Table XIII. Crystallographic Data for $Cp^*Hf(C_6H_{10})Cl \bullet py$ and $Cp^*Hf(C_6H_{10})Cl$

formula	$C_{21}H_{30}HfClN$	$C_{16}H_{25}HfCl$
mol wt	510.4	431.3
space group	$Pna2_1$	C_2
a, Å	17.412 (3)	8.820 (3)
b, Å	8.164 (3)	12.767 (3)
c, Å	14.837 (3)	14.486 (3)
α, deg	90.0	90.0
β, deg	90.0	102.59 (1)
γ, deg	90.0	90.0
V, Å^3	2109.1	1592.1
Z	4	4
D_{calcd}, g cm^{-3}	1.607	1.799
μ, cm^{-1}	50.3	66.5
$F(000)$, e	504	840
T, K	293	100
cryst dimens, mm	0.10 × 0.27 × 0.50	0.45 × 0.49 × 0.106
radiation	Mo Kα	Mo Kα
scan mode	$\omega-2\theta$	$\omega-2\theta$
θ range, deg	1.0–27.0	1.0–38.0
hkl range	22,10,18	15,22,±25
std refl	$\bar{8}\bar{4}2$	$1\bar{1}\bar{7},\bar{1}36,620$
refl measd	2391	4457
refl obsd	2025 ($I \geq 2\sigma(I)$)	4010 ($I \geq 3\sigma(I)$)
no. of parameters refined	216	164
R	0.036	0.036
R_w (w = 1)	0.059	0.049

temperature and for **6** by slowly cooling a pentane solution to −30 °C. A crystal of **6**·py was sealed under dinitrogen in a thin-walled glass capillary. A crystal of **6** was mounted on a goniometer head under dinitrogen and then placed on the diffractometer in a stream of dinitrogen of 100 K. From systematic absences on Weissenberg films the space group of **6**·py was found to be $Pna2_1$ and of **6** was found to be $C2$, Cm, or $C2/m$. In the final state, group $C2$ gave the best fit. The Bragg angles of 24 reflections, with 12° < $\theta \leq$ 15° and 10° $\leq \theta \leq$ 25° for **6**·py and **6**, respectively, were used to obtain the orientation matrix for the intensity data collection and to refine the unit cell parameters. Intensity data were collected by $\theta-2\theta$ scans, with all reflections measured at the same scan speed. The ω scan width was given by $(1.3 + 0.35 \tan \theta)°$ and $(0.8 + 0.35 \tan \theta)°$ and the horizontal opening of the detector by $(3.4 + 1.0 \tan \theta)°$ and $(3.2 + 1.0 \tan \theta)°$ for **6**·py and **6**, respectively. Measuring time background to peak ratio is 1:2. Intensity standard reflections were used during data collection and inspected every 6000 s (fluctuation < 1–2%). The intensities were corrected for Lorentz and polarization effects and absorption (transmission coefficients from 0.601 to 0.269 for **6**·py and from 0.508 to 0.106 for **6**).

Determination and Refinement of the Structures. For **6**·py the Hf atom was located by Patterson synthesis: for **6** the Hf and Cl atoms were found by direct methods (MULTAN 82). The other non-hydrogen atoms were revealed from succeeding difference maps. Attempts to localize the hydrogen atoms from the final difference maps failed. Using anisotropic temperature factors, a full-matrix least squares of F converged for **6**·py to a final R = 0.036 and R_w = 0.059 (w = 1) and for **6** to a final R = 0.036 and R_w = 0.049 (w = 1). All calculations were performed by using CAD4-SDP programs.

Acknowledgment. We thank Professors K. Tatsumi and G. Erker for stimulating discussions. This investigation was supported by the Netherlands Foundation for Chemical Research (SON) with financial aid from the Netherlands Organization for the Advancement of Pure Research (ZWO).

Supplementary Material Available: Tables of elemental analyses of **8**–**14** and Cp*M(diene)Cl·L complexes and positional and thermal parameters and least-squares planes for **6** and **6**·py (8 pages); listings of observed and calculated structure factors for **6** and **6**·py (32 pages). Ordering information is given on any current masthead page.

Hydrido Silyl Complexes. 9.[1] Cr,H,Si Three-Center Bonding in $C_6Me_6(CO)_2Cr(H)SiHPh_2$

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$C_6Me_6(CO)_2Cr(H)SiHPh_2$ (1) contains a Cr,H,Si two-electron three-center bond in its ground state. Comparison of structural and ^{29}Si NMR data with those of the isoelectronic complex $C_5Me_5(CO)_2Mn(H)SiHPh_2$ (2) suggests that Si–H interaction in 1 is slightly stronger than in 2. This is attributed to the increased size of the C_6Me_6 ligand. 1 crystallizes in the monoclinic space group $P2_1/n$ with a = 9.285 (7) Å, b = 15.86 (2) Å, c = 16.05 (2) Å, and β = 94.20 (7)° (Z = 4). Important bond lengths are Cr–Si = 2.456 (1), Cr–H = 1.61 (4), Si–H (bridging) = 1.61 (4), and Si–H (terminal) = 1.39 (3) Å. The Si,Cr,H coupling constant is 70.8 Hz.

Introduction

Complexes containing both a hydride and a silyl ligand, which are formed by oxidative addition of Si–H bonds to transition metals, are important intermediates in metal-catalyzed hydrosilylation reactions.[2] Substantial information on the factors governing these reactions can be obtained from the investigation of metal complexes containing metal–hydrogen–silicon three-center bonds in their ground states. Manganese complexes of the type $(\eta^5\text{-}C_5R_5)(CO)(L)Mn(H)SiR_3$ (L = CO, PR_3, $P(OR)_3$, CNR) are particularly well investigated in this respect; the results have been summarized in the introduction of ref 3.

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[1] Part 8 in this series: Knorr, M.; Schubert, U. *Transition Met. Chem. (Weinheim, Ger.)* **1986**, *11*, 268.

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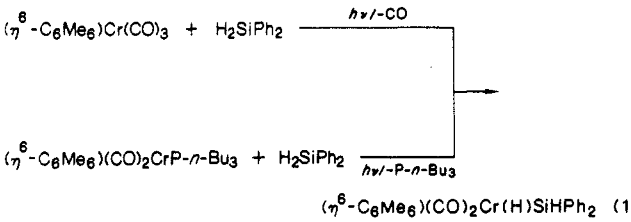
In a series of papers,[3-5] we have shown that the degree of Mn,H,Si three-center bonding (i.e. the degree of Mn–H, Si–H, or Mn–Si interaction) can be influenced by changing substituents at silicon or ligands at the metal. The opening of the Si–H bond is favored by electron-donating ligands, which must not be too bulky, and/or electronegative substituents. These results have been interpreted by a recent molecular orbital (MO) analysis.[6]

We now turned our attention to the question of how the three-center bond is influenced if the *metal* is changed. In this paper we discuss bonding in $(\eta^6\text{-}C_6Me_6)(CO)_2Cr(H)SiHPh_2$ (1) on the basis of spectroscopic and structural data and in comparison with the isoelectronic complex $(\eta^5\text{-}C_5Me_5)(CO)_2Mn(H)SiHPh_2$ (2).[3]

Results and Discussion

1 is prepared by photochemical reaction of $(\eta^6\text{-}C_6Me_6)Cr(CO)_3$ with diphenylsilane (eq 1) as previously described for $(\eta^6\text{-}C_6H_6)(CO)_2Cr(H)SiCl_3$.[7] 1 is also formed upon irradiation of $(\eta^6\text{-}C_6Me_6)(CO)_2CrP\text{–}n\text{–}Bu_3$. In the latter reaction the phosphine is eliminated instead of a CO ligand. This phenomenon was also observed when $MeCp(CO)_2MnPR_3$ complexes were photochemically reacted with H_2SiPh_2: with small PR_3 ligands, $MeCp(CO)(PR_3)Mn(H)SiHPh_2$ was obtained and with bulky ligands (cone angle > 145°[8]), $MeCp(CO)_2Mn(H)SiHPh_2$ instead.[9] Since C_6Me_6 is bulkier than MeCp, elimination of PR_3 from $(C_6Me_6)(CO)_2CrPR_3$ is already favored for smaller phosphines (cone angle of $P\text{–}n\text{–}Bu_3$ is 132° [8]). In the crystalline state the yellow hydrido silyl complex 1 is moderately stable, but in solution it decomposes quite rapidly, particularly if the temperature is raised.



(1)

1

$Cp(CO)(L)Mn(H)SiR_3$ complexes have been shown to eliminate $HSiR_3$ on warming.[4,10] The rate-determining initial step is the dissociation of the silane from the metal moiety. The latter can be trapped in the presence of a phosphine as $Cp(CO)(L)MnPR_3$. We have previously shown that the magnitude of the activation enthalpy for the reductive elimination of $HSiR_3$ correlates with the degree of three-center bonding in the corresponding complex.[3,4]

We therefore attempted to determine the activation parameters for the silane elimination from 1. For this purpose, 1 was reacted with a 10-fold excess of $P\text{–}n\text{–}Bu_3$ (pseudo-first-order conditions) in dibutyl ether (eq 2). The

$$1 + P\text{-}n\text{-}Bu_3 \rightarrow (\eta^6\text{-}C_6Me_6)(CO)_2CrP\text{-}n\text{-}Bu_3 + H_2SiPh_2 \qquad (2)$$

concentration (c) of 1 was monitored with use of IR spectroscopy by means of the intensity of its ν(CO) bands. At 34 °C the plot of ln (c/c_0) vs. time was linear for 3 half-lifes, indicating a first-order rate law. The same rate law had been found for the elimination of silanes from $Cp(CO)(L)Mn(H)SiR_3$ complexes.[4,10] Elimination of H_2SiPh_2 from 1 takes place with a rate constant of $(3.8 \pm 0.1) \times 10^{-4}$ s^{-1} at 34 °C. However, the reaction (eq 2) is influenced by some decomposition products of 1. With samples of 1 that have been stored for some weeks, even at low temperatures, significantly higher rate constants are obtained. Also, if a small amount of the product mixture resulting from thermal decomposition of 1 is added to a solution of freshly prepared, analytically pure 1, the rate constant increases considerably. For this reason we were unable to obtain precise rate constants at higher tem-

Table I. Selected Bond Distances and Bond Angles of 1

	(a) Bond Distances (Å)		
Cr–Si	2.456 (1)	Cr–C(1)	1.818 (4)
Cr–C(3)	2.276 (4)	Cr–C(2)	1.789 (4)
Cr–C(4)	2.293 (4)	C(1)–O(1)	1.163 (5)
Cr–C(5)	2.238 (4)	C(2)–O(2)	1.180 (5)
Cr–C(6)	2.257 (4)	Cr–H(1)	1.61 (4)
Cr–C(7)	2.219 (4)	Si–H(1)	1.61 (4)
C–C(8)	2.224 (4)	Si–H(2)	1.39 (3)
Cr–Cp[a]	1.750	Si–C(10)	1.894 (4)
		Si–C(20)	1.893 (4)
	(b) Bond Angles (deg)		
Cp–Cr–C(1)[a]	122.9	Cr–Si–C(10)	119.2 (1)
Cp–Cr–C(2)[a]	125.4	Cr–Si–C(20)	115.3 (1)
Cp–Cr–H(1)[a]	124.2	Cr–Si–H(1)	40 (1)
Cp–Cr–Si[a]	128.9	Cr–Si–H(2)	108 (1)
H(1)–Cr–Si	40 (1)	H(1)–Si–H(2)	147 (2)
H(1)–Cr–C(1)	83 (1)	H(1)–Si–C(10)	92 (1)
H(1)–Cr–C(2)	103 (1)	H(1)–Si–C(20)	99 (1)
Si–Cr–C(1)	104.8 (1)	H(2)–Si–C(10)	104 (1)
Si–Cr–C(2)	71.9 (1)	H(2)–Si–C(20)	104 (1)
C(1)–Cr–C(2)	85.1 (2)	C(10)–Si–C(20)	105.9 (2)

[a] Cp is the center of the C_6Me_6 ring.

Table II. Fractional Atomic Coordinates of 1

atom	x	y	z
Cr	0.29712 (6)	0.39306 (4)	0.25757 (4)
Si	0.43209 (11)	0.35235 (6)	0.38870 (7)
C(1)	0.3202 (4)	0.3051 (3)	0.1872 (3)
O(1)	0.3337 (4)	0.2518 (2)	0.1387 (2)
C(2)	0.4846 (5)	0.4128 (2)	0.2468 (2)
O(2)	0.6049 (3)	0.4295 (2)	0.2343 (2)
C(3)	0.1991 (4)	0.5066 (2)	0.3191 (3)
C(4)	0.0940 (4)	0.4420 (2)	0.3148 (3)
C(5)	0.0565 (4)	0.4012 (2)	0.2381 (3)
C(6)	0.1148 (4)	0.4292 (3)	0.1637 (3)
C(7)	0.2218 (4)	0.4928 (2)	0.1678 (3)
C(8)	0.2644 (4)	0.5315 (2)	0.2451 (3)
C(10)	0.3301 (4)	0.3308 (2)	0.4843 (2)
C(11)	0.3388 (5)	0.3844 (3)	0.5526 (3)
C(12)	0.2627 (6)	0.3685 (3)	0.6225 (3)
C(13)	0.1778 (5)	0.2989 (4)	0.6250 (3)
C(14)	0.1679 (5)	0.2443 (3)	0.5584 (3)
C(15)	0.2420 (5)	0.2605 (3)	0.4890 (3)
C(20)	0.5607 (4)	0.2607 (2)	0.3804 (2)
C(21)	0.6989 (4)	0.2647 (3)	0.4181 (3)
C(22)	0.7944 (4)	0.1975 (3)	0.4156 (3)
C(23)	0.7524 (5)	0.1250 (3)	0.3741 (3)
C(24)	0.6168 (5)	0.1188 (3)	0.3369 (3)
C(25)	0.5216 (4)	0.1857 (2)	0.3395 (3)
C(31)	0.2315 (6)	0.5517 (3)	0.4007 (3)
C(41)	0.0162 (5)	0.4196 (3)	0.3902 (3)
C(51)	-0.0571 (5)	0.3319 (3)	0.2327 (3)
C(61)	0.0593 (6)	0.3923 (3)	0.0810 (3)
C(71)	0.2855 (6)	0.5209 (3)	0.0890 (3)
C(81)	0.3745 (5)	0.6018 (3)	0.2497 (3)
H(1)	0.299 (4)	0.319 (2)	0.327 (2)
H(2)	0.522 (3)	0.419 (2)	0.413 (2)

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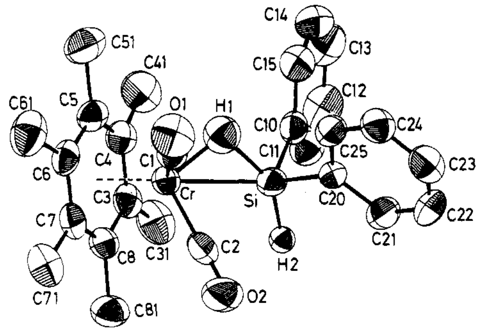

Figure 1. A perspective drawing of $C_6Me_6(CO)_2Cr(H)SiHPh_2$ (**1**). Most hydrogen atoms have been omitted for clarity.

Table III. Comparison of Structural Data of $(C_6Me_6)(CO)_2Cr(H)SiHPh_2$ (1) and $(C_5Me_5)(CO)_2Mn(H)SiHPh_2$ (2)[3] (Distances in Å; Bond Angles in deg)

	1	2
M–Si	2.456 (1)	2.395 (1)
M–H	1.61 (4)	1.52 (3)
M–Cp[a]	1.750	1.768
M–C(CO)	1.818 (4), 1.789 (4)	1.778 (3), 1.768 (4)
C–O	1.163 (5), 1.180 (5)	1.152 (4), 1.165 (5)
Si–H(bridging)	1.61 (4)	1.77 (3)
Si–H(terminal)	1.39 (3)	1.43 (3)
Cp–M–C(CO)[a]	122.9, 125.4	121.1, 123.0
Cp–M–H[a]	124.2	120.0
Cp–M–Si[a]	128.9	124.8
Si–M–C(CO)	104.8 (1), 71.9 (1)	109.7 (1), 75.1 (1)
H–M–C(CO)	103 (1), 83 (1)	111 (1), 80 (1)
C(CO)–M–C(CO)	85.1 (2)	89.2 (2)
M–Si–C(Ph)	119.2 (1), 115.3 (1)	120.7 (1), 112.2 (1)
M–Si–H(terminal)	108 (1)	108 (1)
H(bridging)–Si–H(terminal)	147 (2)	146 (1)
C(Ph)–Si–C(Ph)	105.9 (2)	107.0 (1)

[a] Cp is the center of the C_6Me_6 or C_5Me_5 ring, respectively.

peratures and to determine the activation parameters for the elimination of H_2SiPh_2 from **1**. For comparison, the corresponding parameters of **2** are $\Delta H^{*} = 98.5 \pm 0.7$ kJ/mol and $\Delta S^{*} = 6.5 \pm 8$ J/(mol·K),[3] giving $k = 2.5 \times 10^{-4}$ s^{-1} at 34 °C.

The solid-state structure of **1** (Tables I and II; Figure 1) closely resembles that of **2**.[3] Structural data of both complexes are compared in Table III. As discussed in more detail in another paper of this series,[3] the geometries of a number of $(C_5R_5')(CO)(L)Mn(H)SiR_3$ complexes are nearly identical. Variations of R, R′, and L are mainly reflected in the Mn–Si distances. The structure of the chromium complex **1** is well matched with this series, and all the geometrical details, which are typical for a three-center bonding situation, are found in **1**: (i) The bond angles at Cr, particularly C(1)–Cr–C(2), are typical for a "three-legged piano-stool" geometry, $(C_6Me_6)(CO)_2CrL$, rather than a "four-legged piano-stool" geometry. Therefore H_2SiPh_2 on the whole must be regarded as *one* ligand. (ii) The silane is oriented in such a manner that H(2) is within the Cr,Si,H(1) plane and both carbonyl ligands are below this plane with approximately equal distances to it. (iii) A hypothetical sp^3 orbital at Si and the orbital of $(C_6Me_6)(CO)_2CrL$, which is directed toward the ligand L (the directions of which can be estimated from the geometry of the $(C_6Me_6)(CO)_2Cr$ and the $SiHPh_2$ fragment, respectively), approximately point to the center of the Cr,Si,H(1) triangle.

We were able to refine the positions of H(1) and H(2) located from difference Fourier maps. They are therefore reliable within the accuracy of the method. The bond length between the terminal hydrogen, H(2), and silicon is the same in **1** and **2** within the standard deviations. Contrary to that, the Si–H(1) distance in **1** (1.61 (4) Å) is significantly shorter than the corresponding distance in the manganese complex **2** (1.77 (3) Å). Consequently, Cr–H(1) in **1** (1.61 (4) Å) is longer than Mn–H(1) in **2** (1.52 (3) Å). In fact, the Si–H(1) distance in **1** is shorter than in any of the structurally investigated $(C_5R_5')(CO)(L)Mn(H)SiR_3$ complexes (1.76–1.79 Å)[3] and only about 0.15–0.20 Å longer than the Si–H bond length in tetrahedral silanes.[11] We do not wish to put too much emphasis on hydrogen parameters derived from X-ray data. However, the Cr–Si distance also indicates that the bonding interaction between Si and H(1) in **1** is much stronger than in **2**. We have previously shown that in $Cp(CO)(L)Mn(H)SiR_3$ complexes, the Mn–Si distance correlates quite well with the degree of three-center bonding.[3] Long Mn–Si distances are found in complexes in which there is a strong Si–H interaction, and vice versa. The Cr–Si distance in **1** is 0.06 Å longer than the Mn–Si distance in **2**. Since the covalent radius of Cr(0) should be only 0.01–0.02 Å greater than that of isoelectronic Mn(I),[12] the main difference between the Cr–Si distance in **1** and the Mn–Si distance in **2** should be due to a more delocalized bonding in **1**.

A possible explanation for the stronger Si–H interaction in **1** could be the greater steric bulk of the C_6Me_6 ligand compared with C_5Me_5. The angles between the centroid of the C_6Me_6 ring and the other ligands at chromium are 2–4° larger than the corresponding angles in **2** (Table III). As a consequence, the CO ligands, H(1), and $SiHPh_2$ are pressed together, promoting a stronger Si–H(1) interaction. His interpretation is consistent with our previous findings, that increasing steric bulk of the phosphine ligand in $MeCp(CO)(PR_3)Mn(H)SiHPh_2$ favors reductive elimination of H_2SiPh_2.[4] The same is true if the MeCp ligand in $(C_5H_4Me)(CO)_2Mn(H)SiHPh_2$ (**3**) is replaced by the sterically more demanding C_5Me_5 ligand.[3] We therefore believe that due to steric factors an earlier stage of the oxidative addition of H_2SiPh_2 to the transition metal is observed in **1** than in **2**, regardless of the higher electron density at chromium. ν(CO) in petroleum ether: **1**, 1922, 1868 cm^{-1}; **2**, 1975, 1918 cm^{-1}. Mean C–O distance: **1**, 1.172 Å; **2**, 1.159 Å.

A final indication for the stronger Si–H interaction in **1** is provided by the ^{29}Si NMR spectrum. Although ^1J(SiH) (coupling between Si and the terminal hydrogen H(2)) is slightly smaller in **1** (197.0 Hz) than in **2** (200.3 Hz), indicating that the $C_6Me_6(CO)_6Cr$ moiety is a less electronegative substituent to silicon than $C_5Me_5(CO)_2Mn$, the ^2J(SiCrH) coupling constant is about 5 Hz larger in **1** (70.8 Hz) than in **2** (65.4 Hz). Within a series of complexes, $MeCp(CO)(L)Mn(H)SiHPh_2$, the magnitude of ^2J(SiMnH) can be correlated with changes in the Mn,H,Si three-center bond, induced by variation of L.[3] High absolute values of ^2J(SiMnH) are observed for complexes with a strong Si–H interaction, and vice versa. ^2J(SiMH) is 7.9 Hz in $C_5Me_5Rh(H)_2(SiEt_3)_3$[13] and 20 Hz in $Cp(CO)Fe(H)(SiCl_3)_2$.[14] In the Rh complex the Si–H distance indicates that there is no significant Si–H interaction; in the Fe complex the hydride ligand was not located.[15] On

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the other hand, values up to 69 Hz have been found in manganese complexes containing Mn,H,Si three-center bonds.[3] ^2J(SiCrH) in 1 is even larger, and we attribute this observation to an increased Si–H interaction.

Conclusions

As for the isoelectronic $Cp(CO)_2Mn(H)SiR_3$ complexes, a metal–hydrogen–silicon three-center two-electron bond is also observed in $C_6Me_6(CO)_2Cr(H)SiHPh_2$ (1). Structural and ^{29}Si NMR spectroscopic data suggest that the Si–H interaction is stronger in 1 than in $C_5Me_5(CO)_2Mn(H)SiHPh_2$ (2), probably caused by steric factors rather than the different metals. Thus, in the series of complexes $C_6Me_6(CO)_2Cr(H)SiHPh_2$ (1), $C_5Me_5(CO)_2Mn(H)SiHPh_2$ (2), and $C_5H_4Me(CO)_2Mn(H)SiHPh_2$ (3)[3] the Si–H interaction slightly decreases in going from 1 to 3 as the size of the π-bonded ligand decreases in the same order.

Experimental Section

All manipulations were performed under an atmosphere of dry and oxygen-free nitrogen. All solvents were dried by standard methods and saturated with N_2. Infrared spectra were taken in a NaCl solution cell and were recorded on a Perkin-Elmer 283 spectrometer. Kinetic measurements were performed as previously described.[4] The ^1H NMR spectrum was recorded on a Varian T60 spectrometer and the ^{29}Si NMR spectrum on a JEOL FX90Q spectrometer operating at 17.76 MHz (standard resolution 0.6 Hz).

Synthesis of (η^6-C_6Me_6)$(CO)_2Cr(H)SiHPh_2$ (1). A solution of 1.0 g (3.4 mmol) of $C_6Me_6Cr(CO)_3$ and 4.0 g (21.7 mmol) of H_2SiPh_2 in 250 mL of petroleum ether was irradiated with a high-pressure mercury lamp (Heraeus, 180 W) at −15 °C for 6 h. 1 precipitated during irradiation as a yellow solid, which was filtered off and recrystallized twice from THF/pentane: yield 1.26 g (82%); mp 120 °C dec; IR (cm^{-1}, petroleum ether) ν(CO) 1922 (vs) 1868 (vs); IR (cm^{-1}, THF) ν(SiH) 2016 (w), ν(CO) 1912 (vs), 1854 (vs); ^1H NMR (acetone-d_6, relative to internal Me_4Si) δ 7.1–7.6 (m, 10 H, Ph), 6.1 (d, 1 H, Si-*H*, ^3J(HCrSiH) = 5.6 Hz), 2.1 (s, 18 H, Me), −11.5 (d, 1 H,Cr*H*); ^{29}Si NMR (THF-d_8, relative to internal Me_4Si) δ 21.2, ^1J(SiH) = 197.0 Hz, ^2J(SiCrH) = 70.8 Hz. Anal. Calcd for $C_{26}H_{30}CrO_2Si$: C, 68.68; H, 6.66. Found: C, 68.86; H, 6.93.

X-ray Structure Analysis of 1. Crystals of 1 were obtained from pentane/ether. A crystal (0.3 × 0.35 × 0.25 mm) was mounted on a Syntex $P2_1$ automatic four-circle diffractometer. Mo Kα radiation (λ = 0.71069 Å, graphite monochromator) was used for all measurements. Centering and refinement of 25 reflections from different parts of the reciprocal space resulted in the following unit-cell dimensions: a = 9.285 (7) Å, b = 15.86 (2) Å, c = 16.05 (2) Å, β = 94.20 (7)°, and V = 2360 Å^3. By systematic absences space group $P2_1/n$ was established; d(calcd) = 1.28 g/cm^3 (Z = 4). Diffraction intensities were measured in an ω-scan mode (scan range 0.9°); the scan rate varied as a function of maximum peak intensity from 1.0 to 29.3 min^{-1}. Background radiation was measured on each side of the reflection center for half of the total scan time. Two reference reflections measured every 50 reflections showed no significant deviation in their intensity. A total of 3993 independent reflections were collected ($2° \leq 2\theta \leq 50°$). Intensity data were corrected for Lorentz and polarization effects; an empirical absoption correction was applied (μ = 5.8 cm^{-1}). The structure was solved by the heavy-atom method (Syntex XTL). The positions of the phenyl hydrogen atoms were calculated according to the idealized geometry; the remaining hydrogen positions were located from difference Fourier maps. Atomic coordinates and anisotropic thermal parameters of the non-hydrogen atoms as well as the atomic coordinates and the isotropic temperature factors of H(1) and H(2) were refined by full-matrix least squares with 3548 structure factors ($F_o \geq 2.0\sigma(F_o)$). Final $R_1 = R_2 = 0.062$, where $R_1 = \sum||F_o| - |F_c||/|F_o|$ and $R_2 = \sum w(|F_o| - |F_c|)^2/\sum wF_o^2)^{1/2}$ ($1/w = \sigma(F_o) + 0.000025F_o^2$). The final positional parameters of the non-hydrogen atoms, H(1), and H(2) are listed in Table II. Listings of hydrogen parameters, thermal parameters, and observed and calculated structure factors are available as supplementary material.

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Registry No. 1, 106358-28-5; (η^6-C_6Me_6)$(CO)_2$Cr P-n-Bu_3, 12278-75-0; $C_6Me_6Cr(CO)_3$, 12088-11-8; H_2SiPh_2, 775-12-2; ^{29}Si, 14304-87-1.

Supplementary Material Available: Tables of the atomic coordinates and temperature parameters for all atoms (2 pages); a list of observed and calculated structure factors (20 pages). Ordering information is given on any current masthead page.

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