.

Table II. Anisotropic Thermal Parameters[a]

Atom	$10^4\beta_{11}$	$10^4\beta_{22}$	$10^4\beta_{33}$	$10^4\beta_{12}$	$10^4\beta_{13}$	$10^4\beta_{23}$
C1	29 (6)	90 (16)	55 (9)	2 (8)	1 (6)	2 (10)
Co2	26 (1)	70 (2)	58 (1)	1 (1)	−1 (1)	−7 (2)
Co3	26 (1)	53 (2)	51 (1)	4 (1)	3 (1)	−9 (1)
B4	29 (8)	52 (16)	70 (12)	−1 (9)	−5 (8)	−7 (12)
B5	51 (9)	81 (18)	56 (12)	0 (11)	1 (8)	−14 (12)
B6	15 (7)	92 (19)	52 (10)	7 (9)	1 (6)	−21 (12)
C7	44 (8)	106 (17)	38 (9)	2 (10)	3 (6)	5 (10)
B8	46 (11)	71 (19)	85 (17)	−7 (11)	−1 (10)	−10 (15)
B9	45 (9)	75 (18)	53 (11)	0 (11)	7 (8)	−9 (12)
B10	41 (10)	59 (18)	95 (15)	21 (11)	11 (9)	1 (13)
B11	29 (9)	93 (20)	77 (14)	14 (11)	−10 (9)	12 (14)
B12	45 (11)	97 (20)	67 (12)	−7 (12)	−7 (9)	17 (13)
Cp1	80 (17)	408 (65)	176 (25)	−139 (27)	73 (17)	−173 (34)
Cp2	54 (14)	119 (26)	231 (31)	−42 (15)	−38 (16)	8 (24)
Cp3	71 (13)	243 (36)	136 (20)	−79 (19)	49 (13)	−156 (24)
Cp4	93 (17)	190 (37)	187 (25)	−43 (19)	−78 (16)	33 (25)
Cp5	22 (10)	226 (46)	594 (79)	45 (18)	−43 (23)	−282 (52)
Cp6	37 (8)	116 (20)	108 (14)	37 (11)	11 (9)	8 (14)
Cp7	30 (8)	94 (19)	157 (18)	11 (10)	5 (9)	−30 (15)
Cp8	61 (10)	167 (24)	101 (14)	49 (13)	45 (10)	9 (15)
Cp9	67 (11)	138 (22)	86 (14)	34 (13)	0 (10)	−38 (15)
Cp10	29 (9)	98 (19)	134 (18)	5 (10)	29 (10)	−32 (15)

[a] See footnote *a* of Table I. The anisotropic temperature factor T is defined as $T = \exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)]$. Thermal ellipsoids are depicted in Figure 1.

The cobalt-cobalt distance of 2.387 (2) Å observed here is shorter than those normally observed in cobalt cluster compounds, which range between 2.43 and 2.55 Å,[17,18] and shorter than the 2.489 (1) Å distance observed[4] in $(C_5H_5)_2$·$Co_2C_2B_6H_8$, the only other structurally characterized bimetallocarborane possessing adjacent cobalt atoms. Comparison of metal-metal distances in bridged complexes of different overall geometry is always difficult and therefore a detailed discussion of the metal-metal bonding in this class of metallocarboranes will be deferred until additional experimental evidence becomes available. It should be noted, however, that the absence of abnormal bond lengths and angles (other than the Co-Co distance) suggests that steric

Table IIIa. Interatomic Distances[a]

Atoms	Dist, Å	Atoms	Dist, Å
I. Distances around Cobalt Atoms			
Co2–Co3	2.387 (2)	Co3–C1	2.09 (1)
Co2–C1	2.08 (1)	Co3–B4	2.05 (1)
Co2–B6	2.05 (1)	Co3–C7	2.10 (1)
Co2–C7	2.09 (1)	Co3–B8	2.07 (2)
Co2–B11	2.07 (2)	Co3–Cp6	2.05 (1)
Co2–Cp1	2.00 (2)	Co3–Cp7	2.04 (2)
Co2–Cp2	2.08 (2)	Co3–Cp8	2.05 (1)
Co2–Cp3	2.06 (1)	Co3–Cp9	2.09 (1)
Co2–Cp4	2.03 (2)	Co3–Cp10	2.05 (1)
Co2–Cp5	2.04 (2)		
II. Cyclopentadienyl Ring Distances			
Cp1–Cp2	1.37 (3)	Cp6–Cp7	1.39 (2)
Cp1–Cp5	1.35 (4)	Cp6–Cp10	1.36 (2)
Cp2–Cp3	1.38 (3)	Cp7–Cp8	1.42 (2)
Cp3–Cp4	1.34 (3)	Cp8–Cp9	1.38 (2)
Cp4–Cp5	1.29 (4)	Cp9–Cp10	1.36 (2)
III. Boron-Boron Distances			
B4–B5	1.73 (2)	B8–B9	1.81 (2)
B4–B8	1.84 (2)	B8–B12	1.80 (2)
B4–B9	1.79 (2)	B9–B10	1.77 (2)
B5–B6	1.77 (2)	B9–B12	1.76 (2)
B5–B9	1.77 (2)	B10–B11	1.76 (2)
B5–B10	1.78 (2)	B10–B12	1.75 (2)
B6–B10	1.76 (2)	B11–B12	1.76 (2)
B6–B11	1.80 (2)		
IV. Carbon-Boron Distances			
C1–B4	1.71 (2)	C7–B8	1.72 (2)
C1–B5	1.68 (2)	C7–B11	1.70 (2)
C1–B6	1.71 (2)	C7–B12	1.71 (2)

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

Table IIIb. Average Bond Lengths

Atoms	No.	Range,[a] Å	Av,[b] Å
Co–C	14	2.00 (2)–2.10 (1)	2.06 (3)
Co–B	4	2.05 (1)–2.07 (2)	2.06 (1)
C–C	10	1.29 (4)–1.42 (2)	1.36 (3)
B–B	15	1.73 (2)–1.84 (2)	1.78 (3)
C–B	6	1.68 (2)–1.72 (2)	1.71 (1)

[a] See footnote *a* of Table I. [b] Esd's for average bond lengths were calculated using the equation $\sigma^2 = [\sum_{i=1}^{i=N}(x_i - \bar{x})^2]/(N-1)$, where x_i is the *i*th bond length and $\bar{x}$ is the mean of the N equivalent bond lengths.

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Table IV. Interatomic Angles[a]

Atoms 1-2-3	Angle, deg	Atoms 1-2-3	Angle, deg
I. Angles around Cobalt Atoms			
A. C_5H_5–Co–C_5H_5			
Cp1–Co2–Cp2	39.0 (9)	Cp6–Co3–Cp7	39.9 (6)
Cp1–Co2–Cp3	64.3 (7)	Cp6–Co3–Cp8	66.6 (5)
Cp1–Co2–Cp4	63.3 (9)	Cp6–Co3–Cp9	65.1 (6)
Cp1–Co2–Cp5	38.9 (11)	Cp6–Co3–Cp10	38.8 (6)
Cp2–Co2–Cp3	39.0 (7)	Cp7–Co3–Cp8	40.6 (6)
Cp2–Co2–Cp4	64.6 (7)	Cp7–Co3–Cp9	66.2 (6)
Cp2–Co2–Cp5	65.7 (9)	Cp7–Co3–Cp10	66.1 (6)
Cp3–Co2–Cp4	38.3 (8)	Cp8–Co3–Cp9	39.7 (6)
Cp3–Co2–Cp5	64.2 (8)	Cp8–Co3–Cp10	65.4 (6)
Cp4–Co2–Cp5	37.1 (10)	Cp9–Co3–Cp10	38.4 (5)
B. $C_2B_8H_{10}$–Co–$C_2B_8H_{10}$			
C1–Co2–B6	48.8 (5)	C1–Co3–B4	48.7 (5)
C1–Co2–C7	82.6 (4)	C1–Co3–C7	82.4 (4)
C1–Co2–B11	85.6 (5)	C1–Co3–B8	86.8 (6)
B6–Co2–C7	84.7 (5)	B4–Co3–C7	85.2 (5)
B6–Co2–B11	51.9 (6)	B4–Co3–B8	53.1 (6)
C7–Co2–B11	48.3 (5)	C7–Co3–B8	48.9 (6)
C. Co–Co–$C_2B_8H_{10}$			
Co3–Co2–C1	55.3 (3)	Co2–Co3–C1	54.9 (3)
Co3–Co2–B6	96.5 (4)	Co2–Co3–B4	96.4 (4)
Co3–Co2–C7	55.3 (3)	Co2–Co3–C7	55.2 (4)
Co3–Co2–B11	96.4 (5)	Co2–Co3–B8	97.5 (5)
D. Co–Co–C_5H_5			
Co3–Co2–Cp1	135.1 (11)	Co2–Co3–Cp6	129.5 (5)
Co3–Co2–Cp2	103.1 (6)	Co2–Co3–Cp7	167.6 (4)
Co3–Co2–Cp3	102.9 (6)	Co2–Co3–Cp8	136.0 (5)
Co3–Co2–Cp4	133.1 (10)	Co2–Co3–Cp9	104.6 (5)
Co3–Co2–Cp5	166.9 (6)	Co2–Co3–Cp10	101.5 (5)
E. C_5H_5–Co–$C_2B_8H_{10}$			
Cp1–Co2–C1	106.7 (7)	Cp6–Co3–C1	103.9 (5)
Cp1–Co2–B6	96.8 (7)	Cp6–Co3–B4	97.9 (5)
Cp1–Co2–C7	168.9 (10)	Cp6–Co3–C7	173.6 (5)
Cp1–Co2–B11	125.0 (11)	Cp6–Co3–B8	129.2 (7)
Cp2–Co2–C1	109.6 (7)	Cp7–Co3–C1	127.8 (6)
Cp2–Co2–B6	129.2 (9)	Cp7–Co3–B4	92.3 (6)
Cp2–Co2–C7	144.1 (9)	Cp7–Co3–C7	134.7 (6)
Cp2–Co2–B11	159.8 (7)	Cp7–Co3–B8	94.8 (7)
Cp3–Co2–C1	141.6 (9)	Cp8–Co3–C1	168.5 (6)
Cp3–Co2–B6	159.3 (6)	Cp8–Co3–B4	123.9 (7)
Cp3–Co2–C7	112.2 (6)	Cp8–Co3–C7	107.0 (5)
Cp3–Co2–B11	131.2 (10)	Cp8–Co3–B8	94.2 (7)
Cp4–Co2–C1	169.6 (8)	Cp9–Co3–C1	144.9 (6)
Cp4–Co2–B6	127.1 (10)	Cp9–Co3–B4	158.5 (6)
Cp4–Co2–C7	107.1 (7)	Cp9–Co3–C7	110.5 (5)
Cp4–Co2–B11	98.2 (8)	Cp9–Co3–B8	126.7 (7)
Cp5–Co2–C1	133.3 (13)	Cp10–Co3–C1	111.9 (5)
Cp5–Co2–B6	96.1 (9)	Cp10–Co3–B4	132.7 (7)
Cp5–Co2–C7	130.0 (13)	Cp10–Co3–C7	140.2 (6)
Cp5–Co2–B11	94.3 (9)	Cp10–Co3–B8	158.7 (7)
II. Cyclopentadienyl Ring Angles			
A. C–C–C Angles			
Cp1–Cp2–Cp3	104 (2)	Cp6–Cp7–Cp8	106 (1)
Cp2–Cp3–Cp4	108 (2)	Cp7–Cp8–Cp9	108 (1)
Cp3–Cp4–Cp5	111 (2)	Cp8–Cp9–Cp10	108 (1)
Cp4–Cp5–Cp1	106 (2)	Cp9–Cp10–Cp6	110 (1)
Cp5–Cp1–Cp2	111 (2)	Cp10–Cp6–Cp7	108 (1)
B. C–C–Co Angles			
Cp1–Cp2–Co2	67.3 (11)	Cp6–Cp7–Co3	70.3 (8)
Cp1–Cp5–Co2	69.0 (12)	Cp6–Cp10–Co3	70.4 (8)
Cp2–Cp1–Co2	73.7 (11)	Cp7–Cp6–Co3	69.8 (8)
Cp2–Cp3–Co2	71.6 (9)	Cp7–Cp8–Co3	69.2 (7)
Cp3–Cp2–Co2	69.4 (9)	Cp8–Cp7–Co3	70.2 (8)
Cp3–Cp4–Co2	72.0 (10)	Cp8–Cp9–Co3	69.2 (8)
Cp4–Cp3–Co2	69.7 (9)	Cp9–Cp8–Co3	72.1 (8)
Cp4–Cp5–Co2	70.9 (14)	Cp9–Cp10–Co3	72.3 (9)
Cp5–Cp1–Co2	72.0 (15)	Cp10–Cp6–Co3	70.9 (8)
Cp5–Cp4–Co2	72.0 (13)	Cp10–Cp9–Co3	69.3 (8)

Atoms 1-2-3	Angle, deg	Atoms 1-2-3	Angle, deg
III. $C_2B_8H_{10}$ Cage Angles			
A. B-B-B Angles			
B5-B4-B8	108.5 (10)	B8-B9-B10	108.0 (11)
B5-B4-B9	60.3 (8)	B8-B9-B12	60.4 (9)
B8-B4-B9	59.8 (8)	B10-B9-B12	59.4 (9)
B4-B5-B6	109.0 (9)	B5-B10-B6	59.9 (8)
B4-B5-B9	61.4 (8)	B5-B10-B9	59.8 (9)
B4-B5-B10	109.0 (10)	B5-B10-B11	109.1 (9)
B6-B5-B9	108.1 (9)	B5-B10-B12	108.3 (11)
B6-B5-B10	59.5 (8)	B6-B10-B9	108.6 (10)
B9-B5-B10	59.8 (8)	B6-B10-B11	61.7 (8)
B5-B6-B10	60.6 (8)	B6-B10-B12	109.5 (10)
B5-B6-B11	107.7 (10)	B9-B10-B11	108.6 (10)
B10-B6-B11	59.2 (8)	B9-B10-B12	60.2 (9)
B4-B8-B9	58.6 (8)	B11-B10-B12	60.0 (9)
B4-B8-B12	105.0 (11)	B6-B11-B10	59.1 (8)
B9-B8-B12	58.5 (8)	B6-B11-B12	107.2 (10)
B4-B9-B5	58.3 (8)	B10-B11-B12	59.7 (9)
B4-B9-B8	61.6 (8)	B8-B12-B9	61.1 (9)
B4-B9-B10	106.9 (10)	B8-B12-B10	109.3 (11)
B4-B9-B12	108.9 (9)	B8-B12-B11	108.7 (10)
B5-B9-B10	60.4 (9)	B9-B12-B10	60.4 (8)
B5-B9-B8	108.4 (10)	B9-B12-B11	108.9 (10)
B5-B9-B12	108.1 (11)	B10-B12-B11	60.3 (9)
B. C-B-B Angles			
C1-B4-B5	58.5 (8)	C7-B8-B4	103.9 (11)
C1-B4-B8	107.0 (9)	C7-B8-B9	103.2 (12)
C1-B4-B9	105.8 (10)	C7-B8-B12	57.9 (9)
C1-B5-B4	60.1 (7)	C7-B11-B6	105.5 (9)
C1-B5-B6	59.3 (7)	C7-B11-B10	105.2 (11)
C1-B5-B9	107.9 (9)	C7-B11-B12	59.1 (9)
C1-B5-B10	106.2 (9)	C7-B12-B8	58.8 (8)
C1-B6-B5	57.9 (7)	C7-B12-B9	105.9 (10)
C1-B6-B10	106.0 (10)	C7-B12-B10	105.5 (11)
C1-B6-B11	107.0 (9)	C7-B12-B11	58.9 (8)
C. B–C–B Angles			
B4–C1–B5	61.3 (8)	B8–C7–B11	114.9 (10)
B4–C1–B6	112.7 (9)	B8–C7–B12	63.3 (9)
B5–C1–B6	62.7 (8)	B11–C7–B12	62.0 (9)
D. B-B–Co Angles			
B5-B4–Co3	119.3 (9)	B4-B8–Co3	63.0 (6)
B8-B4–Co3	63.8 (6)	B9-B8–Co3	115.5 (10)
B9-B4–Co3	117.2 (8)	B12-B8–Co3	117.8 (11)
B5-B6–Co2	118.5 (9)	B6-B11–Co2	63.4 (6)
B10-B6–Co2	117.7 (8)	B10-B11–Co2	119.5 (10)
B11-B6–Co2	64.7 (6)	B12-B11–Co2	116.4 (9)
E. C-B–Co Angles			
C1-B4–Co3	66.9 (6)	C7-B8–Co3	66.4 (6)
C1-B6–Co2	66.6 (6)	C7-B11–Co2	66.5 (6)
F. B–C–Co Angles			
B4–C1–Co2	121.6 (7)	B8–C7–Co2	122.7 (8)
B4–C1–Co3	64.4 (6)	B8–C7–Co3	64.7 (6)
B5–C1–Co2	120.9 (7)	B11–C7–Co2	65.2 (7)
B5–C1–Co3	119.6 (8)	B11–C7–Co3	122.3 (8)
B6–C1–Co2	64.6 (6)	B12–C7–Co2	120.8 (8)
B6–C1–Co3	121.2 (7)	B12–C7–Co3	121.0 (8)
G. Co–C–Co Angles			
Co2–C1–Co3	69.7 (3)	Co2–C7–Co3	69.5 (4)

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

Table V. Important Planes in the Molecule[a]

Atom	Dev, Å	Atom	Dev, Å
Cyclopentadienyl Ring: Cp1, Cp2, Cp3, Cp4, Cp5			
$0.7146x + 0.6512y + 0.2555z = 8.2555$			
Cp1	+0.014	Cp4	+0.002
Cp2	−0.012	Cp5	−0.010
Cp3	+0.006		
Cyclopentadienyl Ring: Cp6, Cp7, Cp8, Cp9, Cp10			
$-0.6652x + 0.7308y + 0.1531z = -7.1592$			
Cp6	−0.007	Cp9	−0.012
Cp7	−0.001	Cp10	+0.012
Cp8	+0.008		
Icosahedral Plane: C1, B6, B11, C7, Co3			
$0.5901x + 0.7510y + 0.2946z = 10.6392$			
C1	+0.083	C7	+0.086
B6	−0.040	Co3	−0.086
B11	−0.043		
Icosahedral Plane: B4, B5, B10, B12, B8			
$0.5521x + 0.7769y + 0.3026z = 11.8762$			
B4	−0.004	B12	+0.005
B5	+0.007	B8	−0.001
B10	−0.007		
Icosahedral Plane: C1, Co2, C7, B8, B4			
$-0.5232x + 0.8245y + 0.2156z = -1.7610$			
C1	+0.086	B8	−0.056
Co2	−0.096	B4	−0.035
C7	+0.101		
Icosahedral Plane: B5, B6, B11, B12, B9			
$-0.4925x + 0.8371y + 0.2380z = 0.2809$			
B5	−0.007	B12	+0.002
B6	+0.008	B9	+0.003
B11	−0.006		

[a] Planes are defined as $C_1x + C_2y + C_3z = d$, where x, y, z are orthogonal coordinates (in angstroms) and the axes parallel a, b, c^*.

interactions cannot account for the short metal–metal distance observed in this investigation.

The distortions from idealized icosahedral geometry observed in the $Co_2C_2B_8$ framework are mainly due to the differences in bond lengths of the heavy and light atoms. The five-membered rings Co2-C1-B4-B8-C7 and Co3-C1-B6-B11-C7 show significant deviations from planarity (Table V). The metal atoms are displaced from the least-squares planes through C1-B4-B8-C7 and C1-B6-B11-C7 by 0.29 and 0.32 Å, respectively. The five-membered rings B4-B5-B10-B12-B8 and B6-B5-B9-B12-B11 are planar within experimental error. The dihedral angle between the rings Co2-C1-B4-B8-C7 and B6-B5-B9-B12-B11 is 2.29°, while the dihedral angle between Co3-C1-B6-B11-C7 and B4-B5-B10-B12-B8 is 2.70°.

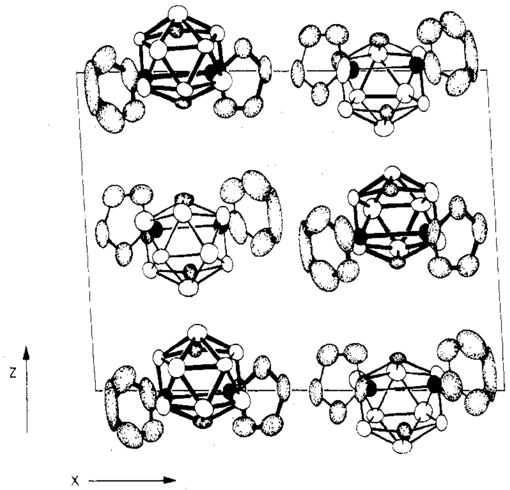

Figure 2. Packing of molecules within the unit cell. Hydrogen atoms have been omitted for clarity.

The cyclopentadienyl rings are planar and the angle between them is 87.7°. They are undergoing a large amount of librational motion, as evidenced by the atomic thermal ellipsoids shown in Figure 1. The orientation of the cyclopentadienyl rings results in short time-averaged intramolecular contacts of Cp3H-Cp9H = 2.27 Å and Cp2H-Cp10H = 2.15 Å. No unusual intermolecular contacts are present in the crystal; a view of the packing in the unit cell is shown in Figure 2.

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Registry No. 2,3-$(\eta\text{-}C_5H_5)_2$-2,3-Co_2-1,7-$C_2B_8H_{10}$, 42612-79-3.

Supplementary Material Available. A listing of observed and calculated structure factor amplitudes will appear following these pages in the microfilm edition of this volume of the journal. Photocopies of the supplementary material from this paper only or microfiche (105 × 148 mm, 24× reduction, negatives) containing all of the supplementary material for papers in this issue may be obtained from the Journals Department, American Chemical Society, 1155 16th St., N.W., Washington, D. C. 20036. Remit check or money order for \$3.00 for photocopy or \$2.00 for microfiche, referring to code number INORG-74-1397.