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The Bonding of Molecular Nitrogen. I. The Crystal and Molecular Structure of Hydridodinitrogentris(triphenylphosphine)cobalt(I)

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The crystal and molecular structure of a molecular nitrogen complex of cobalt, hydridodinitrogentris(triphenylphosphine)cobalt(I), $CoH(N_2)(P(C_6H_5)_3)_3$, has been determined from three-dimensional X-ray data collected by counter methods. There are two independent, but chemically equivalent, molecules in the asymmetric unit, and the coordination around each cobalt atom is trigonal bipyramidal, with the three phosphorus atoms in the equatorial plane. The Co–N–N entity is linear with N–N bond lengths of 1.101 (12) and 1.123 (13) Å and Co–N–N angles of 178 (2) and 178 (1)°, respectively. The nitrogen molecule is very similar to the isoelectronic molecule carbon monoxide in its mode of bonding, with multiple bonding between the metal and the nitrogen atom, as shown by the Co–N bond lengths of 1.784 (13) and 1.829 (12) Å. The hydride hydrogen atom was detected from difference Fourier syntheses at Co–H distances of 1.6 (1) Å. The Co–P distances vary from 2.167 (4) to 2.208 (4) Å. Crystal data: $a = 37.159$ (14) Å, $b = 11.355$ (5) Å, $c = 21.779$ (8) Å, $\beta = 101.3$ (2)°, space group C_{2h}^5-$P2_1/c$, $Z = 8$, and $D_{calcd} = 1.284$ g/cm^3. The structure was refined by least-squares techniques, using 3312 independent reflections for which $F^2 > 3\sigma(F^2)$, and the refinement converged to a conventional R factor (on F) of 6.1%.

Introduction

There has been much interest in molecular nitrogen complexes since Allen and Senoff[1] reported the first preparation of a transition metal complex which contained molecular nitrogen as a ligand. This discovery stimulated structural investigations[2,3] of the salts of $Ru(NH_3)_5(N_2)^{2+}$, but in all reported cases the cation has occupied a site of octahedral symmetry with consequent disorder of the dinitrogen and the ammine groups. Hence, no accurate structural information has been obtained. In 1967, the preparation of a molecular nitrogen complex of cobalt, formulated as $Co(N_2)(P(C_6H_5)_3)_3$, was described by Yamamoto, *et al.*[4] Because it seemed unlikely that there would be disorder in this system, an X-ray study was undertaken. A limited set of visually estimated X-ray intensities was obtained from a crystal grown in diethyl ether as an etherate. This study showed that the bonding of the molecular nitrogen ligand was end-on[5] and that the compound prepared was the hydride $CoH(N_2)(P(C_6H_5)_3)_3 \cdot (C_2H_5)_2O$. A more complete data set could not be obtained at that time owing to crystal decomposition. Further attempts to grow suitable crystals of the same material for the collection of counter data were unsuccessful. In order to obtain suitable crystals, numerous attempts were made using other solvents. We report here the crystal and molecular structure of hydridodinitrogentris(triphenylphosphine)cobalt(I), as grown from di-*n*-butyl ether. A preliminary account of this work has appeared.[6]

Experimental Section

A crystal suitable for X-ray analysis was grown from a di-*n*-butyl ether solution by a significant modification of the originally reported preparation.[4] A mixture of powdered tris(acetylacetonato)cobalt(III) (0.375 g, 0.001 mol) and triphenylphosphine (1.5 g, 0.006 mol) was added to 100 ml of di-*n*-butyl ether. The suspension was cooled in an ice bath, stirred, and flushed with dry nitrogen gas. To the cold suspension, into which a constant stream of dry nitrogen gas was passed, triethylaluminum (0.85 ml) was added drop by drop. The resultant mixture was allowed to warm to room temperature, and a reaction took place, the color of the solution changing from green to reddish brown. The solution was cooled and stirred in an ice bath under a steady nitrogen flow for 45 min. The unreacted tris(acetylacetonato)cobalt(III) was filtered off under a nitrogen atmosphere, and the filtrate was left to stand in a refrigerator at 0°. After 2 days a crop of thin, prismatic crystals was filtered off. A Nujol mull showed two infrared absorption bands at 2085 and 2105 cm^{-1}, which may be ascribed to the N–N stretching mode, but the crystals were not suitable for X-ray analysis. A further crop of crystals was filtered off 2 days later and similarly discarded. After 2 weeks, crystals suitable for X-ray analysis were isolated from the filtrate. An orange-red crystal of approximate dimensions 0.45 × 0.15 × 0.10 mm was mounted in a thin-walled glass capillary.

Collection and Reduction of Intensity Data

A series of Weissenberg and precession photographs taken with Cu K$\bar{\alpha}$ radiation showed the crystal to be monoclinic with $2/m$ Laue symmetry. The systematic extinctions observed were: $h0l$ for l odd and $0k0$ for k odd. These absences are consistent with the space group C_{2h}^5-$P2_1/c$.[7]

The cell constants and their standard deviations were determined at 22° by a least-squares refinement of the setting angles of 11 reflections that had been carefully centered on a Picker four-circle automatic X-ray diffractometer, using procedures previously described.[8] The results (Cu Kα_1 radiation; λ 1.54056 Å) were: $a = 37.159$ (14) Å, $b = 11.355$ (5) Å, $c = 21.779$ (8) Å, β

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$= 101.3\ (2)°$, $V = 9011.0$ Å^3. In an optical study of the crystal, domal faces of the form $\{011\}$ were observed. Two prismatic faces belonged to the form $\{100\}$; the other two were general faces, of indices $(30\bar{2})$ and $(\bar{2}03)$.

The crystal, in a thin-walled glass capillary, was mounted on the diffractometer with the long dimension (010) deliberately offset by 5° from coincidence with the spindle axis in order to minimize the possibility of multiple reflections.

Several ω scans with a narrow source and open counter were taken to check the mosaicity of the crystal. The average width at half-height for strong reflections was approximately 0.11°.

Owing to the large cell, Cu Kα radiation was used for data collection. The intensity data were collected in three separate blocks. The reflections in the range $0° < 2\theta < 65°$ had to be collected in two stages owing to an equipment failure midway through the run, resulting in two blocks of 1600 and 1244 reflections, respectively. A third block of data in the range $65° < 2\theta < 110°$ was collected 5 months later, when it was apparent that additional data were needed to solve the structure. The diffracted beams were filtered through 0.5 mil of Ni foil. A takeoff angle of approximately 1.5° was used. At this angle, the peak intensity of a strong reflection was about 80% of the maximum value as a function of takeoff angle. The counter aperture selected was 3.5 × 3.5 mm and was positioned 29 cm from the crystal. The pulse height analyzer was set for approximately a 90% window, centered on the Cu K$\bar{\alpha}$ peak. The data were collected by the θ–2θ scan technique at a scan rate of 1°/min. An asymmetric scan range of 0.6° on the low side to 0.75° on the high side of the calculated 2θ values (CuKα_1) was used for reflections in the range $0° < 2\theta < 75°$. For the reflections in the range $75° < 2\theta < 110°$ the limits were 0.6° on the low side of the 2θ value calculated for the Cu Kα_1 peak and 0.75° on the high side of the 2θ value calculated for the Cu Kα_2 peak (λ 1.5406 and 1.5444 Å, respectively). Stationary-counter, stationary-crystal background counts of 10 sec were taken at each end of the scan. Attenuators were inserted automatically when the intensity of the diffracted beam exceeded about 7000 counts/sec during the scan; the attenuators were Cu foil, their thickness being chosen to give attenuator factors of approximately 2.2.

Throughout the collection of the data, the intensities of four reference reflections were measured every 200 reflections as a check on electronic and crystal stability. From the values obtained, three separate scale factors were deduced for the three blocks of data. Throughout the data collection, the intensities of the reference reflections remained constant, with no evidence of crystal decomposition.

The unique data set having reflections with $2\theta \leq 65°$ was first processed in the usual manner.[8] A sharpened, origin-removed Patterson function[9] was computed and led to preliminary parameters for the two cobalt and the six phosphorus atoms. These parameters were confirmed by direct-method techniques.[9] However, despite the subsequent apparent location of 18 phenyl rings in geometrically feasible positions, this solution would not refine.

On the assumption that the correct solution could be found more readily if more data were available, data collection was resumed. From the standard reflections it was apparent that no crystal decomposition had occurred during the intervening period. All independent data were collected in the range $65° < 2\theta < 80°$. A set of structure factors was then calculated for reflections with the values $80° < 2\theta < 110°$, using the original cobalt and phosphorus positions. From the values of $|F_c|$, those reflections for which it was believed that I would be greater than $2\sigma(I)$ were collected. In all, 5399 independent reflections were recorded.

All data were processed in a manner previously described.[8] The value of p in the calculation of $\sigma(I)$ was selected as 0.03. The values of I and $\sigma(I)$ were corrected for Lorentz–polarization effects and reflections with $I > 2\sigma(I)$ were corrected for absorption. The absorption coefficient μ of this compound for Cu Kα radiation is 41.9 cm^{-1}, and for the crystal chosen, transmission coefficients were found to range from 0.714 to 0.588. Of the 5399 independent reflections, 3312 had $F^2 > 3\sigma(F^2)$, and only these were used in subsequent calculations.

Solution and Refinement

All least-squares refinements were carried out on F, the function minimized being $\Sigma w(|F_o| - |F_c|)^2$, where $|F_o|$ and $|F_c|$ are the observed and calculated structure amplitudes and the weight w is taken as $4F_o^2/\sigma^2(F_o^2)$. In all calculations of F_c, the atomic scattering factors for cobalt and hydrogen were those calculated by Cromer and Waber[10] and by Stewart, Davidson, and Simpson,[11] respectively; scattering factors for phosphorus, carbon, and nitrogen were taken from the usual tabulation.[7] The effects of anomalous dispersion of the cobalt and phosphorus atoms were included in the calculation of F_c;[12] the values of $\Delta f'$ and $\Delta f''$ used were those calculated by Cromer.[13]

The cell volume of $CoH(N_2)(P(C_6H_5)_3)_3 \cdot (C_2H_5)_2O$ in the previously determined structure[5] is 2496 Å^3. Since there are two molecules in the unit cell (space group P$\bar{1}$), the molecular volume of $CoH(N_2)(P(C_6H_5)_3)_3$ is in the region of 1100 Å^3. Since the cell volume of the present sample is 9011 Å^3, it is apparent that there are eight molecules in the unit cell and two in the asymmetric unit. Therefore, a total of 120 non-

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(9) In addition to various local programs, Patterson functions and Fourier syntheses were calculated using a version of Zalkin's FORDAP. Normalized structure factors were calculated using R. B. K. Dewar's FAME. Sign determination of E values was done by R. E. Long's REL, and absorption corrections were made by a modification of W. C. Hamilton's GONO9. Refinement and structure factor calculations were done by our least-squares program, NUCLS, which, in its nongroup form, resembles the Busing–Levy ORFLS. Errors in derived quantities were obtained from the Busing–Levy ORFFE, and drawings were made with the use of Johnson's ORTEP.

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TABLE I

POSITIONAL, THERMAL, AND GROUP PARAMETERS FOR $CoH(N_2)(P(C_6H_5)_3)_3$

Atom	x	y	z	β_{11} or B[a]	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
				Molecule I					
Co	0.36478 (6)[b]	−0.0554 (2)	0.18755 (9)	0.00048 (2)	0.0062 (3)	0.00107 (6)	0.00004 (7)	0.00016 (3)	−0.00007 (11)
P1	0.3660 (1)	0.1364 (3)	0.1956 (2)	0.00052 (4)	0.0063 (5)	0.0013 (1)	−0.00002 (11)	0.00015 (5)	0.0001 2)
P2	0.3898 (1)	−0.1668 (3)	0.2648 (2)	0.00056 (4)	0.0064 (5)	0.0012 (1)	−0.00009 (11)	0.00012 (5)	−0.0002 (2)
P3	0.3623 (1)	−0.1133 (3)	0.0903 (2)	0.00054 (4)	0.0063 (4)	0.0012 (1)	−0.00004 (11)	0.00013 (5)	−0.0001 (2)
N1	0.3177 (4)	−0.076 (1)	0.1914 (6)	0.0012 (2)	0.008 (2)	0.0013 (3)	−0.0001 (6)	0.0003 (2)	−0.0003 (6)
N2	0.2884 (3)	−0.085 (1)	0.1934 (6)	0.0009 (2)	0.012 (2)	0.0025 (4)	−0.0004 (6)	0.0002 (3)	0.0001 (6)
H	0.405 (3)	−0.046 (10)	0.166 (5)	5.0					
				Molecule II					
Co	0.12076 (6)	0.0539 (2)	0.16620 (9)	0.00064 (3)	0.0085 (3)	0.00209 (7)	0.00019 (8)	0.00027 (3)	0.0001 (1)
P1	0.15509 (9)	−0.0446 (4)	0.2423 (2)	0.00063 (4)	0.0074 (5)	0.0020 (1)	0.0001 (1)	0.00024 (5)	0.0001 (2)
P2	0.13131 (9)	0.0408 (4)	0.0701 (2)	0.00058 (4)	0.0099 (5)	0.0020 (1)	−0.0001 (1)	0.00004 (5)	0.0002 (2)
P3	0.0942 (1)	0.2134 (4)	0.1932 (2)	0.00070 (4)	0.0089 (5)	0.0024 (1)	0.0004 (1)	0.00036 (6)	0.0007 (2)
N1	0.0807 (3)	−0.043 (1)	0.1585 (5)	0.0006 (1)	0.011 (2)	0.0025 (4)	0.0001 (4)	0.0000 (2)	0.0008 (7)
N2	0.0567 (4)	−0.104 (1)	0.1555 (7)	0.0009 (2)	0.012 (2)	0.0052 (5)	−0.0014 (5)	0.0006 (3)	−0.0004 (8)
H	0.161 (3)	0.119 (11)	0.167 (6)	5.0					

Group	x_c[c]	y_c	z	δ	ϵ	η	B, Å^2
			Molecule I				
P1R1	0.2875 (2)	0.2696 (5)	0.1676 (2)	2.714 (8)	2.395 (5)	−0.028 (7)	3.8 (2)
P1R2	0.3972 (1)	0.2512 (5)	0.3313 (3)	−0.725 (6)	2.601 (6)	1.605 (6)	3.8 (2)
P1R3	0.4111 (2)	0.2624 (5)	0.1010 (2)	−2.321 (6)	−3.011 (6)	−2.276 (5)	4.3 (2)
P2R4	0.4456 (2)	−0.3747 (5)	0.2422 (3)	1.909 (11)	2.295 (5)	−2.711 (10)	5.0 (2)
P2R5	0.3325 (1)	−0.3146 (5)	0.3297 (2)	−2.636 (6)	2.922 (5)	0.600 (5)	3.7 (1)
P2R6	0.4414 (1)	−0.0354 (5)	0.3818 (3)	2.443 (7)	−2.283 (6)	1.741 (7)	3.8 (2)
P3R7	0.3048 (2)	0.0483 (5)	−0.0040 (2)	−0.838 (6)	2.930 (5)	−2.673 (5)	3.4 (2)
P3R8	0.4372 (2)	−0.1224 (4)	0.0351 (3)	1.157 (9)	2.139 (6)	−1.272 (9)	4.3 (2)
P3R9	0.3262 (1)	−0.3689 (5)	0.0507 (3)	2.863 (7)	2.459 (7)	1.204 (6)	4.5 (2)
			Molecule II				
P1R1	0.1107 (1)	−0.1083 (6)	0.3523 (3)	2.962 (6)	2.806 (7)	1.064 (5)	5.2 (2)
P1R2	0.2325 (2)	0.0559 (5)	0.3185 (3)	−0.292 (13)	2.080 (6)	0.701 (12)	5.2 (2)
P1R3	0.1837 (2)	−0.2956 (6)	0.2002 (3)	1.691 (9)	2.653 (6)	−2.689 (6)	5.8 (2)
P2R4	0.0582 (2)	−0.0050 (6)	−0.0354 (3)	−0.132 (8)	2.670 (6)	−2.504 (7)	6.1 (2)
P2R5	0.1860 (2)	−0.1645 (5)	0.0388 (3)	−1.184 (10)	−2.346 (6)	−0.461 (9)	5.2 (2)
P2R6	0.1675 (1)	0.2648 (6)	0.0131 (3)	0.374 (9)	−2.242 (6)	−0.863 (9)	4.6 (2)
P3R7	0.0214 (2)	0.1810 (6)	0.2538 (3)	0.447 (8)	2.755 (7)	2.434 (6)	7.3 (2)
P3R8	0.0620 (2)	0.3958 (6)	0.0814 (3)	−0.471 (8)	−2.652 (7)	−2.223 (6)	6.2 (2)
P3R9	0.1431 (2)	0.3919 (5)	0.2924 (3)	−1.923 (9)	2.610 (7)	2.508 (7)	6.7 (2)

[a] The form of the thermal ellipsoid is $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)]$. B is in Å^2. [b] Numbers in parentheses given here and in other tables are estimated standard deviations in the least significant digits. [c] x_c, y_c, and z, are fractional coordinates of the ring center; δ, ϵ, and η (in radians) have been defined by R. Eisenberg and J. A. Ibers, *Inorg. Chem.*, **4**, 773 (1965).

hydrogen atoms must be located and refined. With eight molecules per unit cell, a calculated density of 1.284 g/cm^3 is obtained. A density could not be observed owing to the sensitivity to air and the solubility of the complex. There are no crystallographic symmetry conditions imposed upon the molecules.

A successful solution was obtained by using the entire data set ($2\theta < 110°$) and applying direct-method techniques to locate the cobalt and phosphorus atoms. Values of E (normalized structure factors) were first calculated.[9] The distribution of E values corresponded to the centric one, as judged by their average magnitude and their mean-square value. For the application of the direct-method approach, the 335 reflections for which $E \geqslant 1.8$ were chosen. The following reflections, with their E values in parentheses, were chosen to define the origin: 413 (3.32); $15,4,\bar{1}$ (2.89); $11\bar{1}$ (2.08). Four additional reflections—$25\bar{8}$ (3.54); 7,0,10 (3.53); $41\bar{5}$ (2.80); $17,1,\bar{9}$ (2.87)—were selected and reiterative application of Sayre's equation[9] was carried out on the 16 sets formed by successively assigning phase angles of 0 and 180° to these four reflections. On the basis of the minimum number of cycles for convergence and of the consistency index[9] at convergence, two likely solutions were found. The first solution converged in four cycles to a consistency index of 0.92. An E map based on this solution did not reveal the geometrical features we were anticipating. The second solution, which had converged in five cycles to a consistency index of 0.91, led to an E map on which the two cobalt atoms and six phosphorus atoms, corresponding to a trigonal array of phosphorus atoms about each cobalt atom, could be located from among the ten highest peaks on the map.

The positions so found were consistent with an origin-removed, sharpened Patterson function, with the cobalt atoms at 0.36, −0.06, 0.19 and 0.12, 0.05, 0.17. The original solution (using only data in the range $0° < 2\theta < 65°$) was also derived from a combination of Patterson and direct-method techniques and had

Table II

Derived Parameters for Ring Carbon Atoms

Ring atom	Molecule I				Molecule II			
	x	y	z	B, Å^2	x	y	z	B, Å^2
R1C1[a]	0.3120 (2)[b]	0.2166 (12)	0.1801 (4)	2.8 (2)	0.1309 (2)	−0.0842 (9)	0.3062 (4)	4.0 (2)
R1C2	0.2947 (3)	0.1722 (7)	0.1329 (3)	3.5 (2)	0.1152 (2)	−0.1950 (8)	0.3092 (4)	4.8 (2)
R1C3	0.2603 (2)	0.2251 (10)	0.1203 (3)	4.1 (2)	0.0950 (3)	−0.2192 (7)	0.3553 (5)	5.7 (2)
R1C4	0.2531 (2)	0.3226 (12)	0.1550 (4)	4.5 (2)	0.0905 (2)	−0.1325 (10)	0.3985 (4)	6.3 (2)
R1C5	0.2804 (3)	0.3671 (7)	0.2022 (4)	4.1 (2)	0.1062 (2)	−0.0217 (8)	0.3955 (4)	5.7 (2)
R1C6	0.3148 (2)	0.3141 (10)	0.2148 (3)	3.5 (2)	0.1264 (3)	0.0025 (6)	0.3493 (5)	4.8 (2)
R2C1	0.3851 (3)	0.2012 (8)	0.2726 (3)	3.0 (2)	0.1983 (3)	0.0167 (19)	0.2872 (4)	3.9 (2)
R2C2	0.4100 (2)	0.2945 (8)	0.2796 (4)	3.6 (2)	0.2200 (2)	0.0859 (11)	0.2560 (3)	4.7 (2)
R2C3	0.4220 (2)	0.3444 (7)	0.3383 (5)	4.1 (2)	0.2542 (3)	0.1251 (12)	0.2872 (4)	5.6 (2)
R2C4	0.4092 (3)	0.3012 (9)	0.3900 (3)	4.5 (2)	0.2666 (3)	0.0951 (20)	0.3497 (4)	6.2 (2)
R2C5	0.3844 (2)	0.2080 (8)	0.3830 (4)	4.1 (2)	0.2449 (2)	0.0259 (11)	0.3810 (3)	5.6 (2)
R2C6	0.3723 (2)	0.1580 (7)	0.3243 (5)	3.6 (2)	0.2108 (3)	−0.0133 (12)	0.3497 (4)	4.7 (2)
R3C1	0.3915 (2)	0.2126 (8)	0.1429 (3)	3.3 (2)	0.1718 (3)	−0.1892 (8)	0.2210 (4)	4.4 (2)
R3C2	0.4253 (2)	0.1657 (7)	0.1370 (4)	4.0 (2)	0.1487 (2)	−0.2537 (11)	0.1752 (4)	5.4 (2)
R3C3	0.4450 (2)	0.2155 (9)	0.0952 (5)	4.7 (2)	0.1606 (3)	−0.3602 (9)	0.1544 (4)	6.4 (2)
R3C4	0.4308 (2)	0.3123 (8)	0.0592 (4)	5.1 (2)	0.1956 (4)	−0.4021 (8)	0.1794 (4)	7.1 (2)
R3C5	0.3970 (3)	0.3592 (7)	0.0650 (4)	4.7 (2)	0.2187 (2)	−0.3376 (11)	0.2253 (4)	6.4 (2)
R3C6	0.3773 (2)	0.3093 (8)	0.1069 (4)	4.0 (2)	0.2068 (3)	−0.2311 (9)	0.2461 (4)	5.4 (2)
R4C1	0.4224 (4)	−0.2828 (12)	0.2516 (4)	3.8 (2)	0.0900 (2)	0.0149 (11)	0.0089 (4)	4.6 (2)
R4C2	0.4142 (2)	−0.3512 (12)	0.1977 (4)	4.7 (2)	0.0779 (3)	0.0989 (8)	−0.0372 (5)	5.6 (2)
R4C3	0.4373 (3)	−0.4431 (7)	0.1883 (3)	5.4 (2)	0.0462 (3)	0.0789 (9)	−0.0815 (4)	6.6 (2)
R4C4	0.4687 (4)	−0.4667 (12)	0.2328 (5)	6.0 (2)	0.0264 (2)	−0.0249 (12)	−0.0797 (4)	7.3 (2)
R4C5	0.4770 (2)	−0.3983 (13)	0.2868 (4)	5.4 (2)	0.0384 (3)	−0.1088 (8)	−0.0337 (5)	6.6 (2)
R4C6	0.4538 (3)	−0.3064 (7)	0.2962 (3)	4.7 (2)	0.0702 (3)	−0.0889 (8)	0.0106 (4)	5.6 (2)
R5C1	0.3578 (2)	−0.2523 (8)	0.3027 (3)	2.9 (1)	0.1619 (3)	−0.0775 (11)	0.0508 (4)	4.0 (2)
R5C2	0.3608 (2)	−0.3742 (8)	0.3092 (4)	3.5 (1)	0.1954 (3)	−0.0929 (7)	0.0914 (3)	4.8 (2)
R5C3	0.3356 (3)	−0.4364 (6)	0.3362 (4)	4.0 (1)	0.2195 (2)	−0.1799 (12)	0.0794 (4)	5.6 (2)
R5C4	0.3073 (2)	−0.3768 (8)	0.3567 (4)	4.4 (1)	0.2101 (4)	−0.2515 (12)	0.0268 (5)	6.1 (2)
R5C5	0.3042 (2)	−0.2549 (8)	0.3502 (4)	4.0 (1)	0.1766 (3)	−0.2361 (7)	−0.0138 (4)	5.6 (2)
R5C6	0.3295 (3)	−0.1927 (6)	0.3232 (4)	3.5 (1)	0.1525 (2)	−0.1491 (12)	−0.0018 (4)	4.8 (2)
R6C1	0.4182 (3)	−0.0921 (10)	0.3331 (4)	2.9 (2)	0.1527 (4)	0.1678 (8)	0.0385 (5)	3.6 (2)
R6C2	0.4159 (3)	−0.1169 (8)	0.3949 (5)	3.5 (2)	0.1525 (2)	0.2779 (10)	0.0668 (3)	4.3 (2)
R6C3	0.4392 (2)	−0.0602 (8)	0.4436 (3)	4.1 (2)	0.1674 (4)	0.3749 (6)	0.0414 (5)	5.0 (2)
R6C4	0.4647 (3)	0.0213 (11)	0.4306 (4)	4.5 (2)	0.1823 (4)	0.3618 (8)	−0.0122 (5)	5.5 (2)
R6C5	0.4670 (3)	0.0461 (9)	0.3688 (5)	4.1 (2)	0.1824 (2)	0.2518 (10)	−0.0405 (3)	5.0 (2)
R6C6	0.4437 (2)	−0.0106 (8)	0.3200 (3)	3.5 (2)	0.1676 (4)	0.1548 (7)	−0.0151 (5)	4.3 (2)
R7C1	0.3302 (2)	−0.0252 (7)	0.0326 (3)	2.6 (2)	0.0516 (2)	0.1942 (11)	0.2252 (4)	5.6 (2)
R7C2	0.3415 (2)	0.0811 (8)	0.0105 (4)	3.2 (2)	0.0232 (3)	0.2764 (8)	0.2143 (4)	6.9 (2)
R7C3	0.3161 (3)	0.1546 (6)	−0.0261 (4)	3.7 (2)	−0.0070 (3)	0.2632 (10)	0.2429 (6)	8.0 (2)
R7C4	0.2793 (2)	0.1218 (8)	−0.0406 (3)	4.1 (2)	−0.0088 (2)	0.1678 (12)	0.2824 (5)	8.8 (2)
R7C5	0.2680 (2)	0.0155 (8)	−0.0185 (4)	3.7 (2)	0.0195 (3)	0.0856 (8)	0.2933 (4)	8.0 (2)
R7C6	0.2935 (2)	−0.0580 (6)	0.0181 (4)	3.2 (2)	0.0497 (3)	0.0988 (9)	0.2647 (5)	6.9 (2)
R8C1	0.4046 (2)	−0.1157 (15)	0.0573 (4)	3.3 (2)	0.0762 (3)	0.3212 (9)	0.1308 (4)	4.7 (2)
R8C2	0.4046 (2)	−0.0961 (12)	−0.0058 (4)	4.0 (2)	0.0823 (2)	0.4421 (10)	0.1365 (4)	5.7 (2)
R8C3	0.4372 (3)	−0.1027 (7)	−0.0280 (3)	4.6 (2)	0.0682 (3)	0.5167 (6)	0.0871 (6)	6.7 (2)
R8C4	0.4699 (2)	−0.1290 (16)	0.0129 (5)	5.1 (2)	0.0479 (3)	0.4705 (9)	0.0319 (4)	7.4 (2)
R8C5	0.4699 (2)	−0.1487 (12)	0.0760 (4)	4.6 (2)	0.0417 (2)	0.3496 (10)	0.0262 (4)	6.7 (2)
R8C6	0.4372 (3)	−0.1420 (7)	0.0983 (3)	4.0 (2)	0.0558 (3)	0.2750 (6)	0.0757 (5)	5.7 (2)
R9C1	0.3430 (3)	−0.2609 (7)	0.0680 (5)	3.4 (2)	0.1217 (3)	0.3119 (10)	0.2528 (4)	5.2 (2)
R9C2	0.3236 (2)	−0.3183 (9)	0.1080 (3)	4.2 (2)	0.1592 (3)	0.3203 (8)	0.2533 (5)	6.3 (2)
R9C3	0.3069 (3)	−0.4262 (10)	0.0907 (4)	4.9 (2)	0.1806 (2)	0.4003 (12)	0.2929 (5)	7.3 (2)
R9C4	0.3095 (3)	−0.4768 (7)	0.0334 (5)	5.4 (2)	0.1645 (3)	0.4719 (10)	0.3321 (5)	8.1 (2)
R9C5	0.3288 (2)	−0.4195 (9)	−0.0065 (3)	4.9 (2)	0.1270 (3)	0.4636 (8)	0.3316 (5)	7.3 (2)
R9C6	0.3456 (3)	−0.3116 (10)	0.0108 (4)	4.2 (2)	0.1056 (2)	0.3836 (2)	0.2920 (5)	6.3 (2)

[a] Ring atoms are numbered sequentially, with C1 attached to P. [b] The estimated standard deviations are derived from those of the group parameters.

cobalt atoms at 0.38, 0.45, 0.00 and −0.11, 0.05, 0.14. Thus, a completely different set of parameters was derived from the complete data set. Naturally the final solution must be compatible with the original Patterson function insofar as that function is not distorted by the missing terms. It can only be said that the final solution was not obvious from the original Patterson function. The fact that direct methods, based on the entire data set, led to a solution which was not obvious either from direct methods or from the Patterson function based on the incomplete data set probably results from the availability of an increased number of reflections with large E values.

At first, the positional and isotropic thermal parameters of the two cobalt and six phosphorus atoms were refined. The isotropic thermal parameters on

TABLE III

DERIVED PARAMETERS FOR RING HYDROGEN ATOMS[a]

	Molecule I			Molecule II		
	x	y	z	x	y	z
R1H2[b]	0.299	0.110	0.110	0.118	−0.250	0.282
R1H3	0.242	0.198	0.089	0.085	−0.289	0.358
R1H4	0.230	0.358	0.147	0.078	−0.147	0.430
R1H5	0.275	0.430	0.224	0.104	0.035	0.425
R1H6	0.332	0.343	0.245	0.137	0.074	0.348
R2H2	0.418	0.324	0.247	0.212	0.103	0.216
R2H3	0.438	0.405	0.344	0.268	0.170	0.266
R2H4	0.418	0.332	0.429	0.289	0.123	0.369
R2H5	0.377	0.179	0.417	0.254	0.010	0.422
R2H6	0.356	0.099	0.321	0.198	−0.057	0.371
R3H2	0.435	0.103	0.160	0.126	−0.228	0.158
R3H3	0.467	0.185	0.091	0.146	−0.402	0.123
R3H4	0.444	0.344	0.032	0.204	−0.471	0.164
R3H5	0.388	0.420	0.041	0.241	−0.366	0.241
R3H6	0.356	0.339	0.110	0.221	−0.192	0.276
R4H2	0.394	−0.336	0.169	0.090	0.166	−0.038
R4H3	0.432	−0.489	0.153	0.038	0.132	−0.111
R4H4	0.484	−0.529	0.226	0.006	−0.040	−0.109
R4H5	0.498	−0.417	0.314	0.026	−0.177	−0.033
R4H6	0.460	−0.264	0.330	0.078	−0.143	0.041
R5H2	0.378	−0.414	0.296	0.201	−0.049	0.126
R5H3	0.337	−0.515	0.341	0.241	−0.192	0.106
R5H4	0.291	−0.416	0.375	0.226	−0.308	0.019
R5H5	0.286	−0.216	0.364	0.171	−0.282	−0.048
R5H6	0.328	−0.114	0.319	0.132	−0.139	−0.029
R6H2	0.399	−0.167	0.404	0.144	0.285	0.102
R6H3	0.438	−0.074	0.484	0.168	0.446	0.060
R6H4	0.480	0.059	0.463	0.192	0.427	−0.029
R6H5	0.485	0.099	0.362	0.192	0.247	−0.077
R6H6	0.446	0.006	0.281	0.168	0.086	−0.036
R7H2	0.365	0.103	0.019	0.024	0.337	0.189
R7H3	0.323	0.224	−0.041	−0.026	0.316	0.237
R7H4	0.263	0.169	−0.065	−0.029	0.159	0.302
R7H5	0.244	−0.006	−0.029	0.018	0.023	0.320
R7H6	0.286	−0.127	0.032	0.067	0.045	0.272
R8H2	0.384	−0.082	−0.034	0.095	0.471	0.172
R8H3	0.438	−0.094	−0.070	0.072	0.596	0.092
R8H4	0.491	−0.135	−0.002	0.039	0.522	0.000
R8H5	0.491	−0.164	0.102	0.028	0.324	−0.011
R8H6	0.437	−0.152	0.138	0.052	0.199	0.070
R9H2	0.322	−0.288	0.145	0.170	0.275	0.229
R9H3	0.294	−0.465	0.117	0.205	0.406	0.295
R9H4	0.298	−0.549	0.023	0.178	0.524	0.359
R9H5	0.330	−0.456	−0.044	0.117	0.510	0.358
R9H6	0.358	−0.279	−0.016	0.081	0.379	0.292

[a] All atoms have $B = 5$ Å^2. [b] H2 is attached to C2, H3 to C3, etc.

four of the atoms refined to negative values. Therefore, structure factors with the refined positions and fixed, positive isotropic thermal parameters on the atoms were determined and the usual agreement factors $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$ and R_2 (or weighted R factor) $= (\Sigma w(|F_o| - |F_c|)^2/\Sigma w F_o^2)^{1/2}$ were 0.487 and 0.584, respectively. The four nitrogen atoms and eighteen phenyl rings were found from two successive difference Fourier syntheses. At this time, an absorption correction[9] was applied to the data. A least-squares refinement cycle was carried out in which the two cobalt, six phosphorus, and four nitrogen atoms were refined with isotropic thermal parameters; the eighteen phenyl rings were treated as rigid groups and restricted to their known geometry (D_{6h} symmetry, C–C = 1.392 Å). The variable parameters for a ring included an over-all isotropic thermal parameter, the coordinates of the ring center, and the three orientation angles which have been described previously.[14] The agreement factors so determined were $R_1 = 0.11$ and $R_2 = 0.11$. In this refinement, one phenyl ring moved considerably and therefore was relocated by means of a difference Fourier synthesis. This was followed by a refinement in which nongroup atoms were allowed to refine with anisotropic thermal parameters. This led to agreement factors of $R_1 = 0.094$ and $R_2 = 0.096$. The contributions of the 90 hydrogen atoms of the phenyl rings to F_c were calculated, assuming the known geometry of the ring, a C–H distance of 0.90 Å, and an isotropic thermal parameter of 5.0 Å^2 for each atom. With the inclusion of these contributions to F_c and with the positional and thermal parameters from the previous refinement, a set of structure factors was calculated. The agreement factors were $R_1 = 0.077$ and $R_2 = 0.074$.

The geometry of the model at this point was as found previously and was consistent with the formulation of the compound as a hydride.[5] A difference Fourier synthesis was calculated about each cobalt atom in an attempt to locate the coordinated hydrogen atoms. These were clearly visible in the electron density maps calculated from 3312 structure factors, at an electron density of 0.46 (5) e$^-$/Å^3 on molecule I and 0.42 (5) e$^-$/Å^3 on molecule II. On the map of molecule I, the coordinated hydrogen atom was the most prominent peak (the next peak being at 0.36 (5) e$^-$/Å^3). On the map of molecule II, it was the second most prominent peak (the most prominent peak being at 0.46 (5) e$^-$/Å^3 and the third peak at 0.37 (5) e$^-$/Å^3). These other peaks are in the region of, and apparently due to, residual density from ring carbon atoms. When similar maps were calculated from structure factors for which $\theta < 32.5°$, the coordinated hydrogen atoms were the most prominent peaks on the maps at electron densities of 0.38 (3) e$^-$/Å^3 (the next peak at 0.20 (3) e$^-$/Å^3) and 0.39 (3) e$^-$/Å^3 (the next peak at 0.24 (3) e$^-$/Å^3) for molecule I and molecule II, respectively.

Up to this point, the refinement had proceeded with one over-all isotropic thermal parameter per phenyl ring. As may be seen by examining other structures in which phenyl ring carbon atoms are allowed to refine with individual isotropic thermal parameters, the *meta*- and *para*-carbon atoms of the ring often vibrate more than the other atoms in the ring. We could not refine the carbon atoms in such a manner in this structure because full-matrix refinements prior to this stage involved 235 variables and occupied the entire central memory of the computer. When an over-all thermal parameter for a ring is refined in the program NUCLS,[9] each ring atom is given the over-all value as an individual isotropic thermal parameter. In order to approximate more closely the "flapping" ring motion observed in other structures, a percentage correction was made to the individual thermal parameter

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(14) R. Eisenberg and J. A. Ibers, *Inorg. Chem.*, **4**, 773 (1965).

TABLE IV

OBSERVED AND CALCULATED STRUCTURE AMPLITUDES ×10 (IN ELECTRONS)

L	H	FO	FC
***** K = 0 *****			
-22	3	579	606
-22	7	458	410
-22	10	530	472
-22	14	470	526
-22	18	603	506
-20	2	443	451
-20	6	565	501
-20	10	638	549
-20	17	446	471
-18	1	444	435
-18	2	768	717
-18	3	619	668
-18	4	550	413
-18	6	828	772
-18	13	581	574
-18	22	616	566
-18	30	451	451
-16	2	1110	1120
-16	3	777	781
-16	4	542	481
-16	6	846	959
-16	7	836	869
-16	8	521	595
-16	10	785	762
-16	11	446	613
-16	14	714	708
-16	18	409	289
-16	22	651	647
-14	2	1398	1466
-14	3	622	667
-14	4	1059	895
-14	6	956	1008
-14	7	694	698
-14	8	1177	1160
-14	9	656	563
-14	10	773	729
-14	13	444	509
-14	14	757	812
-14	15	626	714
-14	16	486	525
-14	17	471	533
-14	18	454	553
-14	19	697	761
-14	20	479	451
-14	21	428	546
-14	22	431	491
-12	1	1050	1139
-12	2	1629	1673
-12	3	683	643
-12	4	287	338
-12	5	304	272
-12	6	1107	1111
-12	8	581	548
-12	9	613	777
-12	10	1429	1517
-12	13	1271	1275
-12	14	1329	1297
-12	15	523	520
-12	17	922	1008
-12	18	411	448
-12	19	384	470
-12	21	629	664
-12	23	636	534
-12	25	559	486
-12	26	426	461
-10	1	2906	2913
-10	3	656	608
-10	5	1020	980
-10	7	360	389
-10	8	687	678
-10	9	307	251
-10	10	376	413
-10	11	1246	1182
-10	12	661	708
-10	13	318	346
-10	14	482	674
-10	15	380	388
-10	16	459	473
-10	17	662	613
-10	18	1815	1819
-10	19	419	464
-10	21	370	366
-10	22	2112	2113
-10	23	1806	1808
-10	26	2118	2143
-10	27	687	907
-10	30	1003	931
-8	2	802	752
-8	3	606	639
-8	4	2054	2042
-8	5	678	812
-8	6	445	434
-8	7	1296	1358
-8	8	765	794
-8	9	1204	1209
-8	10	1422	1375
-8	11	277	353
-8	12	773	847
-8	13	2167	2209
-8	14	1664	1700
-8	15	516	471
-8	16	810	917
-8	17	1255	1261
-8	18	1599	1701
-8	19	397	468
-8	20	330	328
-8	21	1658	1610
-8	22	1674	1733
-8	23	343	277
-8	25	1014	1069
-8	26	1653	1670
-8	27	504	569
-8	28	385	297
-8	29	958	1005
-8	30	1042	1099
-8	33	588	715
-6	1	1262	1178
-6	2	1784	1633
-6	3	1081	1004
-6	4	836	882
-6	5	3926	4045
-6	6	506	487
-6	8	296	277
-6	9	1252	1292
-6	10	703	712
-6	11	1422	1491
-6	12	433	377
-6	13	1538	1651
-6	14	623	631
-6	15	867	832
-6	16	375	400
-6	17	367	288
-6	18	1270	1186
-6	19	1082	1092
-6	21	1136	1022
-6	22	1289	1190
-6	24	742	734
-6	25	1254	1247
-6	28	403	368
-6	29	955	1030
-6	33	1098	1116
-4	1	1684	1665
-4	2	902	987
-4	3	363	342
-4	4	1058	996
-4	5	1286	1283
-4	6	2767	2740
-4	7	878	813
-4	8	1048	1047
-4	9	840	784
-4	10	678	612
-4	11	605	610
-4	12	1002	1000
-4	13	305	302
-4	14	1829	1752
-4	16	814	882
-4	17	789	901
-4	18	1976	2029
-4	21	1509	1436
-4	22	538	591
-4	24	701	586
-4	28	367	387
-4	32	517	754
-4	36	811	753
-4	37	367	97
-2	1	2869	2830
-2	3	1074	1151
-2	4	2951	2891
-2	5	2983	2932
-2	6	1091	1116
-2	8	3724	3636
-2	9	510	585
-2	10	2269	2254
-2	11	1616	1574
-2	12	824	790
-2	13	2524	2446
-2	15	922	924
-2	16	1138	1075
-2	17	1078	1152
-2	19	1242	1299
-2	20	766	805
-2	22	312	382
-2	23	966	1072
-2	24	1029	1112
-2	26	929	925
-2	28	1002	1076
-2	29	433	380
-2	31	418	353
0	2	613	636
0	3	645	541
0	4	6795	7193
0	5	603	549
0	7	1032	994
0	8	1212	1340
0	9	233	230
0	10	960	918
0	11	745	687
0	12	1006	950
0	15	712	822
0	16	285	413
0	18	763	762
0	19	1704	1576
0	20	826	885
0	21	862	873
0	24	822	760
0	25	1283	1318
0	26	577	734
0	28	401	301
0	29	1394	1472
0	33	767	776
0	37	738	796
2	0	2862	2898
2	1	2592	2705
2	2	378	422
2	3	1351	1330
2	4	284	273
2	5	391	382
2	7	217	235
2	8	2869	2834
2	9	1499	1523
2	10	481	476
2	12	1866	1857
2	13	1683	1720
2	14	1185	1115
2	15	371	422
2	16	479	386
2	17	1043	1098
2	18	354	369
2	19	1544	1475
2	20	420	420
2	21	597	627
2	22	334	370
2	23	508	496
2	24	571	573
2	25	677	839
2	26	596	584
2	27	577	651
2	28	827	812
2	29	976	1016
2	32	625	557
2	33	696	932
2	36	564	669
2	37	705	770
4	0	1878	1873
4	1	192	298
4	2	311	372
4	3	757	729
4	4	2194	2237
4	5	2922	2924
4	6	2789	2651
4	7	666	676
4	8	762	719
4	9	1796	1862
4	10	1330	1362
4	11	460	409
4	12	2125	2084
4	13	810	774
4	14	690	612
4	16	2228	2194
4	18	487	474
4	19	318	247
4	20	715	703
4	21	602	655
4	23	349	414
4	24	1182	1281
4	26	531	441
4	28	650	726
6	0	2113	2064
6	1	988	919
6	2	1338	1272
6	3	735	761
6	4	2527	2596
6	5	1200	1175
6	6	555	507
6	7	487	416
6	8	432	391
6	9	718	680
6	10	329	226
6	11	631	563
6	12	1006	931
6	13	901	962
6	14	532	513
6	15	1524	1578
6	16	1668	1561
6	17	538	588
6	18	324	175
6	19	665	708
6	20	1566	1499
6	23	552	519
6	24	730	763
6	25	441	369
6	26	502	438
8	0	1530	1483
8	1	1166	1149
8	2	1540	1611
8	3	1674	1674
8	4	1825	1866
8	6	1013	978
8	7	1766	1805
8	8	1253	1282
8	9	1166	1137
8	10	702	649
8	11	1562	1557
8	12	2146	2048
8	15	1285	1246
8	16	1131	1217
8	17	360	307
8	19	439	357
8	20	879	876
8	22	1108	1191
8	23	1357	1413
8	27	472	571
10	0	729	784
10	3	3002	3076
10	4	1061	961
10	5	839	849
10	6	628	633
10	7	3205	3161
10	8	353	434
10	9	994	959
10	10	475	498
10	11	2674	2698
10	12	344	325
10	13	885	898
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TABLE IV (*Continued*)

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1	20	920	916
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-7	6	403	434
-7	7	762	723
-7	8	351	357
-7	10	850	813
-7	11	1055	1072
-7	14	764	748
-7	15	792	817
-7	18	1020	1032
-7	19	655	580
-7	22	627	609
-7	24	431	319
-6	2	305	409
-6	4	492	389
-6	5	410	375
-6	6	330	415
-6	9	365	273
-6	15	387	397
-6	16	445	361
-5	2	1082	1106
-5	3	402	415
-5	4	266	275
-5	5	979	994
-5	6	797	735
-5	7	509	469
-5	9	339	202
-5	10	333	288
-5	11	700	619
-5	13	780	735
-5	14	656	759
-5	16	420	419
-5	17	951	833
-5	18	772	783
-5	19	556	417
-5	20	450	421
-5	21	430	419
-5	22	502	535
-5	23	551	568
-4	1	278	285
-4	3	749	754
-4	4	548	608
-4	9	635	666
-4	14	369	387
-4	15	440	455
-4	16	347	287
-4	19	424	499
-3	1	444	406
-3	2	544	664
-3	5	688	694
-3	6	510	592
-3	7	290	290
-3	8	899	965
-3	9	696	758
-3	10	412	269
-3	11	440	567
-3	12	328	322
-3	13	383	425
-3	15	581	556
-3	18	501	480
3	19	843	832
-3	20	390	374
-2	2	353	320
-2	4	351	376
-2	7	375	471
-2	8	414	510
-2	11	424	425
-2	18	490	503
-2	19	575	559
-2	20	367	381
-2	22	467	402
-1	1	663	593
-1	2	521	491
-1	3	882	955
-1	4	435	462
-1	5	548	611
-1	7	753	721
-1	9	575	579
-1	11	534	523
-1	12	455	428
-1	13	390	352
-1	15	1180	1182
-1	19	744	791
-1	27	571	535
0	1	424	446
0	2	363	283
0	5	327	370
0	6	664	646
0	7	377	372
0	11	303	247
0	12	293	236
0	13	828	784
0	14	593	662
0	17	431	563
0	18	434	406
1	1	651	668
1	2	794	792
1	3	298	229
1	5	1042	1051
1	6	1606	1605
1	8	356	370
1	9	951	938
1	10	1342	1291
1	13	489	578
1	14	1321	1334
1	15	435	444
1	18	752	751
1	19	827	817
1	21	541	596
1	22	675	778
1	23	739	892
1	27	629	793
2	1	634	841
2	2	352	284
2	4	312	352
2	5	1325	1406
2	6	374	363
2	9	649	718
2	10	281	226
2	11	346	295
2	13	537	453
2	15	523	517
2	18	398	403
2	22	397	287
3	0	1485	1598
3	1	325	328
3	2	1209	1161
3	3	280	377
3	4	1292	1278
3	6	1996	1912
3	7	384	381
3	8	724	802
3	10	1443	1468
3	11	313	330
3	14	860	877
3	15	425	425
3	17	789	831
3	18	789	793
3	21	1043	1045
3	22	410	403
3	31	438	365
4	1	280	253
4	3	525	473
4	6	318	321
4	7	355	227
4	8	407	437
4	9	307	373
4	11	304	206
4	12	297	204
4	13	569	585
4	14	566	532
4	15	502	599
5	1	772	788
5	2	1067	1115
5	3	314	485
5	5	941	914
5	6	865	875
5	7	806	826
5	9	678	743
5	10	551	628
5	11	506	626
5	12	493	509
5	13	1097	1094
5	16	426	341
5	17	700	641
5	18	506	600
5	20	724	703
6	0	588	612
6	2	604	667
6	4	543	641
6	10	536	611
6	11	363	339
6	14	536	567
6	15	431	413
6	19	464	355
7	1	1461	1486
7	3	1066	1188
7	5	1128	1086
7	7	958	1001
7	10	625	608
7	11	451	499
7	12	485	508
7	15	375	340
7	16	568	677
7	18	470	363
8	0	757	817
8	4	768	738
8	6	283	152
9	1	1154	1121
9	2	669	680
9	3	396	367
9	5	1033	1085
9	6	516	522
9	7	330	282
9	10	650	667
9	11	382	310
10	0	323	244
10	3	566	594
11	1	768	750
11	3	370	226
11	4	562	565
11	6	580	617
11	8	815	930
11	12	758	698
11	13	696	648
11	17	781	720
12	1	348	287
12	3	501	648
12	6	419	433
12	7	382	239
13	3	598	544
13	5	630	601
13	9	994	1032
13	13	896	850
13	17	672	646
13	21	562	564
15	4	697	605
15	7	422	484
15	8	700	704
15	12	684	754
16	16	643	554
17	6	520	420
17	10	504	527
***** K = 7 *****			
-16	12	548	412
-13	15	492	426
-12	2	391	101
-12	3	620	658
-12	4	522	435
-12	7	450	354
-11	4	419	356
-10	2	370	402
-10	3	477	434
-10	4	382	299
-10	5	375	439
-10	6	781	868
-10	7	641	588
-10	9	433	372
-10	10	804	719
-10	15	549	540
-9	3	376	373
-9	5	496	506
-9	7	511	606
-9	21	537	488
-9	28	408	251
-8	1	615	528
-8	2	460	413
-8	3	525	670
-8	5	587	625
-8	6	473	529
-8	9	402	380
-7	1	794	834
-7	3	714	761
-7	4	393	450
-7	5	327	201
-7	7	501	458
-7	8	445	495
-7	17	449	416
-7	24	411	154
-7	26	412	390
-6	2	695	802
-6	3	322	370
-6	4	556	443
-6	5	518	623
-6	8	900	958
-6	9	379	358
-6	11	692	755
-5	2	757	817
-6	13	429	359
-6	14	557	583
-6	15	726	748
-6	18	460	274
-6	19	615	724
-6	31	456	366
-5	1	378	384
-5	3	401	374
-5	4	335	375
-5	10	310	257
-4	1	298	340
-4	3	686	699
-4	4	837	865
-4	7	628	662
-4	8	749	752
-4	10	567	622
-4	11	633	659
-4	12	417	461
-4	14	1214	1299
-4	15	399	455
-4	17	372	289
-4	18	521	583
-4	23	474	404
-4	26	455	380
-3	5	636	566
-3	9	324	352
-3	15	597	643
-2	3	901	882
-2	4	299	243
-2	6	633	573
-2	7	417	354
-2	9	422	330
-2	10	459	417
-2	12	350	332
-2	13	464	437
-2	14	473	442
-1	1	1075	1084
-1	2	593	608
-1	5	331	297
-1	6	558	583
-1	7	417	407
-1	10	390	370
0	1	569	516
0	2	355	285
0	3	766	769
0	6	546	672
0	7	384	373
0	10	542	574
0	11	330	271
0	13	485	448
0	14	679	794
0	17	867	894
0	19	516	475
1	1	348	293
1	2	692	671
1	3	361	271
1	4	674	671
1	5	493	474
1	17	427	512
1	18	457	212
1	19	449	453
2	1	1015	1161
2	2	342	303
2	3	327	357
2	4	903	879
2	5	301	349
2	6	375	350
2	8	568	482
2	9	661	633
2	12	394	408
2	13	445	507
2	14	547	448
2	15	439	392
2	19	546	536
3	0	1010	1063
3	2	529	575
3	4	711	735
3	5	400	366
3	8	687	725
3	9	342	342
3	14	434	318
4	0	541	576
4	1	1141	1126
4	2	344	326
4	5	1077	1082
4	9	554	579
4	11	549	533
4	14	672	617
4	15	452	513
4	18	936	1059
5	0	726	697
5	3	729	796
5	7	567	563
5	11	543	431
5	17	393	262
6	1	307	424
6	2	867	860
6	6	700	714
6	7	374	434
6	8	349	292
6	11	402	357
6	12	477	468
6	13	466	490
6	25	543	527
7	1	619	627
7	3	521	444
7	4	607	637
7	5	359	401
7	6	741	689
7	7	476	349
7	10	481	471
7	12	485	535
8	2	432	355
8	3	734	668
8	4	418	494
8	5	387	428
8	12	436	467
8	20	427	146
9	4	534	595
9	5	334	152
9	6	437	488
9	8	626	623
9	9	532	492
9	10	373	290
9	12	560	588
10	0	380	375
11	4	518	487
11	5	532	448
12	0	552	564
12	5	402	486
***** K = 8 *****			
-14	6	584	616
-14	10	405	300
-12	2	743	804
-12	6	425	334
-10	11	620	744
-9	2	770	715
-9	5	537	570
-9	6	719	764
-9	9	548	560
-8	2	371	239
-8	3	516	504
-8	7	560	600
-8	11	420	338
-8	16	673	625
-8	18	559	479
-8	22	485	594
-6	3	416	403
-6	5	615	552
-6	9	852	889
-6	13	727	759
-6	17	556	559
-5	1	448	465
-5	2	338	296
-5	4	458	516
-5	5	714	797
-4	1	602	586
-4	3	356	309
-4	4	503	515
-4	5	422	439
-4	8	395	433
-4	9	460	397
-4	12	431	291
-4	13	475	548
-4	19	438	323
-3	4	579	569
-3	8	433	368
-2	1	463	583
-2	4	794	825
-2	14	570	560
-1	5	356	354
-1	8	412	408
-1	18	430	414
0	0	739	675
0	4	773	804
0	5	410	359
0	11	570	632
0	13	387	315
1	1	365	426
1	8	410	472
1	9	469	316
1	12	493	426
1	13	882	853
2	0	922	950
2	1	494	697
2	2	407	460
2	4	385	258
2	6	428	449
2	9	451	459
3	0	561	548
3	4	617	635
3	9	793	765
3	10	507	471
3	11	422	372
3	13	531	657
4	1	423	283
4	3	544	551
4	6	398	401
4	8	464	468
4	12	414	388
4	16	608	559
4	20	621	718
5	2	467	544
5	5	342	466
5	8	383	378
6	3	618	660
6	7	615	686
6	8	407	409
7	3	401	392
7	4	412	408
7	6	444	358
7	7	418	480
7	9	716	736
8	1	470	536
8	5	431	346
8	7	410	340
9	0	600	625
10	3	602	611
10	7	534	432
***** K = 9 *****			
-15	9	678	576
-13	1	534	510
-13	5	455	492
-9	5	416	229
-9	9	550	567
-9	21	511	486
-7	9	756	772
-7	13	903	832
-7	20	523	384
-7	24	478	427
-5	6	449	415
-5	8	667	737
-5	12	611	658
-5	14	479	424
-5	16	780	809
-5	22	378	160
-4	1	471	537
-4	3	540	597
-4	7	418	381
-3	2	646	558
-3	6	454	377
-3	8	456	432
-3	9	484	460
-3	10	585	555
-3	13	467	493
-3	14	471	469
-3	21	453	257
-2	2	510	552
-1	1	636	599
-1	4	402	400
-1	5	710	779
-1	8	474	502
-1	9	625	595
-1	13	496	362
1	3	658	724
1	5	519	483
1	7	514	453
1	9	447	426
1	24	443	492
2	0	380	46
2	6	557	449
3	2	649	724
3	3	432	376
3	5	513	474
3	6	465	618
3	7	429	413
3	12	510	392
4	1	507	642
4	3	473	529
5	11	658	682
5	15	441	420
5	17	575	452
5	21	617	689
7	20	457	366
-3	3	472	430
***** K = 10 *****			
-10	5	460	513
-8	12	593	536
-8	16	[illegible]	350
-6	15	429	351
-6	17	637	532
-4	5	735	684
-4	9	707	683
-4	13	522	607
-3	4	461	577
-2	8	469	435
-2	9	466	425
-2	10	516	530
-2	14	651	612
0	4	570	492
0	8	469	499
***** K = 11 *****			
-3	4	566	553
3	0	569	676
3	4	577	527

of each ring atom. Thus, taking the refined over-all thermal parameter, 26% was subtracted for the carbon atom attached to the phosphorus atom, 7.5% was subtracted for the *ortho*-carbon atoms, 9.5% was added for the *meta*-carbon atoms, and 22% was added for the *para*-carbon atom. These percentage corrections were average values derived from a series of group refinements in this laboratory. In subsequent calculations, only the over-all value was refined.

A cycle of least-squares refinement was carried out in which the two cobalt, six phosphorus, and four nitrogen atoms were refined anisotropically and the eighteen phenyl rings were refined as groups with the described individual thermal parameters. This refinement, which had not converged, gave agreement factors of $R_1 = 0.072$ and $R_2 = 0.069$.

In the final cycle of refinement, the calculated contributions of the two hydride atoms were included ($B = 5.0$ Å^2), and an extinction parameter was varied. The extinction parameter was found to be negligible, and the refinement converged at values of $R_1 = 0.065$ and $R_2 = 0.061$. A statistical analysis[9] of R_2 showed no unusual trends with $|F_o|$, $\lambda^{-1} \sin \theta$, or various combinations of Miller indices. For the 236 variables and 3312 observations, the error in an observation of unit weight was 1.80 e$^-$. A final difference Fourier synthesis showed no peak higher than 0.37 (5) e$^-$/Å^3. The largest peaks in this map were associated with phenyl ring carbon atoms. The agreement factors based on $F_o{}^2$ are $R_1 = 0.090$ and $R_2 = 0.121$. Structure factors for reflections with $I < 3\sigma(I)$ were calculated, and a statistical analysis showed no unusual trends. For those reflections in the region $0° < 2\theta \leqslant 80°$, in which all independent data were collected, there were only three reflections whose calculated values were greater than $3\sigma(F_o)$. In the range $80° < 2\theta \leqslant 110°$ only data based on the first, incorrect solution were collected, so no complete analysis can be made, but only four reflections were observed with an error greater than $3\sigma(F_o)$.

The positional, thermal, and group parameters derived from the last cycle of refinement are presented in Table I, along with the associated standard deviations in these parameters as estimated from the inverse of the normal equations matrix. The positional parameters of the hydride hydrogen atoms are also included, as derived from the interpolated peak positions on the Fourier syntheses. The positional and thermal parameters of the ring carbon atoms and the positional parameters of the phenyl hydrogen atoms (which were

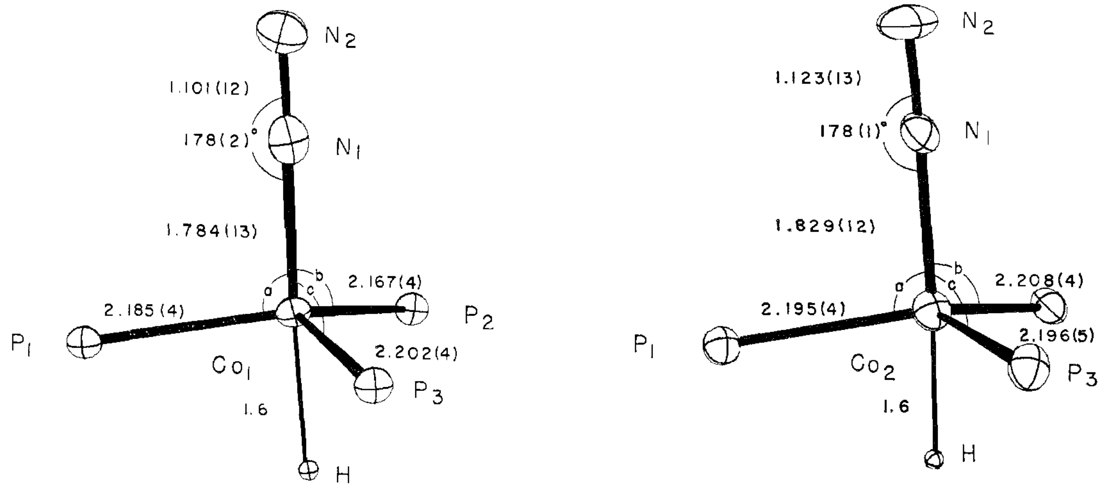

Figure 1.—Inner coordination spheres of the two molecules. Thermal ellipsoids are drawn at a 50% probability level. The N–Co–P angles are: molecule I, $a = 97.5$ (5), $b = 99.6$ (4), $c = 98.4$ (4)°; molecule II, $a = 96.3$ (4), $b = 99.3$ (4), $c = 96.9$ (4)°.

not refined) are listed in Tables II and III. The final values of $10|F_o|$ and $10|F_c|$ (in electrons) are given in Table IV for the 3312 reflections which were used in the refinement.

Description of the Structure

The structure consists of discrete, nearly identical molecules of $CoH(N_2)(P(C_6H_5)_3)_3$. The inner coordination sphere of each of the independent molecules in the cell is shown in Figure 1. The coordination about each cobalt atom is that of a trigonal bipyramid, with the three phosphorus atoms in the equatorial plane and the hydrogen atom and one atom of the nitrogen molecule occupying the apical positions. This coordination is essentially the same, but is more accurately determined than that reported in the earlier structure of $CoH(N_2)(P(C_6H_5)_3)_3 \cdot (C_2H_5)_2O$.[5]

The volume per triphenylphosphine group in the present structure is 375 Å^3, almost identical with that of 374 Å^3 for the closely related compound $RhH(CO)(P(C_6H_5)_3)_3$[15] and slightly larger than that in triphenylphosphine itself (364 Å^3).[16] Accordingly, the packing of the molecules is primarily determined by interactions of the bulky phenyl rings, the closest such intermolecular interaction being between ring hydrogen atoms at a distance of 2.3 Å. Figure 2 illustrates the overall molecular structure of molecule I (molecule II is very similar). It is clear that the cobalt atom is distinctly five-coordinate, the closest interactions between cobalt and ring hydrogen atoms being 3.13 Å for molecule I and 3.17 Å for molecule II.

A selection of intramolecular bond distances and angles, together with estimated standard deviations in parentheses, as derived with the inclusion of correlation effects, is given in Tables V and VI. The root-mean-square amplitudes of vibration along the principal axes of vibration for the atoms in the inner coordination spheres are given in Table VII. The directions of vibration may be discerned from Figure 1.

TABLE V
BOND DISTANCES

Atoms	Distance, Å	
	Molecule I	Molecule II
Co–P1	2.185 (4)	2.195 (4)
Co–P2	2.167 (4)	2.208 (4)
Co–P3	2.202 (4)	2.196 (5)
Co–N1	1.784 (13)	1.829 (12)
Co–N2	2.884 (12)	2.951 (12)
Co–H	1.64 (11)	1.67 (12)
N1–N2	1.101 (12)	1.123 (13)
P1–P2	3.795 (5)	3.811 (5)
P1–P3	3.632 (5)	3.730 (6)
P2–P3	3.791 (5)	3.789 (6)
P1–N1	2.996 (15)	3.007 (12)
P2–N1	3.028 (14)	3.085 (13)
P3–N1	3.029 (13)	3.021 (14)
P1–N2	3.820 (14)	3.841 (13)
P2–N2	3.901 (14)	3.977 (14)
P3–N2	3.877 (13)	3.890 (14)
P1–H	2.67 (11)	2.52 (12)
P2–H	2.69 (11)	2.36 (12)
P3–H	2.19 (11)	2.87 (12)
P1–R1C1	1.846 (7)	1.849 (9)
P1–R2C1	1.845 (10)	1.850 (15)
P1–R3C1	1.839 (9)	1.847 (10)
P2–R4C1	1.849 (12)	1.855 (10)
P2–R5C1	1.847 (9)	1.857 (11)
P2–R6C1	1.855 (11)	1.842 (12)
P3–R7C1	1.852 (8)	1.861 (11)
P3–R8C1	1.848 (12)	1.857 (11)
P3–R9C1	1.852 (11)	1.863 (11)

From the data of Table V it is clear that there are significant differences in certain bond distances and angles. We take but one example: on the assumption that the six P · · · P distances are equal, one derives a standard deviation of a single observation of 0.069 Å, over 10 times that derived from the least-squares procedure. Although it is possible that the standard deviations derived from the least-squares procedure may be too small, there certainly is no evidence from this or similar studies that they are too small by a factor of 10. In fact, in the present case we would expect the standard deviations to be too large, because of the higher residuals resulting from the restriction of

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(15) S. J. La Placa and J. A. Ibers, *Acta Cryst.*, **18**, 511 (1965).

(16) J. J. Daly, *J. Chem. Soc.*, 3799 (1964).

TABLE VI
BOND ANGLES

Atoms	Angle, deg Molecule I	 Molecule II
Co–N1–N2	178 (2)	178 (1)
N1–Co–H	166 (4)	168 (4)
P1–Co–H	87 (3)	80 (3)
P2–Co–H	89 (3)	73 (4)
P3–Co–H	68 (4)	95 (4)
P1–Co–P2	121.4 (2)	119.9 (2)
P1–Co–P3	111.7 (2)	116.3 (2)
P2–Co–P3	120.4 (2)	118.7 (2)
P1–Co–N1	97.5 (5)	96.3 (4)
P2–Co–N1	99.6 (4)	99.3 (4)
P3–Co–N1	98.4 (4)	96.9 (4)
Co–P1–R1C1	118.3 (3)	113.3 (3)
Co–P1–R2C1	118.0 (3)	121.9 (5)
Co–P1–R3C1	115.1 (3)	116.0 (4)
Co–P2–R4C1	119.4 (4)	114.8 (4)
Co–P2–R5C1	115.9 (3)	119.4 (4)
Co–P2–R6C1	116.7 (4)	117.9 (4)
Co–P3–R7C1	113.3 (3)	117.5 (4)
Co–P3–R8C1	119.8 (4)	117.7 (4)
Co–P3–R9C1	117.7 (4)	117.9 (4)
R1C1–P1–R2C1	98.2 (4)	101.1 (6)
R1C1–P1–R3C1	101.5 (4)	102.0 (5)
R2C1–P1–R3C1	103.0 (4)	99.6 (7)
R4C1–P2–R5C1	101.1 (5)	100.5 (5)
R4C1–P2–R6C1	99.3 (5)	102.3 (5)
R5C1–P2–R6C1	101.4 (4)	99.0 (5)
R7C1–P3–R8C1	103.2 (5)	97.9 (5)
R7C1–P3–R9C1	98.3 (4)	101.7 (5)
R8C1–P3–R9C1	101.5 (5)	100.8 (5)

TABLE VII
ROOT-MEAN-SQUARE AMPLITUDES OF VIBRATION (IN Å)

	Molecule I			Molecule II		
Atom	Min	Intermed	Max	Min	Intermed	Max
Co	0.156 (5)	0.179 (5)	0.202 (4)	0.203 (4)	0.220 (4)	0.238 (4)
P1	0.170 (8)	0.187 (7)	0.203 (8)	0.203 (7)	0.214 (7)	0.223 (4)
P2	0.162 (8)	0.196 (7)	0.206 (7)	0.190 (7)	0.225 (6)	0.256 (6)
P3	0.163 (7)	0.192 (7)	0.204 (7)	0.206 (8)	0.221 (7)	0.261 (7)
N1	0.17 (2)	0.23 (2)	0.29 (2)	0.19 (2)	0.24 (2)	0.28 (2)
N2	0.24 (2)	0.24 (2)	0.29 (2)	0.19 (3)	0.32 (2)	0.35 (2)

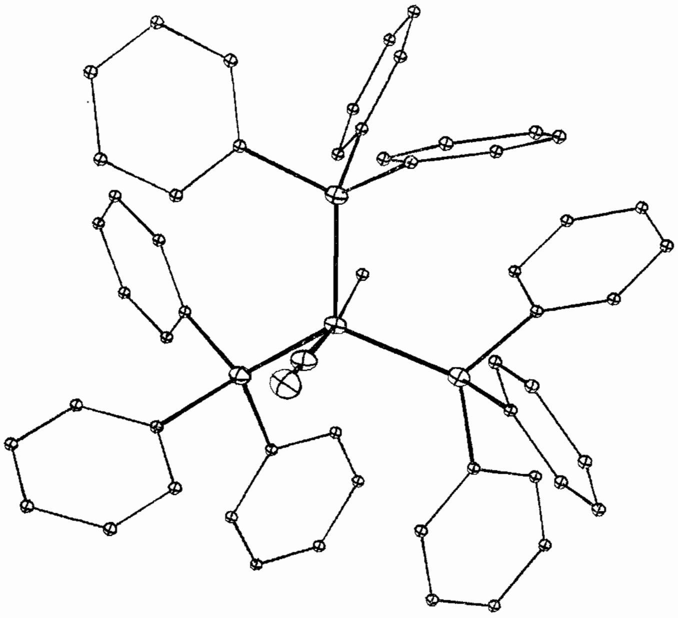

Figure 2.—Over-all view of molecule I. The thermal ellipsoids of the ring carbon atoms have been reduced for clarity.

TABLE VIII
LEAST-SQUARES PLANES

	Molecule I	Molecule II
	Eq of plane $36.622x + 1.864y - 5.008z = 12.478$	Eq of plane $29.350x + 6.830y - 0.732z = 3.941$
Atom	Dev from plane, Å	Dev from plane, Å
Co	−0.161 (2)	−0.150 (2)
P1	+0.200 (4)	+0.129 (4)
P2	+0.160 (4)	+0.140 (4)
P3	+0.127 (4)	+0.141 (4)

a significant fraction of the scattering matter, namely, the 18 phenyl rings, to a fixed geometry. We thus conclude that there are significant differences among certain bond distances or angles, but we can offer no convincing explanation for these differences. In the ensuing discussion we will often, for convenience, talk about average values, even though averaging is not always strictly valid.

Although there are significant variations among the Co–P bonds, the mean distance of 2.192 (6) Å is comparable with that of 2.18 (2) Å in $[Co(CO)_3P(n\text{-}C_4H_9)_3]_2$.[17] The N–Co–P angles are all greater than 97°. In molecule I the cobalt atom lies 0.321 Å above the plane of the three phosphorus atoms toward the N_2 ligand; in molecule II this distance is 0.283 Å. The best, weighted least-squares planes through the cobalt and three phosphorus atoms of each molecule are given in Table VIII.

Of great interest in this structure is the geometry of the Co–N1–N2 entity. The attachment of the nitrogen molecule is end-on, the Co–N1–N2 angles of 178 (2) and 178 (1)° representing an arrangement that does not deviate significantly from linearity. Such an arrangement seems probable also in the $Ru(NH_3)_5(N_2)^{2+}$ cation,[2,3] but owing to disorder of the NH_3 and N_2 groups, no accurate bond distances or angles could be determined.

The Co–N mean distance is 1.807 (23) Å. This distance is compared with a number of metal–nitrogen distances in Table IX for a series of rhenium(V) and osmium(VI)–phosphine complexes. It is clear from the trend observed in this series and a comparison with the Co–N distance of 1.95 Å measured in $[Co(NH_3)_6]I_3$ that there is some multiple bonding between the cobalt atom and the nitrogen atom. In fact, the Co–N distance is comparable with known Co–C distances in carbonyl complexes such as 1.753 (33) Å found in $[Co(CO)_3P(n\text{-}C_4H_9)_3]_2$.[17]

The N–N distances of 1.101 (12) and 1.123 (13) Å average 1.112 (11) Å. These are compared with other N–N distances in Table X. Although the evidence is not incontrovertible, there is a reasonable trend to suggest that the N–N bond has been weakened slightly over that in molecular nitrogen.

Thus the over-all picture that arises for the bonding of molecular nitrogen to the cobalt atom is very similar to that envisioned for the isoelectronic carbonyl group. Presumably there is donation from the nitrogen mole-

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(17) J. A. Ibers, *J. Organometal. Chem.* (Amsterdam), **14**, 423 (1968).

Table IX

Summary of Metal–Nitrogen Bond Lengths

Bond type	Dist, Å	Ref
M≡N	1.60	*a, b*
M=N–	1.70	*c–e*
M—N<	1.95–2.15	*f*
Co—N$\overline{\cdots}$N	1.807 (23)	This work
Co—N<	1.95	*g*

[a] See ref 8. [b] D. Bright and J. A. Ibers, *Inorg. Chem.*, **8,** 709 (1969). [c] D. Bright and J. A. Ibers, *ibid.*, **7,** 1099 (1968). [d] D. Bright and J. A. Ibers, *ibid.*, **8,** 703 (1969). [e] J. Strähle and H. Bärnighausen, *Z. Anorg. Allgem. Chem.*, **357**, 325 (1968). [f] D. Bright and J. A. Ibers, *Inorg. Chem.*, **8,** 1078 (1969). [g] N. E. Kime and J. A. Ibers, *Acta Cryst.*, **B25**, 168 (1969), and references therein.

Table X

Summary of N–N Bond Lengths

Species	Dist, Å	Bond order	Ref
N_2(g)	1.098	3.0	*a*
N_2^+	1.116		*b*
N_2O	1.126	2.5	*c*
HN_3	1.134	2.5	*d*
	1.240	1.5	*d*
Co—N$\overline{\cdots}$N	1.112 (11)	~2.5	This work

[a] P. G. Wilkinson and N. B. Houk, *J. Chem. Phys.*, **24**, 528 (1956). [b] P. G. Wilkinson, *Can. J. Phys.*, **34**, 250 (1956). [c] A. E. Douglas and C. K. Moller, *J. Chem. Phys.*, **22**, 275 (1954). [d] E. Amble and B. P. Dailey, *ibid.*, **18**, 1422 (1950).

cule to the metal with consequent back-bonding from the metal into the π^* antibonding orbitals of the ligand. This results in a slight weakening of the N–N bond and some multiple bonding in the Co–N linkage.

This structure also offers additional proof for the attachment of a hydrogen atom to the cobalt atom. The hydrogen atom parameters were not included in the refinement as variables but as fixed values derived from interpolated peak positions in the difference Fourier syntheses. The Co–H distances are 1.64 (11) and 1.67 (12) Å, with N–Co–H angles of 166 (4) and 168 (4)° for molecule I and molecule II, respectively. These values are comparable with the Rh–H distance of 1.60 (12) Å and the C–Rh–H angle of 170 (5)° found in $RhH(CO)(P(C_6H_5)_3)_3$[15] and the Mn–H distance of 1.601 (16) Å found in $HMn(CO)_5$.[18] The closest approach of a ring hydrogen atom to a hydride hydrogen atom is 1.90 Å.

An nmr study[19] revealed that when benzene solutions of this complex are equilibrated with deuterium gas, the nitrogen ligand is replaced and all *ortho* protons of the phenyl rings exchange, as well as the hydride hydrogen atom. A rapid equilibrium is postulated, in which there is formation of a bond between the *ortho*-carbon atom of a phenyl ring and the cobalt atom. On breakage of this bond, a carbon–deuterium bond is formed, the final product being the *o*-deuterioaryl analog of $CoD_3(P(C_6H_5)_3)_3$ reported by Sacco and Rossi.[20] The structural details reported here do not preclude such an equilibrium process, but the molecules are clearly five-coordinate in the solid state, and there is no tendency toward six-coordination of the cobalt atom through the close approach of a phenyl ring hydrogen atom.

The molecular structure reported here, of the material grown from di-*n*-butyl ether solution, is similar to that reported earlier for $CoH(N_2)(P(C_6H_5)_3)_3 \cdot (C_2H_5)_2O$. In that complex, no phenyl hydrogen atom approached to within 3.0 Å of the cobalt atom, and this was adduced as evidence for the presence of a hydride hydrogen atom. The similarity between the present over-all geometry of the phenyl rings relative to the cobalt atom and that of the earlier study suggests that the formulation of the material as $CoH(N_2)(P(C_6H_5)_3)_3 \cdot (C_2H_5)_2O$ was correct. In view of the similarity between the two studies and our inability to grow suitable crystals of the original material, we do not intend to enlarge upon our previous communication.[5]

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(18) S. J. La Placa, W. C. Hamilton, J. A. Ibers, and A. Davison, *Inorg. Chem.*, **8**, 1928 (1969).

(19) G. W. Parshall, *J. Am. Chem. Soc.*, **90**, 1669 (1968).

(20) A. Sacco and M. Rossi, *Chem. Commun.*, 316 (1967).