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STRUCTURE AND CHARACTERIZATION OF
$(C_5H_5)_2Zr(H)BH_3CH_3$

W.K. Kot, N.M. Edelstein, and A. Zalkin

September 1986

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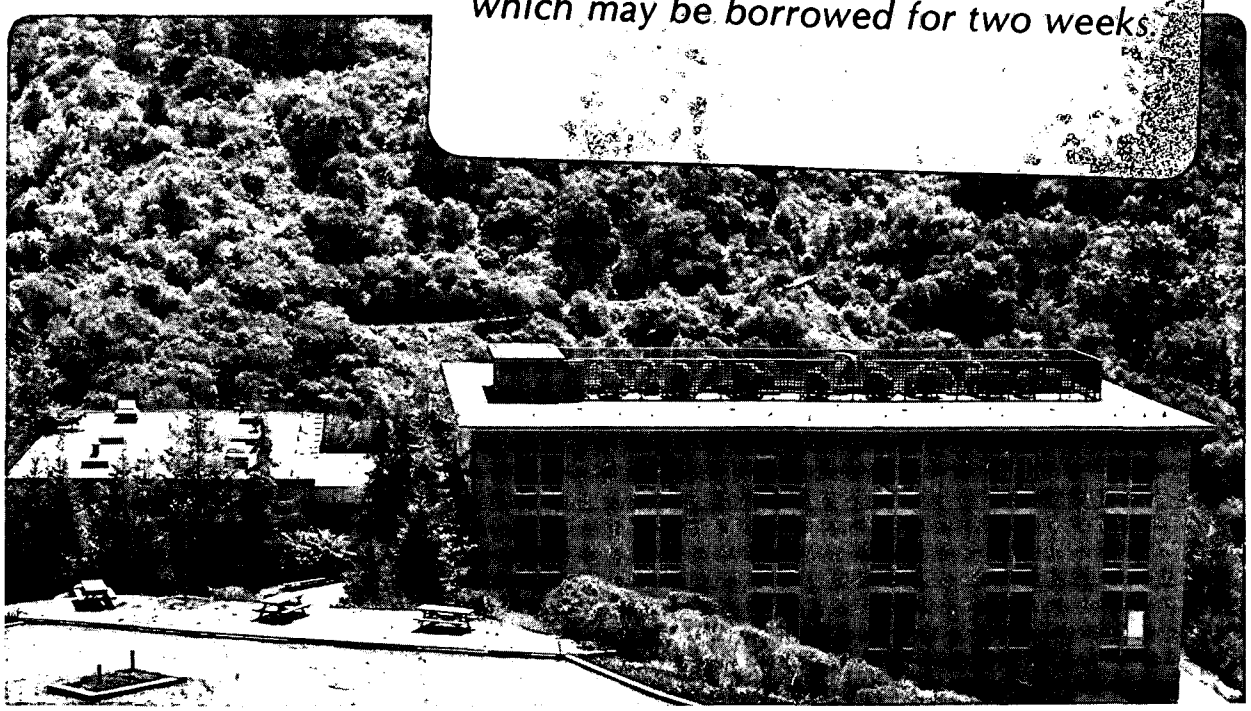

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LBL-22223

Contribution from the Materials and Molecular Research Division, Lawrence Berkeley Laboratory, and the Department of Chemistry, University of California, Berkeley, California 94720

Structure and Characterization of $(C_5H_5)_2Zr(H)BH_3CH_3$

Wing K. Kot, Norman M. Edelstein and Allan Zalkin

Abstract

The monomeric hydride, $(\eta^5\text{-}C_5H_5)Zr(H)BH_3CH_3$, has been prepared by reacting $(\eta^5\text{-}C_5H_5)_2ZrCl_2$ with $LiBH_3CH_3$, and its molecular structure has been determined by single crystal x-ray diffraction. Mass spectroscopy, infrared spectroscopy and nuclear magnetic resonance data are presented. The orthorhombic crystal belongs to the space group $Cmc2_1$ with unit cell parameters a = 13.775(3)A, b = 9.520(3)A, c = 8.816(2)A and R = 0.018. The methyltribydroborato group acts as a bidentate ligand. The Zr-terminal H distance is 1.79 ± 0.04A and the Zr-B distance is 2.558 ± 0.004A.

Most well-characterized zirconium hydrides are obtained as derivatives of bis(cyclopentadienyl)-zirconium; the first of which was prepared by treating $Cp_2Zr(BH_4)_2$ with trimethylamine (Cp = η^5-C_5H_5).[1] Other zirconium hydrides have also been synthesized by reacting $LiAlH_4$, $LiAl(O\text{-tert-}C_4H_9)_3H$, $LiBH_4$ and $CH(CH_3)_2MgCl$ with various starting materials.[2] Most of these hydrides are polymeric and hence insoluble in organic solvents, thereby limiting studies of their physical and chemical properties. Consequently, very little structural information is available. The monomeric hydride $Cp_2Zr(H)BH_3CH_3$ has been isolated and structurally characterized during our unsuccessful attempt to synthesize $Cp_2Zr(BH_3CH_3)_2$.

Experimental Section

All manipulations were conducted under inert atmosphere on a Schlenk line or in an inert atmosphere glovebox. Solvents were dried and purged according to standard procedures. The ^1H (89.5 MHz), ^{11}B (28.7MHz) NMR spectra were recorded on a JEOL FX-90Q spectrometer in deuterated toluene and referenced to tetramethylsilane and boron trifluoride etherate respectively. The IR spectra were recorded on a Perkin-Elmer 297 spectrometer. Mass spectra were obtained with Atlas MS-12 and Consolidated 12-110 instruments at the U.C. Berkeley mass spectroscopy laboratory.

Preparation of $Cp_2Zr(H)BH_3CH_3$ and $Cp_2Zr(D)BD_3CH_3$

Commerically available Cp_2ZrCl_2(1.2g, 4.1mmole) (Alfa Inorganic) was mixed with $LiBH_3CH_3$[3](0.36g, 10mmole) and stirred for 12 hours in either diethyl ether or chlorobenzene. After removal of the solvent by vacuum, the pale yellow residue was sublimed at 60°C and white needle-shaped crystals were collected on a 0°C cold finger. Alternatively, CpNa(10 mmole) was added to a 1.04g (5 mmole) sample of $Zr(BH_3CH_3)_4$[3] in diethyl ether. Similar work-up procedures yielded the same product. The average yield in both cases is 35%. The deuterated compound $Cp_2Zr(D)BD_3CH_3$ was made by substituting $LiBH_3CH_3$ with $LiBD_3CH_3$ which in turn was prepared by reacting $LiAlD_4$ with $(CH_3)_3B$.

X-ray diffraction

A white air-sensitive single crystal fragment with dimensions 0.18 × 0.12 × 0.65 mm was placed inside a 0.3 mm quartz capillary in an argon filled drybox; the capillary was sealed to protect the crystal from the atmosphere. A modified Picker FACS-1 automated diffractometer using graphite monochromated Mo Kα radiation (λ $K\alpha_1$, $K\alpha_2$; 0.70930, 0.71359 Å) was used to collect 5169 θ-2θ scanned intensities; data were collected to a maximum 2θ limit of 55° using a scan width of (1.50 + 0.693tanθ)° on 2θ. Three standard reflections were measured at every 250th reflection; the intensities decayed 3% and were corrected accordingly. The data were corrected for Lorentz and polarization effects and absorption (analytical

method)[4]; the absorption corrections range varied from 1.11 to 1.19. Cell dimensions and other crystal data are given in Table I.

The Zr atom position was located with the use of three-dimensional Patterson maps; subsequent least-squares refinements and electron density maps revealed the locations of the other atoms. The structure was refined by full-matrix least-squares using anisotropic thermal parameters on the non-hydrogen atoms and isotropic thermal parameters on the hydrogen atoms. The atoms of the methyltrihydroborato group are disordered across a mirror plane and were placed in general positions of the space group with one-half occupancy factors. Scattering factors[5] were adjusted for anomalous dispersion. The H^{-1} scattering factors were used for the hydride ion, and neutral H values were used for the other hydrogen atoms. The positional parameters of H(3) would not converge; these parameters were not varied in the final refinements. The statistical results of the least-squares are shown in Table I and the positional parameters in Table II.

Results and Discussion

The formation of $Cp_2Zr(H)BH_4$ was reported to be a result of the bridge-clevage reaction of $Cp_2Zr(BH_4)_2$ with $(CH_3)_3N$.[1] It is, however, apparent that a different mechanism must be involved here since the hydride can be obtained in the absence of a base. Our experience with $U(BH_4)_4$ and $U(BH_3CH_3)_4$ indicates that the methyltrihydroborato group is less susceptible to attack by a base, presumably because it is partially shielded by the methyl group.[6] We have been unable to isolate $Cp_2Zr(BH_3CH_3)_2$ as an intermediate in the formation of the hydride. In contrast, both $Cp_2U(BH_4)_2$[7] and $Cp_2U(BH_3CH_3)_2$[6] have been prepared and found to contain only tridentate tetrahydroborato and methyltrihydroborato groups respectively. The hydride could not have resulted from the thermal decomposition of $Cp_2Zr(BH_3CH_3)_2$ during sublimation since similar NMR and IR spectra were obtained before and after the sublimation. These spectral data are given in Tables IV and V.

The mass spectrum of $Cp_2Zr(H)BH_3CH_3$ consists of three groups of proportional peaks which correspond to the presence of five zirconium and two boron isotopes. The largest group peaks at 249 which is expected for the fragment $Cp_2{}^{90}Zr^{11}BH_3CH_3^+$; metal tetrahydroborates and related compounds are found not to show a very strong parent ion.[1] The other two groups peak at 235 and 221, corresponding to the loss of a CH_3 and a BH_3CH_3 fragment respectively.

The ^1H NMR spectrum shows very similar chemical shifts to that of $Cp_2Zr(H)BH_4$, whereas the deuterated compound $Cp_2Zr(D)BD_3CH_3$ gives the expected spectrum with marked decrease in intensities of the hydride and BH_3 peaks. The multiplicities of the BH_3 peak and the ^{11}B spectrum clearly indicate that the three hydrogens bonded to the boron atom are equivalent in

solution; no detectable difference can be observed at a temperature of $-60^{o}C$. Dynamic interchange of Cp and BH_3 protons has also been shown to exist.[8] The IR spectrum is rather complicated and shows a great similarity to the spectrum of $Cp_2TiBH_3CH_3$ (prepared by a similar reaction between Cp_2TiCl_2 and $LiBH_3CH_3$) except for the presence of a broad peak at $1595cm^{-1}$. This band is hence assigned as the Zr-hydride stretch which upon deuteration is shifted to $1150cm^{-1}$ ($\nu M-H/\nu M-D = 1.387$). This assignment is in good agreement with those found in $Cp_2Zr(H)BH_4$ ($1620cm^{-1}$)[9] and $(\eta^5-C_5Me_5)_2ZrH_2$ ($1555cm^{-1}$).[10] As the compound $Cp_2Ti(BH_4)_2$ was found to contain only double hydrogen-bridge bond between the metal ion and the boron atom,[11] one can rule out from the IR data the possibility that, in both $Cp_2TiBH_3CH_3$ and $Cp_2Zr(H)BH_3CH_3$, the methyltrihydroborato group acts as a tridentate ligand.[9] The tridentate ligation mode had been the sole ligation mode in all but one of the known methyltrihydroborate compounds.[6] The bidentate ligation in $Cp_2Zr(H)BH_3CH_3$ was confirmed by X-ray crystal structure determination.

The zirconium atom is at the center of a distorted tetrahedron consisting of the centers of two cyclopentadienyl rings, a hydride ion, and the boron atom of the methyltrihydroborato group; and is bridge-bonded to the boron atom via two hydrogen atoms (see Figure 1). The zirconium atom and hydride ion are in special positions on the mirror plane. The cyclopentadienyl rings bonded to the zirconium atom are across the mirror plane from each other and therefore in a rigorously eclipsed configuration when viewed down the a axis. The methyltrihydroborato group is disordered across the mirror plane, and is randomly located on one side of mirror plane or the other.

The zirconium-terminal hydrogen distance of 1.79Å is considerably longer than that found in $(\eta^5\text{-}C_8H_{11})Zr(H)(dmpe)_2$ (dmpe = 1,2-bis(dimethylphosphino)ethane).[12] Such a difference probably cannot be explained by steric crowding alone as the average Zr-C and the Zr-ring centroid distances in $Cp_2Zr(H)BH_3CH_3$ are both shorter than those found in comparable compounds such as Cp_2ZrF_2[13] and Cp_2ZrCl_2.[14] However, it is in good agreement with the Zr-H bond lengths found in $(\eta\text{-}C_5Me_5)Zr(\eta\text{-}C_8H_8)H$ (1.81 and 1.78Å)[2c] and $\{ZrH(\mu\text{-}H)(\eta\text{-}C_5H_4Me)_2\}_2$ (1.78Å);[15] it is also consistent with the covalent radii of the elements[16] (the Bragg-Slater radii of hydrogen and zirconium are 0.25Å and 1.55Å respectively).[17] The Zr-B distance of 2.558Å is indicative of a bidentate methyltrihydroborato group as compared to 2.335Å and 2.31Å in the triply hydrogen-bridged $Zr(BH_3CH_3)_4$[2] and $Zr(BH_4)_4$ respectively.[18]

We have been unable to isolate $Cp_2Zr(BH_3CH_3)_2$ by the synthetic route with which $Cp_2U(BH_3CH_3)_2$ is prepared. This may be due to the smaller ionic radius of Zr(IV) (0.19Å smaller than that of U(IV)),[19] which results in a larger coordination number about U(IV), as evidenced by the difference in molecular structure between $Zr(BH_4)_4$ and $U(BH_4)_4$.[20] Moreover, we have also been unable to isolate the compound $Cp_2U(H)BH_3CH_3$.

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Supplementary Material. Tables of thermal parameters, additional distances and angles, least-squares plane, calculated powder parttern, observed structure factors and their discrepancies from the calculated values, and addtional ORTEP drawings (12 pages). Ordering information is given on any current masthead page.

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Table I. Crystal Data and Least-Squares Summary

a, Å[a]	13.775(3)	μ, cm^{-1}	8.97
b, Å	9.520(3)	no. unique data	1387
c, Å	8.816(2)	no. non-zero wght data	1365 [$F^2 > \sigma(F^2)$]
cryst syst	orthorhombic	p[b]	0.025
space group	$Cmc2_1$	no. parameters	116
volume, $Å^3$	1156.1	R (non-zero wtd dat)[c]	0.018
d_{calcd}, g/cm^3	1.604	R_w[d]	0.017
Z	4	R (all data)	0.020
temp, (°C)	23.0	goodness of fit[e]	1.01
empirical formula	$C_{11}H_{17}BZr$	max shift/esd	0.04
f(000)	576	max/min diff map ($e/Å^3$)	0.2-0.1
fw	279.15		

[a] Unit cell parameters were derived by a least-squares fit to the setting angles of the unresolved MoKα components of 31 reflections ($20^o < 2\theta < 35^o$).

[b] In the least-squares, the assigned weights to the data are $1.0/[\sigma(F)]^2$ were derived from $\sigma(F)^2 = [S^2 + (pF^2)^2]$, where S^2 is the variance due to counting statistics and p is assigned a value that adjusts the weights of the stronger reflections such that their weighted residuals are comparable to those of the weak ones.

[c] $R = \Sigma(|Fobs| - |Fcal|) / \Sigma|Fobs|$

[d] $R_w = \sqrt{[\Sigma w(|Fobs|-|Fcal|)^2 / \Sigma\, wFobs^2]}$

[e] σ_1 = error in observation of unit weight = $\sqrt{[\Sigma(w(|Fobs| - |Fcal|)^2) / (no - nv)]}$, where no is the number of observations and nv is the number of variables.

Table II. Positional Parameters with Estimated Standard Deviations

Atom	x	y	z
Zr	0	0.29393(2)	0.250
H-	0	0.480(4)	0.222(5)
B	0.0225(3)	0.2178(4)	-0.0260(5)
C(1)	-0.0562(7)	0.1871(7)	-0.1530(8)
C(2)	0.16155(21)	0.1800(4)	0.2682(10)
C(3)	0.17928(18)	0.3170(4)	0.2183(4)
C(4)	0.15337(19)	0.4051(4)	0.3400(4)
C(5)	0.11813(20)	0.3263(3)	0.4569(4)
C(6)	0.12288(27)	0.1845(4)	0.4145(5)
H(1)	0.011(6)	0.146(4)	0.084(4)
H(2)	0.0219(26)	0.337(4)	0.031(4)
H(3)	0.105(8)	0.282(10)	-0.055(14)
H(4)	-0.112(4)	0.186(6)	-0.083(8)
H(5)	-0.046(6)	0.106(12)	-0.192(9)
H(6)	-0.048(4)	0.26777)	0.240(29)
H(7)	0.1622(28)	0.104(4)	0.211(5)
H(8)	0.208(3)	0.339(4)	0.113(5)
H(9)	0.1624(25)	0.515(5)	0.348(4)
H(10)	0.0979(24)	0.366(4)	0.550(4)
H(11)	0.0972(19)	0.142(3)	0.474(4)

Table III. Selected Distances and Angles

Atoms	d(Å)	Atoms	d(Å)
Zr - H-	1.79(4)	Zr - C(6)	2.461(3)
Zr - H(1)	2.04(4)	Zr - B	2.558(4)
Zr - H(2)	2.00(3)	B - C(1)	1.585(8)
Zr - C(2)	2.481(2)	B - H(1)	1.19(4)
Zr - C(3)	2.495(2)	B - H(2)	1.24(4)
Zr - C(4)	2.493(2)	B - H(3)	1.32(10)
Zr - C(5)	2.464(2)	Cp - Zr	2.177

Atoms	angle(°)
H^- - Zr - B	98.6(14)
Zr - B - C(1)	130.4(4)
H^- - Zr - Cp	95.7
B - Zr - Cp	102.6
B - Zr - Cp'	116.9
Cp - Zr - Cp'	137.1

[f] Cp represents the center of cyclopentadienyl ring C(2)-C(6); Cp' represents the equivalent group at -x,y,z.

Table IV. Nuclear Magnetic Resonance Data for $Cp_2Zr(H)BH_3CH_3$

Nucleus	Chemical Shift[g]
^1H	+5.61 (10H, s), +4.16 (1H, s)
	+0.51 (3H, s), -1.20 (3H, br, quart)
^{11}B	+20.2 (quart)

[g] Shifts are in ppm from Me_4Si and $BF_3.OC_2H_5$ respectively. Positive sign indicates a downfield shift.

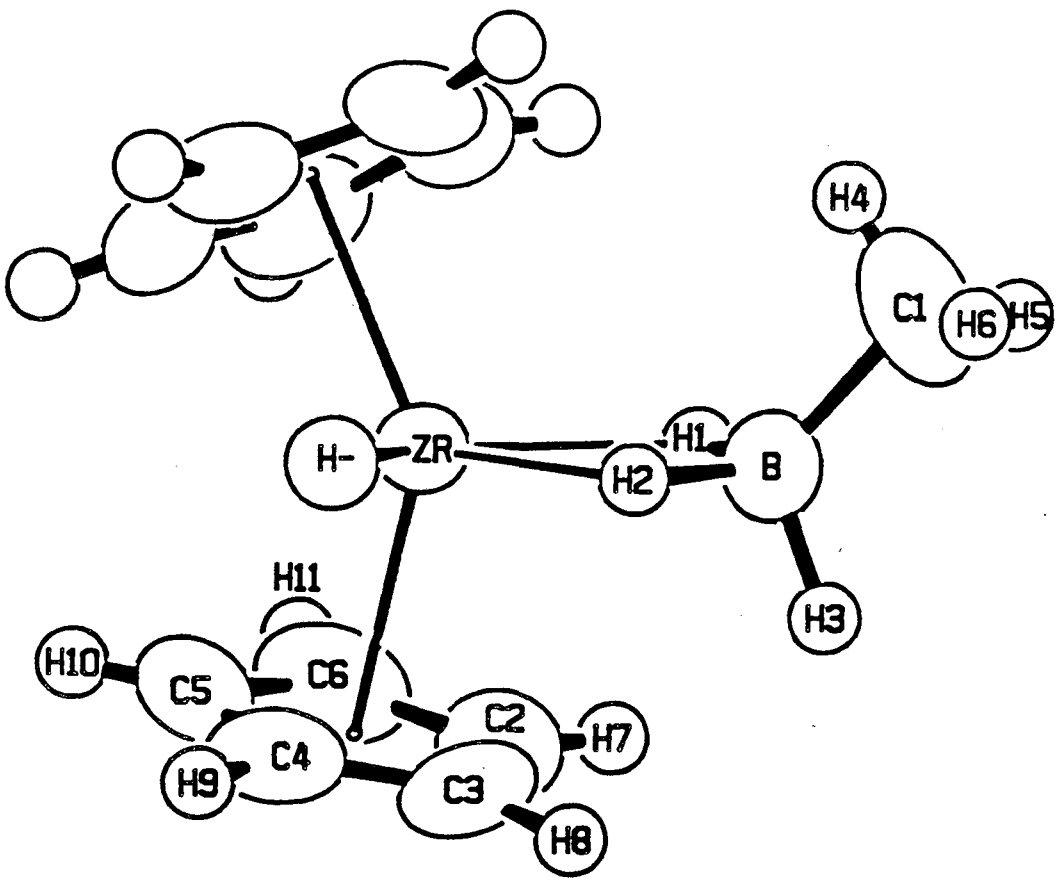
Table V. Infrared Spectroscopic Data (cm^{-1}) for $Cp_2Zr(H)BH_3CH_3$ and $Cp_2Zr(D)BD_3CH_3$[h]

Compound	Frequencies
$Cp_2Zr(H)BH_3CH_3$	2388s, 2240w, 2078w, 1903s, 1850m, 1810sh, 1720w, 1610m, 1595sh, 1290w, 1260w, 1125s, 1065w, 1010s, 993w, 855w, 830sh, 808s
$Cp_2Zr(D)BD_3CH_3$	1775m, 1720m, 1610m, 1290w, 1260w, 1205w, 1150m, 1115w, 1065w, 1030s, 1010s, 972w, 910w, 830sh, 808s, 735m, 720m

[h] Nujol mull in KBr disks.

Figure Caption

Fig 1. ORTEP drawing of $(C_5H_5)_2Zr(H)BH_3CH_3$. Only one conformation of the disorderd methyltrihydrobarate is shown.



Supplementary Material

Contribution from the Materials and Molecular Research Division, Lawrence Berkeley Laboratory, and the Department of Chemistry, University of California, Berkeley, California 94720

Structure and Characterization of $(C_5H_5)_2Zr(H)BH_3CH_3$

Wing K. Kot, Norman M. Edelstein and Allan Zalkin

Supplementary Table I. Table of Thermal Parameters[a] with Estimated Standard Deviations for $(C_5H_5)_2Zr(H)BH_3CH_3$

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Zr	3.238(7)	3.166(7)	3.684(7)	0	0	0.122(24)
B	5.4(3)	4.56(16)	4.02(14)	-0.59(14)	0.40(13)	-0.14(12)
C(1)	10.9(5)	5.44(24)	5.49(24)	-0.91(24)	-2.13(28)	0.04(19)
C(2)	5.25(10)	9.31(19)	10.3(4)	3.71(12)	-2.45(22)	-4.2(3)
C(3)	3.67(7)	10.29(21)	7.6(3)	-0.17(9)	1.27(11)	-0.22(16)
C(4)	3.85(9)	7.48(15)	9.41(18)	-1.35(10)	-0.18(10)	-1.09(14)
C(5)	4.74(10)	8.03(15)	6.40(13)	0.79(10)	-1.96(9)	-1.51(12)
C(6)	6.20(14)	7.24(16)	8.40(19)	1.05(12)	-2.97(14)	1.72(15)

Atom	$B(Å^2)$	Atom	$B(Å^2)$
H^-	3.6(8)	H(6)	8.9(18)
H(1)	4.9(9)	H(7)	9.5(11)
H(2)	3.3(8)	H(8)	8.8(9)
H(3)	9.9(26)	H(9)	9.3(9)
H(4)	5.0(11)	H(10)	7.5(8)
H(5)	12.7(32)	H(11)	4.9(7)

[a] The anisotropic temperature factor has the form: $T = -1/4\sum h_i h_j B_{ij} a_i^* a_j^*$

The isotropic temperature factor has the form: $T = -B(\sin\theta/\lambda)^2$

Supplementary Table II. Least-squares Plane and Deviations from it

Plane Equation: 12.74095 a - 0.62045 b + 3.30160 c = 2.81658

Distances (Å) Atoms to Plane:

Atoms in the Plane	
C(2)	0.016(10)
C(3)	-0.009(6)
C(4)	0.009(5)
C(5)	-0.005(4)
C(6)	0.003(6)
Atoms Not in Plane	
Zr	-2.174(2)

Supplementary Table III. Additional Distances and Angles

Atoms	d(Å)	Atoms	d(Å)
C(2)-C(3)	1.398(7)	C(1)-H(4)	0.99(6)
C(3)-C(4)	1.409(5)	C(1)-H(5)	0.86(11)
C(4)-C(5)	1.364(5)	C(1)-H(6)	1.09(19)
C(5)-C(6)	1.402(4)	C(2)-H(7)	0.89(4)
C(6)-C(2)	1.396(10)	C(3)-H(8)	1.03(4)
B -H(1)	1.19(4)	C(4)-H(9)	1.05(4)
B -H(2)	1.24(4)	C(5)-H(10)	0.95(4)
B -H(3)	1.32(10)	C(6)-H(11)	0.75(3)

Atoms	angle(°)
C(2)-C(3)-C(4)	105.8(5)
C(3)-C(4)-C(5)	109.8(3)
C(4)-C(5)-C(6)	108.2(3)
C(5)-C(6)-C(2)	107.1(4)
C(6)-C(2)-C(3)	109.2(4)

Supplementary Table IV. Calculated Powder Pattern for $(C_5H_5)_2Zr(H)BH_3CH_3$

X-ray Wavelength = 1.5418A

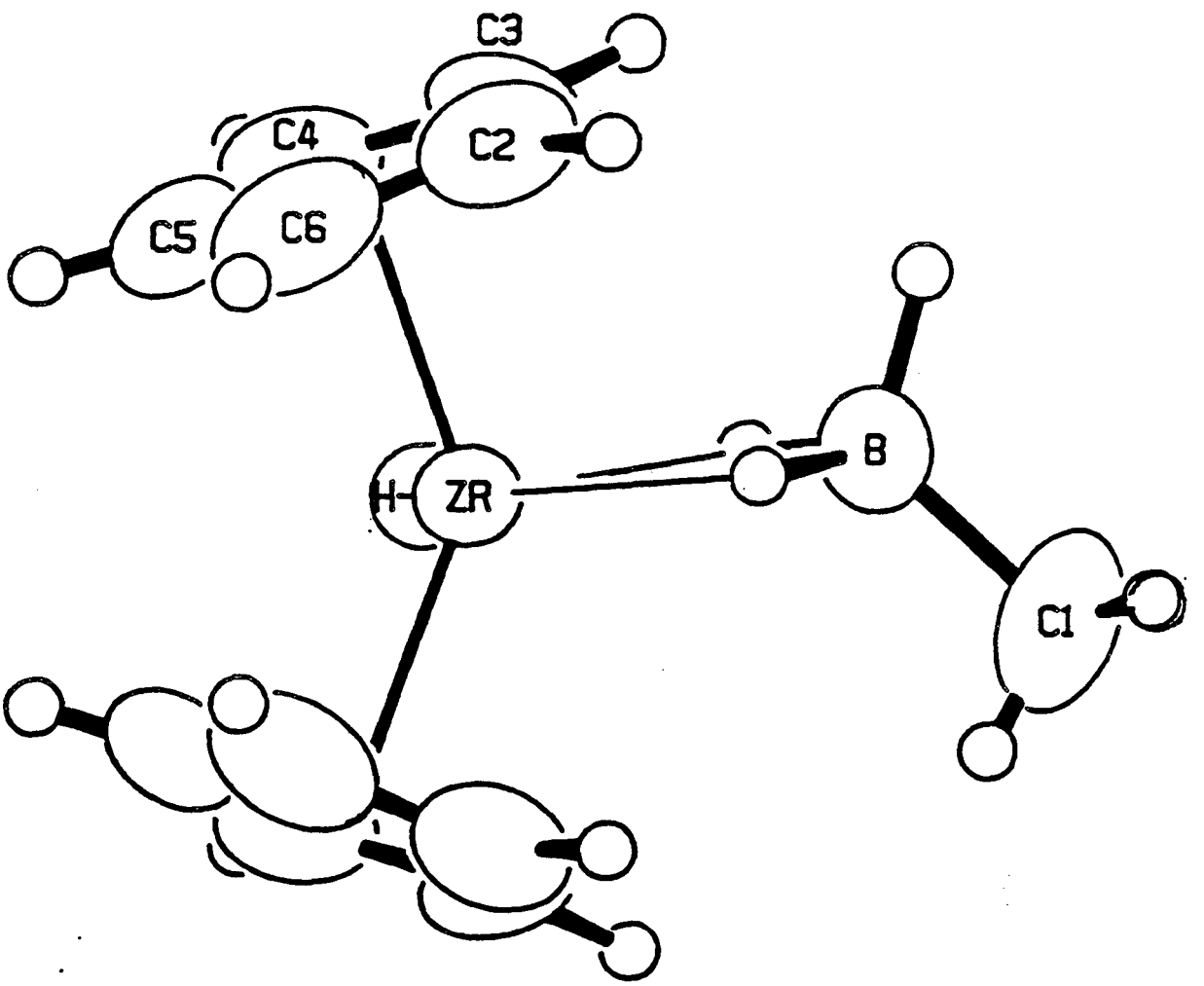
A = 13.775 B = 9.520 C = 8.816

Alpha = 90.00 Theta = 90.00 Gamma = 90.00

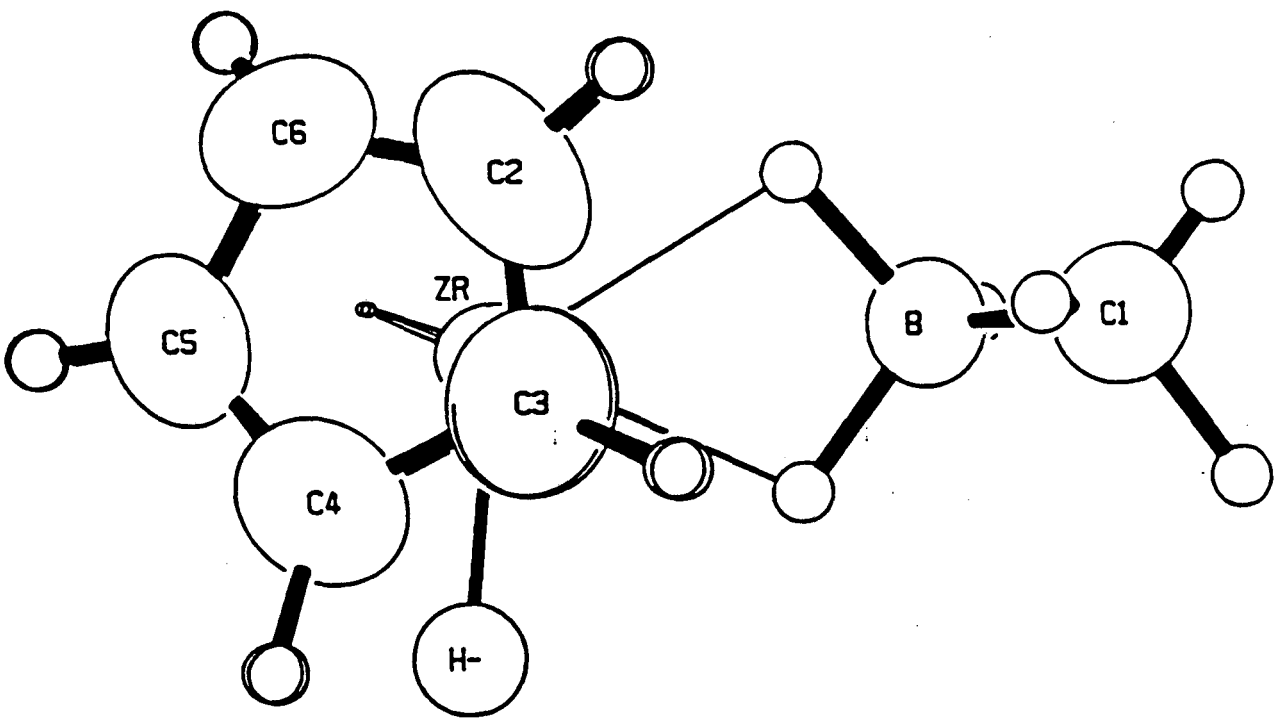
h	k	l	d	I	2 THETA	SINSQ
1	1	0	7.832	76.	11.30	0.00969
2	0	0	6.888	166.	12.85	0.01253
1	1	1	5.855	1993.	15.13	0.01734
0	2	0	4.760	265.	18.64	0.02623
0	0	2	4.408	284.	20.14	0.03059
0	2	1	4.188	157.	21.21	0.03388
3	1	0	4.136	0.	21.40	0.03474
2	2	0	3.916	85.	22.71	0.03876
1	1	2	3.841	32.	23.15	0.04027
3	1	1	3.744	95.	23.76	0.04239
2	0	2	3.713	55.	23.97	0.04311
2	2	1	3.579	81.	24.88	0.04640
4	0	0	3.444	0.	25.87	0.05011
0	2	2	3.234	75.	27.58	0.05681
1	3	0	3.092	15.	28.87	0.06215
3	1	2	3.016	18.	29.62	0.06533
2	2	2	2.928	73.	30.54	0.06934
1	3	1	2.918	62.	30.64	0.06979

4	2	0	2.790	15.	32.08	0.07634
1	1	3	2.751	131.	32.54	0.07851
4	0	2	2.714	103.	33.01	0.08070
4	2	1	2.660	46.	33.69	0.08399
5	1	0	2.646	5.	33.87	0.08486
3	3	0	2.611	12.	34.35	0.08720
5	1	1	2.535	190.	35.41	0.09250
1	3	2	2.532	55.	35.46	0.09273
3	3	1	2.503	56.	35.87	0.09485
0	2	3	2.501	13.	35.91	0.09505
3	1	3	2.396	74.	37.54	0.10356
0	4	0	2.380	0.	37.80	0.10492
4	2	2	2.358	81.	38.17	0.10693
2	2	3	2.350	26.	38.29	0.10757
0	4	1	2.298	30.	39.21	0.11256
6	0	0	2.296	27.	39.24	0.11275
5	1	2	2.269	12.	39.73	0.11544
2	4	0	2.249	6.	40.08	0.11744
3	3	2	2.246	52.	40.14	0.11779
0	0	4	2.204	26.	40.95	0.12234
2	4	1	2.180	65.	41.43	0.12509
1	3	3	2.130	33.	42.43	0.13096
1	1	4	2.122	5.	42.61	0.13203
2	0	4	2.099	28.	43.09	0.13487
0	4	2	2.094	6.	43.20	0.13550
5	3	0	2.080	10.	43.50	0.13731
6	2	0	2.068	13.	43.78	0.13898

Supplementary Figure 1. ORTEP view of molecule perpendicular to the mirror plane.



Supplementary Figure 2. ORTEP drawing of the molecule more or less edge on to the rings.



OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X12.0)
(C5H5)2ZR(BH3CH3)H F(0,0,0) = 2929

SG = Estimated standard deviation of Fob. DEL = /Fob/- /Fca/, where
Fob and Fca are the observed and calculated structure factors.
* indicates zero weighted data.

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K=		0,	0	6	130	2	-1	0	188	3	-1	3	389	5	6	-7	86	2	4
-10	139	3	5	7	158	2	0	1	60	3	-1	4	390	5	2	-6	82	2	2
-8	218	4	3	8	88	2	-2	2	155	3	0	5	297	4	3	-5	127	2	1
-6	376	5	5	9	141	3	-1	3	53	3	-1	6	222	3	-2	-4	84	2	-2
-4	665	9	12	10	43	4	-1	4	126	2	0	7	190	3	0	-3	152	2	1
-2	1063	0	57*	H,K=		0,	6	5	58	3	7	8	130	2	-1	-2	145	2	-3
2	1059	0	39*	-10	8	29	-2	6	90	3	1	9	87	2	-1	-1	178	2	1
4	652	8	3	-9	116	3	0	H,K=		0,	12	10	80	2	-1	0	128	2	-3
6	383	5	10	-8	19	23	8	-2	91	3	0	11	58	3	2	1	180	3	3
8	209	3	-3	-7	147	2	-3	-1	15	27	-6	H,K=		1,	5	2	145	2	-3
10	138	3	3	-6	48	3	-4	0	94	3	-3	-10	83	2	-1	3	151	2	1
H,K=		0,	2	-5	255	4	-6	1	29	18	9	-9	26	9	6	4	84	2	-2
-11	34	12	-10	-4	63	3	-1	2	93	3	2	-8	150	2	1	5	126	2	-1
-10	107	2	2	-3	355	5	3	H,K=		1,	1	-7	41	4	-8	6	80	2	0
-9	106	2	-1	-2	43	3	-2	-11	89	2	4	-6	246	3	-4	7	84	2	1
-8	178	3	-2	-1	398	5	-4	-10	28	9	-8	-5	12	21	-1	H,K=		1,	11
-7	97	2	-1	0	191	3	0	-9	140	2	0	-4	391	5	1	-5	91	2	1
-6	329	10	2	1	401	5	-2	-8	53	2	1	-3	116	2	-2	-4	7	23	3
-5	175	3	1	2	50	3	4	-7	281	4	4	-2	460	6	4	-3	119	2	-1
-4	553	15	-17	3	349	5	-1	-6	80	2	1	-1	87	1	0	-2	25	10	4
-3	281	8	1	4	59	3	-4	-5	515	8	6	0	376	5	1	-1	128	2	0
-2	549	0	39*	5	254	4	-9	-4	151	2	1	1	84	1	0	0	19	20	7
-1	595	0	34*	6	46	4	-7	-3	575	10	2	2	455	6	3	1	125	2	-3
0	1269	0	-9*	7	145	2	-3	-2	205	0	10*	3	119	2	-1	2	14	22	-7
1	605	0	40*	8	0	27	-11	-1	1028	0	30*	4	390	5	2	3	118	2	-1
2	557	0	42*	9	119	3	3	0	269	0	-21*	5	18	10	7	4	16	23	12
3	281	4	2	10	19	29	10	1	1032	0	30*	6	249	3	-1	5	90	2	0
4	556	7	-10	H,K=		0,	8	2	207	0	12*	7	46	3	-3	H,K=		2,	0
5	175	3	1	-8	61	3	2	3	579	7	9	8	149	2	-1	-10	125	2	2
6	335	5	7	-7	96	2	1	4	153	2	3	9	11	22	-9	-8	212	3	3
7	91	2	-2	-6	97	2	-3	5	519	7	11	10	86	2	3	-6	302	4	-1
8	178	3	-1	-5	131	2	-1	6	81	2	2	H,K=		1,	7	-4	508	6	-3
9	106	2	0	-4	140	2	3	7	279	4	0	-9	35	6	3	-2	393	0	15*
10	104	2	-1	-3	182	3	-5	8	49	2	-3	-8	109	2	-1	0	766	0	75*
11	45	4	1	-2	164	2	-1	9	140	2	0	-7	57	2	0	2	395	0	13*
H,K=		0,	4	-1	237	3	-3	10	39	3	4	-6	167	2	-2	4	507	6	-5
-10	43	5	-1	0	244	3	-4	11	85	2	0	-5	125	2	0	6	306	4	0
-9	142	2	0	1	238	3	-4	H,K=		1,	3	-4	224	3	-2	8	210	3	2
-8	88	2	-2	2	163	2	-4	-11	56	3	1	-3	103	2	2	10	125	2	1
-7	159	2	-2	3	185	3	-5	-10	78	2	-3	-2	322	4	-2	H,K=		2,	2
-6	130	2	0	4	138	2	2	-9	87	2	-1	-1	135	2	0	-11	46	3	5
-5	332	9	5	5	134	2	1	-8	132	2	0	0	287	4	-4	-10	101	2	1
-4	237	3	5	6	98	2	-2	-7	190	3	1	1	137	2	2	-9	92	2	1
-3	437	8	1	7	93	3	-1	-6	220	3	-4	2	319	4	-5	-8	171	2	2
-2	235	3	3	8	59	3	0	-5	296	4	1	3	100	2	2	-7	124	2	-1
-1	473	6	1	H,K=		0,	10	-4	390	7	0	4	224	3	-4	-6	231	3	-1
0	84	1	0	-6	91	3	1	-3	391	7	6	5	126	2	1	-5	215	3	2
1	475	6	4	-5	51	4	0	-2	410	5	2	6	168	2	0	-4	377	7	-8
2	234	3	4	-4	121	2	-5	-1	386	5	17	7	56	2	-2	-3	310	6	3
3	431	6	0	-3	54	3	-1	0	347	4	3	8	108	2	-1	-2	409	5	15
4	233	3	2	-2	153	3	-2	1	380	5	14	9	19	23	-13	-1	363	0	28*
5	333	5	7	-1	58	3	-3	2	403	5	1	H,K=		1,	9	0	661	0	33*

STRUCTURE FACTORS continued for
(C5H5)2ZR(BH3CH3)H

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
1	365	0	27*	-6	76	2	0	9	138	2	3	-1	73	2	1	-5	215	3	1
2	413	5	14	-5	155	2	-1	10	25	11	0	0	276	4	-1	-4	370	5	4
3	312	4	3	-4	108	2	0	11	83	2	1	1	68	2	-3	-3	306	4	13
4	378	5	-8	-3	181	3	0	H,K=		3,	3	2	276	4	-3	-2	545	7	8
5	217	3	3	-2	134	2	-2	-10	71	2	3	3	88	2	-3	-1	358	5	8
6	235	3	2	-1	209	3	-2	-9	85	2	0	4	217	3	-2	0	386	5	10
7	126	2	0	0	159	2	0	-8	150	2	-3	5	44	4	-1	1	353	5	5
8	168	2	0	1	212	3	0	-7	149	2	-3	6	190	3	3	2	537	7	3
9	92	2	1	2	135	2	-2	-6	242	3	-7	7	28	9	-14	3	306	4	12
10	100	2	0	3	177	2	-2	-5	161	2	-4	8	103	2	-1	4	376	5	5
11	39	5	-3	4	110	2	1	-4	300	4	-3	9	25	13	-7	5	216	3	2
H,K=		2,	4	5	156	2	0	-3	344	4	0	H,K=		3,	9	6	202	3	-3
-10	45	3	1	6	78	2	1	-2	451	6	-2	-7	78	2	2	7	153	2	-3
-9	132	2	0	7	93	2	-2	-1	423	5	7	-6	74	2	-3	8	165	2	-2
-8	78	2	-2	8	58	3	2	0	383	5	10	-5	106	2	2	9	70	2	0
-7	179	2	0	H,K=		2,	10	1	421	5	5	-4	99	2	0	10	90	2	1
-6	108	2	-2	-6	88	2	2	2	457	6	1	-3	143	2	2	11	41	4	3
-5	288	4	-1	-5	49	3	-1	3	348	4	0	-2	123	2	-1	H,K=		4,	4
-4	186	3	-2	-4	122	2	-1	4	304	4	-3	-1	132	2	1	-10	40	5	-2
-3	386	5	-6	-3	52	3	-4	5	165	2	-1	0	109	2	-1	-9	105	2	0
-2	246	3	2	-2	146	2	5	6	244	3	-6	1	132	2	2	-8	70	2	1
-1	524	7	3	-1	58	2	-3	7	148	2	-4	2	123	2	0	-7	195	3	-1
0	311	4	5	0	160	2	3	8	151	2	-5	3	142	2	2	-6	104	2	-2
1	527	7	2	1	60	2	-1	9	85	2	0	4	97	2	-2	-5	256	3	-6
2	248	3	3	2	144	2	3	10	71	2	2	5	109	2	4	-4	171	2	-1
3	386	5	-9	3	52	2	-3	H,K=		3,	5	6	75	2	-2	-3	379	5	6
4	186	3	-2	4	122	2	0	-10	86	2	3	7	76	2	0	-2	216	3	-1
5	291	4	0	5	46	3	-4	-9	18	21	0	H,K=		3,	11	-1	537	7	-4
6	107	2	-4	6	86	2	0	-8	153	2	1	-4	12	22	6	0	372	5	4
7	177	2	-1	H,K=		2,	12	-7	42	3	-2	-3	115	2	2	1	537	7	-6
8	80	2	0	-2	95	2	4	-6	248	3	-6	-2	16	22	-2	2	221	3	1
9	129	2	-2	-1	20	23	2	-5	68	2	0	-1	127	2	3	3	381	5	4
10	47	3	3	0	105	2	2	-4	292	4	-1	0	0	22	-13	4	171	2	-1
H,K=		2,	6	1	20	22	1	-3	83	2	1	1	129	2	5	5	255	3	-7
-9	115	2	2	2	95	2	4	-2	469	6	3	2	18	20	-1	6	105	2	-2
-8	11	22	3	H,K=		3,	1	-1	178	2	4	3	116	2	3	7	195	3	-2
-7	161	2	0	-11	86	2	3	0	494	6	-1	4	15	23	9	8	72	2	3
-6	17	20	12	-10	28	9	3	1	178	2	3	H,K=		4,	0	9	105	2	0
-5	256	3	0	-9	136	2	2	2	472	6	4	-10	103	2	-2	10	41	5	-2
-4	23	14	2	-8	69	2	-3	3	84	2	2	-8	219	3	3	H,K=		4,	6
-3	322	4	3	-7	265	3	0	4	296	4	1	-6	280	4	-3	-9	97	2	-1
-2	13	18	-15	-6	132	2	2	5	68	2	0	-4	497	6	0	-8	13	22	-1
-1	427	6	4	-5	300	4	-8	6	249	3	-4	-2	760	10	26	-7	160	2	1
0	26	6	-8	-4	178	2	-2	7	45	3	1	0	45	0	0*	-6	11	21	-10
1	425	6	-1	-3	506	6	5	8	153	2	0	2	738	9	15	-5	243	3	-4
2	17	18	-13	-2	203	3	9	9	11	20	-7	4	497	6	-3	-4	62	2	1
3	323	4	3	-1	385	0	25*	10	84	2	1	6	280	4	-2	-3	284	4	-3
4	27	7	5	0	19	0	1*	H,K=		3,	7	8	216	3	0	-2	75	2	-1
5	254	3	-3	1	359	0	22*	-9	27	13	-4	10	104	3	-2	-1	388	5	4
6	14	21	9	2	201	3	10	-8	103	2	0	H,K=		4,	2	0	47	2	2
7	161	2	0	3	503	6	0	-7	42	4	0	-11	40	6	2	1	389	5	4
8	6	22	-3	4	177	2	-3	-6	188	3	1	-10	90	2	1	2	76	2	0
9	111	2	-2	5	304	4	-5	-5	48	2	4	-9	68	2	-1	3	282	4	-4
H,K=		2,	8	6	134	2	4	-4	220	3	0	-8	167	2	0	4	62	2	0
-8	58	3	2	7	262	3	-4	-3	89	2	0	-7	153	2	-2	5	243	3	-3
-7	93	2	-2	8	75	2	2	-2	276	4	-4	-6	200	3	-6	6	20	18	0

STRUCTURE FACTORS continued for
(C5H5)2ZR(BH3CH3)H

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
7	162	2	2	6	88	2	-4	-2	246	3	-5	-4	390	5	3	9	86	2	3
8	17	22	2	7	262	3	-8	-1	117	2	3	-3	204	3	0	H,K=		6,	8
9	98	2	0	8	49	2	-3	0	247	3	-3	-2	506	6	7	-7	70	2	-2
H,K=		4,	8	9	127	2	1	1	114	2	1	-1	320	4	-2	-6	84	2	0
-8	60	3	5	10	16	22	-8	2	243	3	-7	0	512	6	5	-5	114	2	0
-7	81	2	-1	H,K=		5,	3	3	126	2	-1	1	321	4	-1	-4	115	2	-1
-6	72	2	2	-10	65	2	2	4	188	3	-3	2	502	6	5	-3	153	2	3
-5	158	2	2	-9	79	2	-2	5	57	2	-3	3	203	3	-2	-2	152	2	2
-4	109	2	0	-8	120	2	-2	6	156	2	2	4	386	5	0	-1	187	3	0
-3	166	2	3	-7	159	2	-4	7	56	2	2	5	156	2	1	0	138	2	-3
-2	152	2	2	-6	219	3	-3	8	90	2	2	6	251	3	-1	1	185	3	-2
-1	174	2	-2	-5	211	3	2	H,K=		5,	9	7	92	2	-1	2	149	2	1
0	106	2	1	-4	237	3	-1	-7	75	2	0	8	145	2	-1	3	150	2	0
1	174	2	-3	-3	355	5	6	-6	60	2	-2	9	60	2	0	4	114	2	-1
2	151	2	2	-2	431	6	6	-5	98	2	1	10	79	2	2	5	114	2	-1
3	161	2	0	-1	381	5	1	-4	87	2	1	H,K=		6,	4	6	82	2	-2
4	111	2	1	0	426	5	-4	-3	146	2	1	-10	31	9	-6	7	74	2	2
5	157	2	1	1	380	5	1	-2	114	2	3	-9	91	2	2	H,K=		6,	10
6	73	2	3	2	430	6	6	-1	155	2	-1	-8	64	2	-3	-5	34	8	-5
7	85	2	3	3	358	5	8	0	105	2	-2	-7	154	2	3	-4	104	2	1
8	56	3	1	4	236	3	-1	1	154	2	-1	-6	111	2	-1	-3	43	4	-2
H,K=		4,	10	5	209	3	1	2	112	2	1	-5	264	3	-3	-2	127	2	-2
-6	84	2	1	6	215	3	-5	3	145	2	0	-4	173	2	-1	-1	53	3	-2
-5	29	9	-15	7	162	2	-1	4	84	2	-3	-3	323	4	-3	0	143	2	1
-4	121	2	3	8	121	2	-2	5	100	2	2	-2	134	2	0	1	55	2	-1
-3	49	3	0	9	81	2	0	6	63	2	1	-1	330	4	-3	2	126	2	-3
-2	137	2	-1	10	64	2	1	7	74	2	-1	0	160	2	-2	3	42	5	-3
-1	50	3	-6	H,K=		5,	5	H,K=		5,	11	1	329	4	-1	4	103	2	0
0	140	2	0	-10	76	2	1	-4	10	22	-1	2	133	2	1	5	35	6	-4
1	53	2	-4	-9	15	22	-2	-3	100	2	-3	3	320	4	-2	H,K=		7,	1
2	137	2	0	-8	128	2	0	-2	19	23	5	4	169	2	-3	-10	28	11	-3
3	48	3	-1	-7	31	5	-1	-1	121	2	1	5	261	3	-4	-9	109	2	-1
4	119	2	1	-6	232	3	-2	0	0	22	-6	6	113	2	0	-8	36	5	-2
5	40	3	-5	-5	64	2	2	1	118	2	-1	7	154	2	2	-7	198	3	0
6	84	2	1	-4	262	3	-4	2	8	22	-7	8	62	2	-5	-6	38	4	-5
H,K=		4,	12	-3	31	5	-7	3	100	2	-2	9	88	2	-1	-5	290	4	3
-1	16	24	0	-2	405	5	6	4	18	22	7	10	27	11	-10	-4	72	2	2
0	105	2	4	-1	89	2	1	H,K=		6,	0	H,K=		6,	6	-3	373	5	5
1	11	23	-6	0	400	5	-5	-10	92	3	-3	-9	87	2	3	-2	136	2	0
H,K=		5,	1	1	92	2	1	-8	177	3	0	-8	11	22	-7	-1	643	8	13
-10	29	9	4	2	402	5	4	-6	288	4	-1	-7	128	2	-1	0	187	3	-1
-9	126	2	0	3	34	3	-3	-4	457	6	7	-6	37	4	4	1	646	8	14
-8	52	2	0	4	260	3	-5	-2	820	11	24	-5	216	3	-2	2	137	2	-2
-7	267	4	-4	5	61	2	0	0	921	12	21	-4	43	3	-1	3	374	5	2
-6	90	2	-4	6	231	3	-2	2	816	10	19	-3	269	4	-8	4	73	2	2
-5	310	4	-3	7	25	10	-8	4	459	6	8	-2	79	2	0	5	289	4	3
-4	99	2	0	8	129	2	0	6	286	4	-2	-1	287	4	-3	6	43	3	0
-3	685	9	18	9	11	21	-7	8	172	3	-4	0	13	20	-12	7	193	3	-4
-2	212	3	0	10	74	2	0	10	94	3	1	1	283	4	-6	8	30	6	-7
-1	775	10	18	H,K=		5,	7	H,K=		6,	2	2	76	2	-1	9	110	2	1
0	229	3	7	-8	88	2	0	-10	76	2	0	3	266	3	-9	10	30	6	0
1	764	10	15	-7	56	2	2	-9	58	2	-3	4	34	3	-9	H,K=		7,	3
2	211	3	-1	-6	155	2	2	-8	146	2	1	5	216	3	-2	-10	69	2	0
3	687	9	18	-5	56	2	-3	-7	92	2	-2	6	35	3	2	-9	72	2	2
4	98	2	0	-4	189	3	-2	-6	250	3	-3	7	127	2	-2	-8	99	2	3
5	311	4	0	-3	126	2	0	-5	158	2	1	8	18	22	-1	-7	137	2	-1

STRUCTURE FACTORS continued for
(C5H5)2ZR(BH3CH3)H

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-6	145	2	0	-6	63	2	4	-7	118	2	1	0	107	2	2	2	272	4	-2
-5	203	3	-2	-5	84	2	-1	-6	76	2	0	1	49	4	1	3	89	2	1
-4	220	3	-1	-4	72	2	-2	-5	227	3	-2	2	98	2	3	4	217	3	2
-3	251	3	6	-3	105	2	-1	-4	121	2	-2	3	41	3	2	5	18	21	-6
-2	249	3	2	-2	112	2	0	-3	257	3	-6	4	87	2	3	6	133	2	-1
-1	240	3	-2	-1	145	2	2	-2	147	2	2	H,K=		9,	1	7	35	5	4
0	266	3	-2	0	105	2	0	-1	251	3	1	-9	103	2	4	8	106	2	1
1	240	3	0	1	146	2	2	0	136	2	4	-8	41	3	2	H,K=		9,	7
2	249	3	2	2	112	2	0	1	251	3	2	-7	144	2	2	-7	28	10	6
3	246	3	3	3	106	2	-1	2	143	2	-2	-6	63	2	-1	-6	110	2	0
4	215	3	-4	4	74	2	-1	3	255	3	-7	-5	247	3	-1	-5	44	3	0
5	203	3	-1	5	85	2	0	4	120	2	-3	-4	108	2	0	-4	147	2	4
6	145	2	1	6	60	3	0	5	228	3	-3	-3	202	3	0	-3	18	20	-1
7	139	2	0	H,K=		7,	11	6	76	2	0	-2	86	2	2	-2	186	3	2
8	96	2	1	-2	21	15	7	7	117	2	-1	-1	292	4	0	-1	79	2	-1
9	71	2	1	-1	100	2	1	8	53	3	-3	0	80	2	-1	0	184	3	0
10	71	2	2	0	13	21	7	9	94	2	1	1	296	4	0	1	81	2	-1
H,K=		7,	5	1	100	2	2	H,K=		8,	6	2	82	2	-1	2	184	3	1
-9	18	21	2	2	13	21	-2	-8	0	22	-11	3	197	3	-2	3	17	20	-4
-8	109	2	-1	H,K=		8,	0	-7	113	2	-1	4	106	2	-2	4	145	2	1
-7	24	10	-7	-10	90	3	4	-6	29	7	-2	5	244	3	-5	5	45	3	1
-6	174	2	0	-8	125	2	1	-5	177	2	-2	6	62	2	-3	6	108	2	0
-5	22	10	-6	-6	244	3	-3	-4	20	14	-3	7	144	2	0	7	23	18	1
-4	255	3	-3	-4	300	4	3	-3	239	3	-1	8	38	5	-1	H,K=		9,	9
-3	67	2	0	-2	250	3	6	-2	34	4	4	9	102	2	3	-5	75	2	2
-2	295	4	-5	0	510	7	2	-1	256	3	-3	H,K=		9,	3	-4	64	2	2
-1	46	2	4	2	259	4	5	0	29	7	-8	-9	65	2	3	-3	80	2	1
0	270	4	-1	4	296	4	2	1	256	3	-4	-8	95	2	0	-2	79	2	-1
1	35	4	-6	6	247	3	-3	2	32	5	2	-7	90	2	1	-1	98	2	2
2	291	4	-7	8	125	2	0	3	237	3	-4	-6	129	2	-1	0	67	2	-2
3	68	2	1	10	86	3	0	4	8	18	-14	-5	129	2	0	1	95	2	-1
4	254	3	-4	H,K=		8,	2	5	181	3	2	-4	223	3	2	2	76	2	-3
5	21	12	-7	-10	71	2	3	6	29	6	-3	-3	172	2	-3	3	80	2	1
6	173	2	0	-9	68	2	2	7	113	2	-1	-2	228	3	-1	4	63	2	1
7	22	15	-8	-8	106	2	1	8	12	23	1	-1	241	3	-1	5	76	2	3
8	109	2	-1	-7	73	2	2	H,K=		8,	8	0	272	4	3	H,K=		10,	0
9	15	22	-1	-6	195	3	-1	-7	75	2	0	1	242	3	-1	-8	122	2	3
H,K=		7,	7	-5	161	2	-1	-6	70	2	3	2	226	3	-4	-6	205	3	2
-8	86	2	2	-4	251	3	2	-5	100	2	3	3	174	2	-3	-4	314	4	-4
-7	38	5	-7	-3	171	2	4	-4	79	2	0	4	220	3	-3	-2	241	3	-2
-6	114	2	-3	-2	205	3	-2	-3	136	2	-1	5	128	2	-2	0	301	4	3
-5	71	2	-2	-1	161	2	1	-2	80	2	1	6	131	2	-1	2	232	3	-6
-4	171	2	3	0	357	5	-1	-1	158	2	1	7	89	2	0	4	312	4	-2
-3	66	2	-2	1	161	2	-1	0	114	2	0	8	95	2	0	6	207	3	3
-2	241	3	-1	2	210	3	-1	1	160	2	3	9	63	3	1	8	119	2	0
-1	98	2	-4	3	166	2	1	2	80	2	0	H,K=		9,	5	H,K=		10,	2
0	232	3	-4	4	245	3	-3	3	139	2	2	-8	107	2	1	-9	53	3	1
1	100	2	-4	5	160	2	-3	4	78	2	0	-7	30	6	-2	-8	100	2	5
2	239	3	-3	6	197	3	-1	5	96	2	-1	-6	133	2	-1	-7	88	2	3
3	67	2	-1	7	72	2	0	6	72	2	5	-5	15	19	-10	-6	143	2	1
4	171	2	0	8	106	2	0	7	76	2	1	-4	216	3	3	-5	143	2	-1
5	72	2	-1	9	67	2	2	H,K=		8,	10	-3	88	2	0	-4	220	3	-1
6	114	2	-3	10	73	2	5	-4	90	2	5	-2	270	4	-2	-3	183	3	-4
7	39	5	-6	H,K=		8,	4	-3	41	3	2	-1	72	2	0	-2	234	3	0
8	83	2	-1	-9	94	2	2	-2	99	2	4	0	305	4	-7	-1	163	2	-2
H,K=		7,	9	-8	54	2	-1	-1	46	3	-2	1	68	2	-2	0	307	4	-1

STRUCTURE FACTORS continued for
(C5H5)2ZR(BH3CH3)H

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
1	163	2	-1	-2	87	2	2	5	35	3	4	-5	115	2	0	-5	95	2	2
2	234	3	0	-1	37	5	3	6	116	2	-1	-4	76	2	1	-4	79	2	0
3	181	3	-5	0	89	2	4	7	21	22	-3	-3	146	2	-3	-3	118	2	1
4	219	3	-1	1	42	3	8	H,K=	11,		7	-2	80	2	1	-2	118	2	2
5	142	2	-3	2	90	2	5	-6	91	2	2	-1	168	2	-2	-1	104	2	3
6	145	2	2	H,K=	11,		1	-5	39	3	-1	0	88	2	2	0	109	2	-1
7	88	2	3	-9	86	2	3	-4	115	2	2	1	167	2	-2	1	102	2	2
8	95	2	1	-8	31	8	-2	-3	62	2	-1	2	81	2	3	2	117	2	1
9	52	3	0	-7	128	2	-1	-2	122	2	0	3	146	2	-3	3	117	2	1
H,K=	10,		4	-6	44	4	-4	-1	67	2	1	4	76	2	1	4	76	2	-2
-8	43	5	-2	-5	198	3	-1	0	136	2	-2	5	111	2	-1	5	92	2	-1
-7	112	2	-1	-4	69	2	-2	1	68	2	3	6	61	2	0	6	76	2	-2
-6	58	2	0	-3	311	4	-1	2	120	2	-1	7	96	2	1	7	69	2	2
-5	168	2	1	-2	92	2	-2	3	60	2	-2	H,K=	12,		6	H,K=	13,		5
-4	94	2	4	-1	311	4	-1	4	114	2	1	-6	18	23	11	-6	95	2	0
-3	231	3	0	0	86	2	-3	5	35	7	-5	-5	111	2	-1	-5	26	10	-2
-2	148	2	3	1	309	4	-2	6	91	2	2	-4	21	20	-6	-4	116	2	-2
-1	285	4	-7	2	91	2	-3	H,K=	11,		9	-3	128	2	0	-3	23	12	8
0	155	2	-3	3	308	4	-2	-3	87	2	2	-2	36	5	-6	-2	129	2	0
1	283	4	-10	4	67	2	-3	-2	58	3	4	-1	145	2	-1	-1	27	9	-4
2	146	2	0	5	198	3	-1	-1	89	2	0	0	17	20	15	0	119	2	-3
3	232	3	-1	6	48	3	1	0	60	3	-1	1	146	2	0	1	23	15	-8
4	95	2	4	7	125	2	-3	1	87	2	-1	2	31	7	-12	2	127	2	-2
5	170	2	2	8	31	6	-1	2	56	3	1	3	126	2	-2	3	16	21	2
6	58	2	0	9	84	2	1	3	90	2	5	4	26	7	-2	4	114	2	-3
7	111	2	-1	H,K=	11,		3	H,K=	12,		0	5	111	2	-1	5	26	10	-1
8	50	3	5	-8	74	2	-2	-8	102	3	0	6	21	22	14	6	97	2	2
H,K=	10,		6	-7	79	2	-1	-6	132	2	1	H,K=	12,		8	H,K=	13,		7
-7	106	2	3	-6	105	2	0	-4	222	3	2	-4	65	2	0	-4	93	2	2
-6	10	21	4	-5	114	2	0	-2	329	5	-1	-3	76	2	0	-3	48	4	-6
-5	145	2	1	-4	148	2	-1	0	276	4	1	-2	83	2	0	-2	109	2	1
-4	9	21	-1	-3	179	2	3	2	325	5	-3	-1	96	2	0	-1	32	6	-8
-3	180	3	3	-2	213	3	-3	4	220	3	-3	0	68	2	3	0	126	2	1
-2	13	21	1	-1	210	3	-1	6	128	2	-2	1	100	2	3	1	39	3	0
-1	221	3	3	0	234	3	-2	8	103	3	2	2	82	2	-1	2	111	2	3
0	30	6	-4	1	209	3	-1	H,K=	12,		2	3	81	2	4	3	52	3	-2
1	217	3	-2	2	211	3	-4	-8	82	2	1	4	62	3	-3	4	89	2	-2
2	18	20	5	3	179	2	2	-7	65	2	1	H,K=	13,		1	H,K=	14,		0
3	177	2	0	4	148	2	-1	-6	113	2	-2	-7	99	2	1	-6	97	3	0
4	16	21	7	5	114	2	0	-5	63	2	2	-6	21	14	-5	-4	105	2	-1
5	142	2	-1	6	102	2	-2	-4	179	2	3	-5	103	2	-3	-2	174	3	-1
6	18	21	11	7	81	2	2	-3	106	2	-1	-4	22	11	0	0	151	2	2
7	106	2	4	8	72	2	-3	-2	240	3	0	-3	206	3	1	2	175	3	-2
H,K=	10,		8	H,K=	11,		5	-1	137	2	0	-2	59	2	-1	4	104	2	-5
-5	89	2	2	-7	26	11	2	0	201	3	1	-1	214	3	2	6	102	2	5
-4	74	2	2	-6	117	2	0	1	136	2	0	0	66	2	0	H,K=	14,		2
-3	97	2	1	-5	30	6	0	2	236	3	-3	1	211	3	0	-6	90	2	3
-2	69	2	-2	-4	154	2	1	3	110	2	2	2	61	2	0	-5	51	3	0
-1	97	2	-3	-3	25	9	-3	4	178	2	1	3	206	3	-1	-4	94	2	0
0	85	2	0	-2	203	3	0	5	59	2	-1	4	15	21	-9	-3	64	2	-3
1	98	2	-2	-1	37	3	1	6	115	2	1	5	106	2	-1	-2	129	2	0
2	71	2	-1	0	238	3	-1	7	63	2	-1	6	24	9	0	-1	77	2	-2
3	95	2	0	1	37	3	0	8	82	2	0	7	102	2	4	0	103	2	0
4	73	2	2	2	205	3	1	H,K=	12,		4	H,K=	13,		3	1	79	2	1
5	88	2	2	3	30	6	2	-7	94	2	0	-7	66	2	-1	2	128	2	-1
H,K=	10,		10	4	153	2	0	-6	62	2	1	-6	79	2	1	3	67	2	-1

STRUCTURE FACTORS continued for
(C5H5)2ZR(BH3CH3)H

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
4	94	2	0	-2	120	2	3												
5	52	2	1	-1	31	6	3												
6	92	2	5	0	123	2	-1												
H,K=	14,		4	1	32	7	4												
-6	38	6	-4	2	120	2	3												
-5	96	2	2	3	15	23	-9												
-4	56	2	3	4	102	2	4												
-3	108	2	-3	H,K=	16,		0												
-2	55	2	1	-4	109	3	-3												
-1	106	2	-2	-2	117	2	5												
0	58	2	1	0	131	2	0												
1	104	2	-3	2	113	2	2												
2	54	2	0	4	107	3	-3												
3	110	2	-2	H,K=	16,		2												
4	54	2	2	-4	82	2	1												
5	94	2	0	-3	74	2	1												
6	36	7	-5	-2	104	2	2												
H,K=	14,		6	-1	66	2	-3												
-4	5	23	-5	0	124	2	0												
-3	112	2	1	1	67	2	-2												
-2	21	21	8	2	105	2	2												
-1	122	2	1	3	69	2	-3												
0	15	22	4	4	83	2	3												
1	120	2	0	H,K=	16,		4												
2	19	22	7	-3	101	2	3												
3	113	2	2	-2	62	2	4												
4	20	23	10	-1	116	2	-3												
H,K=	15,		1	0	61	2	1												
-6	29	10	-2	1	119	2	0												
-5	103	2	3	2	60	3	2												
-4	32	7	-8	3	101	2	3												
-3	105	2	1	H,K=	17,		1												
-2	31	6	-6	-3	95	2	1												
-1	126	2	0	-2	31	6	3												
0	37	3	-1	-1	117	2	1												
1	125	2	-2	0	26	12	-4												
2	31	7	-6	1	116	2	0												
3	102	2	-1	2	23	16	-5												
4	30	8	-10	3	93	2	1												
5	101	2	2	H,K=	17,		3												
6	22	19	-10	-2	68	2	-4												
H,K=	15,		3	-1	87	2	3												
-5	64	2	2	0	91	2	0												
-4	96	2	2	1	84	2	0												
-3	75	2	2	2	72	2	0												
-2	95	2	-2																
-1	90	2	-1																
0	99	2	-2																
1	91	2	0																
2	94	2	-4																
3	75	2	2																
4	92	2	-2																
5	64	2	2																
H,K=	15,		5																
-4	99	2	1																
-3	27	9	2																

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