ORGANOMETALLICS
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Experimental Section

General. All manipulations were performed using glovebox or double manifold vacuum line techniques. Solvents were purified by distillation over sodium/benzophenone (toluene) and $LiAlH_4$ (hexanes) under a nitrogen atmosphere followed by vacuum transfer from "titanocene". NMR solvents were purified by vacuum transfer from sodium/benzophenone. Elemental analyses were performed in the micro-analytical laboratory , Department of Chemistry, University of Calgary.

$Cp_2Zr[\eta^3\text{-}CH_2CH_2BH(C_6F_5)_2]$ (2a) Toluene (10 mLs) was condensed into a flask containing $Cp_2Zr(CH_2CH_2)PMePh_2$ (0.22 g, 0.48 mmol) and $HB(C_6F_5)_2$ (0.34 g, 0.97 mmol) at -78°C. After stirring for 30 min. at -78°C, the reaction was warmed to room temperature and stirred for another 30 min. Solvent was removed under vacuum and the residue extracted with a 1:1 mixture of toluene and hexane (ca. 6mL). Cooling the solution at -78°C gave crystalline compopund **1** (0.22 g, 52%.) which was contaminated with about 30% $Ph_2MeP{\bullet}HB(C_6F_5)_2$.

$Cp_2Zr[\eta^3\text{-}CH(C_2H_5)CH_2BH(C_6F_5)_2]$ (2b) Toluene (8 mLs) was condensed into a flask containing $Cp_2Zr[CH(C_2H_5)CH_2]{\bullet}PMePh_2$ (0.19 g, 0.4 mmol) and $HB(C_6F_5)_2$ (0.28 g, 0.8 mmol) at -78°C. After stirring for 30 min. at -78°C, the reaction was warmed to room temperature and stirred for another 30 min. Solvent was removed under vacuum and yellow residue was extracted with hexane (15 mLs) with addition 0.5 mL benzene. The extract was cooled at -78°C and filtered cold to afford yellow crystals of compound **2b** (0.11 g, 44%) Anal. Calcd. for $C_{26}H_{19}F_{10}BZr$: C, 50.10; H, 3.07. Found: C, 50.43; H, 3.52.

$Cp_2Zr[\eta^3\text{-}CH(Ph)CH_2BH(C_6F_5)_2]$ (2c) Toluene (10 mLs) was condensed into a flask containing $Cp_2Zr[CH(Ph)CH_2]{\bullet}PMePh_2$ (0.19 g, 0.35 mmol) and $HB(C_6F_5)_2$ (0.25 g, 0.7 mmol) at -78°C. The reaction was stirred for 30 minutes at -78°C and warmed to room temperature while stirring for 1 hour. Solvent was removed *in vacuo* and the residue was triturated with hexane (12mL). Extraction with a mixture of hexane and toluene (9:1) and cooling the solution at -33°C yielded material contaminated with about 15% $Ph_2MeP{\bullet}HB(C_6F_5)_2$.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{24}H_{15}BF_{10}Zr$
Formula Weight	595.40
Crystal Color, Habit	yellow, irregular
Crystal Dimensions	0.20 X 0.25 X 0.45 mm
Crystal System	monoclinic
Lattice Type	Primitive
No. of Reflections Used for Unit	
Cell Determination (2θ range)	25 (45.7 - 53.0°)
Omega Scan Peak Width	
at Half-height	0.38°
Lattice Parameters	a = 15.005(2)Å b = 7.505(1) Å c = 20.9320(8) Å β = 108.459(5)°
	V = 2236.0(4) Å^3
Space Group	$P2_1/n$ (#14)
Z value	4
D_{calc}	1.769 g/cm^3
F_{000}	1176
μ(CuKα)	50.53 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC6S

Radiation	CuKα (λ = 1.54178 Å) graphite monochromated
Take-off Angle	6.0°
Detector Aperture	6.0 mm horizontal 6.0 mm vertical
Crystal to Detector Distance	285 mm
Voltage, Current	45 kV, 25 mA
Temperature	21.0°C
Scan Type	ω-2θ
Scan Rate	16.0°/min (in ω) (up to 9 scans)
Scan Width	(1.05 + 0.20 tan θ)°
$2\theta_{max}$	155.4°
No. of Reflections Measured	Total: 5083 Unique: 4898 (R_{int} = 0.037)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.442 - 1.000) Secondary Extinction (coefficient: 1.32(9) x 10^{-6})

C. Structure Solution and Refinement

Structure Solution	Patterson Methods (DIRDIF92 PATTY)
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma w(\|Fo\| - \|Fc\|)^2$
Least Squares Weights	$w = \frac{1}{\sigma^2(Fo)} = [\sigma_c^2(Fo) + \frac{p^2}{4}Fo^2]^{-1}$
p-factor	0.0000
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	2397
No. Variables	346
Reflection/Parameter Ratio	6.93

Residuals: R; Rw	0.037 ; 0.035
Goodness of Fit Indicator	1.87
Max Shift/Error in Final Cycle	0.002
Maximum peak in Final Diff. Map	0.34 $e^-/\AA^3$
Minimum peak in Final Diff. Map	-0.49 $e^-/\AA^3$

Table 2. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Zr(1)	0.31677(3)	0.50748(8)	0.10864(2)	3.528(9)
F(1)	0.4699(3)	0.3075(5)	0.2838(2)	5.5(1)
F(2)	0.5310(3)	0.2868(6)	0.4165(2)	7.0(1)
F(3)	0.5876(3)	0.5843(6)	0.4924(2)	7.8(1)
F(4)	0.5786(3)	0.9034(6)	0.4312(2)	7.5(1)
F(5)	0.5193(3)	0.9278(5)	0.2970(2)	6.1(1)
F(6)	0.6167(3)	0.4199(7)	0.2168(2)	8.1(1)
F(7)	0.7746(3)	0.498(1)	0.1913(2)	13.7(2)
F(8)	0.7970(3)	0.8204(10)	0.1406(2)	15.0(2)
F(9)	0.6541(5)	1.0609(8)	0.1128(3)	14.6(2)
F(10)	0.4969(4)	0.9852(7)	0.1370(3)	9.9(2)
C(1)	0.1838(4)	0.516(1)	0.1583(3)	5.0(2)
C(2)	0.2574(5)	0.4196(8)	0.2029(3)	4.7(2)
C(3)	0.2693(5)	0.2634(8)	0.1711(3)	4.8(2)
C(4)	0.2046(5)	0.2603(9)	0.1069(4)	5.6(2)
C(5)	0.1523(4)	0.418(1)	0.0989(3)	5.9(2)
C(6)	0.4060(6)	0.583(1)	0.0286(3)	6.1(2)
C(7)	0.3109(6)	0.576(1)	-0.0097(4)	5.7(2)
C(8)	0.2797(5)	0.402(1)	-0.0091(3)	5.4(2)
C(9)	0.3558(6)	0.2968(10)	0.0298(4)	5.9(2)
C(10)	0.4329(6)	0.411(1)	0.0525(3)	6.1(2)
C(11)	0.2880(5)	0.7938(9)	0.1093(4)	5.0(2)
C(12)	0.3629(5)	0.7760(8)	0.1783(3)	4.3(2)
C(13)	0.4912(4)	0.6198(8)	0.2839(3)	3.9(1)

Table 2. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(14)	0.4957(4)	0.4605(7)	0.3175(3)	4.0(2)
C(15)	0.5267(5)	0.4476(9)	0.3867(4)	5.1(2)
C(16)	0.5552(5)	0.596(1)	0.4244(3)	5.3(2)
C(17)	0.5520(4)	0.757(1)	0.3934(4)	5.1(2)
C(18)	0.5209(4)	0.7665(9)	0.3251(3)	4.4(2)
C(19)	0.5485(4)	0.6960(10)	0.1796(3)	4.9(2)
C(20)	0.6230(5)	0.582(1)	0.1906(3)	6.2(2)
C(21)	0.7060(5)	0.617(2)	0.1784(4)	8.5(3)
C(22)	0.7167(6)	0.781(2)	0.1533(5)	10.0(4)
C(23)	0.6451(8)	0.900(2)	0.1386(4)	9.4(3)
C(24)	0.5647(5)	0.859(1)	0.1536(4)	6.6(2)
B(1)	0.4576(5)	0.6404(9)	0.2022(3)	3.8(2)
H(1)	0.1591	0.6307	0.1673	6.0
H(2)	0.2941	0.4563	0.2485	5.7
H(3)	0.3157	0.1704	0.1908	5.7
H(4)	0.1969	0.1656	0.0734	6.7
H(5)	0.1019	0.4539	0.0582	7.1
H(6)	0.4462	0.6894	0.0371	7.3
H(7)	0.2727	0.6765	-0.0329	6.8
H(8)	0.2158	0.3598	-0.0319	6.5
H(9)	0.3546	0.1689	0.0390	7.1
H(10)	0.4960	0.3766	0.0809	7.3
H(11)	0.303(4)	0.856(8)	0.077(3)	5(1)
H(12)	0.230(4)	0.845(7)	0.109(3)	5(1)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(13)	0.394(4)	0.884(7)	0.186(2)	3(1)
H(14)	0.330(4)	0.775(7)	0.210(2)	3(1)
H(15)	0.440(3)	0.490(6)	0.182(2)	3.0(9)

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Table 3. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zr(1)	0.0438(2)	0.0482(3)	0.0503(2)	0.0015(4)	0.0267(2)	0.0023(4)
F(1)	0.087(3)	0.052(2)	0.070(2)	0.003(2)	0.025(2)	0.001(2)
F(2)	0.114(4)	0.086(3)	0.068(3)	0.013(3)	0.029(3)	0.021(2)
F(3)	0.092(3)	0.141(4)	0.058(2)	0.002(3)	0.012(2)	-0.010(2)
F(4)	0.080(3)	0.096(3)	0.102(3)	-0.014(3)	0.016(3)	-0.040(3)
F(5)	0.077(3)	0.058(2)	0.095(3)	-0.012(2)	0.027(2)	-0.005(2)
F(6)	0.075(3)	0.148(4)	0.099(3)	0.055(3)	0.046(3)	0.028(3)
F(7)	0.057(2)	0.356(9)	0.116(3)	0.041(6)	0.041(2)	-0.017(6)
F(8)	0.094(4)	0.385(9)	0.119(4)	-0.131(5)	0.073(3)	-0.096(5)
F(9)	0.223(7)	0.191(6)	0.188(6)	-0.128(6)	0.130(5)	-0.022(5)
F(10)	0.135(4)	0.085(3)	0.168(4)	-0.021(4)	0.068(4)	0.040(4)
C(1)	0.055(3)	0.065(4)	0.084(4)	-0.008(5)	0.043(3)	-0.010(5)
C(2)	0.065(4)	0.062(4)	0.069(4)	-0.007(4)	0.044(4)	0.003(4)
C(3)	0.071(4)	0.049(4)	0.072(4)	-0.002(4)	0.039(4)	0.012(4)
C(4)	0.081(5)	0.061(4)	0.087(5)	-0.020(4)	0.049(4)	-0.015(4)
C(5)	0.042(3)	0.107(6)	0.079(5)	-0.022(4)	0.026(3)	0.006(5)
C(6)	0.090(7)	0.105(6)	0.056(5)	-0.012(5)	0.054(5)	0.008(4)
C(7)	0.075(6)	0.097(6)	0.051(4)	0.005(5)	0.030(4)	0.009(4)
C(8)	0.061(5)	0.092(5)	0.055(4)	-0.010(5)	0.023(4)	-0.008(4)
C(9)	0.093(6)	0.081(5)	0.068(5)	0.019(5)	0.050(5)	-0.008(4)
C(10)	0.057(4)	0.133(7)	0.053(5)	0.022(5)	0.035(4)	0.006(5)
C(11)	0.066(5)	0.049(4)	0.075(5)	0.008(4)	0.022(4)	0.012(4)
C(12)	0.055(4)	0.044(4)	0.071(4)	-0.002(3)	0.027(4)	0.000(4)
C(13)	0.039(3)	0.049(4)	0.065(4)	0.004(3)	0.025(3)	0.001(3)

Table 3. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(14)	0.047(3)	0.047(5)	0.064(4)	0.004(3)	0.025(3)	-0.004(3)
C(15)	0.055(4)	0.076(6)	0.063(4)	0.017(4)	0.020(4)	0.009(4)
C(16)	0.046(4)	0.099(6)	0.054(4)	0.006(4)	0.013(4)	-0.001(5)
C(17)	0.042(4)	0.082(5)	0.068(5)	-0.004(4)	0.014(4)	-0.032(4)
C(18)	0.045(3)	0.056(4)	0.070(4)	-0.001(3)	0.023(3)	-0.003(4)
C(19)	0.042(3)	0.086(5)	0.064(4)	-0.007(4)	0.025(3)	0.004(4)
C(20)	0.052(4)	0.140(7)	0.048(4)	0.007(5)	0.023(4)	0.002(4)
C(21)	0.046(4)	0.22(1)	0.062(5)	-0.002(6)	0.025(4)	-0.022(6)
C(22)	0.051(5)	0.27(2)	0.068(6)	-0.061(8)	0.032(5)	-0.052(8)
C(23)	0.117(8)	0.167(10)	0.087(6)	-0.096(8)	0.053(6)	-0.019(6)
C(24)	0.070(5)	0.108(7)	0.079(5)	-0.031(5)	0.029(4)	-0.008(5)
B(1)	0.044(4)	0.048(4)	0.059(4)	-0.007(3)	0.026(3)	-0.006(4)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table 4. Bond Lengths(Å)*

atom	atom	distance	atom	atom	distance
Zr(1)	C(1)	2.526(5)	Zr(1)	C(2)	2.496(5)
Zr(1)	C(3)	2.483(6)	Zr(1)	C(4)	2.497(6)
Zr(1)	C(5)	2.502(6)	Zr(1)	C(6)	2.518(6)
Zr(1)	C(7)	2.503(7)	Zr(1)	C(8)	2.478(7)
Zr(1)	C(9)	2.486(6)	Zr(1)	C(10)	2.496(7)
Zr(1)	C(11)	2.193(7)	Zr(1)	C(12)	2.455(7)
Zr(1)	Cp(1)	2.20	Zr(1)	Cp(2)	2.19
Zr(1)	B(1)	2.584(7)	F(1)	C(14)	1.339(6)
F(2)	C(15)	1.351(7)	F(3)	C(16)	1.355(7)
F(4)	C(17)	1.342(7)	F(5)	C(18)	1.343(7)
F(6)	C(20)	1.347(8)	F(7)	C(21)	1.32(1)
F(8)	C(22)	1.346(8)	F(9)	C(23)	1.35(1)
F(10)	C(24)	1.351(9)	C(1)	C(2)	1.399(8)
C(1)	C(5)	1.390(8)	C(2)	C(3)	1.387(8)
C(3)	C(4)	1.386(9)	C(4)	C(5)	1.402(9)
C(6)	C(7)	1.40(1)	C(6)	C(10)	1.397(10)
C(7)	C(8)	1.384(9)	C(8)	C(9)	1.416(9)
C(9)	C(10)	1.40(1)	C(11)	C(12)	1.530(9)
C(12)	B(1)	1.689(9)	C(13)	C(14)	1.378(7)
C(13)	C(18)	1.382(8)	C(13)	B(1)	1.629(8)
C(14)	C(15)	1.377(8)	C(15)	C(16)	1.351(9)
C(16)	C(17)	1.365(9)	C(17)	C(18)	1.358(8)
C(19)	C(20)	1.369(9)	C(19)	C(24)	1.392(9)
C(19)	B(1)	1.634(8)	C(20)	C(21)	1.375(10)

Table 4. Bond Lengths(Å)* (continued)

atom	atom	distance	atom	atom	distance
C(21)	C(22)	1.37(1)	C(22)	C(23)	1.36(2)
C(23)	C(24)	1.374(10)			

*Here and elsewhere Cp(1,2) refer to the unweighted centroids of the C(1-5) and C(6-10) cyclopentadienyl rings, respectively

Table 5. Bond Lengths($\AA$) Involving Hydrogen

atom	atom	distance	atom	atom	distance
Zr(1)	H(15)	2.01(4)	C(1)	H(1)	0.98
C(2)	H(2)	0.98	C(3)	H(3)	0.98
C(4)	H(4)	0.98	C(5)	H(5)	0.98
C(6)	H(6)	0.98	C(7)	H(7)	0.98
C(8)	H(8)	0.98	C(9)	H(9)	0.98
C(10)	H(10)	0.98	C(11)	H(11)	0.91(5)
C(11)	H(12)	0.94(6)	C(12)	H(13)	0.92(5)
C(12)	H(14)	0.94(5)	B(1)	H(15)	1.20(5)

Table 6. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(11)	Zr(1)	C(12)	37.9(2)	C(11)	Zr(1)	Cp(1)	106.0
C(11)	Zr(1)	Cp(2)	107.0	C(12)	Zr(1)	Cp(1)	104.4
C(12)	Zr(1)	Cp(2)	124.0	C(2)	C(1)	C(5)	107.3(6)
C(1)	C(2)	C(3)	108.1(6)	C(2)	C(3)	C(4)	108.8(6)
C(3)	C(4)	C(5)	107.2(6)	C(1)	C(5)	C(4)	108.7(6)
C(7)	C(6)	C(10)	107.1(8)	C(6)	C(7)	C(8)	108.6(7)
C(7)	C(8)	C(9)	108.6(7)	C(8)	C(9)	C(10)	106.3(7)
C(6)	C(10)	C(9)	109.4(8)	Zr(1)	C(11)	C(12)	80.4(4)
Zr(1)	C(12)	C(11)	61.7(3)	Zr(1)	C(12)	B(1)	74.6(3)
C(11)	C(12)	B(1)	129.1(5)	C(14)	C(13)	C(18)	114.8(6)
C(14)	C(13)	B(1)	124.5(6)	C(18)	C(13)	B(1)	120.7(6)
F(1)	C(14)	C(13)	121.1(6)	F(1)	C(14)	C(15)	116.0(6)
C(13)	C(14)	C(15)	122.9(6)	F(2)	C(15)	C(14)	120.0(6)
F(2)	C(15)	C(16)	120.3(7)	C(14)	C(15)	C(16)	119.7(6)
F(3)	C(16)	C(15)	120.3(7)	F(3)	C(16)	C(17)	120.1(7)
C(15)	C(16)	C(17)	119.5(6)	F(4)	C(17)	C(16)	119.1(7)
F(4)	C(17)	C(18)	121.0(7)	C(16)	C(17)	C(18)	119.8(7)
F(5)	C(18)	C(13)	119.2(6)	F(5)	C(18)	C(17)	117.6(6)
C(13)	C(18)	C(17)	123.2(7)	C(20)	C(19)	C(24)	112.6(7)
C(20)	C(19)	B(1)	120.2(6)	C(24)	C(19)	B(1)	127.0(6)
F(6)	C(20)	C(19)	118.4(7)	F(6)	C(20)	C(21)	115.6(8)
C(19)	C(20)	C(21)	126.0(9)	F(7)	C(21)	C(20)	121(1)
F(7)	C(21)	C(22)	120.5(8)	C(20)	C(21)	C(22)	117.8(10)
F(8)	C(22)	C(21)	119(1)	F(8)	C(22)	C(23)	120(1)

Table 6. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(21)	C(22)	C(23)	120.0(8)	F(9)	C(23)	C(22)	120.6(9)
F(9)	C(23)	C(24)	119(1)	C(22)	C(23)	C(24)	119(1)
F(10)	C(24)	C(19)	120.4(6)	F(10)	C(24)	C(23)	115.5(9)
C(19)	C(24)	C(23)	124.0(9)	C(12)	B(1)	C(13)	108.7(5)
C(12)	B(1)	C(19)	117.5(5)	C(13)	B(1)	C(19)	108.6(5)

Table 7. Bond Angles(°) Involving Hydrogen

atom	atom	atom	angle	atom	atom	atom	angle
C(11)	Zr(1)	H(15)	101(1)	C(12)	Zr(1)	H(15)	65(1)
C(2)	C(1)	H(1)	126.4	C(5)	C(1)	H(1)	126.4
C(1)	C(2)	H(2)	125.9	C(3)	C(2)	H(2)	125.9
C(2)	C(3)	H(3)	125.6	C(4)	C(3)	H(3)	125.6
C(3)	C(4)	H(4)	126.4	C(5)	C(4)	H(4)	126.4
C(1)	C(5)	H(5)	125.7	C(4)	C(5)	H(5)	125.7
C(7)	C(6)	H(6)	126.4	C(10)	C(6)	H(6)	126.4
C(6)	C(7)	H(7)	125.7	C(8)	C(7)	H(7)	125.7
C(7)	C(8)	H(8)	125.7	C(9)	C(8)	H(8)	125.7
C(8)	C(9)	H(9)	126.9	C(10)	C(9)	H(9)	126.9
C(6)	C(10)	H(10)	125.3	C(9)	C(10)	H(10)	125.3
Zr(1)	C(11)	H(11)	113(3)	Zr(1)	C(11)	H(12)	125(3)
C(12)	C(11)	H(11)	118(3)	C(12)	C(11)	H(12)	116(3)
H(11)	C(11)	H(12)	103(4)	Zr(1)	C(12)	H(13)	148(3)
Zr(1)	C(12)	H(14)	107(3)	C(11)	C(12)	H(13)	105(3)
C(11)	C(12)	H(14)	106(3)	B(1)	C(12)	H(13)	98(3)
B(1)	C(12)	H(14)	110(3)	H(13)	C(12)	H(14)	103(4)
C(12)	B(1)	H(15)	113(2)	C(13)	B(1)	H(15)	103(1)
C(19)	B(1)	H(15)	104(1)	Zr(1)	H(15)	B(1)	104(2)

Table 8. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Zr(1)	C(11)	C(12)	B(1)	34.3(6)	Zr(1)	C(12)	B(1)	C(13)	-128.3(4)
Zr(1)	C(12)	B(1)	C(19)	108.0(5)	F(1)	C(14)	C(13)	C(18)	-179.4(5)
F(1)	C(14)	C(13)	B(1)	-1.5(8)	F(1)	C(14)	C(15)	F(2)	1.0(9)
F(1)	C(14)	C(15)	C(16)	179.1(6)	F(2)	C(15)	C(14)	C(13)	-178.8(5)
F(2)	C(15)	C(16)	F(3)	-0.6(10)	F(2)	C(15)	C(16)	C(17)	178.8(6)
F(3)	C(16)	C(15)	C(14)	-178.7(5)	F(3)	C(16)	C(17)	F(4)	-2.1(10)
F(3)	C(16)	C(17)	C(18)	179.0(5)	F(4)	C(17)	C(16)	C(15)	178.5(6)
F(4)	C(17)	C(18)	F(5)	1.2(9)	F(4)	C(17)	C(18)	C(13)	-178.8(5)
F(5)	C(18)	C(13)	C(14)	179.9(5)	F(5)	C(18)	C(13)	B(1)	1.9(8)
F(5)	C(18)	C(17)	C(16)	-179.8(6)	F(6)	C(20)	C(19)	C(24)	178.9(6)
F(6)	C(20)	C(19)	B(1)	3.7(10)	F(6)	C(20)	C(21)	F(7)	0(1)
F(6)	C(20)	C(21)	C(22)	-178.4(7)	F(7)	C(21)	C(20)	C(19)	179.4(7)
F(7)	C(21)	C(22)	F(8)	1(1)	F(7)	C(21)	C(22)	C(23)	178.2(8)
F(8)	C(22)	C(21)	C(20)	-180.0(7)	F(8)	C(22)	C(23)	F(9)	-1(1)
F(8)	C(22)	C(23)	C(24)	-178.2(7)	F(9)	C(23)	C(22)	C(21)	-178.9(8)
F(9)	C(23)	C(24)	F(10)	3(1)	F(9)	C(23)	C(24)	C(19)	179.2(7)
F(10)	C(24)	C(19)	C(20)	177.2(7)	F(10)	C(24)	C(19)	B(1)	-8(1)
F(10)	C(24)	C(23)	C(22)	-179.8(8)	C(1)	C(2)	C(3)	C(4)	0.5(7)
C(1)	C(5)	C(4)	C(3)	-1.0(7)	C(2)	C(1)	C(5)	C(4)	1.2(7)
C(2)	C(3)	C(4)	C(5)	0.3(7)	C(3)	C(2)	C(1)	C(5)	-1.0(7)
C(6)	C(7)	C(8)	C(9)	-0.2(8)	C(6)	C(10)	C(9)	C(8)	0.0(8)
C(7)	C(6)	C(10)	C(9)	-0.1(8)	C(7)	C(8)	C(9)	C(10)	0.1(8)
C(8)	C(7)	C(6)	C(10)	0.2(9)	C(11)	Zr(1)	C(12)	B(1)	-153.0(5)
C(11)	C(12)	Zr(1)	B(1)	153.0(5)	C(11)	C(12)	B(1)	C(13)	-159.3(6)

Table 8. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(11)	C(12)	B(1)	C(19)	77.0(8)	C(12)	B(1)	C(13)	C(14)	120.3(6)
C(12)	B(1)	C(13)	C(18)	-62.0(7)	C(12)	B(1)	C(19)	C(20)	-172.4(6)
C(12)	B(1)	C(19)	C(24)	13.1(10)	C(13)	C(14)	C(15)	C(16)	-0.7(10)
C(13)	C(18)	C(17)	C(16)	0.1(10)	C(13)	B(1)	C(19)	C(20)	63.8(8)
C(13)	B(1)	C(19)	C(24)	-110.6(7)	C(14)	C(13)	C(18)	C(17)	-0.1(8)
C(14)	C(13)	B(1)	C(19)	-110.9(6)	C(14)	C(15)	C(16)	C(17)	0(1)
C(15)	C(14)	C(13)	C(18)	0.4(8)	C(15)	C(14)	C(13)	B(1)	178.3(5)
C(15)	C(16)	C(17)	C(18)	0(1)	C(17)	C(18)	C(13)	B(1)	-178.1(5)
C(18)	C(13)	B(1)	C(19)	66.9(7)	C(19)	C(20)	C(21)	C(22)	0(1)
C(19)	C(24)	C(23)	C(22)	-4(1)	C(20)	C(19)	C(24)	C(23)	1(1)
C(20)	C(21)	C(22)	C(23)	-2(1)	C(21)	C(20)	C(19)	C(24)	0(1)
C(21)	C(20)	C(19)	B(1)	-175.2(7)	C(21)	C(22)	C(23)	C(24)	4(1)
C(23)	C(24)	C(19)	B(1)	176.8(7)					