is much smaller than that predicted for pure D_{4d} symmetry upon theoretical considerations. The inclusion of a significant amount of d_{z^2} character in the ground-state orbital would lead to the prediction of less anisotropy in the g tensor and, hence, a smaller Δg, as well as to the correct ordering of the g-tensor components. The fact that $g_{\parallel}$ does not equal 2.0023 as predicted from theory lends further support to the idea of intermediate D_2 symmetry as well as to the notion of extensive covalent bonding.

In the final analysis, a full calculation of the anisotropic g values including both orbital mixing and covalent bonding appears necessary but beyond the scope of the present study. On the basis of the structural results and the constant isotropic g value of $Mo(CN)_8^{3-}$ in a variety of samples, we conclude that the esr parameters for this system are not indicative of the molecular geometry as predicted from crystal field considerations.

Acknowledgments.—This work was supported by the National Science Foundation and the Advanced Research Projects Agency. We also wish to thank the Brown University Computer Center for its help and support. In the course of this research, we have had a number of helpful discussions with the following people whom we wish to acknowledge: Professor Gene B. Carpenter, Professor Philip Rieger, Mr. Cortlandt Pierpont, Professor S. J. Lippard, Professor T. V. Long, and Professor J. L. Hoard. B. J. C. thanks the National Science Foundation for a graduate traineeship.

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Structural Studies of Derivatives of Methinyltricobalt Enneacarbonyls. I. The Crystal Structure of $CH_3CCo_3(CO)_8P(C_6H_5)_3$

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Received July 25, 1969

The crystal and molecular structure of $CH_3CCo_3(CO)_8P(C_6H_5)_3$ has been determined by three-dimensional X-ray analysis. Crystals of the compound are monoclinic, space group C_{2h}^5-$P2_1/c$, with four molecules in a cell of dimensions $a = 12.19$ (2), $b = 16.11$ (2), $c = 17.19$ (4) Å; $\beta = 120.0$ (1)°. X-Ray data were collected by conventional film techniques using Co Kα radiation, the intensities of 2189 independent reflections being measured photometrically. The structure has been refined isotropically by modified full-matrix least-squares techniques to a conventional R factor of 0.099. The monomeric molecular structure closely resembles the parent compound $CH_3CCo_3(CO)_9$ being based on a Co_3 triangle. The $P(C_6H_5)_3$ unit has simply replaced one of the *equatorial* carbonyl groups, causing small distortions in the remainder of the molecule. Co–Co bond lengths are in the range 2.490–2.510 (6) Å.

Introduction

Substituted methinyltricobalt enneacarbonyls, $YCCo_3(CO)_9$ (where Y may be halogen, alkyl, aryl, CO_2H, CF_3, etc.) are of interest for a number of reasons. First, they are very readily synthesized and have high air stability.[2] Second, they possess the unique structural feature of a tetrahedral carbon atom triply bridging a triangle of bonded metal atoms.[3] Third, there is mass spectral evidence that the Co–C bridge bonds are unusually strong.[4] Following the initial structure determination of the parent compound ($Y = CH_3$) by Sutton and Dahl,[3] the structures of $Co_3(CO)_{10}BH_2N(C_2H_5)_3$[5] and $[CCo_3(CO)_9]_2CO$[6] have been reported. Both these compounds contain the basic $-CCo_3(CO)_9$ unit as in the parent compound, with only slight distortions. Recent studies by Robinson and coworkers[7,8] indicate that methinyltricobalt enneacarbonyls undergo a number of facile chemical reactions with the production of a variety of stable products including the carbonyl carbides $Co_5(CO)_{15}C_3H$, $Co_6(CO)_{18}C_4$, and $Co_8(CO)_{24}C_6$[9] and the complexes $YCCo_3(CO)_6$(arene). We have undertaken a systematic study of the structures of these products and report here the first detailed results.

It has been found[7] that alkyl- and arylphosphines and -arsines react reversibly with $YCCo_3(CO)_9$ (where $Y = Cl, Br, CH_3, C_6H_5$) to give a range of complexes $YCCo_3(CO)_8L$ and $YCCo_3(CO)_7L_2$ which are air stable, volatile, and soluble without decomposition in nonpolar solvents. The solution infrared spectrum[7] of $CH_3CCo_3(CO)_8P(C_6H_5)_3$ showed bands in the bridging carbonyl region. This suggested the possibility of a rearrangement of CO groups similar to that which oc-

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[1] To whom inquiries should be addressed.

[2] For a summary of references to general properties and methods of synthesis, see B. H. Robinson and W. S. Tham, *J. Chem. Soc., A*, 1784 (1968).

[3] P. W. Sutton and L. F. Dahl, *J. Am. Chem. Soc.*, **89**, 261 (1967).

[4] See the reference cited in footnote 2.

[5] F. Klanberg, W. B. Askew, and L. J. Guggenberger, *Inorg. Chem.*, **7**, 2265 (1968).

[6] G. Allegra and S. Valle, *Acta Cryst.*, **B25**, 107 (1969).

[7] B. H. Robinson and W. S. Tham, *J. Organometal. Chem.* (Amsterdam), **16**, 45 (1969).

[8] B. H. Robinson, J. Spencer, and R. Hodges, *Chem. Commun.*, 1480 (1968).

[9] R. J. Dellaca and B. R. Penfold, *Acta Cryst.*, **A25**, S170 (1969).

curs when some of the groups in $Ir_4(CO)_{12}$ are replaced by phosphines. In that case the resulting structures[10] contain three bridging CO groups as in $Co_4(CO)_{12}$.[11] Similar possibilities exist in the present compound although there are no bands in the bridging carbonyl region in the solid-state spectrum. One of the aims of this analysis was therefore to determine the effect of $P(C_6H_5)_3$ substitution on the molecular structure as a whole.

Experimental Section

Analyzed samples of $CH_3CCo_3(CO)_8P(C_6H_5)_3$ were kindly supplied by Dr. B. H. Robinson, having been prepared by reaction of $CH_3CCo_3(CO)_9$ with $P(C_6H_5)_3$ at 60° in hexane followed by repeated recrystallizations from light petroleum ether (bp 50–70°). The crystals were dark maroon, but because of the very small light transmission all the larger pieces appeared black.

Crystallographic Data.—For $Co_3PC_{28}O_8H_{18}$ of molecular weight 690.3 the crystals are monoclinic: $a = 12.19\ (2)$, $b = 16.11\ (2)$, $c = 17.19\ (4)$ Å; $\beta = 120.0\ (1)°$; $V = 2921.7$ Å^3; $Z = 4$, $d_{\text{calcd}} = 1.57$ g/cm^3; μ for Co Kα radiation is 44.7 cm^{-1}. The space group consistent with systematic absences of X-ray reflections (($0k0$) for k odd and ($h0l$) for l odd) is $P2_1/c$. The cell edges were obtained from measurements of the separation of reciprocal lattice rows on ($hk0$), ($0kl$), and ($h0l$) precession photographs taken with Polaroid film using Co Kα radiation (λ 1.7902 Å). The angle β was the difference in precession camera dial settings for ($hk0$) and ($0kl$) photographs. The error estimates are from our experience with this procedure. (Here and throughout this paper, the uncertainties given in parentheses are estimated standard deviations in the least significant digits quoted.) Because of the rapid solution of the crystals in all available flotation liquids, no accurate density measurement was made, but the approximate value obtained (1.5 g/cm^3) confirmed the number of molecules per cell as 4.

The two crystals used for data collection were both fragments of larger well-formed crystals and both were of irregular shape. They could be approximated to rectangular parallelepipeds, the larger fragment with dimensions 0.25 mm (parallel to b) × 0.3 mm (parallel to a) × 0.1 mm and the smaller fragment with dimensions 0.2 mm (parallel to a) × 0.1 × 0.07 mm.

X-Ray intensity data were recorded at room temperature (21 ± 2°) on a two-dimensionally integrating equiinclination Weissenberg camera using Fe-filtered Co Kα radiation. The plateaus of the integrated spots and adjacent background areas were measured using a single-beam photometer and a galvanometer calibrated to indicate intensities directly. A total of 2189 independent reflections were recorded and measured in the levels (hnl), with n = 0–9, using the larger crystal. Another 803 reflections were below the threshold of observation and were excluded from all refinement procedures. Subsequent structure factor calculations for these unobserved reflections showed that there was only one for which F_c was greater than 3 times the threshold value ($F_{\min}$), there were 15 for which $2F_{\min} < F_c < 3F_{\min}$, and there were 111 for which $F_{\min} < F_c < 2F_{\min}$. Data required for the approximate correlation of the 10 reciprocal lattice levels were obtained using the smaller crystal to record the ($0kl$) and ($1kl$) levels under conditions similar to those of the main data set. At an appropriate point in the refinement, corrections were made for crystal absorption using the Gaussian quadrature method. For the larger crystal, transmission factors ranged from 0.36 to 0.55, and following the corrections there was a drop of 1.1% in the conventional R factor. The effect on the data obtained from the smaller crystal was barely detectable.

All calculations were carried out on an IBM 360/44 computer with 16K words of core storage and twin 2315 disk drives. Programs used to produce atomic parameters and all derived quantities were local modifications of DP3 (data processing) by J. A. Ibers, WABS (Weissenberg absorption corrections, for any crystal whose shape can be described by the intersections of planes) by C. W. Burnham and J. A. Ibers, FORDAP (Fourier summations) by A. Zalkin, and ORFLS (full-matrix least-squares refinement) and ORFFE (interatomic distances and bond angles with estimated standard deviations) both by W. R. Busing, K. O. Martin, and H. A. Levy.

Determination and Refinement of Structure

The three-dimensional Patterson function immediately revealed the positions of the three Co atoms in the asymmetric unit. All remaining atom positions were obtained through systematic application of standard difference Fourier procedures aided by calculations of interatomic distances and angles at each stage. Least-squares refinement of parameters was then achieved by means of a modified full-matrix procedure. With all atoms treated isotropically, there were 172 parameters (including 12 scale factors) to refine, and this number well exceeded the dimensions of the program permitted by the available core storage in our computer. Parameters were therefore refined in three blocks, each of which contained the scale factors, 51 positional parameters, and 18 isotropic thermal parameters. For each of 17 atoms refined in each block, all 4 parameters—x, y, z, B—were varied and all parameters for Co and P atoms were varied in each block. In four complete cycles, R_1 and R_2 were reduced to 0.099 and 0.142, respectively.[12] Finally, scale factors and positional parameters only were varied in two blocks but R factors were not reduced further. Maximum parameter shifts as fractions of their esd's in the final cycle in which each was varied were 0.03 for scale factors, 0.10 for positional parameters, and 0.83 for thermal parameters.

In a final electron density difference map the height of the largest residual peak was 1.1 e$^-$/Å^3 which is just half of the density at which the last carbon atom was detected from earlier maps. Hydrogen atoms were not located. An anisotropic model for some of the atoms would no doubt have led to a reduction of the R factors but no pronounced anisotropic motion was indicated by the difference maps and for practical reasons of limited computer storage, quite apart from the questionable validity of such a procedure when more than one scale factor was involved, anisotropic refinement of this structure was out of the question.

The least-squares refinement minimized $\Sigma w(|F_o| - k|F_c|)^2$, where k is the scale factor associated with each Weissenberg layer. The weight w was derived from the formula suggested by Cruickshank[13]

$$w = (a + |F_o| + b|F_o|^2)^{-1}$$

values of $a = 25$ and $b = 0.0085$ leading to approximate constancy of the mean value of the minimized function over the complete range of F_c. The usual atomic scattering factors[14] were used, those for Co only being corrected for anomalous dispersion using the interpolated

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[10] V. Albano, P. Bellon, and V. Scatturin, *Chem. Commun.*, 730 (1967).

[11] C. H. Wei and L. F. Dahl, *J. Am. Chem. Soc.*, **88**, 1821 (1966).

[12] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $R_2 = [\Sigma w(|F_o| - |F_c|)^2/\Sigma w|F_o|^2]^{1/2}$.

[13] D. W. J. Cruickshank in "Computing Methods in Crystallography," J. S. Rollett, Ed., Pergamon Press, Oxford, 1965, p 114.

[14] "International Tables for X-Ray Crystallography," Vol. 3, The Kynoch Press, Birmingham, England, 1962.

Table I

Positional and Thermal Parameters for $CH_3CCo_3(CO)_8P(C_6H_5)_3$

Atom	x	y	z	B, Å^2
Co(1)	−0.1151 (2)	0.2553 (1)	0.1859 (1)	2.87 (5)
Co(2)	−0.0291 (2)	0.1171 (2)	0.2580 (1)	3.54 (6)
Co(3)	0.0751 (2)	0.2474 (2)	0.3392 (1)	3.87 (6)
P	−0.3056 (3)	0.2300 (3)	0.0642 (2)	2.53 (7)
C(1)	−0.033 (1)	0.274 (1)	0.125 (1)	3.9 (3)
C(2)	0.075 (2)	0.098 (1)	0.214 (1)	5.3 (4)
C(3)	0.192 (2)	0.267 (1)	0.309 (1)	4.9 (4)
C(4)	−0.159 (1)	0.354 (1)	0.199 (1)	4.2 (3)
C(5)	−0.163 (2)	0.057 (1)	0.191 (1)	4.6 (3)
C(6)	0.025 (2)	0.052 (1)	0.351 (1)	5.6 (4)
C(7)	0.160 (2)	0.199 (1)	0.441 (1)	5.5 (4)
C(8)	0.062 (2)	0.344 (1)	0.381 (1)	6.0 (4)
C(9)	−0.096 (1)	0.206 (1)	0.293 (1)	3.1 (3)
C(10)	−0.169 (1)	0.206 (1)	0.341 (1)	4.4 (3)
C(11)	−0.311 (1)	0.164 (1)	−0.024 (1)	2.8 (3)
C(12)	−0.419 (1)	0.163 (1)	−0.110 (1)	4.0 (3)
C(13)	−0.422 (1)	0.110 (1)	−0.178 (1)	4.6 (3)
C(14)	−0.323 (1)	0.065 (1)	−0.162 (1)	4.5 (3)
C(15)	−0.209 (1)	0.066 (1)	−0.076 (1)	3.5 (3)
C(16)	−0.207 (1)	0.115 (1)	−0.008 (1)	3.3 (3)
C(21)	−0.379 (1)	0.325 (1)	−0.002 (1)	3.4 (3)
C(22)	−0.506 (2)	0.346 (1)	−0.031 (1)	5.6 (4)
C(23)	−0.561 (2)	0.418 (1)	−0.083 (1)	6.2 (4)
C(24)	−0.488 (2)	0.467 (1)	−0.105 (1)	7.1 (4)
C(25)	−0.364 (2)	0.448 (1)	−0.079 (1)	6.1 (4)
C(26)	−0.307 (2)	0.378 (1)	−0.025 (1)	5.1 (4)
C(31)	−0.426 (1)	0.190 (1)	0.086 (1)	3.2 (3)
C(32)	−0.448 (1)	0.234 (1)	0.149 (1)	3.6 (3)
C(33)	−0.542 (2)	0.206 (1)	0.165 (1)	4.8 (3)
C(34)	−0.620 (2)	0.140 (1)	0.118 (1)	5.1 (4)
C(35)	−0.601 (2)	0.095 (1)	0.056 (1)	4.8 (3)
C(36)	−0.503 (1)	0.121 (1)	0.040 (1)	3.9 (3)
O(1)	0.024 (1)	0.282 (1)	0.089 (1)	5.8 (3)
O(2)	0.139 (1)	0.089 (1)	0.183 (1)	6.2 (3)
O(3)	0.269 (1)	0.279 (1)	0.288 (1)	8.2 (4)
O(4)	−0.196 (1)	0.417 (1)	0.206 (1)	5.7 (3)
O(5)	−0.252 (1)	0.014 (1)	0.153 (1)	7.0 (3)
O(6)	0.054 (2)	0.007 (1)	0.412 (1)	8.8 (4)
O(7)	0.220 (1)	0.166 (1)	0.514 (1)	7.5 (3)
O(8)	0.058 (1)	0.407 (1)	0.412 (1)	8.5 (4)

values for $\Delta f'$ and $\Delta f''$ quoted by Cotton and Eiss.[15] Final positional and thermal parameters, with esd's, are listed in Table I and observed and calculated structure factors are compared in Table II.

Description and Discussion of Structure

The crystal structure consists of well-separated monomeric molecules of $CH_3CCo_3(CO)_8P(C_6H_5)_3$, no intermolecular contact being unusually short. To a first approximation the structure is derived from that of $CH_3CCo_3(CO)_9$ simply by replacing one *equatorial* CO group by $P(C_6H_5)_3$, a Co–P bond being formed at the expense of a Co–(CO) bond but with no accompanying molecular rearrangement. In Figures 1 and 2 are two views of the molecule, the first normal to the Co_3 triangle and the second parallel to it. (Parentheses have been omitted from atom labels to simplify the diagrams but the numbering scheme is the same as in Table I.) They show particularly the configuration of the $P(C_6H_5)_3$ ligand with respect to the rest of the molecule. None of the phenyl rings shows significant departures from planarity. Bond distances are listed

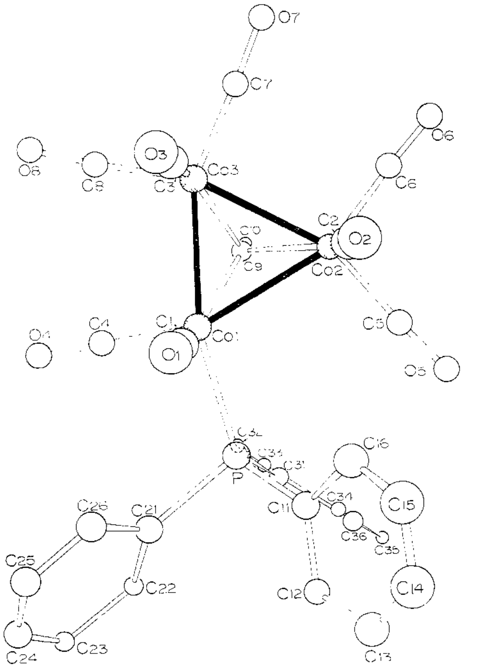

Figure 1.—The molecule viewed normal to the plane of the Co_3 triangle.

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[15] F. A. Cotton and R. Eiss, *J. Am. Chem. Soc.*, **90**, 38 (1968).

TABLE II

OBSERVED AND CALCULATED STRUCTURE FACTORS IN ELECTRONS (COLUMN HEADINGS ARE h, l, $|F_o|$, $|F_o|$)

**** K = 0 ****			
1	0	194	238
2	0	135	155
4	0	12	6
5	0	45	36
6	0	24	19
0	2	41	100
1	2	158	167
2	2	44	99
3	2	96	106
4	2	122	129
5	2	72	63
6	2	12	5
7	2	16	20
8	2	31	28
9	2	35	31
-1	2	256	422
-2	2	306	311
-3	2	41	39
-4	2	74	72
-5	2	76	75
-6	2	71	66
-7	2	23	21
0	4	57	52
1	4	35	34
2	4	164	173
3	4	12	8
4	4	50	50
5	4	37	32
7	4	38	51
10	4	24	14
-1	4	122	125
-2	4	23	16
-4	4	45	40
-5	4	22	16
-6	4	129	119
-7	4	78	68
0	6	73	67
1	6	57	57
2	6	59	49
3	6	121	124
4	6	108	104
5	6	100	101
6	6	72	68
-1	6	39	28
-2	6	116	111
-3	6	112	106
-4	6	38	26
-7	6	28	24
-9	6	33	33
0	8	89	86
1	8	30	21
2	8	107	99
3	8	113	112
4	8	110	101
6	8	23	23
7	8	23	23
-1	8	15	14
-2	8	19	14
-3	8	22	30
-4	8	64	56
-5	8	55	53
-6	8	34	32
-7	8	16	8
-8	8	29	30
-9	8	47	44
-10	8	31	21
1	10	76	62
2	10	69	59
3	10	81	78
4	10	71	72
-1	10	65	58
-3	10	26	21
-4	10	14	6
-5	10	37	37
-6	10	59	51
-7	10	12	8
-8	10	31	26
-9	10	17	12
-10	10	32	33
0	12	67	61
1	12	22	22
4	12	43	9
-1	12	58	57
-2	12	23	21
-4	12	27	25
-5	12	52	44
-6	12	40	39
-7	12	27	19
-8	12	24	25
-9	12	24	28
-10	12	35	33
-11	12	27	22
-12	12	45	46
-1	14	14	10
-2	14	36	32
-3	14	14	14
-4	14	13	11
-5	14	22	21
-6	14	19	20
-7	14	40	34
-8	14	15	13
-9	14	16	16
-10	14	49	46
-12	14	20	12
**** K = 1 ****			
1	0	125	113
2	0	53	61
3	0	6	8
4	0	16	10
5	0	83	75
6	0	74	72
7	0	15	17
8	0	31	30
9	0	10	5
10	0	73	64
11	0	43	45
0	1	32	28
1	1	44	45
2	1	27	33
3	1	33	32
4	1	40	40
5	1	42	41
7	1	16	19
8	1	10	11
9	1	24	25
10	1	20	12
-1	1	27	18
-2	1	65	65
-3	1	18	15
-4	1	72	72
-5	1	47	40
-6	1	56	47
-7	1	14	15
-8	1	38	34
-9	1	31	25
-11	1	15	15
1	2	76	74
2	2	106	117
3	2	62	63
4	2	53	48
5	2	11	11
6	2	50	45
7	2	55	45
8	2	49	43
9	2	72	68
10	2	33	32
-1	2	47	45
-2	2	127	154
-3	2	92	102
-4	2	32	38
-5	2	5	2
-6	2	30	28
-7	2	89	83
-8	2	38	33
-9	2	11	14
-10	2	22	20
-11	2	35	29
0	3	60	60
1	3	36	34
2	3	37	32
3	3	34	33
4	3	16	15
5	3	21	17
7	3	21	25
8	3	21	21
9	3	10	11
-1	3	53	49
-2	3	46	44
-3	3	31	34
-4	3	30	38
-5	3	65	68
-6	3	68	67
-7	3	11	14
-8	3	30	29
-9	3	28	22
-10	3	34	36
-11	3	19	16
0	4	23	23
1	4	27	34
2	4	48	44
3	4	37	40
4	4	25	17
5	4	22	17
6	4	53	45
7	4	41	31
8	4	46	45
9	4	20	25
-1	4	28	25
-2	4	58	62
-4	4	195	218
-5	4	46	50
-6	4	42	37
-8	4	69	63
-9	4	50	41
-10	4	12	7
-11	4	15	11
-12	4	15	18
0	5	14	8
1	5	18	15
2	5	10	8
3	5	30	24
4	5	38	36
6	5	21	18
7	5	24	23
8	5	15	15
-1	5	22	17
-2	5	47	37
-3	5	69	76
-4	5	77	79
-5	5	53	50
-7	5	36	33
-8	5	31	30
-9	5	24	26
-10	5	40	40
-11	5	15	16
0	6	42	37
0	6	42	37
1	6	33	31
3	6	20	22
5	6	20	16
6	6	17	17
7	6	29	33
-1	6	41	44
-2	6	7	4
-3	6	67	57
-4	6	139	144
-5	6	136	154
-6	6	59	74
-7	6	55	55
-10	6	41	35
-12	6	19	15
0	7	27	25
1	7	12	11
2	7	15	17
3	7	26	25
4	7	12	10
5	7	10	9
-1	7	22	19
-2	7	15	14
-3	7	55	60
-4	7	42	40
-5	7	33	32
-6	7	30	30
-7	7	41	41
-8	7	28	24
-9	7	36	33
-10	7	17	13
-11	7	18	21
0	8	42	38
2	8	13	14
3	8	14	16
4	8	31	28
5	8	15	19
6	8	40	42
-1	8	97	91
-2	8	31	30
-3	8	17	16
-4	8	15	18
-5	8	88	95
-6	8	93	99
-7	8	92	94
-8	8	90	90
-9	8	63	59
-10	8	33	30
-11	8	23	21
-12	8	17	16
0	9	45	42
1	9	23	23
2	9	18	17
5	9	15	13
-1	9	21	18
-2	9	42	35
-3	9	10	6
-4	9	18	20
-5	9	41	44
-6	9	41	41
-7	9	31	25
-8	9	27	29
-9	9	25	15
-10	9	26	25
0	10	49	48
1	10	14	14
2	10	36	29
3	10	52	49
4	10	11	14
5	10	29	31
-1	10	23	17
-2	10	58	60
-3	10	59	57
-4	10	13	8
-5	10	30	28
-6	10	49	51
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-8	10	80	77
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1	3	43	39
2	3	21	17
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7	3	14	15
-1	3	6	10
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-5	3	27	26
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6	4	17	11
7	4	23	24
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-4	4	69	76
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-7	4	30	25
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0	5	22	16
1	5	22	17
2	5	24	18
4	5	55	58
5	5	46	46
6	5	16	11
7	5	7	11
-1	5	34	33
-2	5	8	9
-3	5	45	39
-4	5	42	36
-5	5	21	22
-6	5	23	19
-7	5	62	54
-8	5	30	26
-9	5	13	8
-10	5	34	26
0	6	18	23
1	6	25	27
6	6	16	17
-1	6	26	24
-2	6	16	11
-3	6	40	37
-4	6	71	77
-5	6	81	84
-6	6	58	58
-7	6	30	28
-9	6	36	32
1	7	12	17
3	7	43	48
4	7	17	13
5	7	16	12
6	7	14	18
-1	7	27	27
-2	7	52	60
-3	7	14	18
-5	7	70	74
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0	10	16	17
1	10	15	13
2	10	16	19
3	10	16	12
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-7	15	14	18
-8	15	12	12
-5	16	5	6
-6	16	17	20
-7	16	10	11
**** K =10 ****			
0	0	56	52
1	0	25	26
0	1	63	46
-1	1	20	18
-1	2	62	65
1	3	59	61
-1	3	44	36
0	4	48	48
1	4	98	99
-1	4	26	26
0	5	56	48
1	5	49	47
0	6	80	74
1	6	91	92
-1	6	50	49
1	7	35	26
-1	7	46	40
0	8	32	33
1	8	27	24
-1	8	54	59
0	9	31	40
**** K =11 ****			
0	3	32	35
0	4	32	37
-1	5	28	46
0	6	65	50
-1	6	48	37
-1	8	56	59
**** K =12 ****			
0	0	50	44
1	0	28	22
0	1	41	43
1	1	51	55
1	2	28	27
0	3	32	31
0	4	32	37
1	4	76	74
0	6	60	60
1	7	40	17
0	8	29	38
-1	8	44	49
**** K =13 ****			
1	1	28	24
0	6	30	31
**** K =14 ****			
0	0	44	46
0	1	31	35
0	2	31	27
0	3	30	29
**** K =16 ****			
0	0	25	31
0	2	25	27
0	6	18	18

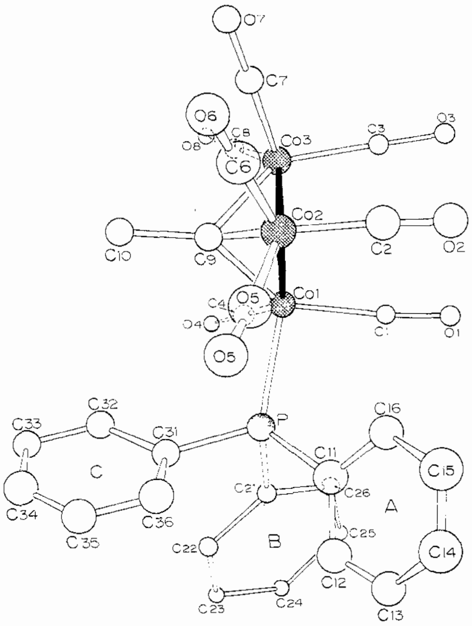

Figure 2.—The molecule viewed parallel to the plane of the Co_3 triangle.

TABLE III

BOND DISTANCES (Å)[a]

Co(1)–Co(2)	2.510 (6)	P–C(11)	1.83 (1)
Co(1)–Co(3)	2.495 (5)	P–C(21)	1.84 (2)
Co(2)–Co(3)	2.490 (6)	P–C(31)	1.80 (1)
			1.82 (2)
Co(1)–P	2.253		
		C(11)–C(12)	1.41 (2)
Co(1)–C(1)	1.79 (1)	C(12)–C(13)	1.42 (2)
Co(2)–C(2)	1.80 (2)	C(13)–C(14)	1.32 (2)
Co(3)–C(3)	1.78 (2)	C(14)–C(15)	1.43 (2)
Co–C(ax.)	*1.79 (1)*	C(15)–C(16)	1.40 (2)
		C(16)–C(11)	1.40 (2)
Co(1)–C(4)	1.72 (2)		*1.40 (4)*
Co(2)–C(5)	1.75 (2)		
Co(2)–C(6)	1.74 (2)	C(21)–C(22)	1.41 (2)
Co(3)–C(7)	1.72 (2)	C(22)–C(23)	1.42 (3)
Co(3)–C(8)	1.75 (2)	C(23)–C(24)	1.38 (3)
Co–C(eq.)	*1.74 (1)*	C(24)–C(25)	1.38 (3)
		C(25)–C(26)	1.40 (2)
Co(1)–C(9)	1.90 (1)	C(26)–C(21)	1.42 (2)
Co(2)–C(9)	1.89 (2)		*1.40 (2)*
Co(3)–C(9)	1.93 (1)		
	1.91 (2)	C(31)–C(32)	1.43 (2)
		C(32)–C(33)	1.39 (2)
C(9)–C(10)	1.50 (2)	C(33)–C(34)	1.39 (2)
		C(34)–C(35)	1.38 (2)
		C(35)–C(36)	1.42 (2)
C(1)–O(1)	1.15 (2)	C(36)–C(31)	1.41 (2)
C(2)–O(2)	1.16 (2)		*1.40 (2)*
C(3)–O(3)	1.18 (2)		
C(4)–O(4)	1.15 (2)		
C(5)–O(5)	1.17 (2)		
C(6)–O(6)	1.17 (2)		
C(7)–O(7)	1.21 (2)		
C(8)–O(8)	1.16 (2)		
	1.17 (2)		

[a] Mean values of bonds assumed chemically equivalent are italicized and their associated uncertainties are rms deviations given by the expression $(\Sigma^n(x_i - \bar{x})^2/n)^{1/2}$, where there are n observations. The estimated standard deviations of individual bonds were calculated using variances and covariances in positional parameters and variances only in cell parameters. They may be underestimates because of the neglect of anisotropic thermal motion.

TABLE IV

SELECTED NONBONDED INTRAMOLECULAR DISTANCES (Å)

C(5)···C(6)	2.56	C(1)···C(2)	3.17
C(7)···C(8)	2.60	C(2)···C(3)	3.14
C(1)···C(4)	2.75	C(3)···C(1)	3.00
C(2)···C(5)	2.80	C(4)···C(8)	2.94
C(2)···C(6)	2.81	C(6)···C(7)	2.85
C(3)···C(7)	2.72		
C(3)···C(8)	2.73	C(1)···C(16)	3.37
		C(4)···C(21)	3.17
		C(5)···C(16)	3.32
		C(10)···C(32)	3.39

in Table III, selected intramolecular nonbonded contacts in Table IV, and bond angles in Table V.

The most interesting feature of the structure is that the $P(C_6H_5)_3$ substitution has occurred preferentially in an equatorial orientation relative to the Co_3 triangle rather than in one of the alternative axial orientations. This is almost certainly a steric preference, for the bulky phosphine group has only one close carbonyl neighbor

TABLE V

BOND ANGLES (DEG)[a]

Co(1)–Co(2)–Co(3)	59.9 (1)	Co(1)–Co(2)–C(6)	149.3 (6)
Co(2)–Co(3)–Co(1)	60.5 (1)	Co(1)–Co(3)–C(7)	150.4 (6)
Co(3)–Co(1)–Co(2)	59.7 (1)	Co(2)–Co(3)–C(8)	148.7 (5)
	59.9 (4)	Co(2)–Co(1)–C(4)	146.3 (6)
		Co(3)–Co(2)–C(5)	152.2 (2)
Co(1)–C(9)–Co(2)	83.1 (5)	Co(3)–Co(1)–P	162.4 (6)
Co(2)–C(9)–Co(3)	81.3 (5)		
Co(3)–C(9)–Co(1)	81.3 (5)	Co(1)–Co(2)–C(5)	98.2 (6)
	82 (1)	Co(1)–Co(3)–C(8)	99.2 (6)
		Co(2)–Co(1)–P	106.3 (2)
C(9)–Co(1)–Co(2)	48.3 (4)	Co(2)–Co(3)–C(7)	93.8 (6)
C(9)–Co(2)–Co(1)	48.7 (4)	Co(3)–Co(1)–C(4)	95.4 (5)
C(9)–Co(2)–Co(3)	50.3 (4)	Co(3)–Co(2)–C(6)	98.0 (6)
C(9)–Co(3)–Co(1)	48.8 (4)		
C(9)–Co(3)–Co(2)	48.5 (4)	Co(1)–Co(2)–C(2)	98.8 (6)
C(9)–Co(1)–Co(3)	50.0 (4)	Co(1)–Co(3)–C(3)	98.1 (5)
	49 (1)	Co(2)–Co(1)–C(1)	102.5 (6)
		Co(2)–Co(3)–C(3)	104.3 (6)
C(10)–C(9)–Co(1)	136 (1)	Co(3)–Co(1)–C(1)	97.5 (5)
C(10)–C(9)–Co(2)	130 (1)	Co(3)–Co(2)–C(2)	96.6 (6)
C(10)–C(9)–Co(3)	126 (1)		
		Co(1)–C(1)–O(1)	176 (1)
C(9)–Co(1)–P	113 (4)	Co(2)–C(2)–O(2)	176 (2)
		Co(3)–C(3)–O(3)	179 (2)
C(9)–Co(1)–C(4)	98.7 (7)	Co(1)–C(4)–O(4)	176 (2)
C(9)–Co(2)–C(5)	103.1 (7)	Co(2)–C(5)–O(5)	174 (1)
C(9)–Co(2)–C(7)	101.2 (7)	Co(2)–C(6)–O(6)	176 (2)
C(9)–Co(3)–C(7)	103.9 (7)	Co(3)–C(7)–O(7)	179 (2)
C(9)–Co(3)–C(8)	100.2 (7)	Co(3)–C(8)–O(8)	177 (2)
			178 (1)
C(9)–Co(1)–C(1)	142.5 (6)		
C(9)–Co(2)–C(2)	140.2 (8)	Co(1)–P–C(11)	118.0 (4)
C(9)–Co(3)–C(3)	142.7 (6)	Co(1)–P–C(21)	112.3 (5)
		Co(1)–P–C(31)	116.1 (4)
C(1)–Co(1)–P	96.0 (5)		
C(1)–Co(1)–C(4)	103.2 (7)	C(11)–P–C(21)	99.8 (6)
C(2)–Co(2)–C(5)	104.1 (7)	C(21)–P–C(31)	103.3 (6)
C(2)–Co(2)–C(6)	105.1 (8)	C(31)–P–C(11)	105.2 (6)
C(3)–Co(3)–C(7)	102.7 (8)		
C(3)–Co(3)–C(8)	101.9 (9)		
P–Co(1)–C(4)	92.5 (5)		
C(5)–Co(2)–C(16)	94.4 (8)		
C(7)–Co(3)–C(8)	97.0 (9)		

[a] See footnote to Table III.

from a neighboring Co atom whereas in an axial orientation it would have two. Relative to the Co–(CO) equatorial bonds, the Co–P bond is significantly bent closer to the Co_3 plane as illustrated, *e.g.*, by the reduction of the angle C(1)–Co(1)–P to 96° and the accompanying increase of the angle Co(3)–Co(1)–P to 162°. As a result a nice balance has been achieved in the nonbonded contacts between the phosphine group and external atoms, the four closest contacts involving four sterically distinct carbon atoms and all being in the range 3.17–3.39 Å. Thus C(4)···C(21) involves the equatorial carbon bonded to the same Co atom, C(5)···C(16) an equatorial carbon bonded to an adjacent Co atom, C(1)···C(16) the axial carbon bonded to the same Co atom, and C(10)···C(32) the terminal methyl group.

The terminal methyl group has been bent significantly away from the phosphine group as can be seen from the angles of the type C(10)–C(9)–Co. Otherwise the molecule (apart from the phosphine group) conforms to its idealized symmetry of C_{3v} as also observed in $CH_3CCo_3(CO)_9$[3] and $Co_3(CO)_{10}BH_2N(C_2H_5)_3$.[5] Likewise the molecular dimensions are in general agreement with those reported for these two compounds and for $[CCo_3(CO)_9]_2CO$.[6] However two particular features are to be noted. The Co–Co bonds in both the phosphine and borane derivatives are 0.03 Å longer than in the other two compounds. Also the Co–C(axial) bonds are systematically longer than the Co–C(equatorial) bonds in the phosphine and borane derivatives but not in the other two compounds. A better assessment of these differences can be made when similar bonds are compared in the related compounds whose detailed structures we have determined.

This structure determination supports the infrared spectral evidence[7] that there exists in solution a different isomer from that found in the solid state. On the other hand, these same spectral studies suggest a different solid-state structure (containing bridging carbonyls) for the $P(C_6H_{11})_3$ derivative, a structure analysis of which is in progress.

Acknowledgment.—The close cooperation of Dr. B. H. Robinson at all stages of this study is gratefully acknowledged. The work was supported by grants for equipment from the Research Committee of the New Zealand Universities Grants Committee.

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The Crystal Structure of the Tetramethylammonium Salt of the Octahydrotriborotetracarbonylchromium Anion, $(CO)_4CrB_3H_8^-$

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Received June 23, 1969

The crystal structure of tetramethylammonium octahydrotriborotetracarbonylchromium, $[(CH_3)_4N][(CO)_4CrB_3H_8]$, has been determined from three-dimensional X-ray counter data. The crystal structure consists of the packing of discrete $(CH_3)_4N^+$ cations and $(CO)_4CrB_3H_8^-$ anions. The $(CO)_4CrB_3H_8^-$ ion has an octahedrally hybridized chromium atom coordinated to two axial carbonyl groups, two equatorial carbonyl groups, and a B_3H_8 moiety bonded through two boron–hydrogen–chromium bonds with Cr–H distances of 1.78 Å. The equatorial and average axial Cr–C distances are 1.824 (7) and 1.900 (10) Å, respectively. Molecular orbital calculations indicate that the difference in equatorial and axial Cr–CO distances results from increased π bonding between the chromium atom and the equatorial carbonyl groups. Crystals of $[(CH_3)_4N][(CO)_4CrB_3H_8]$ are monoclinic, space group $P2_1/m$, with two formula units per cell of dimensions $a = 11.074 \pm 0.004$ Å, $b = 8.938 \pm 0.002$ Å, $c = 7.784 \pm 0.003$ Å, and $\beta = 98.12 \pm 0.04°$. The individual ions have space-group-imposed C_s point symmetry. The structure was refined by least squares to a conventional R of 0.077.

Introduction

The metal atom in metalloborane chemistry has a variety of different and sometimes novel roles. It can occupy a coordination site on the surface of a polyhedral boron fragment[1,2] linking two boron polyhedra in some cases, it may be the nucleus of a cation in forming complexes with borane anions,[3] or it may be coordinated to basic boron hydride fragments *via* metal–boron[4] or metal–hydrogen–boron bonds. The crystal and molecular structures of $[(CH_3)_4N][(CO)_4CrB_3H_8]$ reported here exemplify the latter case wherein a $B_3H_8^-$ moiety is bonded to a chromium atom *via* Cr–H–B bonds. A preliminary account of this work was reported earlier.[5]

Another case of metal–hydrogen–boron bonding occurs with the borohydride ion, BH_4^-, which bonds to metal atoms through double hydrogen bridges in cases such as $(H_3C)_3N \cdot Al(BH_4)_3$[6] and $[(C_6H_5)_3P]_2CuBH_4$[7] and apparently through triple hydrogen bridges in

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