shorter than the corresponding distance in the chloro derivative, supporting the hypothesis of a (d $\rightarrow$ d) π bond between these atoms. The other distances which Robinson and Ibers suggested[1] might provide additional evidence for such a bond were not significantly different in the two compounds.

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CONTRIBUTION FROM THE DEPARTMENT OF CHEMISTRY,
NORTHWESTERN UNIVERSITY, EVANSTON, ILLINOIS 60201

The Crystal Structure of Solvated Hydridochloro(trichlorosilyl)bis(triphenylphosphine)rhodium, $RhHCl(SiCl_3)(P(C_6H_5)_3)_2 \cdot xSiHCl_3$

BY KENNETH W. MUIR AND JAMES A. IBERS

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The crystal structure of solvated hydridochloro(trichlorosilyl)bis(triphenylphosphine)rhodium, $RhHCl(SiCl_3)(P(C_6H_5)_3)_2 \cdot xSiHCl_3$, has been determined by X-ray diffraction methods. The compound crystallizes in the space group C_i^1-$P\bar{1}$ of the triclinic system. There are two molecules of $RhHCl(SiCl_3)(P(C_6H_5)_3)_2$ in a unit cell of dimensions a = 11.727 (5) Å, b = 12.952 (6) Å, c = 13.365 (5) Å, α = 104.65 (2)°, β = 98.08 (2)°, γ = 94.43 (2)°. The structure has been refined by least-squares methods to a conventional R factor of 0.064 over 2485 counter-diffractometric data. It consists of discrete monomeric molecules of $RhHCl(SiCl_3)(P(C_6H_5)_3)_2$ and $SiHCl_3$. The latter are disordered over four different sites; the $SiHCl_3$:Rh ratio is 0.397 (7). The rhodium coordination polyhedron may be described as a highly distorted trigonal bipyramid, with *trans* phosphines at the apices and H, Cl, and $SiCl_3$ in the trigonal plane. Alternatively, the coordination about the formally d^6 Rh(III) ion is distorted octahedral if one chooses to include at the sixth coordination site the contact of 2.79 Å with an *ortho*-hydrogen atom on a phenyl ring of a triphenylphosphine group. The short Rh–Si distance of 2.203 (4) Å is consistent with back-donation of electrons from the metal to the silyl group.

Introduction

The nature of metal–silicon bonding in transition metal–silyl complexes is at present a subject of debate.[1,2] Structural details have been published only for the cobalt complexes $Co(SiR_3)(CO)_4$ (R = F,[3] Cl,[4] H[5]) and for $Mn(Si(CH_3)_3)(CO)_5$.[6] It is our contention that a fruitful discussion of such problems as the relative importance of d_π–d_π back-bonding and electronegativity differences in stabilizing metal–silicon bonds and whether the metal–silicon bond may appropriately be considered as a metal–metal bond will only be possible if adequate structural data are at hand on a sufficient number of representative metal–silyl complexes.

Accordingly, we have determined the crystal structure of the formally d^6 complex hydridochloro(trichlorosilyl)bis(triphenylphosphine)rhodium(III), $RhHCl(SiCl_3)(P(C_6H_5)_3)_2$. This compound was chosen because we believed that back-donation to silicon would be favored by the presence of a second- as opposed to a first-row transition metal and by the absence of strongly π-bonding ligands such as carbonyl. In addition, this compound contains five-coordinate rhodium(III). Five-coordination is much less common in d^6 systems than it is in d^0, d^8, or d^{10} systems;[7] the only d^6 complexes for which structural data are available are the ruthenium(II) complexes $RuXCl(P(C_6H_5)_3)_3$ (X = Cl,[8] H[9]) and $Rh(CH_3)I_2(P(C_6H_5)_3)_2$.[10] Further motives for our interest in this molecule were the presence of a metal–hydrogen bond and the relationship between the structure of the molecule and its postulated role as an intermediate in the catalytic hydrosilation of olefins.

The compound $RhHCl(SiCl_3)(P(C_6H_5)_3)_2$ has been prepared independently by two groups. Haszeldine, Parish, and Parry[11] obtained an unsolvated complex. While this work was underway, de Charentenay, Osborn, and Wilkinson[12] reported a slightly different preparation which yields solvated complexes; these authors suggested that the complexes containing free

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chlorosilanes might involve weak coordination of the substituted silane molecule *via* chlorine to the rhodium atom of $RhHCl(SiCl_3)(P(C_6H_5)_3)_2$.

Collection and Reduction of the X-Ray Data

Two samples of $RhHCl(SiCl_3)(P(C_6H_5)_3)_2$ were kindly given to us by Dr. R. V. Parish. The first, prepared by the original method of Haszeldzine, Parish, and Parry,[11] proved not to contain crystals suitable for a diffraction study. All X-ray measurements were therefore made on crystals from the second sample, which was prepared by treating trichlorosilane with solid chlorotris(triphenylphosphine)rhodium and subsequently pumping off the volatile products. The crystals decompose rapidly in air. Those used in the present work were mounted in well-dried glass capillaries under dry nitrogen.

Preliminary optical and photographic examination of the crystals suggested that they belong to the triclinic system. The dimensions of the Delaunay reduced cell, determined at 22° by the least-squares method outlined below, are $a = 11.727$ (5) Å, $b = 12.952$ (6) Å, $c = 13.365$ (5) Å, $\alpha = 104.65$ (2)°, $\beta = 98.08$ (2)°, $\gamma = 94.43$ (2)° (λ Mo Kα_1) 0.70930 Å). The density calculated for two solvent-free molecules per unit cell is 1.373 g cm^{-3}. Owing to the instability of the crystals in air, their density was not measured. The centrosymmetric triclinic space group C_i^1-$P\bar{1}$ was assumed to be the correct one; this assumption has been confirmed by a successful structure analysis.

Intensity measurements were made on a Picker four-circle diffractometer using procedures which have already been described in detail.[13] A crystal of dimensions 0.14 mm × 0.20 mm × 0.33 mm (in the a^*, b^*, and c^* directions) was mounted on the diffractometer so that c^* was roughly coincident with the ϕ axis. The mean half-width of a number of narrow source–open counter ω scans[14] was 0.30°, indicating that the mosaicity of the specimen was relatively high. These scans were, however, free of fine structure. Fourteen reflections in the range $10° < 2\theta$ (Mo Kα_1) $\leq 30°$ were carefully centered through a top–bottom device and then through a narrow vertical slit at a takeoff angle at 0.5° to yield values of χ, ϕ, and 2θ for each reflection. These observations were used to determine the crystal orientation and cell dimensions by the method of least squares.[13,15] Intensity measurements were made with the θ–2θ scan technique at a takeoff angle of 2.8°. Each peak was scanned from -1.0 to $+1.0°$ in 2θ from the Mo Kα_1 center at a scan rate of 1°/min. The background was counted for 20 sec at each extreme of the scan range. Molybdenum radiation was used, in conjunction with a 3-mil niobium β filter and a pulse-height analyzer set to accept approximately a 90% window, centered on the Mo Kα peak. The distances of the crystal from the source and from the counter were, respectively, 21 and 30 cm. The dimensions of the counter aperture were 6 mm vertically and 4 mm horizontally. Coincidence losses were cut by inserting copper foil attenuators into the diffracted beam until the maximum counting rate during a scan was less than 7000 counts/sec.

The intensities of 3342 independent reflections in the range 2θ(Mo Kα_1) $\leq 39°$ were measured. In the range $36° \leq 2\theta$(Mo Kα_1) $\leq 39°$ few reflections were found to be significantly above background. The intensities of four strong reflections were measured periodically throughout the experiment in order to monitor crystal and electronic stability. The intensities of these standards gradually decreased, until they were about 90% of their initial values, presumably owing to decomposition of the specimen. The observed peak intensities were corrected on the assumption that decomposition was linear with time. The integrated intensities and their standard deviations were derived as before.[13] A value of $p = 0.04$ was assumed, where $\sigma(I)/I$ approaches p as the counting errors become negligible.[13] The intensities of 2485 reflections were greater than three times their estimated standard deviations. Only these reflections were used in the subsequent analysis. In order to apply corrections for absorption, the dimensions of the crystal were determined and then the faces of the crystal were indexed on the diffractometer. All members of the forms $\{100\}$, $\{010\}$, and $\{001\}$ were exhibited. The calculated transmission coefficients, based on a linear absorption coefficient of 8.4 cm^{-1} for Mo K$\bar{\alpha}$ radiation, ranged from 0.76 to 0.90. It was subsequently found (*vide infra*) that the cell contains about 0.4 molecule of $SiHCl_3$ per molecule of the rhodium complex. The calculated density then becomes 1.46 g/cm^3 and the linear absorption coefficient becomes 9.4 cm^{-1}. The relative errors in the transmission coefficients introduced by this change in the linear absorption coefficient are negligible.

Structure Determination

The positions of the rhodium atom and of the atoms of the trichlorosilyl ligand were determined from the three-dimensional Patterson function. The sites of the remaining nonhydrogen atoms were obtained from subsequent electron density syntheses. The model so obtained was refined by the method of full-matrix least squares. The function minimized was $\Sigma w\Delta^2$, where $\Delta = |F_o| - |F_c|$, $|F_o|$ and $|F_c|$ are, respectively, the observed and calculated structure amplitudes, and $w = 1/\sigma^2(F_o) = 4F_o^2/\sigma^2(F_o^2)$. The atomic scattering factors used throughout the analysis were taken from ref 16, with the exceptions of those for Rh[17] and H.[18] The real and imaginary anomalous scattering corrections of

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TABLE I

POSITIONAL, THERMAL, AND GROUP PARAMETERS FOR $RhHCl(SiCl_3)(P(C_6H_5)_3)_2 \cdot xSiCl_3$

Atom	x	y	z	β_{11} or B_{iso}[a]	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Rh	0.19467(10)[b]	0.12720(8)	−0.22192(8)	789(14)	651(11)	643(11)	52(7)	87(7)	156(7)
Si	0.3382(4)	0.2019(3)	−0.2795(3)	882(43)	893(37)	1016(40)	−107(31)	238(32)	111(30)
Cl(1)	0.3228(4)	0.3487(4)	−0.3098(4)	1489(54)	1305(45)	1530(49)	−43(38)	477(40)	718(38)
Cl(2)	0.3984(5)	0.1198(4)	−0.4094(4)	1852(65)	1722(56)	1802(58)	−616(47)	1163(50)	−494(44)
Cl(3)	0.4835(4)	0.2341(4)	−0.1650(4)	946(43)	1274(44)	1727(52)	−209(33)	−245(36)	351(37)
Cl	0.2398(3)	0.1019(3)	−0.0506(3)	1008(39)	864(32)	667(28)	108(26)	−17(25)	229(23)
P(1)	0.1185(3)	0.2841(3)	−0.1434(3)	866(37)	560(28)	672(30)	44(25)	144(25)	156(22)
P(2)	0.2103(3)	−0.0522(3)	−0.3018(3)	849(38)	653(30)	656(30)	112(26)	24(25)	119(23)
Si(S)[c]	$^1/_2$	$^1/_2$	$^1/_2$	26.8(9)					
Cl(S1)	0.461(2)	0.356(1)	0.438(1)	26.2(7)					
Cl(S2)	0.322(2)	0.517(1)	0.493(1)	24.6(7)					
H	0.15	0.14	−0.33						

Groups	x_c[d]	y_c	z_c	δ	ϵ	η
P(1)R(1)[e]	0.2695(6)	0.4304(5)	0.0731(5)	−1.253(8)	2.459(6)	−1.438(7)
P(1)R(2)	0.0411(5)	0.4448(5)	−0.2806(5)	2.544(8)	2.369(6)	2.347(8)
P(1)R(3)	−0.1261(5)	0.2111(4)	−0.0817(4)	0.263(5)	0.147(5)	0.428(5)
P(2)R(1)	0.3956(6)	−0.1725(6)	−0.1884(5)	−0.676(6)	0.230(6)	2.780(6)
P(2)R(2)	0.2336(5)	−0.1190(5)	−0.5456(5)	0.681(6)	3.093(6)	1.654(6)
P(2)R(3)	−0.0389(5)	−0.1663(4)	−0.2886(5)	−1.090(7)	2.396(5)	1.385(8)

[a] The β_{ij} have been multiplied by 10^5; the form of the anisotropic temperature factor 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] Throughout this paper limits of errors are estimated standard deviations. They are given in units of the least significant digits of the quantity to which they refer. [c] Si(S), Cl(S1), and Cl(S2) are the independent atoms of the disordered $SiHCl_3$ solvent in the cell. [d] x_c, y_c, z_c are fractional coordinates of the phenyl-ring centroids; the angles δ, ϵ, η (radians) have been defined previously.[24] [e] P(1)R(1): phenyl ring 1 bonded to phosphorus atom P(1).

Cromer[19] for Rh, Cl, P, and Si were applied to the calculated structure factors.[20] In all refinement calculations the phenyl rings were constrained to D_{6h} symmetry and the C–C bond length was assumed to be 1.392 Å. In the initial refinement the nongroup atoms were constrained to isotropic vibration, and a single isotropic vibrational parameter was adjusted for each group. This refinement converged to values of R and R_w of 0.12 and 0.15, respectively, where the reliability indices are $R = \Sigma|\Delta|/\Sigma|F_o|$ and $R_w = (\Sigma w\Delta^2/\Sigma wF_o^2)^{1/2}$.

The reasons for the poor agreement at this stage of the analysis were apparent on inspection of a difference map. Situated close to the center of symmetry at ($^1/_2$, $^1/_2$, $^1/_2$) were three independent peaks, each about 2 e$^-$/Å^3 in height. Since these peaks were not within bonding distance of any atoms of the $RhHCl(SiCl_3)(P(C_6H_5)_3)_2$ molecule, we concluded that they were due to the presence of solvent of crystallization. We were unable to perform any experiments on the crystal to determine the nature of the solvent. However, the samples of $RhHCl(SiCl_3)(P(C_6H_5)_3)_2$ prepared by Wilkinson and his coworkers[12] by direct reaction of trichlorosilane with $RhCl(P(C_6H_5)_3)_3$ contained one-third of a molecule of trichlorosilane per rhodium. In the absence of definitive analytical data for the crystal used in the present work we have assumed that the residual peaks on the difference map are due to highly disordered trichlorosilane molecules. It was also apparent from this difference map that the motions of several of the heavier atoms, in particular those of the trichlorosilyl ligand, were highly anisotropic.

In a further round of calculations the positional parameters of the group and nongroup atoms were again adjusted; anisotropic thermal parameters for the nongroup atoms and individual isotropic thermal parameters for the carbon atoms of the phenyl rings were refined. In these calculations reflections for which $\lambda^{-1} \sin\theta < 0.29$ Å^{-1} were assigned weights of zero. This course was adopted for the following reason. Inspection of the results of isotropic refinements with and without solvent contributions indicated, as expected, that scattering from the disordered solvent molecules made little or no contribution to the high-angle data. The positional and thermal parameters for the $RhHCl(SiCl_3)(P(C_6H_5)_3)_2$ molecule derived from the high-angle data alone should thus be relatively unbiased by our failure to correct for the solvent scattering or by the adoption of an inadequate model for such scattering. The high-angle refinement led to values of R and R_w of 0.062 and 0.068 for the 1804 high-angle data and to values of 0.084 and 0.133 for all 2485 data.

In an attempt to account for the solvent scattering, a trichlorosilane group was next introduced into the calculations. An Si–Cl distance of 2.01 Å was assumed, as were tetrahedral angles within the molecule. The ratio of solvent to rhodium complex was taken to be 1:3. The refinement converged after two cycles to values of R and R_w of 0.079 and 0.106 (146 variables, 2485 data). The resultant positions of the atoms within the solvent molecule are consistent with those three peaks found on the previous difference Fourier map. Two of those peaks correspond to two of the chlorine atoms. The third peak (the one nearest to $^1/_2$, $^1/_2$, $^1/_2$) results from the overlap of the silicon atom with the third chlorine atom, yet this description of the solvent scattering is still unsatisfactory, for the major features in a subsequent difference Fourier map were all in the region of this molecule, the highest peak being 1.7 e$^-$/Å^3. Attempts to reduce these residual peaks

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by variation in the amount of trichlorosilane in the cell were not successful. The best agreement with the data is achieved when a ratio of one molecule of solvent to three molecules of the rhodium complex is used.

A careful examination of the electron density in the vicinity of $^1/_2$, $^1/_2$, $^1/_2$ on the original difference Fourier map suggests that the solvent molecules are arranged in a more complex manner than the simple disordering of a molecule across a center of symmetry assumed above. Although no unique description is possible, a model in which there is equal disordering of two independent solvent molecules about the center of symmetry, leading to four orientations of four half-molecules, reproduces well the main features of the density map. Yet such a model seems too elaborate and too uncertain to justify the direct refinement of two independent trichlorosilane groups. Rather we chose to simulate this model by placing individual atoms in the positions corresponding to the three main peaks on the difference Fourier map. The silicon atom was placed at $^1/_2$, $^1/_2$, $^1/_2$, near the position of one of the peaks. This atom was assigned a multiplier α which was initially given the value $^1/_3$. The two remaining solvent peaks were assumed to be chlorine atoms. Each chlorine atom was assigned a multiplier 1.5α to obtain the overall stoichiometry Si:Cl = 1:3. In this refinement all data were again used, and the positional and thermal parameters were adjusted for all the nonhydrogen atoms. The occupancy parameter α was also refined. Also in this final refinement fixed contributions for the scattering of the hydrogen atoms of the phenyl rings were introduced.

This refinement led to values of R and R_w of 0.064 and 0.079 (156 variabless, 2485 data). The final positional and thermal parameters are presented in Tables I and II, and the final values $10|F_0|$ and $10|F_o|$ (in electrons) are given in Table III. The parameters of the $RhHCl(SiCl_3)(P(C_6H_5)_3)_2$ molecule given in Tables I and II differ in most cases by less than three times their estimated standard deviations from the corresponding values obtained from the high-angle data alone. The differences from the group refinement are even smaller. Thus any systematic errors resulting from possibly incorrect treatment of the solvent scattering is small. No important conclusion from the analysis would be altered if the results of the high-angle refinement were used instead of those given in Tables I and II.

The standard deviation of an observation of unit weight is 2.4, suggesting either that the errors in $|F_o|$ have been underestimated or, more probably, that the solvent model is not wholly adequate since the mean $\Sigma w\Delta^2$ shows no systematic variation with $|F_o|$ but decreases steadily with increasing $\lambda^{-1} \sin \theta$. For none of the low-intensity reflections excluded from the analysis was $F_c^2/\sigma(F_o^2) > 2.5$. The highest peak in a difference map calculated with all 2485 data was 1.0 e$^-$/Å^3 or 25% of the mean height of a carbon atom in an observed electron density synthesis. This peak is associated with the disordered solvent. In a difference map based on the data for which $\lambda^{-1} \sin \theta < 0.30$ Å^{-1} the top two peaks were again associated with the solvent. However, the third highest peak, with $\rho = 0.55$ e/Å^3, is 1.5 Å from the rhodium atom, in a position consistent with its being due to the hydridic hydrogen atom. Positional parameters obtained from this map are given for the hydridic hydrogen H in Table I. The bond distances and angles derived from them (Table IV) are necessarily of extremely low accuracy.

TABLE II

DERIVED PARAMETERS FOR GROUP ATOMS

Atom	x	y	z	B, Å^2
		P(1)R(1)		
C(1)[a]	0.2028 (9)	0.3670 (9)	−0.0198 (6)	4.6 (3)
C(2)	0.1591 (7)	0.3831 (9)	0.0739 (8)	6.0 (4)
C(3)	0.2258 (9)	0.4464 (7)	0.1667 (6)	6.8 (4)
C(4)	0.3363 (9)	0.4937 (10)	0.1659 (7)	7.1 (4)
C(5)	0.3800 (7)	0.4777 (10)	0.0722 (9)	8.0 (4)
C(6)	0.3132 (8)	0.4143 (7)	−0.0206 (6)	7.0 (4)
		P(1)R(2)		
C(1)	0.0772 (13)	0.3765 (7)	−0.2201 (6)	4.7 (3)
C(2)	0.1013 (7)	0.4873 (8)	−0.1789 (6)	6.0 (3)
C(3)	0.0652 (12)	0.5556 (5)	−0.2394 (8)	7.3 (4)
C(4)	0.0051 (13)	0.5131 (8)	−0.3410 (7)	7.5 (4)
C(5)	−0.0191 (8)	0.4023 (8)	−0.3822 (5)	7.4 (4)
C(6)	0.0170 (11)	0.3339 (5)	−0.3218 (7)	5.6 (3)
		P(1)R(3)		
C(1)	−0.0220 (6)	0.2426 (6)	−0.1103 (6)	3.7 (3)
C(2)	−0.1009 (7)	0.3164 (5)	−0.0865 (7)	5.0 (3)
C(3)	−0.2050 (6)	0.2849 (6)	−0.0579 (7)	5.8 (3)
C(4)	−0.2302 (6)	0.1796 (7)	−0.0531 (7)	5.0 (3)
C(5)	−0.1513 (7)	0.1058 (5)	−0.0770 (7)	5.3 (3)
C(6)	−0.0472 (6)	0.1373 (6)	−0.1056 (6)	4.4 (3)
H(6)	0.010	0.085	−0.121	
		P(2)R(1)		
C(1)	0.3136 (8)	−0.1215 (7)	−0.2379 (7)	5.2 (3)
C(2)	0.4183 (10)	−0.0638 (6)	−0.1823 (8)	7.3 (4)
C(3)	0.5003 (7)	−0.1149 (9)	−0.1329 (8)	9.3 (5)
C(4)	0.4776 (9)	−0.2236 (9)	−0.1390 (8)	8.9 (5)
C(5)	0.3728 (10)	−0.2812 (6)	−0.1945 (9)	8.3 (4)
C(6)	0.2909 (7)	−0.2302 (7)	−0.2440 (7)	5.8 (3)
		P(2)R(2)		
C(1)	0.2221 (8)	−0.0939 (7)	−0.4402 (5)	4.7 (3)
C(2)	0.2936 (8)	−0.1703 (7)	−0.4785 (7)	6.0 (4)
C(3)	0.3050 (8)	−0.1955 (7)	−0.5840 (8)	7.4 (4)
C(4)	0.2450 (9)	−0.1442 (8)	−0.6511 (5)	6.9 (4)
C(5)	0.1735 (8)	−0.0677 (8)	−0.6128 (7)	7.0 (4)
C(6)	0.1621 (7)	−0.0426 (6)	−0.5073 (7)	5.5 (3)
		P(2)R(3)		
C(1)	0.0701 (7)	−0.1213 (9)	−0.2966 (7)	4.3 (3)
C(2)	0.0428 (7)	−0.1215 (10)	−0.1986 (5)	5.2 (3)
C(3)	−0.0661 (8)	−0.1664 (7)	−0.1905 (6)	6.1 (3)
C(4)	−0.1478 (7)	−0.2112 (10)	−0.2805 (8)	7.1 (4)
C(5)	−0.1206 (7)	−0.2110 (11)	−0.3786 (6)	7.1 (4)
C(6)	−0.0117 (8)	−0.1661 (7)	−0.3866 (5)	5.6 (3)

[a] In each group C(1) is bonded to a phosphorus atom and C(4) is *para* to C(1).

Description of the Structure

The crystal structure is built from discrete monomeric molecules of composition $RhHCl(SiCl_3)(P(C_6H_5)_3)_2$. Figures 1 and 2, respectively, show perspective views of the entire molecule, and of the coordination around the rhodium atom. The structure also con-

TABLE III

OBSERVED AND CALCULATED STRUCTURE AMPLITUDES (IN ELECTRONS × 10) FOR $RhHCl(SiCl_3)(P(C_6H_5)_3)_2 \cdot xSiCl_3$

K	L	FO	FC
***** H = 0 *****			
0	0		7969
0	1	419	428
0	2	1236	1078
0	3	535	613
0	4	160	236
0	5	248	214
0	6	174	199
0	7	288	297
0	8	200	210
0	11	325	330
0	12	183	174
1	-11	239	215
1	-10	156	150
1	-7	225	217
1	-6	725	748
1	-4	111	112
1	-3	384	299
1	-2	1238	1114
1	-1	1434	1259
1	0	1034	896
1	1	1142	997
1	2	71	35
1	3	275	230
1	4	590	534
1	5	369	414
1	6	111	115
1	7	244	215
1	10	333	344
1	11	206	202
2	-12	147	158
2	-8	218	206
2	-6	675	684
2	-5	744	768
2	-4	687	771
2	-3	118	99
2	-2	109	132
2	-1	766	673
2	0	525	500
2	1	189	123
2	2	838	816
2	3	306	244
2	5	637	672
2	6	800	777
2	7	511	510
2	8	410	422
2	10	208	219
3	-12	202	160
3	-10	124	159
3	-9	193	167
3	-8	249	226
3	-7	640	628
3	-6	488	465
3	-5	1230	1233
3	-4	278	323
3	-3	687	700
3	-2	949	854
3	-1	82	47
3	0	1640	1452
3	2	113	92
3	3	482	510
3	4	311	356
3	6	1045	1046
3	7	140	116
3	8	352	341
3	10	193	170
4	-12	283	304
4	-11	395	386
4	-10	129	102
4	-9	619	618
4	-8	222	202
4	-7	654	647
4	-6	473	445
4	-5	448	450
4	-4	734	736
4	-3	911	860
4	-1	242	178
4	0	1033	1026
4	1	121	72
4	2	392	366
4	4	460	446
4	5	602	582
4	6	568	587
4	7	427	420
4	9	158	155
4	10	106	97
5	-11	353	348
5	-10	441	425
5	-9	435	391
5	-7	420	403
5	-6	222	276
5	-5	261	213
5	-4	303	321
5	-3	205	222
5	-2	137	76
5	-1	477	441
5	0	820	807
5	1	1065	1069
5	2	374	335
5	3	771	776
5	5	467	495
5	7	223	231
5	8	249	283
6	-12	217	196
6	-10	367	349
6	-9	157	122
6	-8	342	347
6	-7	264	256
6	-6	517	461
6	-5	94	94
6	-3	152	141
6	-2	242	223
6	-1	118	140
6	1	669	714
6	2	310	296
6	4	197	211
6	5	214	215
6	6	174	167
6	8	156	144
7	-9	324	320
7	-7	350	348
7	-6	113	190
7	-5	600	550
7	-4	155	105
7	-3	414	447
7	-1	622	638
7	1	207	208
7	2	266	276
7	3	338	340
7	4	170	178
7	5	191	190
7	6	323	341
7	7	218	181
8	-8	153	120
8	-7	181	181
8	-6	155	171
8	-5	459	467
8	-4	472	455
8	-3	428	425
8	-2	415	439
8	-1	301	291
8	0	516	498
8	1	189	167
8	2	138	131
8	3	192	211
8	5	237	232
8	6	151	165
9	-10	222	235
9	-9	190	191
9	-8	247	257
9	-7	126	137
9	-6	395	383
9	-4	545	519
9	-3	239	237
9	-2	265	275
9	-1	185	143
9	0	174	210
9	1	219	236
9	2	126	119
9	3	170	169
9	5	175	164
10	-8	322	299
10	-6	342	352
10	-3	135	130
10	-2	134	137
10	-1	113	127
10	1	320	326
10	2	152	152
10	3	124	102
10	4	149	134
11	-7	228	174
11	-6	125	61
11	[illegible]	245	[illegible]
11	-3	174	169
11	-2	140	179
11	-1	166	146
11	0	190	191
11	1	212	229
11	2	314	310
12	-5	133	120
12	-4	355	371
12	-2	313	292
***** H = 1 *****			
-12	3	402	384
-12	5	183	162
-11	-1	318	316
-11	0	218	218
-11	1	133	132
-11	2	210	188
-11	3	135	147
-11	4	243	206
-11	6	223	190
-10	-4	174	180
-10	-3	202	198
-10	-2	198	219
-10	0	214	205
-10	5	157	156
-10	7	109	106
-10	8	126	146
-10	9	221	247
-9	-4	250	252
-9	-2	192	139
-9	1	151	143
-9	2	197	164
-9	4	307	301
-9	5	455	430
-9	6	108	47
-9	7	281	276
-9	8	137	154
-9	9	325	299
-9	10	203	158
-8	-6	416	429
-8	-4	281	271
-8	-2	269	268
-8	-1	113	67
-8	0	102	137
-8	1	264	286
-8	3	499	501
-8	4	245	217
-8	5	641	652
-8	6	408	391
-8	7	208	214
-8	8	154	129
-8	9	289	305
-8	10	231	255
-7	-8	268	275
-7	-7	376	386
-7	-6	156	147
-7	-5	182	210
-7	-4	167	167
-7	-2	469	447
-7	-1	249	276
-7	0	123	122
-7	1	383	343
-7	3	493	484
-7	4	748	803
-7	5	95	54
-7	6	529	463
-7	7	109	83
-7	8	220	249
-7	10	213	222
-7	11	261	232
-6	-7	182	195
-6	-6	214	235
-6	-4	130	169
-6	-3	451	514
-6	-1	176	191
-6	0	358	427
-6	1	283	290
-6	2	310	340
-6	4	248	241
-6	5	337	384
-6	7	123	103
-6	8	166	145
-6	9	209	203
-6	11	399	409
-5	-9	221	209
-5	-8	113	110
-5	-7	104	105
-5	-6	280	254
-5	-4	686	673
-5	-3	278	268
-5	-2	747	822
-5	-1	325	290
-5	0	982	975
-5	1	545	542
-5	2	746	759
-5	3	237	179
-5	4	198	246
-5	6	259	239
-5	8	157	127
-5	9	274	256
-5	10	303	284
-5	11	275	256
-5	12	267	253
-4	-7	167	142
-4	-6	507	525
-4	-5	414	413
-4	-4	654	684
-4	-3	88	33
-4	-2	842	818
-4	-1	914	898
-4	0	854	815
-4	1	1636	1647
-4	2	538	521
-4	3	620	586
-4	5	765	766
-4	6	502	510
-4	7	133	149
-4	8	372	351
-4	10	513	524
-4	11	178	190
-4	12	259	241
-3	-8	398	360
-3	-7	455	455
-3	-6	250	249
-3	-5	870	898
-3	-4	321	290
-3	-3	544	584
-3	-2	775	798
-3	-1	1080	991
-3	0	477	463
-3	1	485	490
-3	2	376	318
-3	3	283	291
-3	4	978	992
-3	5	356	379
-3	6	858	864
-3	8	361	382
-3	10	211	225
-3	11	253	250
-3	12	120	105
-2	-11	201	214
-2	-9	310	310
-2	-8	266	254
-2	-7	523	544
-2	-6	434	426
-2	-5	583	623
-2	-4	449	439
-2	-3	939	922
-2	-1	68	39
-2	0	102	48
-2	1	226	192
-2	2	2000	1826
-2	3	85	85
-2	4	679	640
-2	5	776	817
-2	6	279	303
-2	7	300	300
-2	8	232	260
-2	11	129	98
-2	12	117	57
-1	-11	221	238
-1	-9	417	379
-1	-8	127	156
-1	-7	298	288
-1	-6	231	244
-1	-5	394	427
-1	-4	785	850
-1	-3	506	441
-1	-2	111	76
-1	-1	720	657
-1	0	1212	999
-1	1	1094	1036
-1	2	949	872
-1	3	633	632
-1	4	335	367
-1	5	586	568
-1	6	170	165
-1	8	124	139
-1	11	177	164
-1	12	254	265
0	-11	289	268
0	-10	340	342
0	-9	170	156
0	-8	176	182
0	-7	566	555
0	-6	216	264
0	-5	655	625
0	-4	242	238
0	-2	598	557
0	-1	1424	1291
0	0	672	623
0	1	2369	2002
0	2	494	443
0	3	1039	992
0	4	320	336
0	5	530	542
0	7	243	222
0	9	172	203
0	10	466	455
1	-12	322	303
1	-11	135	131
1	-10	206	216
1	-8	344	339
1	-6	149	184
1	-5	1008	1051
1	-4	302	376
1	-3	131	112
1	-2	119	110
1	-1	1569	1337
1	0	697	595
1	1	486	447
1	2	2024	1791
1	3	130	143
1	4	182	174
1	5	95	115
1	6	200	220
1	7	178	178
1	8	424	458
1	10	354	373
1	11	171	149
2	-12	224	191
2	-11	223	202
2	-9	200	161
2	-8	128	115
2	-7	551	597
2	-6	426	417
2	-5	912	884
2	-4	866	890
2	-3	488	528
2	-2	372	378
2	-1	104	19
2	0	249	278
2	1	824	789
2	2	429	405
2	3	297	301
2	4	208	161
2	5	131	175
2	6	703	703
2	7	476	466
2	8	361	347
2	9	249	233
2	10	166	161
2	11	226	206
3	-11	203	202
3	-10	140	138
3	-9	275	257
3	-8	107	109
3	-7	460	432
3	-6	435	482
3	-5	308	326
3	-4	720	692
3	-3	274	220
3	-2	502	446
3	-1	832	726
3	0	429	402
3	1	619	573
3	2	187	208
3	3	116	142
3	4	240	213
3	5	1141	1129
3	6	155	121
3	7	791	784
3	8	230	236
3	9	237	249
3	10	109	110
4	-12	150	159
4	-11	266	293
4	-10	500	511
4	-9	201	189
4	-8	325	345
4	-7	421	434
4	-6	537	553
4	-5	422	457
4	-4	254	251
4	-2	194	137
4	-1	113	132
4	0	173	168
4	1	633	645
4	2	140	115
4	3	574	621
4	5	741	757
4	6	408	404
4	7	272	275
4	8	251	257
5	-12	333	312
5	-11	176	201
5	-10	550	582
5	-9	263	240
5	-8	313	311
5	-7	291	299
5	-6	192	213
5	-5	584	597
5	-4	151	31
5	-1	159	178
5	0	463	456
5	1	968	1004
5	2	396	404
5	3	416	397
5	4	551	553
5	6	503	506
5	7	202	194
5	8	119	140
5	9	118	91
6	-12	171	150
6	-11	384	395
6	-9	256	244
6	-7	256	258
6	-5	728	711
6	-4	111	173
6	-3	390	453
6	-2	134	156
6	-1	567	600
6	0	585	617
6	1	239	227
6	2	785	790
6	3	451	431
6	5	324	313
6	7	229	233
7	-11	234	246
7	-8	160	111
7	-7	177	135
7	-6	304	344
7	-5	124	107
7	-4	794	786
7	-3	319	313
7	-2	385	411
7	-1	283	278
7	0	796	828
7	1	302	275
7	3	143	156
7	4	198	209
7	5	105	112
7	6	126	109
7	7	213	189
8	-10	132	128
8	-6	429	411
8	-5	333	359
8	-4	648	668
8	-3	533	530
8	-2	329	341
8	-1	431	449
8	0	291	284
8	1	539	518
8	6	248	248
9	-10	195	197
9	-9	160	153
9	-8	259	273
9	-7	175	162
9	-6	353	359
9	-5	664	679
9	-4	154	107
9	-3	387	374
9	-2	112	69
9	-1	244	243
9	0	315	318
9	1	204	207
9	2	161	157
10	-9	274	294
10	-8	116	85
10	-7	305	330
10	-5	307	307
10	-4	278	274
10	-2	135	131
10	-1	149	134
10	0	229	220
10	2	217	213
11	-7	113	85
11	-6	194	216
11	-4	158	170
11	-3	231	227
11	0	293	281
11	1	146	106
***** H = 2 *****			
-12	2	167	172
-12	4	240	245
-11	-2	351	383
-11	0	185	171
-11	2	242	229
-11	4	250	201
-11	5	170	173
-11	7	173	123
-10	-4	358	348
-10	-3	131	165
-10	-2	380	376
-10	-1	271	274
-10	2	113	174
-10	7	106	101
-10	9	215	190
-9	-5	230	219
-9	-4	249	265
-9	-3	276	302
-9	3	326	293
-9	4	186	182
-9	5	161	167
-9	6	393	382
-9	8	359	351
-9	10	251	243
-8	-7	309	287
-8	-5	314	318
-8	-3	244	252
-8	-2	162	118
-8	-1	294	275
-8	0	130	141
-8	1	246	263
-8	2	175	204
-8	3	372	363
-8	4	851	831
-8	5	296	282
-8	6	572	539
-8	7	323	343
-8	8	295	305
-8	9	168	161
-7	-7	492	488
-7	-6	207	167
-7	-4	124	164
-7	-3	328	312
-7	-2	467	463
-7	-1	496	459
-7	0	294	331
-7	2	327	319
-7	3	175	202
-7	4	523	510
-7	5	441	448
-7	7	203	207
-7	9	161	159
-7	11	173	156
-6	-9	140	135
-6	-8	350	328
-6	-5	221	175
-6	-4	119	95
-6	-2	656	692
-6	-1	507	474
-6	0	383	365
-6	1	572	598
-6	2	563	589
-6	3	948	962
-6	4	307	305
-6	5	315	266
-6	6	392	413
-6	7	117	105
-6	10	249	217
-5	-8	120	91
-5	-7	125	115
-5	-5	180	181
-5	-4	312	320
-5	-3	708	704
-5	-2	415	390
-5	-1	1294	1365
-5	0	170	152
-5	1	1280	1374
-5	2	300	370
-5	3	485	492
-5	5	129	93
-5	7	177	171
-5	8	134	163
-5	9	114	76
-5	10	310	313
-5	11	212	190
-4	-9	129	128
-4	-8	141	143
-4	-7	231	214
-4	-6	154	145
-4	-5	546	549
-4	-4	228	222
-4	-3	1001	1063
-4	-2	635	614
-4	-1	1209	1179
-4	0	448	473
-4	1	530	562
-4	3	562	603
-4	4	426	479
-4	6	186	167
-4	8	265	281
-4	9	224	241
-4	10	452	496
-4	11	342	359
-3	-11	132	116
-3	-10	180	168
-3	-7	519	529
-3	-6	400	389
-3	-5	311	323
-3	-4	937	943
-3	-3	450	461
-3	-2	674	707
-3	0	157	133
-3	1	703	679
-3	2	108	171
-3	3	444	451
-3	4	815	767
-3	5	536	561
-3	6	261	296
-3	7	659	649
-3	8	116	154
-3	9	524	547
-3	10	121	86
-3	11	175	151
-2	-11	119	133
-2	-9	367	382
-2	-8	350	329
-2	-7	466	483
-2	-6	829	823
-2	-5	112	130
-2	-4	648	698
-2	-3	737	684
-2	-2	1086	1028
-2	-1	1781	1585
-2	0	169	198
-2	1	1302	1252
-2	3	139	193
-2	4	740	788
-2	5	762	776
-2	6	341	331
-2	7	494	503
-2	8	126	123
-2	9	205	158
-1	-10	360	346
-1	-9	140	107
-1	-8	471	500
-1	-6	176	142
-1	-5	111	95
-1	-4	664	719
-1	-3	402	404
-1	-2	96	103
-1	-1	363	312
-1	0	803	695
-1	1	1111	989
-1	2	306	243
-1	3	1426	1393
-1	4	119	102
-1	5	976	1054
-1	6	831	854
-1	7	190	218
-1	10	204	224
-1	11	164	162
0	-12	303	299
0	-11	238	251
0	-10	235	256
0	-6	109	116
0	-4	727	754
0	-3	62	39
0	-2	523	477
0	-1	161	78
0	0	901	848
0	1	327	262
0	2	541	593
0	3	1189	1193
0	4	1616	1644
0	6	450	487
0	7	359	348
0	10	347	356
0	11	261	257
1	-12	125	131
1	-11	361	358
1	-10	130	149
1	-9	235	230
1	-7	632	644
1	-6	700	703
1	-5	302	332
1	-4	772	795
1	-3	874	850
1	-2	805	732
1	-1	846	627
1	0	1264	1084
1	1	402	433
1	2	630	623
1	4	451	490
1	5	742	781
1	6	202	211
1	7	554	517
1	8	174	144
1	9	339	322
1	10	131	155
1	11	353	348
2	-12	163	163
2	-10	158	181
2	-8	224	214
2	-6	620	632
2	-5	237	254
2	-4	627	624
2	-3	612	570
2	-2	1053	1003
2	-1	261	188
2	0	447	449
2	1	625	568
2	3	411	398
2	4	311	270
2	5	223	227
2	6	751	726
2	7	310	298
2	8	192	214
2	9	319	296
2	10	218	212
3	-12	170	156
3	-11	107	99
3	-10	158	136
3	-8	435	428
3	-7	212	209
3	-6	578	581
3	-5	449	470
3	-4	144	167
3	-3	513	522
3	-2	1008	1049
3	-1	478	397
3	0	623	646
3	1	1068	1059
3	2	640	615
3	3	263	292
3	4	127	164
3	5	155	192
3	6	686	718
3	8	404	402
3	10	231	235
4	-11	162	143
4	-10	114	130
4	-9	407	385
4	-8	451	441
4	-7	536	532
4	-6	434	441
4	-5	483	501
4	-4	100	92
4	-3	499	499
4	-2	319	303
4	-1	87	107
4	0	930	925
4	2	414	457
4	3	435	415
4	4	500	482
4	6	451	429
4	7	352	352
4	8	135	128
5	-11	335	339
5	-10	130	182
5	-9	435	430
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2	3	362	389
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9	-4	116	175
9	-3	157	169
9	-2	165	181
9	1	247	257
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-9	3	[illegible]	106
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-8	-4	[illegible]	262
-8	-2	[illegible]	176
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2	-8	131	158
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6	2	252	246
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6	4	227	244
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7	-8	158	150
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7	-5	133	126
7	-4	356	383
7	-3	145	135
7	-2	120	83
7	2	148	149
7	3	110	132
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8	-5	230	236
8	-4	239	217
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TABLE III (*Continued*)

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-8	4	232	269
-7	-5	245	250
-7	-3	196	168
-7	-2	248	237
-7	-1	147	150
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-7	3	249	246
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-6	-7	246	222
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-6	-5	146	146
-6	-4	297	292
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-6	-2	167	145
-6	2	223	206
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-6	5	250	231
-6	7	260	271
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-5	-5	274	266
-5	-3	365	364
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-5	-1	234	205
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-5	2	226	240
-5	3	304	289
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-5	6	224	211
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-4	7	130	145
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-3	-7	115	145
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5	4	230	242
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7	-2	192	164
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3	-6	318	307
3	-2	322	320
3	0	317	293
3	1	120	105
3	3	217	238
4	-7	121	135
4	-6	281	263
4	-5	116	63
4	-4	177	173
4	-2	227	207
4	-1	356	368
4	1	182	194
4	2	135	137
5	-6	170	155
5	-5	209	205
5	-4	187	175
5	-3	292	290
5	-2	169	166
5	-1	214	199
5	0	316	309
6	-5	255	257
6	-4	158	169
6	-3	173	152
6	-2	340	316
***** H = 10 *****			
-5	-3	255	237
-5	-2	265	217
-5	-1	128	83
-5	0	137	112
-5	1	169	164
-4	-4	197	194
-4	-3	142	137
-4	-2	233	245
-4	1	171	167
-4	2	185	181
-3	-4	243	259
-3	-2	167	182
-3	0	135	120
-3	1	153	169
-3	2	240	236
-3	3	344	320
-2	-6	133	76
-2	-4	297	289
-2	0	158	155
-2	1	149	126
-2	3	428	430
-1	-4	129	112
-1	0	133	108
-1	1	234	234
-1	2	289	294
0	-6	129	97
0	-5	254	241
0	-3	160	162
0	-2	143	142
0	0	286	300
0	2	261	281
1	-6	286	310
1	-5	201	200
1	-4	327	313
1	-3	149	135
1	-2	279	277
1	-1	192	188
1	1	130	121
1	2	141	111
2	-6	219	189
2	-5	122	104
2	-4	370	373
2	-3	189	173
2	-2	215	215
2	-1	162	160
3	-5	265	224
3	-4	137	116
3	-3	260	256
3	-1	215	188
4	-3	172	155
4	-2	124	138
***** H = 11 *****			
-1	-2	138	115

TABLE IV

SELECTED INTERATOMIC DISTANCES AND ANGLES

Distances	Value, Å	Angles	Value, deg
Rh-Si	2.203 (4)	Si-Rh-Cl	115.9 (1)
Rh-Cl	2.387 (4)	Si-Rh-P(1)	98.3 (1)
Rh-P(1)	2.344 (4)	Si-Rh-P(2)	98.4 (2)
Rh-P(2)	2.332 (4)	Si-Rh-H	69
Rh-H	1.48[a]	Si-Rh-H_{136}	166
Rh-H_{136}	2.79	Cl-Rh-P(1)	87.2 (1)
Si-Cl(1)	2.057 (6)	Cl-Rh-P(2)	92.1 (1)
Si-Cl(2)	2.042 (6)	Cl-Rh-H	174
Si-Cl(3)	2.063 (6)	Cl-Rh-H_{136}	62
P-C (av of 6)	1.823 (11)	P(1)-Rh-P(2)	161.7 (1)
Si-Cl	3.891 (6)	P(1)-Rh-H	89
Si-P(1)	3.441 (6)	P(1)-Rh-H_{136}	68
Si-P(2)	3.434 (5)	P(2)-Rh-H	90
Si-H	2.2	P(2)-Rh-H_{136}	96
Si-H_{136}	4.96	H-Rh-H_{136}	112
Cl-P(1)	3.261 (5)	Rh-Si-Cl(1)	118.5 (2)
Cl-P(2)	3.398 (5)	Rh-Si-Cl(2)	120.5 (2)
Cl-H	3.86	Rh-Si-Cl(3)	108.5 (2)
Cl-H_{136}	2.70	Cl(1)-Si-Cl(2)	101.6 (3)
P(1)-P(2)	4.616 (5)	Cl(1)-Si-Cl(3)	102.8 (3)
P(1)-H	2.75	Cl(2)-Si-Cl(3)	102.6 (3)
P(1)-H_{136}	2.89	Rh-P-C (av of 6)	114 (3)
H-H_{136}	3.62	C-P-C (av of 6)	104.0 (17)
Cl(1)-Cl(2)	3.177 (7)	Cl(S1)-Si(S)-Cl(S2)	91
Cl(2)-Cl(3)	3.204 (7)		
Cl(3)-Cl(1)	3.219 (6)		
Si(S)-Cl(S1)	1.83		
Si(S)-Cl(S2)	2.11		

[a] No meaningful errors can be assigned to distances and angles involving the hydridic hydrogen atom because of the uncertainties in the coordinates of this atom caused, in large measure, by the difficulties with the solvent scattering.

TABLE V

ROOT-MEAN SQUARE AMPLITUDES OF VIBRATION (Å)

Atom	Min	Intermed	Max
Rh	0.222 (2)	0.232 (2)	0.237 (2)
Si	0.222 (6)	0.267 (6)	0.316 (6)
Cl(1)	0.238 (6)	0.341 (6)	0.372 (6)
Cl(2)	0.242 (6)	0.287 (6)	0.549 (7)
Cl(3)	0.224 (6)	0.331 (6)	0.404 (6)
Cl	0.220 (5)	0.260 (5)	0.277 (5)
P(1)	0.209 (5)	0.234 (5)	0.245 (5)
P(2)	0.220 (5)	0.226 (6)	0.259 (5)

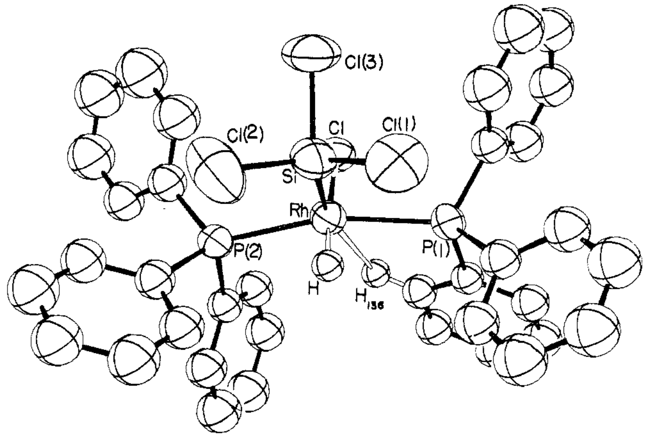

Figure 1.—Perspective view of the $RhHCl(SiCl_3)(P(C_6H_5)_3)_2$ molecule. Here and in Figure 2 the 50% probability ellipsoids are shown except for the hydrogen atoms. Most of the hydrogen atoms have been omitted for clarity.

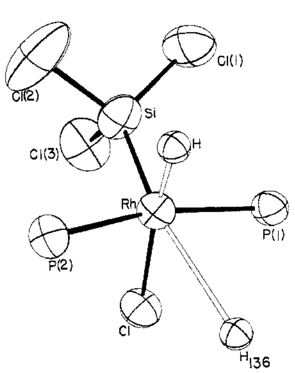

Figure 2.—Perspective view of the coordination polyhedron around the rhodium atom.

tains disordered molecules of solvent which, on the basis of the work of Wilkinson and his coworkers,[12] we believe to be trichlorosilane. Our results are consistent with a disorder in which the trichlorosilane molecule can adopt four orientations in space; in each the silicon atom is less than 0.5 Å from the center of symmetry at ($^1/_2$, $^1/_2$, $^1/_2$). The resulting electron density distribution consists of a peak at the center of symmetry due to silicon and two independent peaks roughly 2 Å from the center due to chlorine atoms. These peaks are necessarily diffuse since they involve at least four noncoincident equilibrium atomic positions. The occupancy parameter α refined in our least-squares calculations leads to a value of 0.397 (7) molecule of

SiHCl$_3$ per Rh, in reasonable agreement with the value of $^1/_3$ of Wilkinson, *et al.*[12] The closest approach of a nonhydrogen atom of the metal complex to ($^1/_2$, $^1/_2$, $^1/_2$) is that made by Cl(1) at 4.24 Å; the four other contacts of less than 5 Å all involve carbon atoms of the phenyl rings. Atom Cl(1) also makes the closest approach to each of the two independent solvent chlorine sites, namely, 3.96 Å to Cl(S1) and 3.82 Å to Cl(S2). The closest approach of the rhodium atom to one of the solvent chlorine sites is 6.97 Å. There is accordingly no reason to suppose that the interactions between the metal complex and the solvent represent anything but van der Waals contacts. Owing to the disorder, the differences between the distances and angles found here for the solvent molecule and the known values for trichlorosilane[21] are without significance.

The vibrational motions of the atoms (Figures 1 and 2 and Tables I, II, and V) show no unexpected features. Only the atoms of the trichlorosilyl group appear to undergo appreciable anisotropic vibration, presumably owing to the proximity of the chlorine atoms, especially Cl(1), to the partially occupied solvent position.

The coordination polyhedron about the rhodium atom may be described as a highly distorted trigonal bipyramid, with apical phosphines, and H, Cl, and SiCl$_3$ in the trigonal plane. A certain artificiality is involved in such a description, particularly since the position of the hydridic hydrogen atom is poorly determined. The coordination polyhedron could also be called a distorted tetragonal pyramid with equal validity. Furthermore, on the assumption of normal phenyl ring geometry, the hydrogen atom H$_{136}$, bonded to carbon C(6) of ring P(1)R(3), makes an intramolecular contact of 2.79 Å with the rhodium atom. If H$_{136}$ is considered as part of the coordination sphere, then the rhodium has distorted octahedral coordination. If a trigonal-bipyramidal description is adopted, then the idealized values of the P–Rh–P and P–Rh–Si angles would be, respectively, 180 and 90°. The departures of the observed bond angles about rhodium from these idealized values can then be ascribed to steric repulsions between the bulky phosphine and silyl ligands. Relief of these repulsions is brought about by opening of the Si–Rh–P angles to 98°, with a corresponding closure of the P–Rh–P angle to 162°. As a result the intramolecular Cl(1)···P(1) and Cl(2) ···P(2) contacts are, respectively, 3.68 and 3.70 Å, close to the sum of the corresponding van der Waals radii; the short H$_{136}$–Rh contact is probably the result of the closure of the P–Rh–P angle, rather than a genuine interaction between H$_{136}$ and Rh.

The mean Si–Cl distance of 2.054 (5) Å in the coordinated silyl group is slightly longer than the value of 2.035 (3) Å found in Co(SiCl$_3$)(CO)$_4$[4] but is within the range of 2.01–2.05 Å found in free chlorosilanes.[21] The coordination around the silicon is distorted tetrahedral, but the distortions are slightly different from those found in the cobalt complexes Co(SiR$_3$)(CO)$_4$ (R = F,[3] Cl[4]). In the cobalt compounds the Co–Si–Cl angles are all around 115° and the Cl–Si–Cl angles are all around 104°. The Rh–Si–Cl(3) angle found here is 109° while the other two Rh–Si–Cl angles are 119 and 121°. These irregularities are a further manifestation of the nonbonded interactions P(1)···Cl(1) and P(2)···Cl(2).

The geometry found here about the rhodium is extremely similar to the corresponding geometries found about ruthenium in the d^6 complexes RuXCl(P(C$_6$H$_5$)$_3$)$_3$ (X = Cl,[8] H[9]). In the ruthenium complexes two phosphine ligands are *trans* to one another, the P–Ru–P angles being 156° when X = Cl and 153° when X = H, and the third phosphine is *cis* to the other two, the angles subtended by *cis* phosphines at the metal being around 100°. In both of these compounds there is a short contact between the metal and a phenyl-ring hydrogen atom[22] (2.59 Å for X = Cl; 2.85 Å for X = H). It has been suggested that the metal–phenyl hydrogen contact stabilizes the unexpected five-coordinate d^6 complex by preventing the approach of a sixth ligand.[8,23] It is interesting to note that on purely steric grounds one would predict that these five-coordinate complexes would adopt a regular trigonal-bipyramidal configuration, with the phosphine or silyl ligands in the trigonal plane, as occurs in RhH(CO)(P(C$_6$H$_5$)$_3$)$_2$.[24]

The fact that the potential sixth coordination site about the Rh atom is blocked by a phenyl hydrogen atom may be of significance in understanding the chemistry of the complex. Thus the complex is not an effective hydrosilation catalyst for olefins,[12] possibly because no coordination site is open for the incoming olefin. Moreover the compound RhHCl(SiCl$_3$)(CO)(P(C$_6$H$_5$)$_3$)$_2$ is not formed by the addition of CO to RhHCl(SiCl$_3$)(P(C$_6$H$_5$)$_3$)$_2$, but rather SiHCl$_3$ is split off and RhCl(CO)(P(C$_6$H$_5$)$_3$)$_2$ is left. Yet through the addition of SiHCl$_3$ to the analogous RhCl(CO)(P(C$_2$H$_5$)$_3$)$_2$ the compound RhHCl(SiCl$_3$)(CO)(P(C$_2$H$_5$)$_3$)$_2$ is apparently formed.[12] It is possible that the blocking of the sixth coordination site is more effective when P(C$_6$H$_5$)$_3$, rather than P(C$_2$H$_5$)$_3$, is employed but, of course, such differences in the chemistry may also be due to the more basic nature of P(C$_2$H$_5$)$_3$.

The similarities in these five-coordinate d^6 complexes also extend to the bond distances involving the metal. The Rh–P distances of 2.344 (4) and 2.332 (4) Å found here are normal; recent determinations of Rh–P bond lengths have given mean values in the range 2.32–2.36 Å.[10,24–28] The Rh–Si distance of 2.203 (4) Å is

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[21] L. E. Sutton, Ed., Special Publication No. 18, The Chemical Society London, 1965.

[22] RuCl$_2$(P(C$_6$H$_5$)$_3$)$_3$ was originally described as a somewhat distorted tetragonal pyramid, while RuHCl(P(C$_6$H$_5$)$_3$)$_3$ was described as having "distorted pentacoordinate" geometry. Nevertheless, these two Ru complexes and the Rh complex described here have remarkably similar coordination about the metal atom.

[23] J. Chatt and A. E. Underhill, *J. Chem. Soc.*, 2088 (1963).

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

[25] J. L. de Boer, D. Rogers, A. C. Skapski, and P. G. H. Troughton, *Chem. Commun.*, 756 (1966).

[26] B. T. Kilbourn and P. G. Owston, private communication.

[27] J. A. McGinnety, N. C. Payne, and J. A. Ibers, *J. Am. Chem. Soc.*, **91**, 3601 (1969).

[28] K. W. Muir and J. A. Ibers, *Inorg. Chem.*, **8**, 1921 (1969).

the shortest yet reported for a metal–silicon bond.[29] In the ruthenium complexes the two Ru–P bonds involving phosphorus atoms which are mutually *trans* to one another are normal, the mean values being 2.393 (6) Å (X = Cl) and 2.345 (4) Å (X = H), whereas the third Ru–P distance, involving the phosphorus atom which is *cis* to the other two, is in each case much shorter, being 2.230 (8) Å (X = Cl) and 2.206 (4) Å (X = H).[8,9] These results may be rationalized if one assumes that transition metal–phosphine and --silyl bonds involve some back-donation from the metal; short metal–phosphorus and metal–silicon distances occur when there is no competing π-bonding ligand in the *trans* position. Since the covalent radius of phosphorus is some 0.07 Å shorter than the covalent radius of silicon, while the covalent radii of Ru and Rh differ by about 0.01 Å,[30] it would then appear, from the near equality of the short Ru–P distance in RuHCl(P(C_6H_5)$_3$)$_2$ with the Rh–Si distance found here, that back-bonding occurs more readily with $SiCl_3$ than with P(C_6H_5)$_3$. Such an explanation is consistent with the relative stabilities of these complexes formed with different substituted silanes.[12]

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[29] Further discussion of metal–silicon bond lengths appears in the following paper: Lj. Manojlović-Muir, K. W. Muir, and J. A. Ibers, *ibid.*, **9**, 447 (1970).

[30] L. Pauling, "The Nature of the Chemical Bond," Cornell University Press, Ithaca, N. Y., 1960.

CONTRIBUTION FROM THE DEPARTMENT OF CHEMISTRY,
NORTHWESTERN UNIVERSITY, EVANSTON, ILLINOIS 60201

The Crystal and Molecular Structure of Hydridobis(trichlorosilyl)carbonyl-π-cyclopentadienyliron, (π-C_5H_5)FeH($SiCl_3$)$_2$(CO)

BY LJUBICA MANOJLOVIĆ-MUIR, KENNETH W. MUIR, AND JAMES A. IBERS

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The crystal structure of hydridobis(trichlorosilyl)carbonyl-π-cyclopentadienyliron, (π-C_5H_5)FeH($SiCl_3$)$_2$(CO), has been determined by X-ray diffraction methods. A monoclinic unit cell of dimensions a = 7.493 (5) Å, b = 11.867 (9) Å, c = 8.651 (5) Å, and β = 99.73 (2)° contains two monomeric molecules; the observed and calculated densities are, respectively, 1.88 (2) and 1.835 g cm^{-3}, and the space group is C_2^2-$P2_1$. The structure has been refined by least-squares methods to a conventional R factor of 0.041 over 1245 counter-diffractometric data. The absolute configuration of the molecules in the crystal used in the analysis has been determined by least-squares methods and Bijvoet ratio tests. The coordination polyhedron around the Fe atom can be regarded as a distorted tetragonal pyramid, with the centroid of the cyclopentadienyl ring at the apex and the remaining ligands in the basal plane. The Fe atom is displaced from the basal plane toward the ring. The two Fe–Si distances are equal at 2.252 (3) Å. This is the first determination of the length of such a bond. Structural data on transition metal-silicon bonds are summarized and arguments are presented in favor of some d_π–d_π back-bonding being involved in these bonds.

Introduction

Although complexes containing metal–silicon bonds are known for a wide variety of transition metals, there is still very little structural information on such compounds. The recent work on silylcobalt complexes of the type Co(SiX_3)(CO)$_4$[1-3] (where X = Cl, F, and H) tends to confirm the suggestion of Hagen and McDiarmid[4] that the empty silicon d orbitals may be involved in the Co–Si bonding. We have pointed out in the previous paper that the Rh–Si distance in RhHCl($SiCl_3$)(P(C_6H_5)$_3$)$_2$ provides evidence that the silicon d orbitals are used in the Rh–Si bonding.[5] In order to obtain further insight into the behavior of substituted silyl groups as ligands in transition metal complexes, we have determined the structure of π-CpFeH($SiCl_3$)$_2$(CO) (Cp = cyclopentadienyl = $C_5H_5^-$). This is the first reported structure of a compound which contains an Fe–Si bond. The work also reflects our interest in the geometries of five-coordinated[6] transition metal complexes and, in particular, those containing a hydridic hydrogen bonded to the transition metal.

Collection and Reduction of Intensity Data

A sample of π-CpFeH($SiCl_3$)$_2$(CO) was kindly supplied by Graham.[7] The crystals are pale yellow needles, moderately stable in air. A preliminary X-ray photographic examination showed that they possess monoclinic symmetry. According to the photographs of the $0kl$, $hk0$, $h0l$, and $h1l$ reciprocal lattice nets, taken with Mo Kα radiation, systematic absences occur only

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[1] W. T. Robinson and J. A. Ibers, *Inorg. Chem.*, **6**, 1208 (1967).

[2] K. Emerson, P. R. Ireland, and W. T. Robinson, *ibid.*, **9**, 436 (1970).

[3] A. G. Robiette, G. M. Sheldrick, R. N. F. Simpson, B. J. Aylett, and J. A. Campbell, *J. Organometal. Chem.* (Amsterdam), **14**, 279 (1968).

[4] A. P. Hagen and A. G. McDiarmid, *Inorg. Chem.*, **6**, 686 (1967).

[5] K. W. Muir and J. A. Ibers, *ibid.*, **9**, 440 (1970).

[6] In this paper the cyclopentadienyl ring is regarded as occupying one vertex of the iron coordination polyhedron. Some authors assume that a cyclopentadienyl ring occupies three vertices of the coordination polyhedron and would therefore describe the iron as heptacoordinate in the present case.

[7] W. A. G. Graham and W. Jetz, Abstracts, 155th National Meeting of the American Chemical Society, San Francisco, Calif., March–April 1968, No. M 082.