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THE UNEXPECTED FORMATION OF A MIXED BIS(η^5-PENTAMETHYLCYCLOPENTADIENYL)TETRACARBONYL-(μ^3-ETHYLIDENE)TRIANGULOTRICOBALT COMPOUND AND ITS STRUCTURAL CHARACTERIZATION

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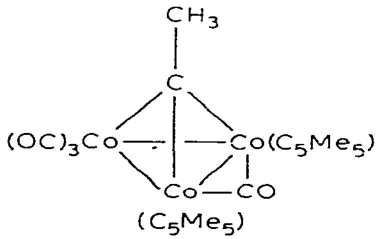
Summary

The title compound was first obtained photolytically from (η^5-Me_5C_5)Co-$(CO)_2$ (by a mechanism not understood) and later by refluxing C_5Me_5H with $Co_3(CO)_9CCH_3$. It was identified and characterized structurally by X-ray crystallography. The crystals belong to space group $P2_1/n$ with a 9.529(2), b 18.325(4), c 14.801(3) Å, β 95.69(2)° with $Z = 4$, making one entire molecule the asymmetric unit. Using 2541 reflections with $F_0^2 > 3\sigma(F_0^2)$ the structure was solved and refined to $R_1 = 0.051$ and $R_2 = 0.067$. It consists of a triangular pyramid with two (η^5-C_5Me_5)Co groups and one $Co(CO)_3$ group in the base and CCH_3 at the apex. The basal edge between the (η^5-C_5Me_5)Co groups has a bridging CO group and a Co—Co distance of 2.405(1) Å, while the other two unbridged Co—Co distances are 2.484(1) and 2.501(1) Å. The distances from the apical C atom to the bridged Co atoms are 1.857(6) and 1.866(6) Å but 1.932(6) Å to the unique Co atom. The C—C distance in the ethylidyne group is 1.497(9) Å. The structure is closely similar to that of the analogous (η^5-C_5H_5)$_2Co_3(CO)_4CCH_3$ compound.

Introduction

In an initial attempt to prepare $(C_5Me_5)_3Co_3(CO)_3$, we obtained instead a different trinuclear compound. The identity and structure of this compound, conclusively established by X-ray crystallography, are as shown schematically in I. Once the identity of the substance was known a rational preparative method was devised and its structure compared to that of (η^5-C_5H_5)$_2Co_3$-$(CO)_4CCH_3$ which had previously been described by Elder, Robinson and Simpson [1] and structurally characterized by McCallum and Penfold [2].



(I)

Experimental

All operations were performed in an atmosphere of dry nitrogen. Non-chlorinated solvents were dried with potassium/benzophenone and distilled under nitrogen immediately prior to use. Chlorinated solvents were dried with molecular sieves and freeze-thaw degassed before use. Dicobaltoctacarbonyl was purchased from Alfa Products, Danvers, Ma. Pentamethylcyclopentadiene was prepared by the method of Whitesides [3].

Preparation by photolysis. 1.84 g (5.24 mmol) $Co_2(CO)_8$ and 2.90 g (21.32 mmol) Me_5C_5H was dissolved in 30 ml CH_2Cl_2. The resulting solution was freeze-thaw degassed and heated to 45°C for 48 h. The reaction mixture was concentrated with a water aspirator and the remaining liquid chromatographed on Florisil. $Me_5C_5Co(CO)_2$ was eluted by developing the column with hexane. The hexane solution of $Me_5C_5Co(CO)_2$ was photolyzed (Hanovia 450 W medium-pressure lamp) in a quartz flask at room temperature. After 5 days the solvent was removed in vacuo leaving a dark solid. Green crystals of $(C_5Me_5)_2Co_3(CO)_4(\mu^3\text{-}CCH_3)$ were obtained from a THF/hexane solvent mixture. Infrared spectrum (hexane): ν(CO) 2030s, 2012s, 2005s, 1830m cm^{-1}.

Second preparative method. Once the identity of the compound was recognized, the following deliberate preparative method was devised, beginning with $Co_3(CO)_9(\mu\text{-}CCH_3)$, which was obtained by a literature method [4]. The purple solid was treated with 2 equivalents of Me_5C_5H in refluxing THF. After heating for 4 h, the solvent was removed in vacuo. The reaction solid was chromatographed on Florisil by elution with hexane to give a green band identified by IR as $(Me_5C_5)_2Co_3(CO)_4(\mu^3\text{-}CCH_3)$. This was then recrystallized as above.

X-ray crystallography. A dark green crystal measuring approximately 0.27 × 0.43 × 0.12 mm was sealed in a glass capillary. Data were collected at 21 ± 3°C on a Syntex P$\bar{1}$ automated diffractometer using Mo-K_α radiation monochromatized with a graphite crystal in the incident beam. The automated centering and auto-indexing procedures have previously been described [5]. Systematic absences $h0l$, $h + l = 2n + 1$ and $0k0$, $k = 2n + 1$ indicated that the space group was $P2_1/n$ (a non-standard setting of $P2_1/c$). The principal crystallographic data are as follows: a 9.529(2), b 18.325(4), c 14.801(3) Å, β 95.69(2)°, V 2571.6(9) Å^3 and $d_{calc} = 1.514$ g/cm^3 for $Z = 4$ and a molecular weight of 586.52. A total of 3534 unique reflections with $0.0° < 2\theta \leqslant 45.0°$ were collected using the $\theta - 2\theta$ scan technique. Mo-K_α linear absorption coefficient for this crystal is 8.79 cm^{-1}. No absorption corrections were made. Data collection methods have previously been described [5].

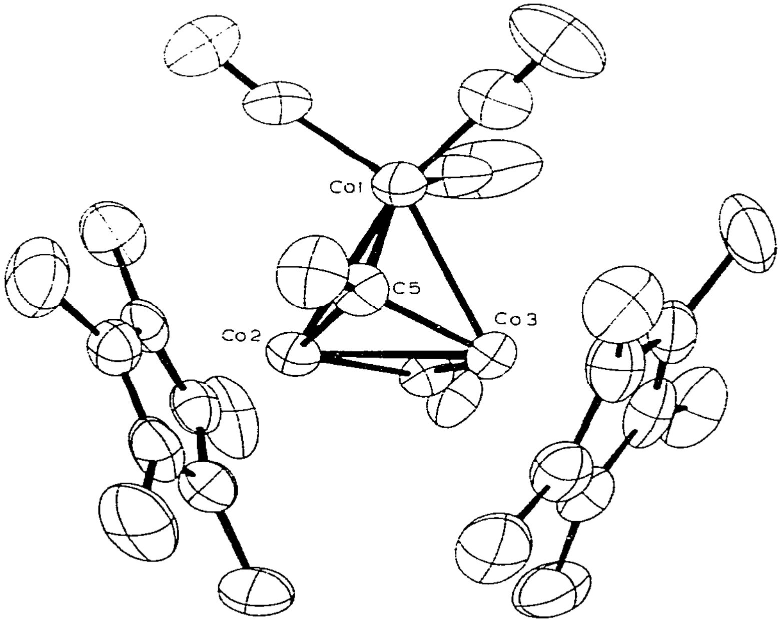


Fig. 1. An ORTEP drawing of the molecule. Atoms are represented by their ellipsoids of thermal vibration scaled to enclose 50% of the electron density.

Solution and refinement [6]. Direct methods using the program MULTAN, revealed the positions of the cobalt atoms. The coordinates of these three atoms were refined by least squares to give discrepancy factors of

$$R_1 = (\sum ||F_0| - |F_c|| / \sum |F_0| = 0.300$$

$$R_2 = [\sum w(|F_0| - |F_c|)^2 / \sum w |F_0|^2]^{1/2} = 0.385$$

The function, $\Sigma w(|F_0| - |F_c|)^2$, was minimized with the weighting factor, w, equal to $4F_0^2/\sigma(F_0^2)$. All structure factor calculations and least squares refinements were executed using those 2541 reflections for which $F_0^2 > 3\sigma(F_0^2)$. Atomic scattering factors were those of Cromer and Waber [7]. Anomalous dispersion effects were included in the calculated scattering factors for cobalt [8]. After refining the three cobalt positions, subsequent difference Fourier maps revealed the remaining non-hydrogen atoms. All non-hydrogen atoms were refined anisotropically to convergence using full-matrix least squares to give final discrepancy factors of $R_1 = 0.051$ and $R_2 = 0.067$ *. The error in an observation of unit weight was 1.492. A final difference Fourier map was essentially featureless.

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* The table of structure factors may be obtained upon request from F.A.C.

TABLE 1

POSITIONAL AND THERMAL PARAMETERS FOR $Cp_2Co_3(CO)_3(\mu^3\text{-}CMe)$ AND THEIR ESTIMATED STANDARD DEVIATIONS [a, b]

Atom	X	Y	Z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Co(1)	0,42970(9)	0,30279(5)	0,37567(7)	0,0081(1)	0,00333(3)	0,00420(5)	0,0003(1)	0,0018(1)	0,00017(7)
Co(2)	0,59018(9)	0,22680(5)	0,29236(6)	0,0092(1)	0,00245(3)	0,00345(5)	0,0002(1)	−0,0003(1)	−0,00050(6)
Co(3)	0,61405(9)	0,35732(5)	0,28717(6)	0,0086(1)	0,00255(3)	0,00317(4)	−0,0003(1)	0,0007(1)	0,00002(6)
O(1)	0,2031(7)	0,1962(4)	0,3766(6)	0,0171(8)	0,0080(3)	0,0136(6)	−0,0137(8)	0,0059(12)	0,0007(8)
O(2)	0,2506(7)	0,4296(4)	0,3781(6)	0,0203(9)	0,0062(3)	0,0133(5)	0,0104(8)	0,0125(11)	0,0026(7)
O(3)	0,5737(8)	0,2951(7)	0,5591(5)	0,0198(10)	0,0229(9)	0,0055(4)	0,0170(15)	−0,0001(11)	−0,0014(10)
O(4)	0,8096(5)	0,2852(3)	0,4180(4)	0,0109(6)	0,0039(2)	0,0059(3)	0,0011(6)	−0,0037(8)	−0,0005(4)
C(1)	0,2940(9)	0,2372(5)	0,3782(7)	0,0154(12)	0,0052(4)	0,0072(6)	−0,0016(12)	0,0045(14)	0,0006(8)
C(2)	0,3254(8)	0,3816(5)	0,3775(6)	0,0136(10)	0,0045(3)	0,0066(5)	0,0022(10)	0,0075(11)	−0,0002(7)
C(3)	0,5191(9)	0,2975(6)	0,4875(6)	0,0104(10)	0,0090(5)	0,0049(5)	0,0045(12)	0,0025(12)	−0,0009(8)
C(4)	0,7116(7)	0,2887(4)	0,3616(5)	0,0083(8)	0,0032(2)	0,0035(3)	0,0006(8)	−0,0012(9)	−0,0010(5)
C(5)	0,4611(7)	0,2975(4)	0,2489(5)	0,0097(8)	0,0029(2)	0,0036(3)	0,0004(8)	−0,0007(9)	−0,0002(5)
C(6)	0,3555(9)	0,3008(5)	0,1671(6)	0,0140(11)	0,0044(3)	0,0055(5)	−0,0006(10)	−0,0072(12)	−0,0005(7)
C(2,1)	0,5562(10)	0,1152(4)	0,3190(6)	0,0199(13)	0,0027(3)	0,0061(5)	0,0013(10)	0,0027(14)	0,0008(6)
C(2,2)	0,7000(9)	0,1310(4)	0,3348(6)	0,0196(12)	0,0028(3)	0,0047(4)	0,0053(9)	−0,0049(13)	−0,0008(6)
C(2,3)	0,7474(8)	0,1592(4)	0,2543(5)	0,0140(10)	0,0030(3)	0,0054(4)	0,0026(9)	0,0011(11)	−0,0023(6)
C(2,4)	0,6295(9)	0,1587(4)	0,1842(5)	0,0156(11)	0,0031(3)	0,0044(4)	0,0019(9)	0,0004(11)	−0,0019(5)
C(2,5)	0,5102(9)	0,1318(4)	0,2243(6)	0,0167(12)	0,0029(3)	0,0054(5)	−0,0017(9)	−0,0014(13)	−0,0023(6)
C(2,6)	0,4653(13)	0,0783(5)	0,3851(7)	0,0358(19)	0,0035(3)	0,0095(6)	−0,0025(14)	0,0148(18)	0,0040(7)
C(2,7)	0,7884(12)	0,1184(5)	0,4230(7)	0,0282(17)	0,0050(4)	0,0062(6)	0,0088(14)	−0,0096(17)	−0,0008(8)
C(2,8)	0,8993(9)	0,1811(6)	0,2427(8)	0,0138(12)	0,0054(4)	0,0108(7)	0,0025(12)	0,0064(15)	−0,0027(9)
C(2,9)	0,6334(11)	0,1795(5)	0,0859(6)	0,0266(16)	0,0049(3)	0,0034(4)	0,0038(13)	0,0029(14)	−0,0013(6)
C(2,10)	0,3669(10)	0,1175(5)	0,1740(8)	0,0147(12)	0,0047(3)	0,0114(7)	−0,0044(11)	−0,0055(16)	−0,0045(9)
C(3,1)	0,6262(8)	0,4700(4)	0,3135(5)	0,0175(11)	0,0023(2)	0,0046(4)	−0,0024(9)	0,0039(11)	−0,0001(5)
C(3,2)	0,7617(8)	0,4423(4)	0,3220(6)	0,0110(9)	0,0031(3)	0,0062(5)	−0,0038(8)	−0,0011(11)	0,0010(6)
C(3,3)	0,7844(8)	0,4094(4)	0,2370(6)	0,0133(10)	0,0033(3)	0,0077(5)	−0,0021(9)	0,0070(12)	0,0015(6)
C(3,4)	0,6595(9)	0,4195(4)	0,1763(5)	0,0197(13)	0,0033(3)	0,0043(4)	−0,0021(10)	0,0023(12)	0,0020(6)
C(3,5)	0,5617(8)	0,4577(4)	0,2228(5)	0,0134(10)	0,0028(2)	0,0038(4)	0,0006(8)	0,0013(10)	0,0005(5)
C(3,6)	0,5639(12)	0,5132(5)	0,3878(6)	0,0341(19)	0,0035(3)	0,0064(5)	−0,0025(13)	0,0129(15)	−0,0029(7)
C(3,7)	0,8707(11)	0,4489(5)	0,4037(7)	0,0245(15)	0,0052(4)	0,0088(6)	−0,0116(12)	−0,0124(16)	0,0022(8)
C(3,8)	0,9305(10)	0,3764(6)	0,2167(8)	0,0171(12)	0,0061(4)	0,0150(8)	0,0005(12)	0,0194(15)	0,0026(10)
C(3,9)	0,6457(13)	0,3979(6)	0,0751(16)	0,0390(22)	0,0053(4)	0,0038(5)	−0,0045(17)	0,0072(16)	−0,0003(7)
C(3,10)	0,4214(11)	0,4864(5)	0,1823(8)	0,0178(14)	0,0046(3)	0,0107(7)	0,0032(12)	−0,0046(17)	0,0050(8)

[a] Numbers in parentheses are estimated standard deviations in the last significant digits. [b] The form of the anisotropic thermal parameter is: $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + \beta_{12}hk + \beta_{13}hl + \beta_{23}kl)]$.

TABLE 2

BOND LENGTHS IN $Cp_2Co_3(CO)_4(\mu^3\text{-}CCH_3)$ [a]

Co(1)—Co(2)	2.484(1)	C(2,1)—C(2,2)	1.398(10)
Co(2)—Co(3)	2.405(1)	C(2,2)—C(2,3)	1.414(10)
Co(3)—Co(1)	2.501(1)	C(2,3)—C(2,4)	1.452(9)
Co(1)—C(1)	1.768(9)	C(2,4)—C(2,5)	1.422(10)
Co(1)—C(2)	1.754(8)	C(2,5)—C(2,1)	1.458(10)
Co(1)—C(3)	1.788(9)	C(3,1)—C(3,2)	1.380(9)
Co(1)—C(5)	1.932(6)	C(3,2)—C(3,3)	1.432(10)
Co(2)—C(4)	1.855(6)	C(3,3)—C(3,4)	1.430(10)
Co(2)—C(5)	1.857(6)	C(3,4)—C(3,5)	1.399(9)
Co(3)—C(4)	1.859(6)	C(3,5)—C(3,1)	1.438(9)
Co(3)—C(5)	1.866(6)	C(2,1)—C(2,6)	1.527(11)
Co(2)—C(2,1)	2.114(7)	C(2,2)—C(2,7)	1.499(10)
Co(2)—C(2,2)	2.108(6)	C(2,3)—C(2,8)	1.528(10)
Co(2)—C(2,3)	2.065(6)	C(2,4)—C(2,9)	1.507(10)
Co(2)—C(2,4)	2.094(6)	C(2,5)—C(2,10)	1.512(10)
Co(2)—C(2,5)	2.116(6)	C(3,1)—C(3,6)	1.523(9)
Co(3)—C(3,1)	2.102(6)	C(3,2)—C(3,7)	1.519(10)
Co(3)—C(3,2)	2.128(6)	C(3,3)—C(3,8)	1.574(11)
Co(3)—C(3,3)	2.083(7)	C(3,4)—C(3,9)	1.543(10)
Co(3)—C(3,4)	2.077(6)	C(3,5)—C(3,10)	1.505(10)
Co(3)—C(3,5)	2.108(6)		
C(1)—O(1)	1.146(9)		
C(2)—O(2)	1.134(8)		
C(3)—O(3)	1.134(10)		
C(4)—O(4)	1.190(7)		
C(5)—C(6)	1.497(9)		

[a] Numbers in parentheses are estimated standard deviations in the last significant digits.

Results

The molecular structure is shown in Fig. 1 and the atom numbering scheme is fully defined in Fig. 2. The atomic positional and thermal parameters are listed in Table 1. Bond distances and angles are given in Tables 2 and 3, respectively. The entire molecule constitutes the asymmetric unit and, hence, no sym-

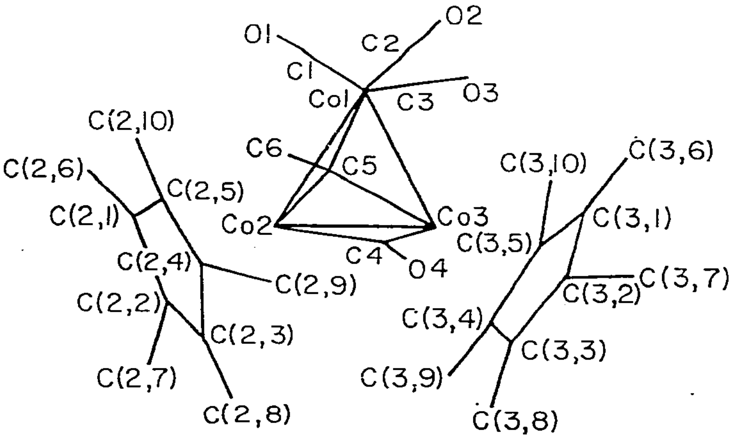

Fig. 2. A schematic drawing of the molecule in which the atomic numbering scheme is defined.

TABLE 3

BOND ANGLES IN $Cp_2Co_3(CO)_4(\mu^3\text{-}CCH_3)$ [a]

Co(2)—Co(1)—Co(3)	57.67(3)	Co(1)—Co(3)—C(5)	50.0(2)	C(3,2)—C(3,3)—C(3,4)	108.0(6)
Co(2)—Co(1)—C(1)	96.7(3)	Co(2)—Co(3)—C(4)	49.6(2)	C(3,3)—C(3,4)—C(3,5)	108.0(6)
Co(2)—Co(1)—C(2)	147.8(3)	Co(2)—Co(3)—C(5)	46.6(2)	C(3,1)—C(3,5)—C(3,4)	107.1(6)
Co(2)—Co(1)—C(3)	99.7(3)	C(4)—Co(3)—C(5)	96.5(3)	C(2,2)—C(2,1)—C(2,6)	126.4(8)
Co(2)—Co(1)—C(5)	47.8(2)	Co(1)—C(1)—O(1)	177.0(8)	C(2,5)—C(2,1)—C(2,6)	125.0(8)
Co(3)—Co(1)—C(1)	146.7(3)	Co(1)—C(2)—O(2)	175.6(8)	C(2,1)—C(2,2)—C(2,7)	124.9(8)
Co(3)—Co(1)—C(2)	96.2(2)	Co(1)—C(3)—O(3)	178.5(8)	C(2,3)—C(2,2)—C(2,7)	126.2(8)
Co(3)—Co(1)—C(3)	102.2(3)	Co(2)—C(4)—O(4)	139.3(5)	C(2,2)—C(2,3)—C(2,8)	125.2(7)
Co(3)—Co(1)—C(5)	47.7(2)	Co(2)—C(4)—Co(3)	80.7(3)	C(2,4)—C(2,3)—C(2,8)	126.6(7)
C(1)—Co(1)—C(2)	98.2(4)	Co(3)—C(4)—O(4)	139.7(5)	C(2,3)—C(2,4)—C(2,9)	126.6(7)
C(1)—Co(1)—C(3)	103.0(4)	Co(1)—C(5)—Co(2)	81.9(2)	C(2,5)—C(2,4)—C(2,9)	126.0(7)
C(2)—Co(1)—C(3)	104.4(4)	Co(1)—C(5)—Co(3)	82.4(2)	C(2,1)—C(2,5)—C(2,10)	127.4(7)
C(5)—Co(1)—C(1)	99.9(3)	Co(1)—C(5)—C(6)	128.8(5)	C(2,4)—C(2,5)—C(2,10)	125.1(7)
C(5)—Co(1)—C(2)	101.4(3)	Co(2)—C(5)—Co(3)	80.5(2)	C(3,2)—C(3,1)—C(3,6)	123.6(7)
C(5)—Co(1)—C(3)	142.3(3)	Co(2)—C(5)—C(6)	132.6(5)	C(3,5)—C(3.1)—C(3,6)	126.5(7)
Co(1)—Co(2)—Co(3)	61.52(3)	Co(3)—C(5)—C(6)	131.7(5)	C(3,1)—C(3,2)—C(3,7)	127.1(7)
Co(1)—Co(2)—C(4)	76.4(2)	C(2,2)—C(2,1)—C(2,5)	108.3(7)	C(3,3)—C(3,2)—C(3,7)	125.6(8)
Co(1)—Co(2)—C(5)	50.4(2)	C(2,1)—C(2,2)—C(2,3)	108.9(6)	C(3,2)—C(3,3)—C(3,8)	122.9(8)
Co(3)—Co(2)—C(4)	49.7(2)	C(2,2)—C(2,3)—C(2,4)	108.1(6)	C(3,4)—C(3,3)—C(3,8)	128.8(8)
Co(3)—Co(2)—C(5)	49.9(2)	C(2,3)—C(2,4)—C(2,5)	107.3(6)	C(3,3)—C(3,4)—C(3,9)	124.2(8)
C(4)—Co(2)—C(5)	96.9(3)	C(2,1)—C(2,5)—C(2,4)	107.3(6)	C(3,5)—C(3,4)—C(3,9)	127.5(7)
Co(1)—Co(3)—Co(2)	60.81(3)	C(3,2)—C(3,1)—C(3,5)	109.7(6)	C(3,1)—C(3,5)—C(3,10)	126.7(7)
Co(1)—Co(3)—C(4)	75.8(2)	C(3,1)—C(3,2)—C(3,3)	107.2(6)	C(3,4)—C(3,5)—C(3,10)	126.0(7)

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[a] Numbers in parentheses are the estimated standard deviation in the last significant digits.

metry is crystallographically imposed. In fact, there is a virtual plane of symmetry containing Co(1), C(5), C(4) and O(4).

The central motif of the structure is a distorted tetrahedron consisting of three cobalt atoms and one carbon atom, C(5). One edge, Co(2)—Co(3), is bridged by a carbonyl group and this metal—metal bond, with a length of 2.405(1) Å is significantly shorter than the other two unbridged edges, with lengths of 2.484(1) and 2.501(1) Å. In a related pattern, there are differences among the Co—C distances in the tetrahedron: The unique one, Co(1)—C(5), is longer, 1.932(6) Å, by a significant amount, than the other two which are essentially equal at 1.857(6) and 1.866(6) Å.

Each of the atoms of the central tetrahedron has certain appendages. A methyl group is attached to the carbon atom, and one of the cobalt atoms, Co(1), has a set of three carbonyl groups, just as in the well-known $Co_3(CO)_9$-CR type structures. Each of the other cobalt atoms has one η^5-C_5Me_5 group plus one bond to the bridging CO group, which, formally, is electronically equivalent to a set of three terminal CO groups.

None of the distances or angles in this molecule can be considered unusual. There are apparent small differences in certain dimensions as compared to those in the $(\eta^5\text{-}C_5H_5)_2Co_3(CO)_4(\mu\text{-}CCH_3)$ analog, but these are only at about the threshold of statistical significance and may not be real. Thus, the C—C distance in the ethylidyne unit, 1.55(3) Å, found in that work is not significantly different from 1.50(1) Å found here. The corresponding Co—Co distances differ by 0.037 Å, for the bridged one and 0.015 Å for the averages of the others. These are, respectively, ca. 10 and ca. 4 times the esds. If they are real, as they appear to be, in a statistical sense, they perhaps indicate a slight expansion of the Co_3 triangle because of steric crowding caused by the C_5Me_5 groups.

The mean planes of the ring and methyl carbon atoms were calculated for each $(\eta^5\text{-}C_5Me_5)$ ring and the distances of the Co atoms from each of these planes. These results showed that the methyl groups are distinctly bent away from the metal atoms. For the ring attached to Co(2) the mean plane of the methyl groups is 0.08(1) Å away from the ring plane and for the ring attached to Co(3) it is 0.11(1) Å away from the ring plane.

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ture and the production of the derived results were done using the Molecular Structure Corporation PDP-11/45 computer and the Enraf-Nonius Structure Determination Package with programs written chiefly by Frenz and Okaya.

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