The Molecular Structure of $Co_3(CO)_9CCH_3$. A Tricyclic Organocobalt Complex Containing a Metal-Coordinated Triply Bridging Aliphatic Carbon Atom[1]

Paul W. Sutton[2] and Lawrence F. Dahl[3]

Contribution from the Department of Chemistry, University of Wisconsin, Madison, Wisconsin 53706. *Received September 6, 1966*

Abstract: A three-dimensional, single-crystal X-ray examination of $Co_3(CO)_9CCH_3$ has afforded the first detailed structural characterization of a tricyclic $Co_3(CO)_9CY$ complex which represents the only known class of compounds containing an aliphatic carbon atom triply bridged to three metal atoms. The crystals of $Co_3(CO)_9CCH_3$ contain two molecules in a reduced triclinic unit cell of symmetry $P\bar{1}$ and of lattice parameters $a = 8.80$ A, $b = 9.33$ A, $c = 12.34$ A; $\alpha = 93.0°$, $\beta = 93.3°$, $\gamma = 128.8°$. A full-matrix, least-squares refinement of the structure gave an unweighted discrepancy factor of $R_1 = 11.7\%$. The molecular configuration ideally possesses C_{3v} symmetry and consists of an apical ethylidyne group, CH_3–C$<$, symmetrically coordinated by three Co–C σ bonds to a basal $Co_3(CO)_9$ fragment containing three identical $Co(CO)_3$ groups positioned at the corners of an equilateral triangle and bonded to one another by cobalt–cobalt bonds. The salient structural features of $Co_3(CO)_9CCH_3$ are discussed, and the stereochemistry of the tricyclic Co_3C(aliphatic) core is compared with that of the skeletal framework of the tricyclic M_3C(carbonyl) fragments embodied in several metal carbonyl complexes. A rationalization of the constrained molecular geometry in terms of bent bonds is given.

Markby, *et al.*,[4] reported the first preparation of a trinuclear cobalt complex of formula $Co_3(CO)_9C_2H_3$ which they isolated from the reaction of a methanolic solution of $Co_2(CO)_6(HC_2H)$ with aqueous sulfuric acid. A triangular arrangement of cobalt tricarbonyl groups was predicted for this diamagnetic complex with a near-zero dipole moment, since its infrared spectrum showed carbonyl absorption bands characteristic of only terminal carbonyl groups. Since the originally reported nmr measurements indicated the presence of two types of protons, the suggested types of organic moieties included a $-CH_2-CH<$ grouping as well as separated CH and CH_2 groups. Markby, *et al.*,[4] also noted that although the 1-pentyne complex, $Co_2(CO)_6(HC_2C_3H_7)$, reacted to give $Co_3(CO)_9C_5H_9$, the corresponding 3-hexyne complex, $Co_2(CO)_6(C_2H_5C_2C_2H_5)$, would not under any conditions yield a trinuclear cobalt complex.

Our initial three-dimensional X-ray investigation of $Co_3(CO)_9C_2H_3$, performed in 1959–1960, established that the three cobalt atoms formed an equilateral triangle with 2.45-A sides. Although our attempts at that time to determine the positions of the carbon and oxygen atoms were unsuccessful, the equivalence of the three Co–Co distances together with the infrared spectrum of the complex in the carbonyl stretching region strongly suggested a C_{3v} symmetry for the $Co_3(CO)_9$ fragment. Furthermore, careful consideration of the various types of hydrocarbon groups which might coordinate to this $Co_3(CO)_9$ fragment strongly implied that only an ethylidyne group, $>$C–CH_3, could satisfy both the closed-shell electronic requirements of each cobalt atom and the stereochemical requirements of a 2.45-A triangle. Since this group was not consistent with the originally reported nmr spectrum, a reinvestigation of the proton magnetic resonances was undertaken which revealed a single line assignable to a methyl group. This single resonance spectrum was independently confirmed by the original investigators.[5]

The formulation of this complex as $Co_3(CO)_9CCH_3$ was independently deduced by chemical investigation. Krüerke and Hübel[6] found that the degradation of $Co_3(CO)_9C_2H_2C_6H_5$ with bromine gave $C_6H_5CH_2CBr_3$ and that the treatment of the same complex with H_2O_2 yielded $C_6H_5CH_2CO_2H$. Hence, they concluded that the hydrocarbon fragment is joined to the heavy atom framework of the complex by three σ bonds and that the acetylene skeleton remains intact during the formation of the complex. The migration of an acetylenic hydrogen during the formation of $Co_3(CO)_9CCH_2R$ from $Co_2(CO)_6(HC_2R)$ is consistent with the earlier observation[4] that the reaction proceeds only for 1-alkyne complexes.

The three-point attachment of an aliphatic carbon atom to three cobalt atoms was also emphasized by the different and more general synthetic method reported by Dent, *et al.*,[7] who treated either dicobalt octacacarbonyl or tetracobalt dodecacarbonyl in ethanol with trihalogenomethyl derivatives, X_3CY, to form a large series of complexes of the type $Co_3(CO)_9CY$ (Y = CH_3, Cl, F, C_6H_5, $CO_2C_2H_5$, CO_2H, $CH(O_2CCH_3)_2$, and CF_3). The reaction product for Cl_3CCH_3 was shown to be identical with the corresponding tricobalt nonacarbonyl complex, $Co_3(CO)_9C_2H_3$, originally synthesized[4] from $CO_2(CO)_6(HC_2H)$. This new synthetic route was independently explored by Bor, Markó, and Markó,[8,9] who not only obtained $Co_3(CO)_9CH$ and $[Co_3(CO)_9C]_2$ in addition to several of the above complexes but also

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(1) Presented in part at the 140th National Meeting of the American Chemical Society, Chicago, Ill., Sept 1961; see Abstracts of Papers, p 48N.

(2) (a) Based in part on a dissertation submitted by P. W. Sutton to the Graduate School of the University of Wisconsin in partial fulfillment of the requirements for the Ph.D. degree; (b) National Science Foundation Predoctoral Fellow.

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isolated $Co_3(CO)_9CCO_2CH_3$ as a by-product involving solvent interaction in methanolic solution. A further characterization of these complexes was made by Ercoli, *et al.*,[10] who proposed a reaction mechanism involving $Co(CO)_4^-$ as a catalyst for the formation of the ester complex from $Co_3(CO)_9CBr$ and alcohol. Subsequently, $Co_3(CO)_9CCH_2C_6H_5$ has been studied as an initiator for vinyl polymerization.[11]

The infrared spectra[7-9] of these $Co_3(CO)_9CY$ complexes containing four absorption bands in the carbonyl stretching region have been analyzed by Bor[12] on the basis of C_{3v} symmetry of the $Co_3(CO)_9C$ radical. The corresponding derivatives, $Co_3(CO)_9SiC_2H_3$,[13a] $[Co_3(CO)_9Si]_2$,[13b] and $Co_3(CO)_9Sn(n\text{-}C_4H_5)$,[14] of the group IV congener elements, silicon and tin, have been reported and tentatively assigned structures similar to their carbon analogs.

Although several polynuclear metal carbonyl complexes containing carbonyl groups symmetrically coordinated to three metal atoms recently have been characterized by X-ray analysis,[15-18] the $Co_3(CO)_9CY$ complexes are the only known examples of such a three-point attachment of an *aliphatic* carbon atom. This single-crystal X-ray diffraction study of $Co_3(CO)_9CCH_3$ provides the first detailed characterization of a complex of this class of compounds. A preliminary report of this investigation has been presented.[1]

Experimental Section

A sample of $Co_3(CO)_9CCH_3$ was generously supplied to us by Drs. I. Wender and H. Sternberg of the Central Experiment Station, Bureau of Mines, U. S. Department of the Interior (Pittsburgh, Pa.). X-Ray photographs revealed that the dark purple crystals belong to the triclinic system. During the collection and processing of intensity data, the reflections were indexed on the basis of a nonreduced primative cell whose reciprocal cell parameters, determined from precession photographs, are $a^{*\prime} = 0.14672 \pm 0.00044$ A^{-1}, $b^{*\prime} = 0.12298 \pm 0.00037$ A^{-1}, $c^{*\prime} = 0.08174 \pm 0.00025$ A^{-1}; $\alpha^{*\prime} = 89.40 \pm 0.05°$, $\beta^{*\prime} = 83.32 \pm 0.05°$, $\gamma^{*\prime} = 61.00 \pm 0.05°$. The calculated density of 1.95 g cm^{-3} for two formula species in this unit cell agrees with the value 1.9 g cm^{-3} obtained by the flotation method. Two crystals were used for obtaining all diffraction data with Zr-filtered Mo Kα radiation by the multiple-exposure precession method and multiple-film equi-inclination Weissenberg method. The first crystal was essentially a cylinder, 0.1 mm in diameter and 0.3 mm in length. Data for the *hk*0 and 0*kl* precession zones and for the *h*0*l*, *h*1*l*, and *h*2*l* Weissenberg levels were gathered with this crystal before it decomposed in the X-ray beam. Since another satisfactory crystal could not be found in the original sample and since attempts to obtain suitable crystals by recrystallization from various solvents were unsuccessful, crystals were grown from sublimed vapor in evacuated glass capillaries. The crystals developed as thin plates that were too fragile to be remounted. In order to make direct use of the evacuated capillary as a crystal mounting, it was necessary to find an isolated single crystal with a reasonable orientation among the more commonly occurring clusters of crystals. After many unsuccessful attempts, a crystal was located which had a thickness of 0.04 mm and a nearly elliptical cross section with maximum and minimum dimensions of 0.8 and 0.6 mm. The *c* axis was approximately normal to this plate. The *h*0*l* precession zone and the *hk*0 through *hk*11 Weissenberg layers were obtained with this crystal.

A relative intensity was assigned to each observation of a reflection by visual comparison with a calibrated set of similarly shaped reflections. Only reflections which could be judged on at least two films in a given set were processed. The intensity data from each set of films were scaled and averaged by a procedure developed by Sutton.[19] The average intensities were corrected for Lorentz-polarization effects, but absorption corrections were neglected. Since the linear absorption coefficient for Mo Kα radiation is 33 cm^{-1}, absorption corrections for the second crystal are warranted in view of its nonuniform cross section (*i.e.*, for an elliptical cross section μR varies from 1.0 to 1.3); the thinness of that crystal, however, precluded the calculation of adequate absorption corrections in that no suitable absorption programs were available then.

In order to record the independent part of each Weissenberg reciprocal lattice layer, intensities from both the upper and lower halves of the films were measured for the nonzero layers. Different scale factors were assigned to reflections from the two halves of these layers, so that the major portion of the systematic error due to the expansion and contraction of spot size would be eliminated. The availability of intersecting zones of Weissenberg and precession data permitted the adjustment of the resulting 31 scale factors by a least-squares method[20] such that all observed structure factors and their estimated standard deviations were reduced to a single relative scale. It is noteworthy that 45% of these merged data were averages of measurements made under two or more independent experimental conditions. It has been shown that such a merging of data which possess unrelated systematic error tends to randomize the error in the resulting average.[21]

The reduced triclinic cell and its Miller indices (unprimed) are related to the nonreduced primitive cell and corresponding indices (primed) used in the intensity measurements by the transformations: $\mathbf{a}^* = \mathbf{a}^{*\prime}$, $\mathbf{b}^* = \mathbf{a}^{*\prime} - \mathbf{b}^{*\prime}$, $\mathbf{c}^* = \mathbf{c}^{*\prime}$. The transformed reciprocal parameters for the reduced cell are: $a^* = 0.14672 \pm 0.00044$ A^{-1}, $b^* = 0.13841 \pm 0.00041$ A^{-1}, $c^* = 0.08174 \pm 0.00025$ A^{-1}, $\alpha^* = 83.45 \pm 0.08°$, $\beta^* = 83.32 \pm 0.05°$, $\gamma^* = 51.00 \pm 0.28°$. A measured value of $\gamma^* = 50.85 \pm 0.05°$, determined directly from precession photographs, was used in place of the less precise transformed value for the calculation of the direct reduced cell parameters which are: $a = 8.80 \pm 0.03$ A, $b = 9.33 \pm 0.03$ A, $c = 12.34 \pm 0.04$ A; $\alpha = 93.02 \pm 0.13°$, $\beta = 93.30 \pm 0.11°$, $\gamma = 128.78 \pm 0.06°$. All results are reported in terms of this reduced primitive cell.

Structural Determination

The centrosymmetric space group $P\bar{1}$ was presumed on the basis of the distribution of Co–Co vectors in the computed Patterson function. This choice was confirmed by the satisfactory refinement of the structure, in which all atoms occupy the general twofold set of positions (2i): $\pm(x, y, z)$.[22]

The first efforts in 1959–1960 to determine the structure were only partially successful. At that point in the investigation the observed structure factors were based on intensity data that had been averaged on a desk calculator. The three independent cobalt atoms were located through the interpretation of Patterson projections for the three principal zones of the nonreduced unit cell. Scale factors for the 31 sets of reflections were determined by a least-squares refinement based on the cobalt atoms alone. A three-dimensional

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[20] P. W. Sutton, Ph.D. Thesis (Appendix A), University of Wisconsin, 1967.

[21] *Cf.* P. Werner, *Acta Chem. Scand.*, 18, 1851 (1964).

[22] "International Tables for X-Ray Crystallography," Vol. 1, The Kynoch Press, Birmingham, England, 1952, p 75.

Fourier synthesis based on these least-squares scale factors and phased on the cobalt atoms could not be interpreted in terms of a satisfactory set of carbon and oxygen atomic positions, and further efforts including difference syntheses failed to reveal the configuration of the light atoms.

Later, computer programs were written to process intensity data in the manner already described, and a revised set of observed structure factors was prepared. A three-dimensional Patterson function calculated with the reprocessed data confirmed the previously determined heavy-atom positions. Since the earlier Fourier synthesis had not been successful, a difference synthesis was prepared which included the 420 unobserved reflections with $\sin^2 \theta/\lambda^2 < 0.28$. Each unobserved structure factor was assigned one-half the minimum observable F value for that point in reciprocal space. The three-dimensional difference synthesis, based on the internally scaled data from which the calculated cobalt contribution had been removed, revealed the positions of the 20 carbon and oxygen atoms. The reasons for the failure of the earlier Fourier synthesis are not understood. The unobserved data were not used in the refinement of the structure.

Two isotropic full-matrix, least-squares cycles were followed by three cycles with anisotropic temperature factors. The positional parameters of a different pair of cobalt atoms were fixed during each of the latter cycles, in order not to exceed the parameter capacity of the computer used in the least-squares refinement. In the third anisotropic least-squares cycle, the average thermal parameter shift was 0.15σ; in 85% of the cases, the thermal parameter shift was less than 0.3σ, while the largest thermal parameter change was 1.0σ. During two final refinement cycles the values of the anisotropic temperature factors were fixed; instead, an over-all temperature factor was varied along with all positional parameters and a scale factor. In the last cycle, every one of these parameters changed by less than 0.1σ. For the 1818 independent reflections the final unweighted and weighted discrepancy factors, $R_1 = [\Sigma||F_o| - |F_c||/\Sigma|F_o|] \times 100$ and $R_2 = [\Sigma w\,||F_o| - |F_c||^2/\Sigma w|F_o|^2]^{1/2} \times 100$ are 11.7 and 14.5%, respectively. A three-dimensional difference synthesis based on the refined structure showed no unusual features.

The final anisotropic thermal parameters for C(1) are not positive-definite. This is not at all surprising in a refinement of photographic data which are known to have systematic errors. It has been generally concluded from other structural determinations as well as from empirical investigations[21,23] that the thermal parameters show an unusual sensitivity to systematic errors, while at the same time these errors do not seriously affect the values of the positional parameters. When systematic errors are present, the thermal parameters tend to lose physical significance as indicators of thermal displacement and to become empirical adjustments for the systematic errors. The essential invariance of the positional parameters to the thermal models is indicated in this least-squares refinement by the equally low positional-thermal correlation coefficients (*i.e.*, <0.1) obtained from the inverse matrices of the isotropic, anisotropic, and final refinement cycles.

All Patterson and Fourier syntheses were calculated on a CDC 1604 computer with the Blount program.[24] The least-squares cycles were performed on an IBM 704 computer with the Busing–Martin–Levy ORFLS program.[25] The refinement was based on the minimization of $\Sigma w_i \Delta F_i^2$, and the weights were assigned according to the estimated standard deviations of the observed structure factors. The calculated structure factors are based on the atomic scattering factors of Freeman and Watson[26] for cobalt, and of Berghuis, *et al.*,[27] for carbon and oxygen.

Final positional parameters and final anisotropic thermal parameters are given in Tables I and II, respectively. Observed and calculated structure factors, based on these parameters, are listed in Table III.

Table I. Fractional Coordinates for $Co_3(CO)_9CCH_3$[a]

Atom	x	y	z
Co(1)	0.2056 (3)	−0.0664 (3)	0.1736 (2)
Co(2)	−0.0849 (3)	−0.1713 (3)	0.2650 (2)
Co(3)	0.0095 (3)	−0.3705 (3)	0.2432 (2)
C(1)	0.0995 (27)	−0.1372 (25)	0.0342 (10)
O(1)	0.0256 (28)	−0.1840 (22)	−0.0493 (11)
C(2)	0.3189 (29)	0.1756 (27)	0.1907 (14)
O(2)	0.3937 (25)	0.3221 (22)	0.2066 (16)
C(3)	0.4286 (36)	−0.0371 (29)	0.1644 (21)
O(3)	0.5673 (27)	−0.0099 (27)	0.1591 (20)
C(4)	−0.2592 (23)	−0.2546 (23)	0.1420 (13)
O(4)	−0.3681 (22)	−0.3077 (23)	0.0732 (12)
C(5)	−0.2489 (30)	−0.2982 (28)	0.3678 (13)
O(5)	−0.3348 (27)	−0.3479 (25)	0.4378 (11)
C(6)	−0.0260 (31)	0.0449 (30)	0.3040(14)
O(6)	0.0150 (27)	0.1847 (21)	0.3333 (13)
C(7)	−0.1444 (32)	−0.5085 (25)	0.1177 (19)
O(7)	−0.2382 (27)	−0.6011 (21)	0.0352 (15)
C(8)	0.2026 (30)	−0.3940 (30)	0.2496 (14)
O(8)	0.3191 (30)	−0.3965 (27)	0.2661 (23)
C(9)	−0.1282 (36)	−0.5225 (28)	0.3409 (20)
O(9)	−0.2134 (32)	−0.6142 (31)	0.4071 (15)
C(10)	0.1543 (27)	−0.1266 (25)	0.3156 (14)
$H_3C(11)$	0.2799 (30)	−0.0385 (35)	0.4269 (20)

[a] Standard deviations of the last significant figures are in parentheses.

Distance and angle calculations were performed with the Busing–Martin–Levy function and error program ORFFE.[28] The full inverse matrix of the last least-squares cycle was used in the error calculations which included the effect of estimated unit cell uncertainties. Intramolecular bond distances and angles are given in Tables IV and V, respectively, while Table VI presents the nonbonding intramolecular C···C distances corresponding to the edges of a polyhedral fragment. Table VII gives the perpendicular distances of atoms from the plane containing the three cobalt atoms.

Discussion

Crystalline $Co_3(CO)_9CCH_3$ contains discrete molecules whose configuration (Figure 1) ideally conforms

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Table II. Anisotropic Thermal Parameters ($\times 10^4$) for $Co_3(CO)_9CCH_3$[a]

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Co(1)	83 (6)	86 (6)	33 (2)	54 (5)	23 (3)	21 (3)
Co(2)	83 (6)	105 (6)	24 (2)	67 (5)	21 (3)	13 (2)
Co(3)	138 (7)	103 (6)	45 (2)	92 (6)	24 (3)	32 (3)
C(1)	281 (60)	292 (59)	−8 (12)	231 (53)	61 (20)	39 (18)
O(1)	444 (70)	277 (50)	44 (15)	251 (51)	35 (24)	12 (19)
C(2)	186 (64)	173 (56)	61 (18)	132 (54)	48 (25)	28 (23)
O(2)	231 (58)	155 (46)	148 (22)	104 (45)	−15 (27)	8 (23)
C(3)	208 (80)	134 (58)	120 (27)	89 (61)	−21 (37)	−42 (30)
O(3)	236 (60)	290 (60)	220 (32)	177 (54)	126 (37)	124 (34)
C(4)	88 (45)	151 (46)	46 (15)	96 (41)	13 (20)	20 (19)
O(4)	199 (48)	273 (50)	82 (15)	159 (43)	−46 (23)	5 (20)
C(5)	219 (66)	208 (57)	32 (16)	126 (54)	6 (25)	3 (22)
O(5)	386 (62)	441 (66)	34 (12)	228 (55)	114 (23)	73 (21)
C(6)	225 (69)	242 (64)	36 (15)	141 (57)	36 (24)	32 (23)
O(6)	405 (71)	186 (45)	95 (17)	197 (49)	65 (27)	−14 (20)
C(7)	186 (68)	65 (47)	106 (23)	17 (50)	63 (31)	−1 (26)
O(7)	297 (61)	180 (47)	121 (19)	146 (47)	−24 (28)	−42 (24)
C(8)	140 (56)	232 (66)	35 (16)	73 (55)	−7(23)	−17 (23)
O(8)	276 (74)	275 (67)	247 (34)	175 (63)	4 (41)	97 (35)
C(9)	261 (77)	136 (54)	114 (26)	132 (57)	−13 (36)	43 (27)
O(9)	474 (84)	522 (80)	101 (20)	299 (71)	181 (35)	171 (33)
C(10)	152 (54)	176 (50)	53 (16)	132 (47)	15 (22)	18 (20)
$H_3C(11)$	99 (56)	308 (79)	99 (24)	46 (57)	−40 (28)	93 (34)

[a] Standard deviations of the last significant figures are in parentheses.

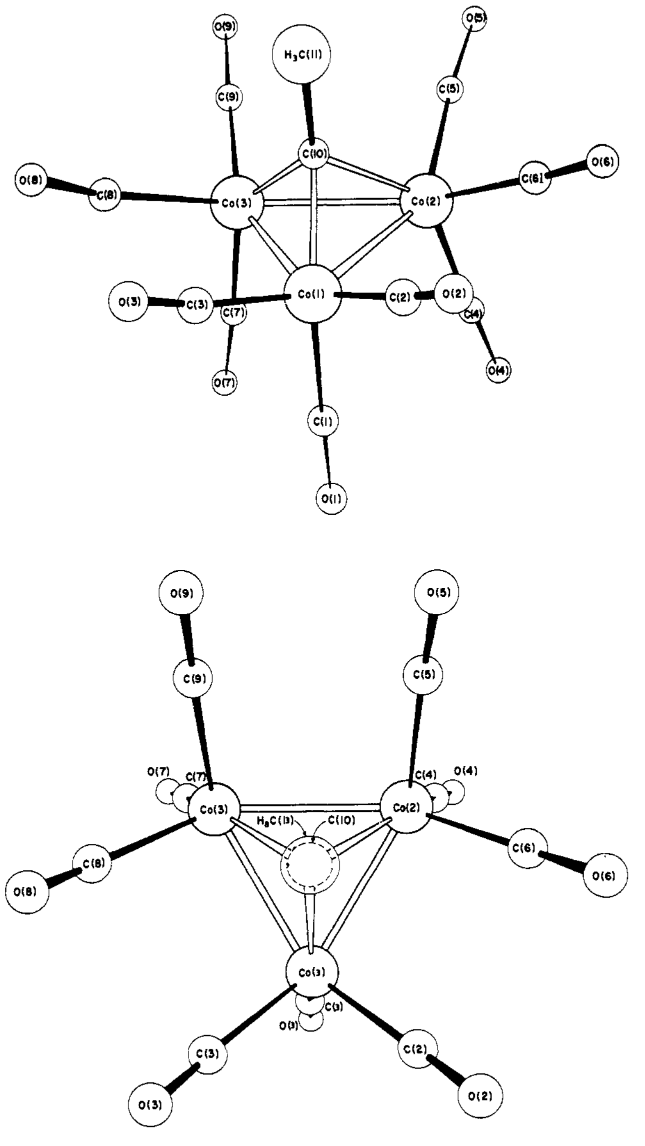

Figure 1. Molecular configuration of $Co_3(CO)_9CCH_3$ corresponding ideally to the trigonal point group C_{3v}-3m.

to C_{3v} molecular symmetry. Each molecule consists of an apical ethylidyne group, $CH_3–C<$, symmetrically coordinated by three carbon–cobalt σ bonds to a $Co_3(CO)_9$ fragment structured of identical equilaterally positioned $Co(CO)_3$ groups joined to one another by metal–metal bonds. Each of the three six-coordinated cobalt atoms, which are equivalent under the above molecular symmetry, attains a closed-shell ground-state electronic configuration consistent with the observed diamagnetism of the compound through bonds to three terminal carbonyl groups, the apical carbon atom, and the two other cobalt atoms. The latter three ligands are constrained to a tricyclic geometry which involves interligand angles of 50 and 60°. A detailed study of the ligand arrangement reveals that the effects of these constraints on the disposition of the terminal carbonyl groups are consistent with generally observed structural features in strained systems (*vide infra*).

Within experimental error, the nonbonding C···C distances listed in Table VI conform to the edges of a 3:6:1 polyhedron of C_{3v} symmetry. The small deviations of the experimentally determined nonhydrogen atoms from the idealized positions required by the C_{3v} point group (see Tables IV through VII) are presumably due to intermolecular forces. However, the observed distances for various types of closest intermolecular contact (*viz.*, CO···OC, 3.14 A; CO···CO, 3.31 A; $CO\cdots CH_3$, 3.62 A; and $H_3C\cdots CH_3$, 3.79 A) indicate that there are no abnormal interactions between molecules. Hence, average values for the molecular parameters based on the idealized C_{3v} symmetry are used throughout the discussion of the structure.

The geometry of $Co_3(CO)_9CCH_3$ can be primarily attributed to the stereochemical constraints imposed by the formation of the Co_3C core. The attachment of the $CH_3C<$ organic moiety to the basal $Co_3(CO)_9$ fragment can be ascribed in valence-bond terminology to the interaction of a tetrahedral-like carbon orbital with an octahedral-like orbital of each of the three cobalt atoms. The three terminal carbonyl groups attached to each cobalt atom are positioned so as to

Table III. Observed and Calculated Structure Factors

H	K	L	FO	FC
1	0	0	90.7	119.8
3	0	0	33.9	29.4
4	0	0	27.5	26.5
5	0	0	34.2	30.9
7	0	0	17.7	-10.9
2	1	0	14.9	12.6
-2	1	0	42.2	-33.2
3	1	0	71.0	-75.2
4	1	0	35.4	-36.7
-4	1	0	33.7	35.2
-6	1	0	37.4	-38.0
-7	1	0	40.3	-44.7
-8	1	0	27.3	-30.5
0	2	0	11.1	5.4
1	2	0	13.1	-9.3
-1	2	0	32.5	-26.9
2	2	0	45.7	-50.5
3	2	0	49.4	-56.1
-3	2	0	38.4	-37.6
4	2	0	26.7	-25.1
-4	2	0	64.3	64.2
-5	2	0	48.8	54.4
0	3	0	24.1	21.9
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3	-4	9	18.1	-18.4
-3	-4	9	15.8	-12.1
4	-4	9	20.4	-24.0
-5	-4	9	18.3	-15.4
7	-4	9	21.1	-18.4
-7	4	9	19.9	-19.4
8	-4	9	18.4	-14.8
-8	4	9	34.5	-34.0
0	5	9	19.6	-17.5
0	-5	9	28.9	24.0
1	5	9	25.2	-23.4
1	-5	9	31.3	35.1
2	-5	9	22.7	23.1
3	-5	9	25.4	21.7
4	-5	9	24.0	24.4
-5	5	9	25.4	25.2
5	-5	9	29.4	24.4
-6	5	9	37.6	34.7
6	-5	9	19.3	17.9
-7	5	9	17.6	14.2
7	-5	9	18.8	-15.6
-8	5	9	18.0	-15.0
0	-6	9	16.2	-9.5
-1	6	9	16.3	11.7
1	-6	9	14.4	-10.0
-1	-6	9	30.1	-24.1
2	-6	9	30.8	-31.8
-2	-6	9	30.4	-34.4
-3	6	9	14.4	-15.1
3	-6	9	22.3	-20.8
-3	-6	9	20.6	-14.7
-5	6	9	29.9	32.2
-6	6	9	42.2	45.3
6	-6	9	13.6	-2.5
-7	6	9	25.7	23.3
7	-6	9	15.5	-9.4
-8	6	9	14.5	11.1
8	-6	9	17.7	-17.0
-9	6	9	17.7	15.3
-2	7	9	17.4	-17.4
2	-7	9	29.0	-26.5
-3	7	9	24.0	-24.4
3	-7	9	20.9	-13.6
-4	7	9	23.5	-22.4
4	-7	9	18.8	17.4
5	-7	9	54.5	33.0
6	-7	9	22.5	20.4
-7	7	9	17.1	-12.2
7	-7	9	17.0	10.6
-8	7	9	15.9	-13.9
8	-7	9	21.0	15.0
-1	-8	9	14.4	18.7
2	-8	9	14.3	-14.0
-4	8	9	18.6	-12.2
4	-8	9	19.8	13.0
1	-9	9	16.6	-15.0
2	-9	9	26.5	-26.1
3	-9	9	16.0	-14.4
-4	9	9	16.0	13.1
5	-9	9	17.0	-14.8
6	-9	9	25.1	-23.1
-7	9	9	22.3	-22.2
7	-9	9	19.1	-21.0
3	-10	9	25.1	22.2
4	-10	9	24.4	21.5
-7	10	9	17.4	-16.1
0	0	10	59.1	-62.9
1	0	10	21.9	-21.5
-1	0	10	55.5	-62.9
2	0	10	23.1	-20.4
-2	0	10	11.7	-10.6
3	0	10	35.4	-33.9
-3	0	10	20.6	20.1
4	0	10	31.8	-29.6
-4	0	10	27.0	23.8
-7	0	10	24.5	-12.4
0	1	10	12.1	-12.7
0	-1	10	23.6	26.4
1	-1	10	20.4	17.2
-2	-1	10	53.4	11.5
-3	1	10	39.3	44.7
3	-1	10	16.8	-16.4
-3	-1	10	29.0	28.5
-4	1	10	37.9	32.0
4	-1	10	20.5	-17.6
-4	-1	10	31.8	33.6
-6	1	10	22.3	16.0
-6	-1	10	21.4	-18.6
-7	1	10	28.1	25.6
-7	-1	10	21.5	-20.6
-8	1	10	27.2	24.6
0	2	10	15.8	-14.6
0	-2	10	29.4	43.4
1	2	10	13.6	12.9
-1	2	10	24.2	-31.7
1	-2	10	39.5	57.8
-1	-2	10	14.0	14.9
2	2	10	22.6	19.0
-2	2	10	23.2	-30.8
2	-2	10	14.0	17.6
3	2	10	14.6	13.7
-3	2	10	11.9	-12.3
-3	-2	10	19.2	17.0
-4	2	10	26.2	-6.9
-4	-2	10	24.5	19.7
-5	2	10	30.1	-30.3
-6	2	10	21.3	-14.4
-7	2	10	18.9	14.6
-7	-2	10	16.5	-12.9
-8	2	10	22.6	20.0
0	-3	10	12.6	10.3
1	-3	10	22.1	23.2
-1	-3	10	16.1	-11.4
2	3	10	28.5	23.0
-2	3	10	17.9	9.2
-2	-3	10	37.7	-41.0
3	3	10	17.6	19.7
3	-3	10	17.2	-16.1
-3	-3	10	40.9	-36.1
-4	3	10	30.4	-31.8
-5	3	10	37.6	-34.2
-6	3	10	24.4	-22.7
-6	-3	10	15.0	-17.2
7	-3	10	27.4	-22.2
-8	3	10	21.2	29.5
8	-3	10	25.8	-20.4
0	4	10	12.6	10.1
0	-4	10	22.7	21.9
1	4	10	21.7	19.1
-1	4	10	22.5	24.8
1	-4	10	16.9	16.2
-1	-4	10	12.2	6.1
2	4	10	25.7	38.4
2	-4	10	22.0	20.4
-2	-4	10	22.2	-21.1
-3	4	10	21.9	23.4
3	-4	10	31.4	27.7
4	-4	10	32.4	24.4
-5	4	10	25.8	-14.5
5	-4	10	37.4	40.2
-5	-4	10	17.4	17.8
6	-4	10	20.0	14.4
7	-4	10	20.2	-4.4
0	5	10	19.1	-17.3
1	-5	10	20.1	-17.8
-2	5	10	17.8	14.5
2	-5	10	32.3	-34.1
-2	-5	10	19.3	-15.7
3	-5	10	23.0	-17.8
-4	5	10	11.7	-13.2
-5	5	10	27.4	-25.4
-6	5	10	14.1	-13.4
-7	5	10	12.9	-7.0
-8	5	10	20.6	-21.2
-9	5	10	34.8	-33.5
-10	5	10	20.0	-20.4
1	-6	10	30.4	-29.4
2	-6	10	34.6	-41.0
-3	6	10	13.3	7.5
3	-6	10	30.4	-26.8
-5	6	10	14.0	19.0
-6	6	10	24.4	28.2
-7	6	10	16.7	15.8
-8	6	10	14.4	-17.2
0	-7	10	25.4	23.1
1	-7	10	14.5	3.5
-1	-7	10	32.4	33.3
-2	-7	10	23.7	23.1
4	-7	10	16.4	10.2
-6	7	10	23.4	25.4
-7	7	10	14.7	15.9
8	-7	10	21.4	22.4
9	-7	10	26.4	14.9
-3	8	10	24.0	-20.8
-4	8	10	24.5	-22.4
5	-8	10	24.0	-20.2
6	-8	10	36.4	-30.0
7	-8	10	30.6	-25.8
8	-8	10	25.3	21.9
4	-9	10	19.7	14.0
3	-10	10	22.1	21.4
4	-10	10	16.9	15.5
0	0	11	26.1	16.4
-2	0	11	12.0	-19.5
3	0	11	26.1	-26.2
-3	0	11	11.3	5.4
-4	0	11	11.7	4.7
-5	0	11	14.5	-14.4
-6	0	11	24.0	-24.0
-7	0	11	30.9	-32.9
-8	0	11	25.4	-20.6
0	1	11	9.6	-5.0
0	-1	11	36.2	51.4
1	-1	11	28.1	37.0
2	1	11	17.9	-21.2
-2	1	11	6.5	9.0
-2	-1	11	10.5	-9.9
3	1	11	24.0	-27.8
-3	1	11	14.0	14.5
-3	-1	11	11.5	-7.3
4	1	11	18.3	-14.7
-4	1	11	35.3	34.2
-5	1	11	17.1	15.1
-5	-1	11	14.2	13.4
-6	1	11	17.3	-14.7
-7	1	11	19.6	-18.5
0	-2	11	9.6	-8.0
1	2	11	14.1	13.8
-1	2	11	11.7	-15.2
-1	-2	11	17.1	-18.5
-2	2	11	8.1	4.3
2	-2	11	10.4	-9.4
-2	-2	11	35.4	-59.3
-3	2	11	29.3	38.0
-3	-2	11	42.4	-50.5
-4	2	11	35.7	43.5
4	-2	11	17.9	17.4
-4	-2	11	20.7	-21.0
-5	2	11	27.8	27.4
-8	2	11	16.3	14.2
0	3	11	23.4	-22.1
0	-3	11	13.3	9.9
-1	3	11	31.5	-36.5
-2	3	11	24.6	-51.4
-2	-3	11	20.6	-25.1
-3	3	11	10.3	-10.4
3	-3	11	11.9	9.4
-3	-3	11	14.8	-17.1
-4	3	11	11.4	-7.2
4	-3	11	30.2	35.1
-5	3	11	18.6	-19.3
5	-3	11	29.4	32.3
-8	3	11	18.8	19.4
0	-4	11	13.4	12.5
1	4	11	19.9	14.0
-1	4	11	15.3	-12.4
1	-4	11	15.5	-15.4
-1	-4	11	20.7	21.0
2	4	11	19.6	13.9
-2	4	11	10.9	-12.4
2	-4	11	20.3	-21.2
-2	-4	11	14.7	14.2
4	-4	11	14.4	13.9
-5	4	11	14.6	-12.2
5	-4	11	14.9	14.3
-7	4	11	15.9	14.8
-8	4	11	30.5	31.6
-9	4	11	24.2	24.0
0	-5	11	12.3	-11.9
1	-5	11	33.0	-35.6
-1	-5	11	15.1	15.3
2	-5	11	39.9	-35.1
3	-5	11	21.1	-20.7
-3	-5	11	16.1	-7.9
-4	5	11	17.4	-18.6
4	-5	11	16.7	-15.3
-5	5	11	26.9	-32.1
5	-5	11	22.0	-25.2
-6	5	11	17.5	-16.5
6	-5	11	18.5	-18.4
0	-6	11	22.7	24.9
-1	-6	11	28.7	32.2
-2	-6	11	20.6	20.5
-3	6	11	12.2	9.7
3	-6	11	16.2	15.6
4	-6	11	12.6	14.0
-5	6	11	21.5	-24.4
6	-6	11	14.4	-13.3
-6	6	11	18.6	-16.5
7	-6	11	17.9	7.1
-9	6	11	21.7	-22.5
-3	7	11	19.6	22.2
3	-7	11	17.4	16.4
-4	7	11	17.3	20.0
5	-7	11	17.4	-14.5
6	-7	11	24.0	-22.4
-7	7	11	14.4	12.9
0	-8	11	16.0	-19.1
3	-8	11	18.7	17.2
-6	8	11	13.5	-6.7
2	-9	11	16.5	18.5
3	-9	11	21.8	24.3
4	-9	11	17.7	18.4
6	-9	11	19.1	14.8
7	-9	11	26.7	24.7
4	-10	11	17.4	-18.0
0	0	12	29.8	28.1
-1	0	12	24.4	17.1
3	0	12	22.4	15.4
-1	0	12	22.7	-24.4
4	0	12	22.1	14.7
1	-1	12	20.7	-26.7
-2	-1	12	20.2	-26.7
-3	-1	12	23.4	-14.0
0	2	12	24.0	26.4
1	-2	12	30.5	-34.7
2	-2	12	28.0	-27.0
-3	-2	12	23.1	-27.3
-4	2	12	29.5	29.5
1	0	13	26.5	-25.8
-5	0	13	22.1	22.6
-6	0	13	26.0	29.1
-7	0	13	27.6	23.9
1	-1	13	26.2	-37.1
-1	-2	13	19.8	22.6
-2	-2	13	27.4	42.5
-3	2	13	18.7	-16.4
-4	2	13	20.1	-26.3
0	0	14	25.9	-24.2
1	0	14	28.1	-26.1
-4	0	15	28.6	-16.6
-6	0	15	29.5	-22.3

Table IV. Bond Distances (A) for $Co_3(CO)_9CCH_3$[a]

Co(1)–Co(2)	2.466 (7.3)	Co(1)–C(10)	1.86 (1.8)
Co(2)–Co(3)	2.475 (7.0)	Co(2)–C(10)	1.93 (1.9)
Co(3)–Co(1)	2.462 (7.1)	Co(3)–C(10)	1.90 (1.9)
Average	2.467	Average	1.90
Co(1)–C(1)	1.79 (1.5)	C(1)–O(1)	1.09 (2.0)
Co(1)–C(2)	1.80 (2.0)	C(2)–O(2)	1.08 (2.2)
Co(1)–C(3)	1.82 (2.8)	C(3)–O(3)	1.09 (2.8)
Co(2)–C(4)	1.84 (1.7)	C(4)–O(4)	1.07 (1.9)
Co(2)–C(5)	1.82 (1.9)	C(5)–O(5)	1.10 (2.2)
Co(2)–C(6)	1.77 (2.4)	C(6)–O(6)	1.14 (2.4)
Co(3)–C(7)	1.80 (2.3)	C(7)–O(7)	1.18 (2.6)
Co(3)–C(8)	1.84 (2.5)	C(8)–O(8)	1.05 (2.7)
Co(3)–C(9)	1.77 (2.2)	C(9)–O(9)	1.14 (2.5)
Average	1.80	Average	1.10
	$H_3C(11)$–C(10)	1.53 (2.8)	

[a] Standard deviations of the last significant figures are in parentheses.

Table V. Bond Angles in Degrees for $Co_3(CO)_9CCH_3$[a]

Co(3)–Co(1)–Co(2)	60.3 (1.4)	C(2)–Co(1)–C(3)	97.1 (10)
Co(1)–Co(2)–Co(3)	59.8 (1.9)	C(5)–Co(2)–C(6)	97.5 (9)
Co(2)–Co(3)–Co(1)	59.9 (2.4)	C(8)–Co(3)–C(9)	97.1 (10)
Average	60.0	Average	97.2
Co(1)–C(10)–Co(2)	81.2 (6.9)		
Co(2)–C(10)–Co(3)	80.5 (7.2)	Co(1)–C(1)–O(1)	176.3 (16)
Co(3)–C(10)–Co(1)	81.7 (7.3)	Co(1)–C(2)–O(2)	175.5 (18)
Average	81.1	Co(1)–C(3)–O(3)	176.2 (21)
		Co(2)–C(4)–O(4)	176.5 (15)
C(10)–Co(1)–Co(2)	50.6 (5.7)	Co(2)–C(5)–O(5)	168.8 (19)
C(10)–Co(2)–Co(1)	48.2 (5.4)	Co(2)–C(6)–O(6)	177.2 (18)
C(10)–Co(2)–Co(3)	49.3 (5.6)	Co(3)–C(7)–O(7)	176.3 (22)
C(10)–Co(3)–Co(2)	50.2 (5.8)	Co(3)–C(8)–O(8)	170.8 (23)
C(10)–Co(3)–Co(1)	48.4 (5.4)	Co(3)–C(9)–O(9)	177.1 (24)
C(10)–Co(1)–Co(3)	49.9 (5.7)	Average	175.0
Average	49.4		
$H_3C(11)$–C(10)–Co(1)	133.2 (13)	Co(1)–Co(2)–C(5)	150.6 (7.0)
$H_3C(11)$–C(10)–Co(2)	129.8 (16)	Co(1)–Co(3)–C(9)	153.2 (8.1)
$H_3C(11)$–C(10)–Co(3)	130.9 (14)	Co(2)–Co(3)–C(8)	149.2 (6.6)
Average	131.3	Co(2)–Co(1)–C(3)	151.6 (8.6)
		Co(3)–Co(1)–C(2)	149.9 (5.4)
C(10)–Co(1)–C(2)	101.3 (08)	Co(3)–Co(2)–C(6)	151.1 (7.4)
C(10)–Co(1)–C(3)	101.9 (10)	Average	151.0
C(10)–Co(2)–C(5)	104.8 (09)		
C(10)–Co(2)–C(6)	102.1 (09)		
C(10)–Co(3)–C(8)	99.9 (09)	Co(1)–Co(2)–C(6)	99.7 (6.6)
C(10)–Co(3)–C(9)	106.2 (10)	Co(1)–Co(3)–C(8)	96.1 (7.0)
Average	102.7	Co(2)–Co(3)–C(9)	98.6 (8.3)
		Co(2)–Co(1)–C(2)	95.9 (5.8)
C(10)–Co(1)–C(1)	143.6 (8.2)	Co(3)–Co(1)–C(3)	97.9 (7.8)
C(10)–Co(2)–C(4)	141.6 (7.3)	Co(3)–Co(2)–C(5)	94.8 (7.3)
C(10)–Co(3)–C(7)	140.5 (8.9)	Average	97.2
Average	141.9		
C(1)–Co(1)–C(2)	103.1 (08)	Co(1)–Co(2)–C(4)	98.0 (5.4)
C(1)–Co(1)–C(3)	101.3 (10)	Co(1)–Co(3)–C(7)	97.8 (6.6)
C(4)–Co(2)–C(5)	101.8 (08)	Co(2)–Co(3)–C(7)	98.5 (8.2)
C(4)–Co(2)–C(6)	101.2 (09)	Co(2)–Co(1)–C(1)	100.2 (5.8)
C(7)–Co(3)–C(8)	104.2 (10)	Co(3)–Co(1)–C(1)	99.4 (5.8)
C(7)–Co(3)–C(9)	101.4 (10)	Co(3)–Co(2)–C(4)	101.6 (5.5)
Average	102.2	Average	99.2

[a] Standard deviations of the last significant figures are in parentheses.

direct the appropriate metal orbital more nearly toward the coordinating apical carbon atom. Other basal $M_3(CO)_9$ fragments stereochemically analogous to the $Co_3(CO)_9$ moiety have been found from X-ray studies of $Ir_4(CO)_{12}$[29] and $Co_3(CO)_9S$,[30] where the apical coordinating groups are $Ir(CO)_3$[31] and S, respectively.

The geometric conformation of the apical aliphatic carbon atom in the skeletal Co_3C framework is similar to that of the carbon atom in the triply bridging metal-coordinated carbonyl groups found in $(C_5H_5)_3Ni_3(CO)_2$,[15] $Rh_6(CO)_{16}$,[16] $[Fe_4(CO)_{13}]^{2-}$,[17] and $[C_5H_5FeCO]_4$.[18] The average Co–C–CH_3 angle of 131° resembles the average triply bridging M–C–O angle of 134° in $(C_5H_5)_3Ni_3(CO)_2$, 132° in $Rh_6(CO)_{16}$, 134° in $[Fe_4(CO)_{13}]^{2-}$, and 132° in $[C_5H_5FeCO]_4$. The average Co–C–Co angle of 81° parallels the corresponding average triply bridging M–CO–M angle of 77° in $(C_5H_5)_3Ni_3(CO)_2$, 79.5° in $Rh_6(CO)_{16}$, 77° in $[Fe_4(CO)_{13}]^{2-}$, and 80° in $[C_5H_5FeCO]_4$. The mode of localized interaction for a case in which the normal tetrahedral internuclear angle has decreased to the acute value observed for the triply bridging alkyl group in $Co_3(CO)_9CCH_3$ can be interpreted in terms of bent bonds (*vide infra*).

The basic tetrahedral valency for the apical carbon atom is reflected in the normal single-bond C–CH_3

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(29) G. R. Wilkes, Ph.D. Thesis, University of Wisconsin, 1965; G. R. Wilkes and L. F. Dahl, to be published.

(30) C. H. Wei and L. F. Dahl, Abstracts of the National Meeting of the American Crystallographic Association, Montana State College, Bozeman, Mont., July 26–31, 1964; submitted to *Inorg. Chem.*

(31) The idealized equivalence of the four $Ir(CO)_3$ groups in $Ir_4(CO)_{12}$ results in cubic T_d rather than trigonal C_{3v} symmetry.

Table VI. Nonbonding Intramolecular Carbon–Carbon Distances (A) Corresponding to Edges of a Closed Polyhedral Fragment in $Co_3(CO)_9CCH_3$[a]

C(1)···C(4)	3.04	C(1)···C(3)	2.79
C(4)···C(7)	3.11	C(1)···C(2)	2.81
C(7)···C(1)	3.00	C(4)···C(6)	2.79
Average	3.05	C(4)···C(5)	2.84
		C(7)···C(9)	2.76
		C(7)···C(8)	2.88
C(2)···C(3)	2.71	Average	2.81
C(5)···C(6)	2.70		
C(8)···C(9)	2.71		
Average	2.71	C(10)···C(3)	2.86
		C(10)···C(2)	2.83
		C(10)···C(6)	2.88
C(2)···C(6)	2.95	C(10)···C(5)	2.97
C(5)···C(9)	2.89	C(10)···C(9)	2.94
C(8)···C(3)	2.91	C(10)···C(8)	2.87
Average	2.92	Average	2.89

[a] Standard deviations for these distances are 0.03 A.

Table VII. Perpendicular Distances (A) of Atoms in $Co_3(CO)_9CCH_3$ from the Plane Containing the Three Cobalt Atoms[a]

$H_3C(11)$	2.79
C(10)	1.25
O(8)	1.16
O(6)	1.11
O(2)	1.04
O(3)	0.97
O(5)	0.92
O(9)	0.89
C(6)	0.65
C(8)	0.64
C(2)	0.60
C(3)	0.60
C(9)	0.51
C(5)	0.49
C(1)	−1.75
C(7)	−1.78
C(4)	−1.80
O(1)	−2.83
O(4)	−2.84
O(7)	−2.93

[a] Standard deviations of these distances are 0.03 A.

distance of 1.53 A. Although no terminal alkyl–cobalt distances are as yet known from which to assess the bond lengths of Co–C σ bonds,[32] the Co–C (triply bridging) σ-bond distance of 1.90 A (individual estimated standard deviation (esd), 0.02 A) in $Co_3(CO)_9CCH_3$ is shorter than the bridging Co–C(alkyl) σ-bond distance of 2.01 A in $Co_2(CO)_4(t\text{-}C_4H_9C_2H)_2(HC_2H)$[34] and the predicted distance of 2.00 A based on covalent radii (*viz.*, 0.77 A for an aliphatic carbon and one-half the observed Co–Co distance in this complex[35]).

A corresponding comparison of the average observed triply bridging M–CO distances with a calculated M–CO distance (based arbitrarily on an *aliphatic* radius for carbon and a metal radius equal to one-half the metal–metal distance[35]) does not show in general a similar shortening for $(C_5H_5)_3Ni_3(CO)_2$ (1.93 *vs.* 1.965 A (calcd)),[15] $Rh_6(CO)_{16}$ (2.17 *vs.* 2.16 A (calcd)),[16] $[Fe_4(CO)_{13}]^{2-}$ (2.00 *vs.* 2.02 A (calcd)),[17] and $[C_5H_5FeCO]_4$ (1.97 *vs.* 2.03 A (calcd)).[18] The comparative shortening of the Co–C(alkyl) bond length implies a greater stability for a Co_3C(alkyl) fragment than for an M_3CO fragment. This trend is not altogether surprising, since the carbon–oxygen bond in the triply bridging carbonyl group maintains some multiple bond character which necessitates either a fractional bond order (from a valence bond standpoint) for a localized triply bridging M–CO bond or a multicenter delocalized MO bonding description in which there is less "electron density" between the carbonyl carbon atom and the three metal atoms.

This symmetrical skeletal arrangement of the tricyclic Co_3C(alkyl) fragment presumably is responsible for most of the salient chemical and physical properties of the $Co_3(CO)_9CY$ class of compounds. Evidence for the high stability of such complexes is manifested in their facile synthesis by two very different types of reaction,[9] in their volatility which is unusually high for trinuclear transition metal derivatives,[36] and in their relative stability to air compared to that of other cobalt carbonyl complexes.[36]

The Co–Co bonding distances of 2.47 A may be compared with those in $Co_2(CO)_8$ (2.52 A),[37] $Co_2(CO)_6(C_6H_5C_2C_6H_5)$ (2.47 A),[38] $Co_2(CO)_6(C_4F_6C_2)$ (2.47 A),[39] triclinic form of $Co_2(CO)_9C_2H_2$ (2.46 A),[15,40] orthorhombic form of $Co_2(CO)_9C_2H_2$ (2.43 A),[15,40] $Co_2(CO)_4(t\text{-}C_4H_9C_2H)_2(C_2H_2)$ (2.45 A),[32] $Co_3(CO)_4(SC_2H_5)_5$ (2.49 and 2.55 A),[41] $SCo_3(CO)_9$ (2.64 A),[30] $Co_4(CO)_{12}$ (2.49 A),[42] $Co_4(CO)_{10}(C_2H_5C_2C_2H_5)$ (2.43 and 2.55 A),[43] $S_2Co_4(CO)_{10}$ (2.48 and 2.60 A),[41] $Co_5(CO)_{10}(SC_2H_5)_5$ (2.43 to 2.53 A),[41] $[SCo_3(CO)_7]_2S_2$ (2.51 A (av)),[44] $SCo_6(CO)_{11}(SC_2H_5)_4$ (2.45 to 2.53 A),[41] and cobalt metal (2.51 A).[45]

Possible differences in the bond lengths for the two nonequivalent types of carbonyl groups cannot be distinguished in this X-ray determination. For all nine terminal carbonyl groups, the average Co–C distances of 1.80 A (individual esd, 0.02 A) and 1.10 A (individual esd, 0.03 A) are normal distances for terminal carbonyl groups in cobalt carbonyl complexes.

Since the orientation of the six ligands about each cobalt atom in $Co_3(CO)_9CCH_3$ conforms to a distorted octahedron, the actual ligand arrangement may ad-

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(32) The wide range of reported Fe–C σ-bond lengths, which vary from 1.94 to 2.10 A in iron carbonyl complexes,[33] no doubt is a result of the different character of the orbitals involved in the bond, the effective charge on each nuclei, the iron coordination number, and steric and electronic factors prescribed by the other iron-coordinating ligands. These variations show that generalizations based on bond length differences are not necessarily reliable without a careful examination of the entire situation.

(33) *Cf.* L. F. Dahl, R. J. Doedens, W. Hübel, and J. Nielsen, *J. Am. Chem. Soc.*, 88, 446 (1966), and references contained therein.

(34) O. S. Mills and G. Robinson, *Proc. Chem. Soc.*, 187 (1964).

(35) The variation of Co–Co bonding distances (*vide infra*) found in cobalt carbonyl complexes makes it difficult to assign a fixed radius to the cobalt atom in such complexes. Accordingly, it was decided that the metal radius in these complexes containing single-bond metal–metal interactions is best approximated by one-half the metal–metal bond length.

(36) R. B. King, "Organometallic Syntheses," Vol. 1, Academic Press Inc., New York, N. Y., 1965, pp 153–155.

(37) G. G. Sumner, H. P. Klug, and L. E. Alexander, *Acta Cryst.*, 17, 732 (1964).

(38) W. G. Sly, *J. Am. Chem. Soc.*, 81, 18 (1959).

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(40) O. S. Mills and G. Robinson, *ibid.*, 156 (1959).

(41) C. H. Wei and L. F. Dahl, to be published.

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(43) L. F. Dahl and D. L. Smith, *J. Am. Chem. Soc.*, 84, 2450 (1962).

(44) D. L. Stevenson, V. R. Magnuson, and L. F. Dahl, to be published.

(45) *Cf.* "Tables of Interatomic Distances and Configuration in Molecules and Ions," Special Publication No. 11, The Chemical Society, London, 1958, p S4.

vantageously be described and correlated with those of related complexes through the formal use of a valence bond directed orbital model to indicate the degree of distortion from an octahedral configuration. The following discussion will employ a formal sequence of deformations which preserve the vertical mirror plane of the idealized C_{3v} molecular symmetry. To begin the description, the triply bridging carbon atom, the cobalt atom, and an axial carbonyl group are placed in vertical alignment in the mirror plane. Two equatorial carbon groups and the two remaining cobalt atoms are related in pairs by the mirror operation and are located in a horizontal plane which also contains the cobalt atom.

The formation of the equilateral metal-atom triangle requires that the Co–Co–Co angle decrease to 60°. There is a concomitant increase of the equatorial–equatorial OC–Co–CO angle to 97.2° (individual esd, 1.0°). This angular increase from 90° is found in general for equatorial $M(CO)_2$ groups which are symmetrically bonded in a triangular array to two other metal atoms. Other examples (with the M–M–M and OC–M–CO angles) include $Ru_3(CO)_{12}$ (60 and 103.3°),[46] $SCo_3(CO)_9$ (60 and 100.9°),[30] $HFe_3(CO)_{11}^-$ (57.2 and 102.3°),[47] and $C_6H_5C_2C_6H_5Fe_3(CO)_9$ (62.4 and 100.1°).[48] This opening of the equatorial OC–M–CO angle from 90° can be rationalized in terms of an adjustment of atomic orbital coefficients in order to achieve maximum overlap (more rigorously minimum molecular energy) for the metal–metal bonds. However, since the adjusted orbitals cannot attain the 60° M–M–M angle, the resulting metal–metal interactions are not axially symmetric. These so-called "bent" bonds have proved to be a useful concept in the discussion of the geometry of transition metal carbonyl complexes.

The remaining distortions in $Co_3(CO)_9CCH_3$ are associated with the bond between the triply bridging carbon atom and each cobalt atom. The geometric constraints are more severe in this case, since the placement of the aliphatic carbon atom above the center of the metal triangle on the principal molecular threefold axis requires that the C–Co–Co angles decrease to approximately 50° (see Table V). A readjustment of LCAO coefficients to maximize cobalt–carbon orbital overlap is evidenced by an increase of the axial–equatorial OC–Co–CO angles from 90 to 102° and by the rotation of the entire set of modified octahedral-like orbitals so as to direct the appropriate orbital more nearly toward the bridging atom. This motion completes the molecular deformations. The mean plane containing the two equatorial carbonyl groups attached to a given cobalt atom now makes an average angle of 29° with respect to the plane of the three cobalt atoms, while the axial carbonyl groups make an average angle of 101° with a line from their respective cobalt atom to the center of the metal triangle.

The isolation of a triply bridging *aliphatic* carbon atom in a transition metal complex outside of the $Co_3(CO)_9CY$ class of complexes may be difficult owing to the rather stringent geometric requirements needed for the formation of the M_3C fragment and to the requirement that the ligands and metal atoms involved allow the complex as a whole to achieve a stable electronic configuration. Of obvious interest is whether the corresponding metal complexes can be isolated for the congener elements rhodium and iridium.

Acknowledgments. We are most grateful to Drs. I. Wender and H. Sternberg for supplying us with a sample of this compound and for their interest in our work. We are greatly indebted to the National Science Foundation for their generous financial support. The extensive use of the CDC 1604 and 3600 computers at the University of Wisconsin Computing Center was largely due to the financial support of NSF and WARF provided through the University Research Committee.

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