H(COT)–C, and H(COT)–Cl contacts did not indicate that these interactions are responsible for the observed deformation. Thus we are led to the conclusion that the distortion of the COT ligand results from the electronic nature of the COT–metal interaction.

Similar conclusions were also reached by Hodgson and Raymond in their analysis of $[C_8H_4(CH_3)_4]_2U$[19] and by Rees and Coppens in their study of $C_6H_6Cr(CO)_3$.[20] In these two compounds the substituents were also located on the metal side of the ring planes. Average substituent angles of 4.1° for the methyl groups[19] and 1.7° for the hydrogen atoms[20] were reported for the former and latter complexes, respectively.

Hodgson and Raymond offered two possible explanations for their observations. The first invoked a rehybridization of the ring carbon atoms from trigonal to slightly pyramidal. The ring carbon π orbitals would then be inclined toward the metal atom; thus better ring–metal overlap would be possible. The second requires a volume contraction and an inward polarization of the π density on the metal side of the ring relative to that on the other side, the electron density in the bonds to the ring substituents being forced away from the noncontracted π-electron density.[19] Rees and Coppens' argument retains the trigonal character of the ring carbon atom hybridization; however, they postulated a tilting of these hybrid orbitals so that the carbon π orbitals are directed more along the metal–carbon vector. This rationalization is quite similar to the first given by Hodgson and Raymond.[20] We might add that the third argument bears some similarity to the explanation of the deformation experienced by π-allyl[21] and butadiene[22] moieties π bonded to transition metals. It should be noted that the above arguments consider only the interaction between the metal atom and the π orbitals of the carbocyclic ring. In some cases interactions between the metal atom and the ring σ system may also be important. A differentiation between these two possibilities cannot be derived from substituent angles alone.

Registry No. II, 50648-05-0.

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 Business Office, Books and Journals Division, American Chemical Society, 1155 16th St., N.W., Washington, D.C. 20036. Remit check or money order for \$4.50 for photocopy or \$2.50 for microfiche, referring to code number AIC50444Y-12-75.

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Crystal and Molecular Structure of 2-Methyl-1,7-bis(η^5-cyclopentadienyl)-1,7,2,4-dicobaltadicarbaheptaborane(7), a Triple-Decked Sandwich Compound

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A single-crystal X-ray diffraction investigation of the dicobalt metallocarborane 2-CH_3-1,7,2,4-(η-C_5H_5)$_2Co_2C_2B_3H_4$ has established the structure as that of a triple-decked sandwich containing a central planar ring formally designated in the parent molecule as $C_2B_3H_5^{4-}$, isoelectronic with $C_5H_5^-$. The compound crystallizes in the orthorhombic space group *Pnam* with $a = 13.596$ (6), $b = 9.968$ (3), and $c = 10.008$ (4) Å and a calculated density of 1.58 g cm^{-3} for $Z = 4$. The structure was refined by full-matrix least-squares procedures to a final R value of 0.046. The 1,7,2,3- and 1,7,2,4-(η-C_5H_5)$_2Co_2C_2B_3H_5$ systems are the only known electrically neutral triple-decked sandwich species, the sole "pure metallocene" member of this class being the (η-C_5H_5)$_3Ni_2^+$ ion.

Introduction

The metallocarboranes 1,7,2,3- and 1,7,2,4-(η^5-C_5H_5)$_2Co_2C_2B_3H_5$ occupy a key position in both metallocene and metallocarborane chemistry and can realistically be viewed as members of both classes. Inasmuch as the only known and characterized triple-decked sandwich metallocene is the (η^5-C_5H_5)$_3Ni_2^+$ cation prepared by Werner and Salzer,[2-4] the (η^5-C_5H_5)$_2Co_2C_2B_3H_5$ species[5-8] are the first electrically neutral examples of true triple-decked complexes containing three planar aromatic rings; in addition, these compounds, in association with the closely related $C_2B_3H_7^{2-}$ complexes,[6,8-10] represent the first metallocarboranes which are direct steric analogs of known metallocenes.[11]

Four isomers of (η^5-C_5H_5)$_2Co_2C_2B_3H_5$ have been isolated and characterized[5-8] and together with the related species $(CO)_6Fe_2C_2B_3H_5$[7] these are the smallest known metallocarboranes having more than one framework metal atom. The thermally least stable isomer, 1,7,2,3-$(\eta^5\text{-}C_5H_5)_2Co_2C_2B_3H_5$, rearranges above 200° to the 1,2,3,5, 1,2,4,5, and ultimately the 1,7,2,4 species.[8,13,14] All four isomers are proposed to have central pentagonal-pyramidal $Co_2C_2B_3$ cages, but only in the 1,7,2,3 and 1,7,2,4 species do both cobalt atoms occupy apical (1,7) vertices,[14] giving a triple-decked sandwich geometry. The structure of the 1,7,2,3 isomer was established from an earlier X-ray diffraction study of its 2-methyl derivative.[5] In order to confirm the triple-decked structure for the 1,7,2,4 isomer, and also to shed further light on some unexplained details of the 1,7,2,3 structure,[5] we have conducted an X-ray study of 2-CH_3-1,7,2,4-$(\eta^5\text{-}C_5H_5)_2Co_2C_2B_3H_4$.

Experimental Section

A sample of the title compound was prepared by thermal rearrangement of 2-CH_3-1,7,2,3-$(\eta^5\text{-}C_5H_5)_2Co_2C_2B_3H_4$ as described earlier,[13] and was recrystallized from heptane to give dark green platelike crystals.[15] As the material is completely stable to air and moisture, all subsequent operations were conducted in air. The crystal selected for precession photography and data collection was a thin plate of irregular shape, 0.22 × 0.13 × 0.024 mm, $V = 3.4 \times 10^{-4}$ mm^3. Precession photographs taken using Cu Kα radiation (λ 1.5418 Å) indicated the conditions limiting possible reflections to be $0kl$: $k + l = 2n$, and $h0l$: $h = 2n$. Possible space groups are thus $Pna2_1$ and $Pnam$. The nonstandard centrosymmetric group $Pnam$ was subsequently found to provide a satisfactory model, and the noncentrosymmetric group $Pna2_1$ was not further tested. The choice of $Pnam$ with $Z = 4$ was consistent with structural characterization based on NMR studies[5,6,13] provided that the molecule contained a mirror plane at $z = 0.25$ on which were located both cobalt atoms, one carbon atom in each of the three rings, and the carbon atom of a methyl group linked to a carbon atom in the central ring. This implied disorder of the remaining central ring carbon atom between two equivalent positions nonadjacent to the methylated carbon atom; the disordered atoms are labeled BC throughout this paper. General equivalent positions in this unconventional setting of the space group are x, y, z; $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} - z$; $\bar{x}, \bar{y}, \frac{1}{2} + z$; $\frac{1}{2} - x, \frac{1}{2} + y, \bar{z}$; and their centrosymmetric equivalents.

Accurate alignment and data collection were carried out on a Hilger and Watts four-circle, computer-controlled diffractometer using Mo Kα (λ 0.7107 Å) radiation at $T = 23°$. Unit cell constants, determined from a least-squares refinement of the setting angles for 12 reflections, were $a = 13.596$ (6) Å, $b = 9.968$ (3) Å, and $c = 10.008$ (4) Å. As the calculated density of 1.58 g cm^{-3} for $Z = 4$ was identical with that of the isomeric compound[5] 2-CH_3-1,7,2,3-$(\eta\text{-}C_5H_5)_2Co_2C_2B_3H_4$, no measurement of the density was made.

The intensity data were collected with a θ–2θ step-scan over a range of $0 < \theta \leq 22°$, for three equivalent members of the form. Stationary-counter 18-sec background counts were taken at the limits of each scan. A symmetric scan range of 0.72° in θ, centered on the calculated peak position was composed of 72 steps, each of 1-sec duration. Reflections with a count rate exceeding 8000/sec were brought within the linear response range of the scintillation counter by means of calibrated attenuators. No significant change in the intensities of the three standard reflections, monitored at regular intervals, was noted during data collection. Data were corrected for Lorentz and polarization (Lp) factors and then for absorption (μ(Mo K$\bar{\alpha}$) = 25.11 cm^{-1}) using gaussian integration.[16] Maximum and minimum absorption corrections were 1.351 and 1.044, respectively. After averaging reflections recorded more than once, as well as those equivalent by symmetry, there remained 896 unique reflections of which 294 had $F^2 \geq 3\sigma(F^2)$, where $\sigma(F^2)$ is defined below. Only these latter reflections were employed in the final refinements of structure parameters.

Solution and Refinement of the Structure

A standard Patterson synthesis contained several strong peaks which were assigned to cobalt–cobalt vectors having both cobalt atoms on the mirror plane ($z = 0.25$), with Co7 at $x = 0.152$ and $y = -0.029$ and Co1 at $x = 0.152$ and $y = 0.294$. The most intense nonorigin peak corresponded to the Co1–Co7 vector with a length of 3.16 Å, close to the expected value based on the known structure of the 1,7,2,3 isomer.[5] Full-matrix least-squares refinement based on F for the cobalt atoms alone produced a conventional R value of 0.348, where $R = \sum(|F_o| - |F_c|)/\sum|F_o|$. The function minimized was $\sum w(|F_o| - |F_c|)^2$, and the weights w were taken as $4F_o^2/\sigma F_o^2$ where $|F_o|$ and $|F_c|$ are observed and calculated structure factor amplitudes. The atomic scattering factors for nonhydrogen atoms were taken from Cromer and Waber[17] and those for hydrogen from Stewart.[18] A difference Fourier synthesis based on these cobalt atom positions gave a number of intense peaks, of which six corresponded to expected nonhydrogen atom positions (two in each of the three rings of the molecule). Least-squares refinement of these positions led to a value of $R = 0.188$. A difference Fourier synthesis based on these refined atom positions revealed the remaining four nonhydrogen atoms in the asymmetric unit, and subsequent least-squares refinement of all nonhydrogen atom positions with all atoms isotropic gave $R = 0.129$ and a weighted $R_w = 0.143$, where $R_w = (\sum w(|F_o| - |F_c|)^2/\sum w|F_o|^2)^{1/2}$.

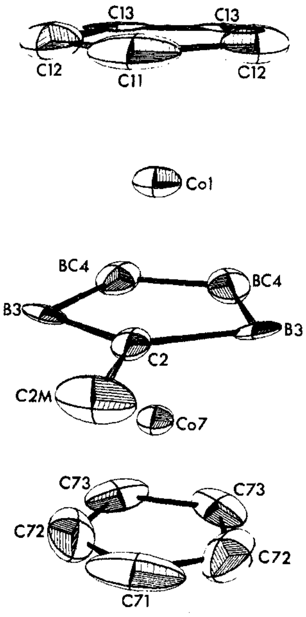

Figure 1. Molecular structure of 2-CH_3-1,7,2,4-$(\eta^5\text{-}C_5H_5)_2Co_2C_2B_3H_4$.

Difference Fourier syntheses taken through the planes of the three rings revealed peaks corresponding to expected hydrogen atom locations on the central ring but were complicated by thermal motion of the carbon atoms on the cyclopentadienyl rings. Hydrogen atom positions, except for those on the methyl group, were calculated assuming bond distances of 0.95, 1.10, and 1.00 Å for C–H, B–H, and (BC)–H, respectively, and the calculated locations and isotropic thermal parameters ($B = 5.0$ Å^2) for the hydrogen atoms were included as nonvarying parameters in all subsequent least-squares calculations. At this point the intensity data were averaged and absorption corrections were applied, with subsequent least-squares refinements converging to $R = 0.096$ and $R_w = 0.105$.

Introduction of anisotropic temperature factors for both cobalt atoms led to an R value of 0.064 after several cycles of full-matrix least-squares refinement. Finally, all nonhydrogen atoms were assigned anisotropic temperature factors and, together with all positional parameters and scale factors, refinements converged with all shift to error ratios less than 0.15. Final values of the agreement factors were $R = 0.046$ and $R_w = 0.053$. In a final difference Fourier synthesis the largest residual peak of 0.099 e/Å^3 can be compared with 0.20 e/Å^3 for the average density at which hydrogen atom positions had been established. The error in an observation of unit weight was 1.28.

No extinction correction was applied since the pattern of positive and negative deviations of observed vs. calculated intensities appeared random.

Final positional and thermal parameters are listed in Table I.

Discussion

The triple-decked sandwich structure of the molecule is illustrated in Figure 1 and the important interatomic distances and angles are summarized in Table II. All bond lengths are within the normal ranges, and the nonmethylated carbon atom in the central ring is disordered between two crystallographically equivalent positions (BC4) nonadjacent to the

Table I. Positional and Thermal Parameters[a]

Atom	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Co1	0.1401 (3)	0.2844 (4)	0.25	0.0050 (3)	0.0043 (5)	0.0121 (7)	0.0007 (3)	0.0000	0.0000
Co7	0.1641 (3)	−0.0285 (4)	0.25	0.0066 (3)	0.0043 (4)	0.0078 (5)	0.0002 (3)	0.0000	0.0000
C2	0.053 (2)	0.113 (3)	0.25	0.008 (3)	0.003 (3)	0.006 (4)	0.002 (3)	0.0000	0.0000
C2M	−0.060 (2)	0.094 (3)	0.25	0.002 (2)	0.010 (4)	0.024 (5)	−0.002 (2)	0.0000	0.0000
B3	0.119 (2)	0.118 (2)	0.118 (2)	0.008 (2)	0.002 (2)	0.011 (3)	−0.001 (2)	0.000 (2)	−0.002 (3)
BC4	0.232 (2)	0.137 (3)	0.174 (2)	0.008 (2)	0.006 (3)	0.011 (3)	0.003 (2)	0.002 (2)	0.000 (3)
C11	0.040 (3)	0.434 (3)	0.25	0.008 (4)	0.005 (4)	0.03 (1)	0.003 (3)	0.0000	0.0000
C12	0.099 (2)	0.445 (2)	0.135 (3)	0.007 (2)	0.006 (3)	0.019 (5)	0.002 (2)	−0.001 (2)	0.000 (3)
C13	0.192 (2)	0.467 (2)	0.179 (2)	0.009 (2)	0.000 (2)	0.023 (5)	−0.001 (2)	0.002 (2)	0.001 (2)
C71	0.087 (4)	−0.196 (4)	0.25	0.007 (4)	0.004 (5)	0.06 (2)	0.001 (3)	0.0000	0.0000
C72	0.145 (3)	−0.196 (3)	0.143 (3)	0.015 (4)	0.011 (4)	0.015 (4)	0.003 (3)	−0.003 (4)	−0.003 (3)
C73	0.239 (2)	−0.188 (2)	0.175 (3)	0.011 (2)	0.004 (3)	0.025 (6)	0.003 (2)	0.009 (3)	0.000 (2)
H11	−0.0301	0.4184	0.25						
H12	0.0777	0.4405	0.0444						
H13	0.2486	0.4791	0.1233						
H71	0.0187	−0.2006	0.25						
H72	0.1204	−0.1985	0.0527						
H73	0.2945	−0.1833	0.1174						
H3	0.0946	0.1089	0.0138						
H4	0.2921	0.1484	0.1164						

[a] All hydrogen atoms isotropic; B fixed at 5.0.

Table II. Selected Distances and Angles[a]

	Distances, Å		
Co1–C11	2.02 (3)	Co7–C73	2.03 (2)
Co1–C12	2.06 (2)	Co7–C2	2.07 (3)
Co1–C13	2.08 (2)	Co7–B3	2.06 (2)
Co1–C2	2.08 (3)	Co7–BC4	2.04 (3)
Co1–B3	2.14 (2)	C11–C12	1.41 (3)
Co1–BC4	2.07 (2)	C12–C13	1.36 (3)
Co1–Co7	3.137 (5)	C13–C13	1.43 (5)
C2M–C2	1.54 (4)	C71–C72	1.32 (3)
C2–B3	1.60 (3)	C72–C73	1.32 (4)
B3–BC4	1.65 (3)	C73–C73	1.49 (6)
BC4–BC4	1.52 (4)	Co1–C2M	3.32 (3)
Co7–C71	1.97 (4)	Co7–C2M	3.28 (3)
Co7–C72	2.00 (3)		
	Angles, Deg		
Co1–C2–C2M	132 (2)	B3–BC4–BC4	110 (1)
Co7–C2–C2M	130 (2)	Co1–C2–Co7	98 (1)
B3–C2–C2M	124 (1)	Co1–B3–Co7	97 (1)
C2–B3–BC4	104 (2)	Co1–BC4–Co7	100 (1)
B3–C2–B3	112 (3)		

[a] Estimated standard deviations of the least significant figure are in parentheses and were derived from the inverse matrix in the course of least-squares refinement.

methylated carbon atom, C2. This situation is clear from the interatomic distances in the central ring, since the established (methylated) carbon atom is 1.60 (3) Å from its nearest ring neighbor (B3), a value typical of a carbon–boron bond in carborane cages. In comparison, the carboranyl C–C distances in the closely related species 2-CH$_3$-1,7,2,3-(η^5-C$_5$H$_5$)$_2$Co$_2$C$_2$B$_3$H$_4$,[5] 2,3-(CH$_3$)$_2$-1,2,3-(η^5-C$_5$H$_5$)-CoC$_2$B$_4$H$_4$,[19] and 1-CH$_3$-1,2,3-GaC$_2$B$_4$H$_6$[20] are 1.44, 1.46, and 1.47 Å, respectively. The observed B3–BC4 and BC4–BC4 distances of 1.65 (3) and 1.52 (4) Å are also consistent with the partial carbon character of BC4. The locations of all nonhydrogen atoms in the Co$_2$C$_2$B$_3$ cage are thus unambiguously established and the molecular geometry is in agreement with that proposed from ^{11}B and ^{1}H NMR studies.[5,6,13] The cyclopentadienyl carbon atom positions are less well defined due to thermal motion of the rings and possibly disorder as well, but these effects are inconsequential in relation to the chemically significant aspects of the structure.

All three rings are planar and nearly parallel, the cyclopentadienyl rings C11–C15 and C71–C75 being tilted by 3.2 and 3.3°, respectively, with respect to the central ring. The direction of the tilt in both cases is *toward* the methyl group, in contrast to the isomeric molecule 2-CH$_3$-1,7,2,3-(η^5-C$_5$H$_5$)$_2$C$_2$B$_3$H$_4$ in which the C$_5$H$_5$ rings were tilted slightly away from the methyl group.[5] No clear rationale for these effects can be offered at present, but a recent X-ray investigation[19] of another seven-vertex cobaltacarborane, 2,3-(CH$_3$)$_2$-1,2,3-(η^5-C$_5$H$_5$)CoC$_2$B$_4$H$_4$, revealed a cyclopentadienyl ring tilt of 7.5° (away from the methyl groups) with respect to the equatorial ring of the pentagonal bipyramid. A possibly related example is found in yet another seven-vertex species, 1-CH$_3$-1,2,3-GaC$_2$B$_4$H$_6$,[20] in which the CH$_3$–Ga vector lies 20° from the normal to the central ring. Packing effects may be responsible for some of these distortions, although in none of the cases cited have particularly close intermolecular contacts been found; in the present structure, the nearest such distance is 3.44 Å between C13 and C72.

The nature of the bonding in the 1,7,2,4- and 1,7,2,3-(η^5-C$_5$H$_5$)$_2$Co$_2$C$_2$B$_3$H$_5$ isomers is a question of some interest since no other triple-decked complexes have been isolated except for the previously mentioned dinickel cation[2-4] (η^5-C$_5$H$_5$)$_3$Ni$_2^+$, a species which differs structurally, electronically, and chemically from the dicobalt systems (vide infra). The 1,7,2,3- and 1,7,2,4-(η^5-C$_5$H$_5$)$_2$Co$_2$C$_2$B$_3$H$_5$ molecules can be regarded either as dicobalt metallocarboranes held together by strong, highly delocalized covalent bonding, or alternatively as complexes containing Co^{3+} ions sandwiched between a pair of C$_5$H$_5^-$ rings and a C$_2$B$_3$H$_5^{4-}$ central ligand. The high thermal and hydrolytic stability of both isomers, and indeed of all four (η^5-C$_5$H$_5$)$_2$Co$_2$C$_2$B$_3$H$_5$ species (see Introduction), is consistent with the general properties of cobalt metallocarboranes.[8] Each of these Co$_2$C$_2$B$_3$ systems is a seven-vertex cage having 16 framework valence electrons, the number required by the "$2n + 2$ rule",[21,22] to fill all available bonding molecular orbitals extending over the Co$_2$C$_2$B$_3$ polyhedral surface. This model is useful in that it (1) underlines the homologous relation of the (η^5-C$_5$H$_5$)$_2$Co$_2$C$_2$B$_3$H$_5$ species to other cobalt metallocarboranes,[8,12,23] (2) emphasizes the participation of the metal atoms in the delocalized cage binding, and (3) illustrates the well-known ability of the (η^5-C$_5$H$_5$)Co group to substitute for BH as a structural member in polyhedra, as shown by the isoelectronic series (η^5-C$_5$H$_5$)$_2$Co$_2$C$_2$B$_3$H$_5$, (η^5-C$_5$H$_5$)CoC$_2$B$_4$H$_6$, and C$_2$B$_5$H$_7$.

The alternative "triple-decked sandwich" description of 1,7,2,3- and 1,7,2,4-(η^5-C$_5$H$_5$)$_2$Co$_2$C$_2$B$_3$H$_5$ is consistent with the diamagnetism of these species since formal cobalt(III) is assumed and is helpful in relating these species directly to the metallocenes. The central planar 2,3- and 2,4-C$_2$B$_3$H$_5^{4-}$ rings are isoelectronic with C$_5$H$_5^-$ and may be regarded as heterocyclic difunctional aromatic ligands containing three filled bonding molecular orbitals similar to those in C$_5$H$_5^-$ and may be considered to be of appropriate symmetry for interaction with p_x, p_y, and sp atomic orbitals on the metals.[20] This conception is strengthened by the existence of complexes[6,8–10] of 2,3-$C_2B_3H_6^{3-}$ and 2,3-$C_2B_3H_7^{2-}$ which are related to 2,3-$C_2B_3H_5^{4-}$ by the formal addition to the latter system of one and two protons, respectively, into B–H–B three-center bond locations. Thus $C_5H_5^-$, $C_2B_3H_5^{4-}$, $C_2B_3H_6^{3-}$, and $C_2B_3H_7^{2-}$ form an isoelectronic series of planar pentagonal aromatic ring systems which are capable of η^5 bonding to metal atoms having suitable valence orbitals. The cyclocarboranyl ligands, unlike $C_5H_5^-$, have not been isolated as salts or observed as free ions, and their heterocyclic nature contrasts with the higher D_{5h} symmetry of the $C_5H_5^-$ ion. Nevertheless, the direct structural and electronic analogy of the X-ray-characterized species 1,7,2,3- and 1,7,2,4-$(\eta^5\text{-}C_5H_5)_2Co_2C_2B_3H_5$ and 1,2,3-$(CO)_3FeC_2B_3H_7$[9] with the metallocenes is quite striking and points up a relationship between the metallocarborane and metallocene areas in a way that is not always obvious—for example, when one considers the large (e.g., icosahedral) boron species[12,24] which have no structural counterparts outside of boron chemistry. The true degree of electronic similarity between the complexes of $C_5H_5^-$ and those of the cyclocarboranyl ring ligands can be elucidated only by detailed quantitative study; current work utilizing pulse Fourier transform ^{11}B, ^{13}C, and ^1H NMR spectroscopy is in progress and will be reported elsewhere.[25]

A brief comparison between the $(\eta^5\text{-}C_5H_5)_2Co_2C_2B_3H_5$ isomers and the $(\eta^5\text{-}C_5H_5)_3Ni_2^+$ ion may be worthwhile. The latter species, isolated as a BF_4^- salt,[2,3] is the only triple-decked metallocene complex to have been actually isolated, and its structure was recently confirmed in an X-ray diffraction study.[4] The chemistry of this ion is dominated by its tendency to expel $(\eta^5\text{-}C_5H_5)Ni^+$ and generate nickelocene, and its salts and those of its substituted derivatives react readily with water and other solvents.[2,3] In contrast, the $(\eta^5\text{-}C_5H_5)_2Co_2C_2B_3H_5$ triple-decked isomers are stable to solvolysis and exhibit no changes on heating below 200° in vacuo.[5,6,8,13] The metal-to-central ring distances in $(\eta^5\text{-}C_5H_5)_3Ni_2^+$ are somewhat greater (1.771 and 1.805 Å) than the corresponding vectors in the two dicobalt species (average value 1.57 Å in both isomers), but the difference is close to that expected on the basis of the larger size of formal Ni^{2+} ion in relation to Co^{3+}, so that direct structural comparisons between the nickel and cobalt species are ambiguous.

Other $(\eta^5\text{-}C_5H_5)_3M_2^{q+}$ triple-decked complexes may be obtainable, but few such species are likely to be characterized. On the other hand, a large family of triple- and multiple-decked metallocarboranes based on the formal $C_2B_3H_5^{4-}$ planar ring system seems well within reach, considering the variety of seven-vertex boron cage systems already characterized. The ultimate extension of this concept would be a linear sandwich polymer consisting of stacked $C_2B_3H_5^{4-}$ rings linked by formal Co^{3+} units but covalently bonded as in the monomeric metallocarboranes. If the degree of electron delocalization is comparable to that evident in both monomeric triple-decked species,[25] such a polymer can be expected to exhibit high electrical conductivity along the polymeric backbone and would represent a new extension of the field of "organic metals" which has attracted considerable interest.[26]

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Registry No. 2-CH_3-1,7,2,4-$(\eta^5\text{-}C_5H_5)_2Co_2C_2B_3H_4$, 56679-06-2.

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, 20× reduction, negatives) containing all of the supplementary material for the papers in this issue may be obtained from the Business Office, Books and Journals Division, American Chemical Society, 1155 16th St., N.W., Washington, D.C. 20036. Remit check or money order for $4.00 for photocopy or $2.50 for microfiche, referring to code number AIC50546O-12-75.

References and Notes

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(15) We are grateful to Dr. Vernon Miller for preparing the crystals used in this study.

(16) Calculations were carried out on a Burroughs B6718 computer. The data processing program HILGOUT is based on programs DRED (J. F. Blount) and PICKOUT (R. J. Doedens). Numerical absorption corrections were applied using program DABS which is a modified version of DATAPH (P. Coppens). Mathematical methods are fully described in "Crystallographic Computing", Munksgaard, Copenhagen, 1970. Structure factor calculations and least-squares refinements were carried out using program CUCLS and Fourier summations using program FOURIER, which are highly modified versions of the programs ORFLS (W. R. Busing, K. O. Martin, and H. A. Levy) and FORDAP (A. Zalkin), respectively.

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