Supplementary Material (ESI) for Dalton Transactions

Novel μ_3-oxo Complexes Prepared From Cp*Zr(BH_3R) (R = H, CH_3) and $B(C_6F_5)_3$ in Ether

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Table S1. Crystal data and structure refinement for $Cp^*Zr(BH_3CH_3)_3$

Empirical formula	$C_{13}H_{33}B_3Zr$	
Formula weight	313.04	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	P4(3)	
Unit cell dimensions	a = 7.8250(3) Å	α = 90°.
	b = 7.8250(3) Å	β = 90°.
	c = 28.7350(11) Å	γ = 90°.
Volume	1759.46(12) $Å^3$	
Z	4	
Density (calculated)	1.182 Mg/m^3	
Absorption coefficient	0.605 mm^{-1}	
F(000)	664	
Crystal size	0.30 x 0.30 x 0.30 mm^3	
Theta range for data collection	2.60 to 27.50°.	
Index ranges	-10<=h<=10, -10<=k<=10, -37<=l<=37	
Reflections collected	17156	
Independent reflections	4028 [R(int) = 0.0366]	
Completeness to theta = 27.50°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8394 and 0.8394	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4028 / 1 / 181	
Goodness-of-fit on F^2	1.052	
Final R indices [I>2sigma(I)]	R1 = 0.0257, wR2 = 0.0632	
R indices (all data)	R1 = 0.0278, wR2 = 0.0643	
Absolute structure parameter	0.04(4)	
Largest diff. peak and hole	0.303 and -0.240 $e.Å^{-3}$	

[a] $R_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$.

[b] $wR_2 = \{\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2\}^{1/2}$.

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $Cp^*Zr(BH_3CH_3)_3$

Atom	x	y	z	U(eq)[a]
Zr	3312(1)	9079(1)	2203(1)	20(1)
B(1)	1099(4)	7000(4)	2285(1)	33(1)
B(2)	5042(4)	7974(4)	1598(1)	37(1)
B(3)	4989(4)	8757(4)	2886(1)	36(1)
C(1)	-616(4)	5945(5)	2316(1)	58(1)
C(2)	6122(5)	7382(6)	1159(2)	63(1)
C(3)	6115(5)	8814(5)	3350(1)	59(1)
C(4)	2848(4)	11606(4)	1685(1)	43(1)
C(5)	1239(4)	11126(4)	1848(1)	32(1)
C(6)	1174(3)	11419(3)	2327(1)	28(1)
C(7)	2742(4)	12078(3)	2467(1)	36(1)
C(8)	3800(4)	12200(3)	2074(1)	45(1)
C(9)	3440(8)	11658(6)	1187(2)	102(2)
C(10)	-246(6)	10568(6)	1550(2)	72(1)
C(11)	-400(5)	11175(5)	2627(1)	59(1)
C(12)	3151(7)	12771(5)	2943(2)	80(2)
C(13)	5550(5)	12976(4)	2054(3)	111(3)

[a] U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Table S3. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $Cp^*Zr(BH_3CH_3)_3$

Atom	U11	U22	U33	U23	U13	U12
Zr	19(1)	18(1)	23(1)	3(1)	-3(1)	0(1)
B(1)	30(1)	30(1)	38(2)	6(1)	-7(1)	-8(1)
B(2)	32(2)	34(2)	46(2)	-5(2)	6(1)	5(1)
B(3)	38(2)	33(2)	38(2)	12(1)	-14(1)	-8(1)
C(1)	45(2)	60(2)	68(3)	11(2)	-5(2)	-28(2)
C(2)	55(2)	70(3)	63(2)	-18(2)	25(2)	3(2)
C(3)	73(3)	58(2)	44(2)	19(2)	-35(2)	-27(2)
C(4)	50(2)	40(2)	39(2)	23(1)	16(1)	25(1)
C(5)	32(1)	32(1)	32(1)	-2(1)	-9(1)	14(1)
C(6)	29(1)	27(1)	28(1)	2(1)	1(1)	10(1)
C(7)	48(2)	19(1)	42(2)	-7(1)	-16(1)	9(1)
C(8)	26(1)	17(1)	91(3)	17(1)	-1(1)	2(1)
C(9)	165(5)	91(3)	51(3)	50(2)	60(3)	77(4)
C(10)	71(3)	73(3)	73(3)	-24(2)	-52(2)	34(2)
C(11)	62(2)	53(2)	64(2)	12(2)	32(2)	21(2)
C(12)	127(4)	47(2)	67(3)	-27(2)	-59(3)	25(2)
C(13)	32(2)	28(2)	273(9)	43(3)	2(3)	-5(1)

Table S4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $Cp^*Zr(BH_3CH_3)_3$

Atom	x	y	z	U(eq)
H(1A)	1320(50)	8050(40)	2567(13)	49
H(1B)	1250(50)	7800(50)	1928(12)	49
H(1C)	2300(40)	6330(40)	2339(12)	49
H(2A)	3640(50)	8300(50)	1536(14)	56
H(2B)	5490(50)	9190(50)	1779(14)	56
H(2C)	4880(50)	6880(50)	1898(14)	56
H(3A)	5570(40)	9720(50)	2614(13)	55
H(3B)	3390(40)	9160(40)	2908(16)	55
H(3C)	4920(50)	7540(50)	2729(13)	55
H(1D)	-357	4759	2399	87
H(1E)	-1198	5974	2014	87
H(1F)	-1358	6448	2554	87
H(2D)	6827	6394	1244	94
H(2E)	6861	8320	1057	94
H(2F)	5345	7064	906	94
H(3D)	6408	7647	3444	88
H(3E)	5462	9370	3599	88
H(3F)	7166	9461	3291	88
H(9A)	3133	12761	1049	153
H(9B)	2890	10734	1012	153
H(9C)	4683	11511	1176	153
H(10A)	-891	11574	1448	108
H(10B)	-995	9816	1731	108
H(10C)	183	9950	1277	108
H(11A)	-1063	12238	2633	89
H(11B)	-53	10875	2944	89
H(11C)	-1104	10255	2497	89
H(12A)	2821	13978	2959	120
H(12B)	4380	12664	3002	120
H(12C)	2518	12123	3179	120
H(13A)	5452	14209	2001	167
H(13B)	6201	12455	1800	167
H(13C)	6142	12772	2350	167

Table S5. Bond lengths [Å] and angles [°] for $Cp^*Zr(BH_3CH_3)_3$

Zr-B(2)	2.367(3)	C(2)-H(2D)	0.9800
Zr-B(3)	2.374(3)	C(2)-H(2E)	0.9800
Zr-B(1)	2.387(3)	C(2)-H(2F)	0.9800
Zr-C(5)	2.498(2)	C(3)-H(3D)	0.9800
Zr-C(8)	2.500(3)	C(3)-H(3E)	0.9800
Zr-C(4)	2.502(3)	C(3)-H(3F)	0.9800
Zr-C(6)	2.506(2)	C(4)-C(5)	1.395(4)
Zr-C(7)	2.507(3)	C(4)-C(8)	1.422(5)
Zr-H(1A)	2.04(4)	C(4)-C(9)	1.503(5)
Zr-H(1B)	2.06(4)	C(5)-C(6)	1.397(4)
Zr-H(1C)	2.33(3)	C(5)-C(10)	1.508(4)
Zr-H(2A)	2.02(4)	C(6)-C(7)	1.390(4)
Zr-H(2B)	2.10(4)	C(6)-C(11)	1.515(4)
Zr-H(2C)	2.29(4)	C(7)-C(8)	1.404(5)
Zr-H(3A)	2.18(4)	C(7)-C(12)	1.506(4)
Zr-H(3B)	2.03(5)	C(8)-C(13)	1.499(5)
Zr-H(3C)	2.31(4)	C(9)-H(9A)	0.9800
B(1)-C(1)	1.578(4)	C(9)-H(9B)	0.9800
B(1)-H(1A)	1.17(4)	C(9)-H(9C)	0.9800
B(1)-H(1B)	1.21(4)	C(10)-H(10A)	0.9800
B(1)-H(1C)	1.09(3)	C(10)-H(10B)	0.9800
B(2)-C(2)	1.586(5)	C(10)-H(10C)	0.9800
B(2)-H(2A)	1.14(4)	C(11)-H(11A)	0.9800
B(2)-H(2B)	1.14(4)	C(11)-H(11B)	0.9800
B(2)-H(2C)	1.22(4)	C(11)-H(11C)	0.9800
B(3)-C(3)	1.600(4)	C(12)-H(12A)	0.9800
B(3)-H(3A)	1.17(4)	C(12)-H(12B)	0.9800
B(3)-H(3B)	1.29(3)	C(12)-H(12C)	0.9800
B(3)-H(3C)	1.06(4)	C(13)-H(13A)	0.9800
C(1)-H(1D)	0.9800	C(13)-H(13B)	0.9800
C(1)-H(1E)	0.9800	C(13)-H(13C)	0.9800
C(1)-H(1F)	0.9800		

B(2)-Zr-B(3)	104.61(13)	B(3)-Zr-C(4)	130.99(12)
B(2)-Zr-B(1)	103.83(12)	B(1)-Zr-C(4)	119.49(11)
B(3)-Zr-B(1)	104.29(11)	C(5)-Zr-C(4)	32.41(10)
B(2)-Zr-C(5)	107.82(11)	C(8)-Zr-C(4)	33.04(12)
B(3)-Zr-C(5)	139.85(11)	B(2)-Zr-C(6)	138.89(11)
B(1)-Zr-C(5)	90.37(10)	B(3)-Zr-C(6)	109.17(11)
B(2)-Zr-C(8)	99.22(12)	B(1)-Zr-C(6)	89.98(10)
B(3)-Zr-C(8)	98.13(12)	C(5)-Zr-C(6)	32.42(9)
B(1)-Zr-C(8)	142.31(10)	C(8)-Zr-C(6)	53.79(9)
C(5)-Zr-C(8)	53.98(10)	C(4)-Zr-C(6)	53.88(9)
B(2)-Zr-C(4)	86.24(11)	B(2)-Zr-C(7)	131.76(12)

B(3)-Zr-C(7)	86.96(11)	B(1)-Zr-H(2B)	132.5(11)
B(1)-Zr-C(7)	118.62(11)	C(5)-Zr-H(2B)	105.4(10)
C(5)-Zr-C(7)	53.67(9)	C(8)-Zr-H(2B)	75.5(11)
C(8)-Zr-C(7)	32.58(11)	C(4)-Zr-H(2B)	75.0(10)
C(4)-Zr-C(7)	54.16(11)	C(6)-Zr-H(2B)	126.6(11)
C(6)-Zr-C(7)	32.21(9)	C(7)-Zr-H(2B)	106.4(11)
B(2)-Zr-H(1A)	132.0(10)	H(1A)-Zr-H(2B)	159.0(14)
B(3)-Zr-H(1A)	87.5(10)	H(1B)-Zr-H(2B)	115.9(15)
B(1)-Zr-H(1A)	29.2(10)	H(1C)-Zr-H(2B)	114.3(13)
C(5)-Zr-H(1A)	88.1(10)	H(2A)-Zr-H(2B)	50.3(14)
C(8)-Zr-H(1A)	125.3(10)	B(2)-Zr-H(2C)	30.4(10)
C(4)-Zr-H(1A)	120.4(10)	B(3)-Zr-H(2C)	86.5(10)
C(6)-Zr-H(1A)	72.9(10)	B(1)-Zr-H(2C)	85.1(10)
C(7)-Zr-H(1A)	94.5(10)	C(5)-Zr-H(2C)	132.5(10)
B(2)-Zr-H(1B)	89.4(10)	C(8)-Zr-H(2C)	126.6(10)
B(3)-Zr-H(1B)	134.3(10)	C(4)-Zr-H(2C)	116.4(10)
B(1)-Zr-H(1B)	30.3(10)	C(6)-Zr-H(2C)	164.3(10)
C(5)-Zr-H(1B)	69.3(10)	C(7)-Zr-H(2C)	156.3(10)
C(8)-Zr-H(1B)	122.6(10)	H(1A)-Zr-H(2C)	108.0(14)
C(4)-Zr-H(1B)	92.5(10)	H(1B)-Zr-H(2C)	84.8(13)
C(6)-Zr-H(1B)	83.5(10)	H(1C)-Zr-H(2C)	63.3(13)
C(7)-Zr-H(1B)	115.6(10)	H(2A)-Zr-H(2C)	49.2(14)
H(1A)-Zr-H(1B)	53.5(13)	H(2B)-Zr-H(2C)	51.1(15)
B(2)-Zr-H(1C)	88.8(8)	B(2)-Zr-H(3A)	91.0(10)
B(3)-Zr-H(1C)	87.2(8)	B(3)-Zr-H(3A)	29.5(10)
B(1)-Zr-H(1C)	26.7(8)	B(1)-Zr-H(3A)	133.6(10)
C(5)-Zr-H(1C)	116.2(8)	C(5)-Zr-H(3A)	126.9(10)
C(8)-Zr-H(1C)	168.8(8)	C(8)-Zr-H(3A)	74.5(10)
C(4)-Zr-H(1C)	141.5(8)	C(4)-Zr-H(3A)	105.0(10)
C(6)-Zr-H(1C)	115.2(8)	C(6)-Zr-H(3A)	107.2(10)
C(7)-Zr-H(1C)	139.0(8)	C(7)-Zr-H(3A)	76.5(10)
H(1A)-Zr-H(1C)	44.8(12)	H(1A)-Zr-H(3A)	115.5(15)
H(1B)-Zr-H(1C)	49.3(13)	H(1B)-Zr-H(3A)	162.5(14)
B(2)-Zr-H(2A)	28.9(11)	H(1C)-Zr-H(3A)	113.3(13)
B(3)-Zr-H(2A)	132.9(11)	H(2A)-Zr-H(3A)	118.6(14)
B(1)-Zr-H(2A)	88.9(10)	H(2B)-Zr-H(3A)	69.3(13)
C(5)-Zr-H(2A)	83.5(11)	H(2C)-Zr-H(3A)	86.8(13)
C(8)-Zr-H(2A)	97.7(11)	B(2)-Zr-H(3B)	136.7(9)
C(4)-Zr-H(2A)	72.1(11)	B(3)-Zr-H(3B)	32.9(9)
C(6)-Zr-H(2A)	115.9(11)	B(1)-Zr-H(3B)	86.8(9)
C(7)-Zr-H(2A)	126.1(11)	C(5)-Zr-H(3B)	114.1(9)
H(1A)-Zr-H(2A)	117.5(14)	C(8)-Zr-H(3B)	96.5(10)
H(1B)-Zr-H(2A)	65.8(14)	C(4)-Zr-H(3B)	125.0(10)
H(1C)-Zr-H(2A)	85.7(14)	C(6)-Zr-H(3B)	81.7(9)
B(2)-Zr-H(2B)	28.8(11)	C(7)-Zr-H(3B)	70.9(10)
B(3)-Zr-H(2B)	92.0(11)	H(1A)-Zr-H(3B)	61.6(13)

H(1B)-Zr-H(3B)	115.0(13)	Zr-B(3)-H(3B)	59(2)
H(1C)-Zr-H(3B)	82.6(12)	H(3A)-B(3)-H(3B)	105(2)
H(2A)-Zr-H(3B)	161.9(15)	C(3)-B(3)-H(3C)	114(2)
H(2B)-Zr-H(3B)	123.6(14)	Zr-B(3)-H(3C)	73(2)
H(2C)-Zr-H(3B)	112.9(14)	H(3A)-B(3)-H(3C)	108(3)
H(3A)-Zr-H(3B)	55.0(14)	H(3B)-B(3)-H(3C)	101(2)
B(2)-Zr-H(3C)	88.8(9)	B(1)-C(1)-H(1D)	109.5
B(3)-Zr-H(3C)	26.0(10)	B(1)-C(1)-H(1E)	109.5
B(1)-Zr-H(3C)	88.5(10)	H(1D)-C(1)-H(1E)	109.5
C(5)-Zr-H(3C)	163.1(9)	B(1)-C(1)-H(1F)	109.5
C(8)-Zr-H(3C)	121.6(10)	H(1D)-C(1)-H(1F)	109.5
C(4)-Zr-H(3C)	151.9(10)	H(1E)-C(1)-H(1F)	109.5
C(6)-Zr-H(3C)	130.7(9)	B(2)-C(2)-H(2D)	109.5
C(7)-Zr-H(3C)	112.8(10)	B(2)-C(2)-H(2E)	109.5
H(1A)-Zr-H(3C)	82.7(13)	H(2D)-C(2)-H(2E)	109.5
H(1B)-Zr-H(3C)	115.1(15)	B(2)-C(2)-H(2F)	109.5
H(1C)-Zr-H(3C)	65.9(13)	H(2D)-C(2)-H(2F)	109.5
H(2A)-Zr-H(3C)	113.3(15)	H(2E)-C(2)-H(2F)	109.5
H(2B)-Zr-H(3C)	87.6(13)	B(3)-C(3)-H(3D)	109.5
H(2C)-Zr-H(3C)	64.2(14)	B(3)-C(3)-H(3E)	109.5
H(3A)-Zr-H(3C)	47.4(15)	H(3D)-C(3)-H(3E)	109.5
H(3B)-Zr-H(3C)	49.0(12)	B(3)-C(3)-H(3F)	109.5
C(1)-B(1)-Zr	168.2(2)	H(3D)-C(3)-H(3F)	109.5
C(1)-B(1)-H(1A)	117.0(18)	H(3E)-C(3)-H(3F)	109.5
Zr-B(1)-H(1A)	58.8(18)	C(5)-C(4)-C(8)	107.2(3)
C(1)-B(1)-H(1B)	113.5(17)	C(5)-C(4)-C(9)	127.3(4)
Zr-B(1)-H(1B)	59.6(17)	C(8)-C(4)-C(9)	125.3(4)
H(1A)-B(1)-H(1B)	102(2)	C(5)-C(4)-Zr	73.61(15)
C(1)-B(1)-H(1C)	118.3(18)	C(8)-C(4)-Zr	73.39(15)
Zr-B(1)-H(1C)	73.6(18)	C(9)-C(4)-Zr	122.8(2)
H(1A)-B(1)-H(1C)	97(2)	C(4)-C(5)-C(6)	108.7(3)
H(1B)-B(1)-H(1C)	107(3)	C(4)-C(5)-C(10)	125.6(3)
C(2)-B(2)-Zr	174.2(3)	C(6)-C(5)-C(10)	125.4(3)
C(2)-B(2)-H(2A)	117(2)	C(4)-C(5)-Zr	73.98(15)
Zr-B(2)-H(2A)	59(2)	C(6)-C(5)-Zr	74.12(15)
C(2)-B(2)-H(2B)	116.2(19)	C(10)-C(5)-Zr	123.1(2)
Zr-B(2)-H(2B)	62.4(19)	C(7)-C(6)-C(5)	108.3(3)
H(2A)-B(2)-H(2B)	100(3)	C(7)-C(6)-C(11)	126.9(3)
C(2)-B(2)-H(2C)	114.1(18)	C(5)-C(6)-C(11)	124.7(3)
Zr-B(2)-H(2C)	71.4(18)	C(7)-C(6)-Zr	73.92(14)
H(2A)-B(2)-H(2C)	100(3)	C(5)-C(6)-Zr	73.46(15)
H(2B)-B(2)-H(2C)	107(3)	C(11)-C(6)-Zr	122.13(19)
C(3)-B(3)-Zr	172.3(3)	C(6)-C(7)-C(8)	108.2(3)
C(3)-B(3)-H(3A)	108.9(18)	C(6)-C(7)-C(12)	125.7(3)
Zr-B(3)-H(3A)	66.2(18)	C(8)-C(7)-C(12)	125.6(3)
C(3)-B(3)-H(3B)	119(2)	C(6)-C(7)-Zr	73.87(14)

C(8)-C(7)-Zr	73.44(16)	H(10B)-C(10)-H(10C)	109.5
C(12)-C(7)-Zr	125.1(2)	C(6)-C(11)-H(11A)	109.5
C(7)-C(8)-C(4)	107.6(2)	C(6)-C(11)-H(11B)	109.5
C(7)-C(8)-C(13)	126.6(4)	H(11A)-C(11)-H(11B)	109.5
C(4)-C(8)-C(13)	125.6(4)	C(6)-C(11)-H(11C)	109.5
C(7)-C(8)-Zr	73.98(15)	H(11A)-C(11)-H(11C)	109.5
C(4)-C(8)-Zr	73.57(16)	H(11B)-C(11)-H(11C)	109.5
C(13)-C(8)-Zr	122.8(2)	C(7)-C(12)-H(12A)	109.5
C(4)-C(9)-H(9A)	109.5	C(7)-C(12)-H(12B)	109.5
C(4)-C(9)-H(9B)	109.5	H(12A)-C(12)-H(12B)	109.5
H(9A)-C(9)-H(9B)	109.5	C(7)-C(12)-H(12C)	109.5
C(4)-C(9)-H(9C)	109.5	H(12A)-C(12)-H(12C)	109.5
H(9A)-C(9)-H(9C)	109.5	H(12B)-C(12)-H(12C)	109.5
H(9B)-C(9)-H(9C)	109.5	C(8)-C(13)-H(13A)	109.5
C(5)-C(10)-H(10A)	109.5	C(8)-C(13)-H(13B)	109.5
C(5)-C(10)-H(10B)	109.5	H(13A)-C(13)-H(13B)	109.5
H(10A)-C(10)-H(10B)	109.5	C(8)-C(13)-H(13C)	109.5
C(5)-C(10)-H(10C)	109.5	H(13A)-C(13)-H(13C)	109.5
H(10A)-C(10)-H(10C)	109.5	H(13B)-C(13)-H(13C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S6. Crystal data and structure refinement for $Cp^*Zr(BH_3Ph)_3$

Empirical formula	$C_{28}H_{39}B_3Zr$	
Formula weight	499.24	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 8.8868(1) Å	α = 90°.
	b = 14.7203(2) Å	β = 91.1669(5)°.
	c = 20.4718(3) Å	γ = 90°.
Volume	2677.49(6) $Å^3$	
Z	4	
Density (calculated)	1.238 Mg/m^3	
Absorption coefficient	0.424 mm^{-1}	
F(000)	1048	
Crystal size	0.25 x 0.25 x 0.20 mm^3	
Theta range for data collection	1.70 to 27.50°..	
Index ranges	-11<=h<=11, -19<=k<=18, -26<=l<=26	
Reflections collected	20179	
Independent reflections	6152 [R(int) = 0.0712]	
Completeness to theta = 27.50°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.940 and 0.867	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6152 / 0 / 326	
Goodness-of-fit on F^2	1.077	
Final R indices [I>2sigma(I)]	R1 = 0.0410, wR2 = 0.0861	
R indices (all data)	R1 = 0.0847, wR2 = 0.1152	
Extinction coefficient	0.0086(7)	
Largest diff. peak and hole	0.791 and -0.663 $e.Å^{-3}$	

[a] $R_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$.
[b] $wR_2 = \{\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2\}^{1/2}$.

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $Cp^*Zr(BH_3Ph)_3$

Atom	x	y	z	U(eq)[a]
Zr	8874(1)	2967(1)	2995(1)	22(1)
B(1)	10909(4)	4015(2)	3216(2)	29(1)
B(2)	9962(4)	1540(2)	3271(2)	27(1)
B(3)	8611(4)	2942(2)	1831(2)	28(1)
C(1)	11897(3)	4813(2)	3501(1)	30(1)
C(2)	11485(4)	5719(2)	3421(2)	42(1)
C(3)	12348(5)	6427(3)	3665(2)	53(1)
C(4)	13647(4)	6249(3)	4007(2)	48(1)
C(5)	14088(4)	5366(3)	4110(2)	47(1)
C(6)	13219(4)	4650(2)	3855(2)	38(1)
C(7)	10662(3)	623(2)	3518(1)	25(1)
C(8)	12034(3)	329(2)	3284(2)	30(1)
C(9)	12748(4)	-448(2)	3519(2)	34(1)
C(10)	12074(4)	-951(2)	3996(2)	38(1)
C(11)	10688(4)	-693(2)	4232(2)	36(1)
C(12)	9997(4)	88(2)	3995(2)	32(1)
C(13)	8186(3)	2937(2)	1077(1)	28(1)
C(14)	7458(4)	2200(2)	786(2)	40(1)
C(15)	7149(4)	2168(2)	120(2)	45(1)
C(16)	7538(4)	2885(2)	-272(2)	44(1)
C(17)	8226(4)	3634(2)	3(2)	43(1)
C(18)	8549(4)	3661(2)	664(2)	36(1)
C(19)	7222(3)	2896(2)	3970(1)	27(1)
C(20)	7510(3)	3831(2)	3862(1)	26(1)
C(21)	6846(3)	4078(2)	3246(1)	28(1)
C(22)	6115(3)	3295(2)	2987(1)	29(1)
C(23)	6361(3)	2562(2)	3426(1)	28(1)
C(24)	7569(4)	2361(2)	4583(2)	38(1)
C(25)	8270(4)	4467(2)	4340(2)	36(1)
C(26)	6812(4)	5004(2)	2941(2)	37(1)
C(27)	5112(4)	3278(2)	2386(2)	40(1)
C(28)	5663(4)	1626(2)	3373(2)	42(1)

[a] U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Table S8. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $Cp^*Zr(BH_3Ph)_3$

Atom	U11	U22	U33	U23	U13	U12
Zr	26(1)	19(1)	21(1)	1(1)	-1(1)	2(1)
B(1)	30(2)	28(2)	30(2)	1(2)	2(2)	1(2)
B(2)	29(2)	23(2)	29(2)	-2(2)	-4(2)	3(2)
B(3)	33(2)	28(2)	22(2)	1(2)	-1(2)	-1(2)
C(1)	33(2)	29(2)	27(2)	-2(1)	5(1)	-2(1)
C(2)	49(2)	30(2)	48(2)	-2(2)	-10(2)	-5(2)
C(3)	69(3)	36(2)	53(2)	-6(2)	-3(2)	-11(2)
C(4)	53(2)	48(2)	45(2)	-17(2)	12(2)	-21(2)
C(5)	30(2)	70(3)	41(2)	-13(2)	0(2)	-10(2)
C(6)	34(2)	43(2)	38(2)	-3(2)	4(2)	-2(2)
C(7)	30(2)	22(2)	23(2)	-4(1)	-5(1)	1(1)
C(8)	35(2)	29(2)	26(2)	-3(1)	-4(1)	0(1)
C(9)	36(2)	34(2)	33(2)	-7(2)	-6(1)	10(1)
C(10)	56(2)	29(2)	30(2)	-1(1)	-13(2)	12(2)
C(11)	57(2)	26(2)	25(2)	3(1)	-2(2)	1(2)
C(12)	40(2)	27(2)	28(2)	-1(1)	2(1)	4(1)
C(13)	28(2)	31(2)	25(2)	1(1)	1(1)	6(1)
C(14)	51(2)	37(2)	31(2)	3(1)	-5(2)	-1(2)
C(15)	52(2)	49(2)	34(2)	-7(2)	-11(2)	-7(2)
C(16)	45(2)	61(2)	25(2)	3(2)	-7(2)	5(2)
C(17)	50(2)	49(2)	28(2)	12(2)	0(2)	-2(2)
C(18)	38(2)	40(2)	31(2)	3(2)	-2(1)	-2(2)
C(19)	30(2)	28(2)	22(2)	1(1)	4(1)	3(1)
C(20)	30(2)	25(2)	23(2)	0(1)	4(1)	6(1)
C(21)	29(2)	28(2)	28(2)	3(1)	3(1)	9(1)
C(22)	23(2)	37(2)	26(2)	4(1)	2(1)	5(1)
C(23)	26(2)	32(2)	26(2)	2(1)	6(1)	0(1)
C(24)	52(2)	37(2)	26(2)	9(1)	1(2)	8(2)
C(25)	44(2)	33(2)	31(2)	-7(1)	3(2)	6(2)
C(26)	47(2)	28(2)	37(2)	6(1)	5(2)	11(2)
C(27)	29(2)	55(2)	37(2)	3(2)	-5(2)	5(2)
C(28)	42(2)	39(2)	45(2)	0(2)	5(2)	-12(2)

Table S9. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $Cp^*Zr(BH_3Ph)_3$

Atom	x	y	z	U(eq)
H(1A)	9880(30)	4282(19)	2928(14)	29(8)
H(1B)	10430(30)	3583(19)	3589(14)	28(8)
H(1C)	11460(30)	3560(20)	2880(15)	40(9)
H(2A)	8750(30)	1407(19)	3037(12)	21(7)
H(2B)	10630(40)	1900(20)	2909(16)	37(9)
H(2C)	9820(40)	2080(20)	3660(16)	41(9)
H(3A)	8380(30)	3667(18)	2095(13)	22(7)
H(3B)	9780(40)	2820(20)	1975(15)	43(9)
H(3C)	7970(30)	2460(20)	2145(14)	25(7)
H(2D)	10575	5856	3190	51
H(3D)	12037	7038	3594	63
H(4A)	14246	6734	4173	58
H(5A)	14984	5241	4354	56
H(6A)	13540	4042	3926	46
H(8A)	12501	672	2951	36
H(9A)	13691	-629	3352	41
H(10A)	12560	-1478	4165	46
H(11A)	10213	-1049	4555	43
H(12A)	9049	262	4161	38
H(14A)	7165	1704	1051	48
H(15A)	6668	1650	-66	54
H(16A)	7333	2864	-728	53
H(17A)	8480	4135	-265	51
H(18A)	9029	4183	844	43
H(24A)	6752	2441	4892	57
H(24B)	8515	2580	4782	57
H(24C)	7667	1716	4474	57
H(25A)	7519	4725	4631	54
H(25B)	8764	4957	4102	54
H(25C)	9024	4132	4600	54
H(26A)	5938	5341	3097	56
H(26B)	6740	4945	2464	56
H(26C)	7736	5333	3062	56
H(27A)	4081	3432	2505	61
H(27B)	5128	2670	2192	61
H(27C)	5475	3722	2068	61
H(28A)	4673	1631	3576	63
H(28B)	6314	1184	3598	63
H(28C)	5549	1458	2912	63

Table S10. Bond lengths [Å] and angles [°] for $Cp^*Zr(BH_3Ph)_3$

Zr-B(2)	2.375(3)	C(9)-C(10)	1.373(5)
Zr-B(3)	2.389(3)	C(9)-H(9A)	0.9500
Zr-B(1)	2.413(4)	C(10)-C(11)	1.385(5)
Zr-C(23)	2.490(3)	C(10)-H(10A)	0.9500
Zr-C(21)	2.495(3)	C(11)-C(12)	1.385(4)
Zr-C(22)	2.498(3)	C(11)-H(11A)	0.9500
Zr-C(19)	2.503(3)	C(12)-H(12A)	0.9500
Zr-C(20)	2.515(3)	C(13)-C(14)	1.391(4)
Zr-H(1A)	2.14(3)	C(13)-C(18)	1.402(4)
Zr-H(1B)	2.04(3)	C(14)-C(15)	1.386(5)
Zr-H(2A)	2.30(3)	C(14)-H(14A)	0.9500
Zr-H(2B)	2.22(3)	C(15)-C(16)	1.373(5)
Zr-H(2C)	2.05(3)	C(15)-H(15A)	0.9500
Zr-H(3A)	2.15(3)	C(16)-C(17)	1.375(5)
Zr-H(3B)	2.26(3)	C(16)-H(16A)	0.9500
Zr-H(3C)	2.04(3)	C(17)-C(18)	1.378(4)
B(1)-C(1)	1.572(4)	C(17)-H(17A)	0.9500
B(1)-H(1A)	1.15(3)	C(18)-H(18A)	0.9500
B(1)-H(1B)	1.09(3)	C(19)-C(20)	1.419(4)
B(1)-H(1C)	1.08(3)	C(19)-C(23)	1.425(4)
B(2)-C(7)	1.567(4)	C(19)-C(24)	1.508(4)
B(2)-H(2A)	1.18(2)	C(20)-C(21)	1.428(4)
B(2)-H(2B)	1.09(3)	C(20)-C(25)	1.505(4)
B(2)-H(2C)	1.14(3)	C(21)-C(22)	1.420(4)
B(3)-C(13)	1.583(4)	C(21)-C(26)	1.500(4)
B(3)-H(3A)	1.22(3)	C(22)-C(23)	1.419(4)
B(3)-H(3B)	1.09(3)	C(22)-C(27)	1.505(4)
B(3)-H(3C)	1.12(3)	C(23)-C(28)	1.514(4)
C(1)-C(6)	1.390(4)	C(24)-H(24A)	0.9800
C(1)-C(2)	1.392(4)	C(24)-H(24B)	0.9800
C(2)-C(3)	1.381(5)	C(24)-H(24C)	0.9800
C(2)-H(2D)	0.9500	C(25)-H(25A)	0.9800
C(3)-C(4)	1.363(5)	C(25)-H(25B)	0.9800
C(3)-H(3D)	0.9500	C(25)-H(25C)	0.9800
C(4)-C(5)	1.372(5)	C(26)-H(26A)	0.9800
C(4)-H(4A)	0.9500	C(26)-H(26B)	0.9800
C(5)-C(6)	1.401(4)	C(26)-H(26C)	0.9800
C(5)-H(5A)	0.9500	C(27)-H(27A)	0.9800
C(6)-H(6A)	0.9500	C(27)-H(27B)	0.9800
C(7)-C(8)	1.388(4)	C(27)-H(27C)	0.9800
C(7)-C(12)	1.395(4)	C(28)-H(28A)	0.9800
C(8)-C(9)	1.390(4)	C(28)-H(28B)	0.9800
C(8)-H(8A)	0.9500	C(28)-H(28C)	0.9800

B(2)-Zr-B(3)	104.75(12)	B(3)-Zr-H(2A)	91.1(6)
B(2)-Zr-B(1)	102.75(12)	B(1)-Zr-H(2A)	131.8(6)
B(3)-Zr-B(1)	104.72(13)	C(23)-Zr-H(2A)	72.9(6)
B(2)-Zr-C(23)	93.90(11)	C(21)-Zr-H(2A)	127.8(6)
B(3)-Zr-C(23)	106.24(11)	C(22)-Zr-H(2A)	98.5(6)
B(1)-Zr-C(23)	139.53(11)	C(19)-Zr-H(2A)	84.2(6)
B(2)-Zr-C(21)	145.40(11)	C(20)-Zr-H(2A)	117.1(6)
B(3)-Zr-C(21)	99.14(11)	H(1A)-Zr-H(2A)	157.8(10)
B(1)-Zr-C(21)	94.82(11)	H(1B)-Zr-H(2A)	117.0(10)
C(23)-Zr-C(21)	55.06(10)	B(2)-Zr-H(2B)	27.2(8)
B(2)-Zr-C(22)	124.58(11)	B(3)-Zr-H(2B)	88.0(8)
B(3)-Zr-C(22)	85.43(11)	B(1)-Zr-H(2B)	86.8(8)
B(1)-Zr-C(22)	127.52(11)	C(23)-Zr-H(2B)	119.6(8)
C(23)-Zr-C(22)	33.05(10)	C(21)-Zr-H(2B)	172.1(9)
C(21)-Zr-C(22)	33.04(10)	C(22)-Zr-H(2B)	145.6(8)
B(2)-Zr-C(19)	90.92(11)	C(19)-Zr-H(2B)	117.2(9)
B(3)-Zr-C(19)	138.36(11)	C(20)-Zr-H(2B)	139.7(8)
B(1)-Zr-C(19)	109.08(11)	H(1A)-Zr-H(2B)	109.9(11)
C(23)-Zr-C(19)	33.17(9)	H(1B)-Zr-H(2B)	83.9(11)
C(21)-Zr-C(19)	54.96(9)	H(2A)-Zr-H(2B)	47.9(10)
C(22)-Zr-C(19)	54.72(9)	B(2)-Zr-H(2C)	28.5(9)
B(2)-Zr-C(20)	118.64(11)	B(3)-Zr-H(2C)	133.0(9)
B(3)-Zr-C(20)	132.26(11)	B(1)-Zr-H(2C)	89.3(9)
B(1)-Zr-C(20)	85.10(11)	C(23)-Zr-H(2C)	88.3(9)
C(23)-Zr-C(20)	54.71(10)	C(21)-Zr-H(2C)	124.5(9)
C(21)-Zr-C(20)	33.13(9)	C(22)-Zr-H(2C)	121.0(9)
C(22)-Zr-C(20)	54.54(9)	C(19)-Zr-H(2C)	71.5(9)
C(19)-Zr-C(20)	32.84(9)	C(20)-Zr-H(2C)	92.8(9)
B(2)-Zr-H(1A)	130.3(8)	H(1A)-Zr-H(2C)	116.9(11)
B(3)-Zr-H(1A)	89.0(8)	H(1B)-Zr-H(2C)	67.9(12)
B(1)-Zr-H(1A)	28.4(8)	H(2A)-Zr-H(2C)	50.1(10)
C(23)-Zr-H(1A)	128.2(8)	H(2B)-Zr-H(2C)	47.6(12)
C(21)-Zr-H(1A)	74.0(8)	B(2)-Zr-H(3A)	134.7(7)
C(22)-Zr-H(1A)	103.6(8)	B(3)-Zr-H(3A)	30.5(7)
C(19)-Zr-H(1A)	110.0(8)	B(1)-Zr-H(3A)	89.7(7)
C(20)-Zr-H(1A)	78.2(8)	C(23)-Zr-H(3A)	104.4(7)
B(2)-Zr-H(1B)	89.1(8)	C(21)-Zr-H(3A)	74.0(7)
B(3)-Zr-H(1B)	130.8(8)	C(22)-Zr-H(3A)	73.5(7)
B(1)-Zr-H(1B)	26.6(8)	C(19)-Zr-H(3A)	126.2(7)
C(23)-Zr-H(1B)	119.8(8)	C(20)-Zr-H(3A)	105.6(7)
C(21)-Zr-H(1B)	94.0(8)	H(1A)-Zr-H(3A)	65.8(10)
C(22)-Zr-H(1B)	124.9(8)	H(1B)-Zr-H(3A)	115.1(11)
C(19)-Zr-H(1B)	86.8(8)	H(2A)-Zr-H(3A)	120.1(9)
C(20)-Zr-H(1B)	71.6(8)	H(2B)-Zr-H(3A)	113.8(11)
H(1A)-Zr-H(1B)	49.9(11)	H(2C)-Zr-H(3A)	161.4(12)
B(2)-Zr-H(2A)	29.2(6)	B(2)-Zr-H(3B)	89.0(8)

B(3)-Zr-H(3B)	27.0(8)	H(2A)-B(2)-H(2C)	107(2)
B(1)-Zr-H(3B)	87.3(8)	H(2B)-B(2)-H(2C)	102(2)
C(23)-Zr-H(3B)	130.1(8)	C(13)-B(3)-Zr	171.8(2)
C(21)-Zr-H(3B)	121.7(8)	C(13)-B(3)-H(3A)	113.5(12)
C(22)-Zr-H(3B)	112.4(8)	Zr-B(3)-H(3A)	63.7(12)
C(19)-Zr-H(3B)	163.2(8)	C(13)-B(3)-H(3B)	118.0(17)
C(20)-Zr-H(3B)	152.3(8)	Zr-B(3)-H(3B)	70.1(17)
H(1A)-Zr-H(3B)	82.5(11)	H(3A)-B(3)-H(3B)	101(2)
H(1B)-Zr-H(3B)	110.0(12)	C(13)-B(3)-H(3C)	116.2(14)
H(2A)-Zr-H(3B)	87.5(9)	Zr-B(3)-H(3C)	58.6(14)
H(2B)-Zr-H(3B)	66.1(11)	H(3A)-B(3)-H(3C)	102.1(19)
H(2C)-Zr-H(3B)	113.7(12)	H(3B)-B(3)-H(3C)	104(2)
H(3A)-Zr-H(3B)	47.7(10)	C(6)-C(1)-C(2)	116.4(3)
B(2)-Zr-H(3C)	91.7(8)	C(6)-C(1)-B(1)	121.6(3)
B(3)-Zr-H(3C)	28.0(8)	C(2)-C(1)-B(1)	122.0(3)
B(1)-Zr-H(3C)	132.4(9)	C(3)-C(2)-C(1)	122.6(3)
C(23)-Zr-H(3C)	82.8(8)	C(3)-C(2)-H(2D)	118.7
C(21)-Zr-H(3C)	98.2(8)	C(1)-C(2)-H(2D)	118.7
C(22)-Zr-H(3C)	72.3(8)	C(4)-C(3)-C(2)	119.9(4)
C(19)-Zr-H(3C)	115.9(8)	C(4)-C(3)-H(3D)	120.1
C(20)-Zr-H(3C)	126.8(8)	C(2)-C(3)-H(3D)	120.1
H(1A)-Zr-H(3C)	115.8(11)	C(3)-C(4)-C(5)	119.8(3)
H(1B)-Zr-H(3C)	157.3(12)	C(3)-C(4)-H(4A)	120.1
H(2A)-Zr-H(3C)	69.4(10)	C(5)-C(4)-H(4A)	120.1
H(2B)-Zr-H(3C)	86.4(11)	C(4)-C(5)-C(6)	120.1(3)
H(2C)-Zr-H(3C)	118.7(12)	C(4)-C(5)-H(5A)	119.9
H(3A)-Zr-H(3C)	51.4(11)	C(6)-C(5)-H(5A)	119.9
H(3B)-Zr-H(3C)	47.3(11)	C(1)-C(6)-C(5)	121.2(3)
C(1)-B(1)-Zr	163.4(2)	C(1)-C(6)-H(6A)	119.4
C(1)-B(1)-H(1A)	111.6(14)	C(5)-C(6)-H(6A)	119.4
Zr-B(1)-H(1A)	62.4(14)	C(8)-C(7)-C(12)	117.0(3)
C(1)-B(1)-H(1B)	113.6(15)	C(8)-C(7)-B(2)	120.2(3)
Zr-B(1)-H(1B)	57.0(14)	C(12)-C(7)-B(2)	122.8(3)
H(1A)-B(1)-H(1B)	104(2)	C(7)-C(8)-C(9)	122.3(3)
C(1)-B(1)-H(1C)	116.1(16)	C(7)-C(8)-H(8A)	118.8
Zr-B(1)-H(1C)	80.4(16)	C(9)-C(8)-H(8A)	118.8
H(1A)-B(1)-H(1C)	105(2)	C(10)-C(9)-C(8)	119.2(3)
H(1B)-B(1)-H(1C)	106(2)	C(10)-C(9)-H(9A)	120.4
C(7)-B(2)-Zr	174.9(2)	C(8)-C(9)-H(9A)	120.4
C(7)-B(2)-H(2A)	109.8(14)	C(9)-C(10)-C(11)	120.2(3)
Zr-B(2)-H(2A)	71.9(13)	C(9)-C(10)-H(10A)	119.9
C(7)-B(2)-H(2B)	114.7(16)	C(11)-C(10)-H(10A)	119.9
Zr-B(2)-H(2B)	68.6(15)	C(10)-C(11)-C(12)	119.8(3)
H(2A)-B(2)-H(2B)	108(2)	C(10)-C(11)-H(11A)	120.1
C(7)-B(2)-H(2C)	115.3(16)	C(12)-C(11)-H(11A)	120.1
Zr-B(2)-H(2C)	59.7(15)	C(11)-C(12)-C(7)	121.4(3)

C(11)-C(12)-H(12A)	119.3	C(21)-C(22)-C(27)	125.3(3)
C(7)-C(12)-H(12A)	119.3	C(23)-C(22)-Zr	73.14(16)
C(14)-C(13)-C(18)	116.5(3)	C(21)-C(22)-Zr	73.33(16)
C(14)-C(13)-B(3)	121.4(3)	C(27)-C(22)-Zr	124.5(2)
C(18)-C(13)-B(3)	122.1(3)	C(22)-C(23)-C(19)	107.9(3)
C(15)-C(14)-C(13)	121.9(3)	C(22)-C(23)-C(28)	126.1(3)
C(15)-C(14)-H(14A)	119.1	C(19)-C(23)-C(28)	125.6(3)
C(13)-C(14)-H(14A)	119.1	C(22)-C(23)-Zr	73.81(16)
C(16)-C(15)-C(14)	120.0(3)	C(19)-C(23)-Zr	73.95(16)
C(16)-C(15)-H(15A)	120.0	C(28)-C(23)-Zr	124.2(2)
C(14)-C(15)-H(15A)	120.0	C(19)-C(24)-H(24A)	109.5
C(15)-C(16)-C(17)	119.5(3)	C(19)-C(24)-H(24B)	109.5
C(15)-C(16)-H(16A)	120.2	H(24A)-C(24)-H(24B)	109.5
C(17)-C(16)-H(16A)	120.2	C(19)-C(24)-H(24C)	109.5
C(16)-C(17)-C(18)	120.5(3)	H(24A)-C(24)-H(24C)	109.5
C(16)-C(17)-H(17A)	119.8	H(24B)-C(24)-H(24C)	109.5
C(18)-C(17)-H(17A)	119.8	C(20)-C(25)-H(25A)	109.5
C(17)-C(18)-C(13)	121.5(3)	C(20)-C(25)-H(25B)	109.5
C(17)-C(18)-H(18A)	119.2	H(25A)-C(25)-H(25B)	109.5
C(13)-C(18)-H(18A)	119.2	C(20)-C(25)-H(25C)	109.5
C(20)-C(19)-C(23)	107.9(2)	H(25A)-C(25)-H(25C)	109.5
C(20)-C(19)-C(24)	127.0(3)	H(25B)-C(25)-H(25C)	109.5
C(23)-C(19)-C(24)	124.6(3)	C(21)-C(26)-H(26A)	109.5
C(20)-C(19)-Zr	74.04(16)	C(21)-C(26)-H(26B)	109.5
C(23)-C(19)-Zr	72.89(16)	H(26A)-C(26)-H(26B)	109.5
C(24)-C(19)-Zr	124.9(2)	C(21)-C(26)-H(26C)	109.5
C(19)-C(20)-C(21)	108.2(3)	H(26A)-C(26)-H(26C)	109.5
C(19)-C(20)-C(25)	125.6(3)	H(26B)-C(26)-H(26C)	109.5
C(21)-C(20)-C(25)	126.1(3)	C(22)-C(27)-H(27A)	109.5
C(19)-C(20)-Zr	73.12(16)	C(22)-C(27)-H(27B)	109.5
C(21)-C(20)-Zr	72.64(16)	H(27A)-C(27)-H(27B)	109.5
C(25)-C(20)-Zr	123.9(2)	C(22)-C(27)-H(27C)	109.5
C(22)-C(21)-C(20)	107.5(3)	H(27A)-C(27)-H(27C)	109.5
C(22)-C(21)-C(26)	125.2(3)	H(27B)-C(27)-H(27C)	109.5
C(20)-C(21)-C(26)	127.1(3)	C(23)-C(28)-H(28A)	109.5
C(22)-C(21)-Zr	73.62(16)	C(23)-C(28)-H(28B)	109.5
C(20)-C(21)-Zr	74.23(16)	H(28A)-C(28)-H(28B)	109.5
C(26)-C(21)-Zr	121.3(2)	C(23)-C(28)-H(28C)	109.5
C(23)-C(22)-C(21)	108.5(3)	H(28A)-C(28)-H(28C)	109.5
C(23)-C(22)-C(27)	125.9(3)	H(28B)-C(28)-H(28C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S11. Crystal data and structure refinement for $Cp^*Zr(BH_4)_3$

Empirical formula	$C_{10}H_{27}B_3Zr$	
Formula weight	270.97	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.0619(8) Å	α = 84.077(2)°.
	b = 8.4186(9) Å	β = 88.589(2)°.
	c = 13.4982(15) Å	γ = 66.427(2)°.
Volume	731.47(14) $Å^3$	
Z	2	
Density (calculated)	1.230 Mg/m^3	
Absorption coefficient	0.717 mm^{-1}	
F(000)	284	
Crystal size	0.20 x 0.20 x 0.10 mm^3	
Theta range for data collection	1.52 to 27.50°.	
Index ranges	-9<=h<=9, -10<=k<=10, -17<=l<=17	
Reflections collected	9665	
Independent reflections	3345 [R(int) = 0.0351]	
Completeness to theta = 27.50°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9318 and 0.8699	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3345 / 0 / 175	
Goodness-of-fit on F^2	1.155	
Final R indices [I>2sigma(I)]	R1 = 0.0364, wR2 = 0.0857	
R indices (all data)	R1 = 0.0401, wR2 = 0.0873	
Largest diff. peak and hole	1.205 and -0.785 $e.Å^{-3}$	

[a] $R_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$.
[b] $wR_2 = \{\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2\}^{1/2}$.

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $Cp^*Zr(BH_4)_3$

Atom	x	y	z	U(eq)[a]
Zr	888(1)	8121(1)	2513(1)	19(1)
B(1)	3057(5)	6033(5)	1484(3)	34(1)
B(2)	1499(6)	10639(5)	1980(3)	35(1)
B(3)	2536(6)	7188(6)	4109(3)	41(1)
C(1)	-2001(4)	7606(3)	1775(2)	21(1)
C(2)	-2650(4)	9437(3)	1738(2)	21(1)
C(3)	-2870(4)	9886(3)	2732(2)	21(1)
C(4)	-2364(4)	8344(3)	3381(2)	22(1)
C(5)	-1807(4)	6924(3)	2792(2)	20(1)
C(6)	-1761(5)	6579(4)	900(2)	31(1)
C(7)	-3242(5)	10696(4)	817(2)	32(1)
C(8)	-3772(5)	11706(4)	3030(2)	33(1)
C(9)	-2576(5)	8221(4)	4494(2)	32(1)
C(10)	-1334(5)	5069(4)	3176(2)	33(1)

[a] U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Table S13. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $Cp^*Zr(BH_4)_3$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zr	16(1)	18(1)	22(1)	-2(1)	2(1)	-7(1)
B(1)	27(2)	31(2)	43(2)	-10(2)	8(1)	-9(1)
B(2)	33(2)	28(2)	50(2)	-6(2)	13(2)	-18(2)
B(3)	35(2)	63(3)	29(2)	3(2)	-7(2)	-26(2)
C(1)	17(1)	23(1)	24(1)	-6(1)	1(1)	-8(1)
C(2)	16(1)	21(1)	24(1)	0(1)	0(1)	-7(1)
C(3)	17(1)	19(1)	26(1)	-5(1)	3(1)	-6(1)
C(4)	18(1)	24(1)	23(1)	-3(1)	3(1)	-8(1)
C(5)	16(1)	18(1)	27(1)	-1(1)	1(1)	-6(1)
C(6)	33(2)	34(2)	30(2)	-14(1)	2(1)	-14(1)
C(7)	33(2)	32(2)	28(2)	6(1)	-4(1)	-11(1)
C(8)	32(2)	22(1)	44(2)	-13(1)	5(1)	-7(1)
C(9)	32(2)	44(2)	22(1)	-5(1)	7(1)	-15(1)
C(10)	34(2)	19(1)	44(2)	2(1)	4(1)	-11(1)

Table S14. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $Cp^*Zr(BH_4)_3$

Atom	x	y	z	U(eq)
H(1A)	2210(50)	5580(40)	2130(20)	33(9)
H(1B)	3990(60)	6600(50)	1810(30)	46(10)
H(1C)	1700(60)	7360(50)	1140(30)	44(10)
H(1D)	3800(60)	5080(50)	990(30)	45(10)
H(2A)	780(50)	10130(50)	1440(30)	43(10)
H(2B)	2940(60)	9710(50)	2150(30)	45(10)
H(2C)	610(60)	10670(50)	2680(30)	50(11)
H(2D)	1440(60)	11940(50)	1760(30)	53(11)
H(3A)	3620(50)	7340(40)	3650(20)	27(8)
H(3B)	1200(60)	8340(50)	3980(30)	39(9)
H(3C)	1960(50)	6330(50)	3810(30)	39(9)
H(3D)	3040(60)	6770(50)	4900(30)	64(12)
H(6A)	-3092	6550	739	47
H(6B)	-738	5387	1066	47
H(6C)	-1298	7130	324	47
H(7A)	-4707	11032	658	49
H(7B)	-2402	10145	261	49
H(7C)	-3006	11734	930	49
H(8A)	-5283	12150	3006	50
H(8B)	-3314	12456	2571	50
H(8C)	-3307	11702	3709	50
H(9A)	-3984	8349	4662	49
H(9B)	-2294	9148	4757	49
H(9C)	-1588	7085	4788	49
H(10A)	-2620	4887	3229	49
H(10B)	-661	4812	3834	49
H(10C)	-410	4294	2716	49

Table S15. Bond lengths [Å] and angles [°] for $Cp^*Zr(BH_4)_3$

Zr-B(2)	2.366(3)	B(3)-H(3C)	1.07(4)
Zr-B(1)	2.369(4)	B(3)-H(3D)	1.11(4)
Zr-B(3)	2.378(4)	C(1)-C(2)	1.417(4)
Zr-C(5)	2.489(3)	C(1)-C(5)	1.421(4)
Zr-C(3)	2.497(2)	C(1)-C(6)	1.501(4)
Zr-C(1)	2.498(3)	C(2)-C(3)	1.420(4)
Zr-C(2)	2.498(2)	C(2)-C(7)	1.497(4)
Zr-C(4)	2.500(3)	C(3)-C(4)	1.411(4)
Zr-H(1A)	2.08(3)	C(3)-C(8)	1.500(4)
Zr-H(1B)	2.29(4)	C(4)-C(5)	1.421(4)
Zr-H(1C)	2.02(3)	C(4)-C(9)	1.503(4)
Zr-H(2A)	2.09(4)	C(5)-C(10)	1.498(4)
Zr-H(2B)	2.34(4)	C(6)-H(6A)	0.9800
Zr-H(2C)	2.11(4)	C(6)-H(6B)	0.9800
Zr-H(3A)	2.33(3)	C(6)-H(6C)	0.9800
Zr-H(3B)	2.03(3)	C(7)-H(7A)	0.9800
Zr-H(3C)	2.13(3)	C(7)-H(7B)	0.9800
B(1)-H(1A)	1.16(3)	C(7)-H(7C)	0.9800
B(1)-H(1B)	1.08(4)	C(8)-H(8A)	0.9800
B(1)-H(1C)	1.20(4)	C(8)-H(8B)	0.9800
B(1)-H(1D)	1.06(4)	C(8)-H(8C)	0.9800
B(2)-H(2A)	1.11(4)	C(9)-H(9A)	0.9800
B(2)-H(2B)	1.02(4)	C(9)-H(9B)	0.9800
B(2)-H(2C)	1.12(4)	C(9)-H(9C)	0.9800
B(2)-H(2D)	1.09(4)	C(10)-H(10A)	0.9800
B(3)-H(3A)	1.02(3)	C(10)-H(10B)	0.9800
B(3)-H(3B)	1.05(4)	C(10)-H(10C)	0.9800
B(2)-Zr-B(1)	103.26(13)	B(1)-Zr-C(2)	107.81(11)
B(2)-Zr-B(3)	103.66(15)	B(3)-Zr-C(2)	140.19(12)
B(1)-Zr-B(3)	104.02(15)	C(5)-Zr-C(2)	54.81(8)
B(2)-Zr-C(5)	144.91(11)	C(3)-Zr-C(2)	33.03(8)
B(1)-Zr-C(5)	97.72(11)	C(1)-Zr-C(2)	32.97(8)
B(3)-Zr-C(5)	98.04(12)	B(2)-Zr-C(4)	121.10(11)
B(2)-Zr-C(3)	91.90(11)	B(1)-Zr-C(4)	130.71(11)
B(1)-Zr-C(3)	139.20(11)	B(3)-Zr-C(4)	86.43(11)
B(3)-Zr-C(3)	108.85(12)	C(5)-Zr-C(4)	33.09(8)
C(5)-Zr-C(3)	54.73(8)	C(3)-Zr-C(4)	32.80(8)
B(2)-Zr-C(1)	121.03(12)	C(1)-Zr-C(4)	54.72(8)
B(1)-Zr-C(1)	85.49(11)	C(2)-Zr-C(4)	54.62(8)
B(3)-Zr-C(1)	130.97(12)	B(2)-Zr-H(1A)	132.2(9)
C(5)-Zr-C(1)	33.11(8)	B(1)-Zr-H(1A)	29.3(9)
C(3)-Zr-C(1)	54.69(8)	B(3)-Zr-H(1A)	90.4(9)
B(2)-Zr-C(2)	91.76(12)	C(5)-Zr-H(1A)	74.0(9)

C(3)-Zr-H(1A)	126.7(9)	B(2)-Zr-H(2C)	28.1(10)
C(1)-Zr-H(1A)	74.9(9)	B(1)-Zr-H(2C)	130.8(11)
C(2)-Zr-H(1A)	106.1(9)	B(3)-Zr-H(2C)	89.1(10)
C(4)-Zr-H(1A)	104.9(9)	C(5)-Zr-H(2C)	127.6(10)
B(2)-Zr-H(1B)	86.0(10)	C(3)-Zr-H(2C)	73.8(10)
B(1)-Zr-H(1B)	26.7(10)	C(1)-Zr-H(2C)	120.8(10)
B(3)-Zr-H(1B)	88.7(9)	C(2)-Zr-H(2C)	87.9(10)
C(5)-Zr-H(1B)	122.0(10)	C(4)-Zr-H(2C)	96.8(11)
C(3)-Zr-H(1B)	162.2(9)	H(1A)-Zr-H(2C)	158.2(15)
C(1)-Zr-H(1B)	111.9(10)	H(1B)-Zr-H(2C)	109.9(14)
C(2)-Zr-H(1B)	129.3(9)	H(1C)-Zr-H(2C)	114.5(15)
C(4)-Zr-H(1B)	152.8(10)	H(2A)-Zr-H(2C)	49.8(14)
H(1A)-Zr-H(1B)	48.3(13)	H(2B)-Zr-H(2C)	44.3(13)
B(2)-Zr-H(1C)	87.5(10)	B(2)-Zr-H(3A)	87.6(8)
B(1)-Zr-H(1C)	30.5(10)	B(1)-Zr-H(3A)	89.7(8)
B(3)-Zr-H(1C)	133.7(11)	B(3)-Zr-H(3A)	24.9(8)
C(5)-Zr-H(1C)	97.2(10)	C(5)-Zr-H(3A)	120.7(8)
C(3)-Zr-H(1C)	115.6(10)	C(3)-Zr-H(3A)	129.2(8)
C(1)-Zr-H(1C)	71.4(10)	C(1)-Zr-H(3A)	151.4(8)
C(2)-Zr-H(1C)	82.6(10)	C(2)-Zr-H(3A)	162.2(8)
C(4)-Zr-H(1C)	126.0(10)	C(4)-Zr-H(3A)	111.1(8)
H(1A)-Zr-H(1C)	52.9(13)	H(1A)-Zr-H(3A)	87.3(12)
H(1B)-Zr-H(1C)	46.7(13)	H(1B)-Zr-H(3A)	68.4(12)
B(2)-Zr-H(2A)	28.1(10)	H(1C)-Zr-H(3A)	115.2(13)
B(1)-Zr-H(2A)	90.1(10)	H(2A)-Zr-H(3A)	112.4(13)
B(3)-Zr-H(2A)	131.4(10)	H(2B)-Zr-H(3A)	67.4(12)
C(5)-Zr-H(2A)	126.2(10)	H(2C)-Zr-H(3A)	83.1(12)
C(3)-Zr-H(2A)	85.9(10)	B(2)-Zr-H(3B)	93.4(10)
C(1)-Zr-H(2A)	95.8(10)	B(1)-Zr-H(3B)	130.0(10)
C(2)-Zr-H(2A)	72.1(10)	B(3)-Zr-H(3B)	26.0(10)
C(4)-Zr-H(2A)	118.7(10)	C(5)-Zr-H(3B)	94.3(10)
H(1A)-Zr-H(2A)	118.0(13)	C(3)-Zr-H(3B)	85.7(10)
H(1B)-Zr-H(2A)	84.0(13)	C(1)-Zr-H(3B)	125.0(10)
H(1C)-Zr-H(2A)	65.8(14)	C(2)-Zr-H(3B)	118.6(10)
B(2)-Zr-H(2B)	25.0(9)	C(4)-Zr-H(3B)	71.1(10)
B(1)-Zr-H(2B)	88.1(9)	H(1A)-Zr-H(3B)	114.2(13)
B(3)-Zr-H(2B)	88.5(9)	H(1B)-Zr-H(3B)	112.1(14)
C(5)-Zr-H(2B)	169.9(9)	H(1C)-Zr-H(3B)	158.7(15)
C(3)-Zr-H(2B)	115.8(9)	H(2A)-Zr-H(3B)	120.1(14)
C(1)-Zr-H(2B)	140.3(9)	H(2B)-Zr-H(3B)	88.2(13)
C(2)-Zr-H(2B)	115.5(9)	H(2C)-Zr-H(3B)	70.9(14)
C(4)-Zr-H(2B)	140.9(9)	H(3A)-Zr-H(3B)	43.7(13)
H(1A)-Zr-H(2B)	113.9(13)	B(2)-Zr-H(3C)	130.2(10)
H(1B)-Zr-H(2B)	65.5(13)	B(1)-Zr-H(3C)	91.6(9)
H(1C)-Zr-H(2B)	83.6(13)	B(3)-Zr-H(3C)	26.8(10)
H(2A)-Zr-H(2B)	45.1(13)	C(5)-Zr-H(3C)	76.1(10)

C(3)-Zr-H(3C)	107.1(9)	C(5)-C(1)-Zr	73.13(14)
C(1)-Zr-H(3C)	107.1(10)	C(6)-C(1)-Zr	123.66(18)
C(2)-Zr-H(3C)	128.6(10)	C(1)-C(2)-C(3)	107.9(2)
C(4)-Zr-H(3C)	76.4(9)	C(1)-C(2)-C(7)	126.0(2)
H(1A)-Zr-H(3C)	69.6(13)	C(3)-C(2)-C(7)	125.8(2)
H(1B)-Zr-H(3C)	87.4(13)	C(1)-C(2)-Zr	73.51(14)
H(1C)-Zr-H(3C)	121.3(14)	C(3)-C(2)-Zr	73.46(14)
H(2A)-Zr-H(3C)	157.1(15)	C(7)-C(2)-Zr	124.26(18)
H(2B)-Zr-H(3C)	112.1(13)	C(4)-C(3)-C(2)	108.2(2)
H(2C)-Zr-H(3C)	114.8(14)	C(4)-C(3)-C(8)	125.9(2)
H(3A)-Zr-H(3C)	44.7(12)	C(2)-C(3)-C(8)	125.4(2)
H(3B)-Zr-H(3C)	45.1(13)	C(4)-C(3)-Zr	73.69(14)
Zr-B(1)-H(1A)	61.2(16)	C(2)-C(3)-Zr	73.51(14)
Zr-B(1)-H(1B)	72(2)	C(8)-C(3)-Zr	125.21(19)
H(1A)-B(1)-H(1B)	107(3)	C(3)-C(4)-C(5)	108.1(2)
Zr-B(1)-H(1C)	58.3(17)	C(3)-C(4)-C(9)	126.4(2)
H(1A)-B(1)-H(1C)	101(2)	C(5)-C(4)-C(9)	125.2(2)
H(1B)-B(1)-H(1C)	98(3)	C(3)-C(4)-Zr	73.51(14)
Zr-B(1)-H(1D)	171(2)	C(5)-C(4)-Zr	73.07(14)
H(1A)-B(1)-H(1D)	114(3)	C(9)-C(4)-Zr	123.91(18)
H(1B)-B(1)-H(1D)	117(3)	C(4)-C(5)-C(1)	107.8(2)
H(1C)-B(1)-H(1D)	117(3)	C(4)-C(5)-C(10)	125.8(2)
Zr-B(2)-H(2A)	62.0(18)	C(1)-C(5)-C(10)	126.0(2)
Zr-B(2)-H(2B)	76(2)	C(4)-C(5)-Zr	73.84(15)
H(2A)-B(2)-H(2B)	107(3)	C(1)-C(5)-Zr	73.76(14)
Zr-B(2)-H(2C)	63(2)	C(10)-C(5)-Zr	123.37(18)
H(2A)-B(2)-H(2C)	105(3)	C(1)-C(6)-H(6A)	109.5
H(2B)-B(2)-H(2C)	105(3)	C(1)-C(6)-H(6B)	109.5
Zr-B(2)-H(2D)	168(2)	H(6A)-C(6)-H(6B)	109.5
H(2A)-B(2)-H(2D)	115(3)	C(1)-C(6)-H(6C)	109.5
H(2B)-B(2)-H(2D)	115(3)	H(6A)-C(6)-H(6C)	109.5
H(2C)-B(2)-H(2D)	109(3)	H(6B)-C(6)-H(6C)	109.5
Zr-B(3)-H(3A)	74.7(18)	C(2)-C(7)-H(7A)	109.5
Zr-B(3)-H(3B)	58.0(19)	C(2)-C(7)-H(7B)	109.5
H(3A)-B(3)-H(3B)	106(3)	H(7A)-C(7)-H(7B)	109.5
Zr-B(3)-H(3C)	63.6(18)	C(2)-C(7)-H(7C)	109.5
H(3A)-B(3)-H(3C)	109(3)	H(7A)-C(7)-H(7C)	109.5
H(3B)-B(3)-H(3C)	97(3)	H(7B)-C(7)-H(7C)	109.5
Zr-B(3)-H(3D)	170(2)	C(3)-C(8)-H(8A)	109.5
H(3A)-B(3)-H(3D)	115(3)	C(3)-C(8)-H(8B)	109.5
H(3B)-B(3)-H(3D)	116(3)	H(8A)-C(8)-H(8B)	109.5
H(3C)-B(3)-H(3D)	112(3)	C(3)-C(8)-H(8C)	109.5
C(2)-C(1)-C(5)	107.9(2)	H(8A)-C(8)-H(8C)	109.5
C(2)-C(1)-C(6)	126.3(2)	H(8B)-C(8)-H(8C)	109.5
C(5)-C(1)-C(6)	125.5(2)	C(4)-C(9)-H(9A)	109.5
C(2)-C(1)-Zr	73.52(14)	C(4)-C(9)-H(9B)	109.5

H(9A)-C(9)-H(9B)	109.5	C(5)-C(10)-H(10B)	109.5
C(4)-C(9)-H(9C)	109.5	H(10A)-C(10)-H(10B)	109.5
H(9A)-C(9)-H(9C)	109.5	C(5)-C(10)-H(10C)	109.5
H(9B)-C(9)-H(9C)	109.5	H(10A)-C(10)-H(10C)	109.5
C(5)-C(10)-H(10A)	109.5	H(10B)-C(10)-H(10C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S16. Crystal data and structure refinement for $[(\mu_3\text{-O})(\mu_2\text{-OC}_2\text{H}_5)_3\{(\text{Cp*Zr}(\text{OC}_2\text{H}_5))_2(\text{BCH}_3)\}][\text{HB}(\text{C}_6\text{F}_5)_3]$.

Empirical formula	$C_{49}H_{59}B_2F_{15}O_6Zr_2$	
Formula weight	1233.02	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 10.5767(5) Å	α = 90°.
	b = 16.4862(8) Å	β = 93.389(1)°.
	c = 32.1655(17) Å	γ = 90°.
Volume	5598.9(5) $Å^3$	
Z	4	
Density (calculated)	1.463 Mg/m^3	
Absorption coefficient	0.466 mm^{-1}	
F(000)	2504	
Crystal size	0.50 x 0.32 x 0.20 mm^3	
Theta range for data collection	1.27 to 27.50°.	
Index ranges	-13<=h<=12, -21<=k<=17, -41<=l<=41	
Reflections collected	49575	
Independent reflections	12748 [R(int) = 0.0591]	
Completeness to theta = 27.50°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9126 and 0.8005	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12748 / 4 / 689	
Goodness-of-fit on F^2	1.089	
Final R indices [I>2sigma(I)]	R1 = 0.0695, wR2 = 0.1928	
R indices (all data)	R1 = 0.0997, wR2 = 0.2137	
Largest diff. peak and hole	2.181 and -0.568 $e.Å^{-3}$	

Table S17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for [(μ_3-O)(μ_2-OC_2H_5)$_3${(Cp*Zr(OC_2H_5))$_2$(BCH_3)}][$HB(C_6F_5)_3$]. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Zr(1)	1625(1)	7071(1)	1901(1)	29(1)
Zr(2)	577(1)	6907(1)	895(1)	34(1)
O(1)	2245(3)	7128(2)	1278(1)	34(1)
O(2)	335(4)	6366(2)	1491(1)	39(1)
O(3)	239(3)	7487(2)	2190(1)	43(1)
O(4)	2014(4)	8273(2)	1659(1)	41(1)
O(5)	1308(4)	8140(2)	904(1)	49(1)
O(6)	-1105(4)	7338(3)	871(1)	57(1)
B(1)	2395(7)	8002(4)	1228(2)	43(2)
C(1)	-947(7)	6091(5)	1580(2)	64(2)
C(2)	-972(8)	5445(6)	1880(3)	96(3)
C(3)	-661(6)	7786(4)	2466(2)	57(2)
C(4)	-1788(7)	8129(5)	2240(3)	76(2)
C(5)	2284(6)	9075(4)	1812(2)	58(2)
C(6)	1290(30)	9380(20)	2075(9)	88(11)
C(6')	1090(20)	9500(20)	1890(9)	74(8)
C(7)	839(8)	8928(4)	796(2)	70(2)
C(8)	575(14)	9018(7)	352(3)	149(6)
C(9)	-2362(8)	7638(6)	816(3)	112(3)
C(10)	-2259(9)	8329(6)	515(3)	97(3)
C(11)	3698(6)	8361(5)	1098(2)	63(2)
C(12)	2266(5)	6227(3)	2523(2)	39(1)
C(13)	2831(5)	6995(3)	2595(2)	34(1)
C(14)	3766(5)	7104(3)	2303(2)	34(1)
C(15)	3771(5)	6407(4)	2048(2)	41(1)
C(16)	2848(6)	5861(3)	2181(2)	43(1)
C(17)	1299(6)	5836(4)	2792(2)	59(2)
C(18)	2535(6)	7550(4)	2944(2)	47(1)
C(19)	4687(5)	7796(4)	2296(2)	49(2)
C(20)	4690(6)	6245(5)	1721(2)	59(2)
C(21)	2618(8)	5025(4)	2013(2)	67(2)
C(22)	1960(6)	5999(4)	487(2)	48(2)
C(23)	1529(6)	6600(4)	214(2)	48(1)
C(24)	205(6)	6525(4)	146(2)	52(2)
C(25)	-178(7)	5854(5)	383(2)	67(2)
C(26)	945(9)	5534(4)	598(2)	63(2)
C(27)	3351(8)	5859(6)	620(2)	86(3)
C(28)	2348(9)	7199(5)	-7(3)	82(3)
C(29)	-661(10)	7023(6)	-142(2)	97(3)
C(30)	-1504(9)	5517(7)	379(3)	124(5)

C(31)	1001(13)	4776(5)	866(2)	121(5)
B(2)	3289(6)	2407(4)	1547(2)	40(1)
C(32)	4082(5)	1568(4)	1659(2)	45(1)
C(33)	3876(6)	1153(4)	2022(2)	49(2)
C(34)	4528(6)	464(4)	2151(2)	54(2)
C(35)	5434(6)	166(4)	1910(2)	58(2)
C(36)	5682(6)	543(4)	1547(2)	59(2)
C(37)	5011(6)	1233(4)	1428(2)	54(2)
C(38)	1814(5)	2230(3)	1380(2)	38(1)
C(39)	1333(6)	1519(4)	1205(2)	45(1)
C(40)	78(6)	1410(4)	1072(2)	49(1)
C(41)	-761(5)	2039(4)	1109(2)	44(1)
C(42)	-334(6)	2757(3)	1274(2)	41(1)
C(43)	916(5)	2828(3)	1404(2)	39(1)
C(44)	4002(5)	2995(3)	1223(2)	41(1)
C(45)	3864(6)	2934(4)	797(2)	50(2)
C(46)	4476(6)	3420(5)	526(2)	58(2)
C(47)	5270(6)	4013(4)	680(2)	56(2)
C(48)	5449(6)	4115(4)	1102(2)	55(2)
C(49)	4810(5)	3616(4)	1364(2)	43(1)
F(2)	2972(4)	1412(2)	2273(1)	59(1)
F(3)	4248(4)	83(2)	2505(1)	70(1)
F(4)	6081(4)	-508(2)	2032(2)	83(1)
F(5)	6571(4)	240(3)	1308(2)	87(1)
F(6)	5304(4)	1564(3)	1064(1)	73(1)
F(7)	2105(3)	875(2)	1149(1)	65(1)
F(8)	-321(4)	696(2)	904(2)	77(1)
F(9)	-1989(3)	1943(3)	982(1)	65(1)
F(10)	-1148(3)	3381(2)	1306(1)	59(1)
F(11)	1259(3)	3551(2)	1578(1)	50(1)
F(12)	3132(4)	2342(3)	621(1)	63(1)
F(13)	4296(4)	3322(3)	108(1)	81(1)
F(14)	5877(4)	4499(3)	414(2)	82(1)
F(15)	6240(4)	4694(3)	1255(2)	81(1)
F(16)	5029(3)	3753(2)	1775(1)	56(1)

Table S18. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[(\mu_3\text{-}O)(\mu_2\text{-}OC_2H_5)_3\{(Cp^*Zr(OC_2H_5))_2(BCH_3)\}][HB(C_6F_5)_3]$. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... \quad + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zr(1)	31(1)	29(1)	27(1)	-4(1)	1(1)	0(1)
Zr(2)	42(1)	34(1)	26(1)	-4(1)	1(1)	-3(1)
O(1)	35(2)	35(2)	32(2)	-2(1)	4(1)	-1(2)
O(2)	50(2)	36(2)	31(2)	-3(2)	3(2)	-15(2)
O(3)	37(2)	47(2)	44(2)	-5(2)	8(2)	3(2)
O(4)	48(2)	30(2)	47(2)	-4(2)	-2(2)	-4(2)
O(5)	55(3)	37(2)	53(2)	7(2)	-12(2)	-2(2)
O(6)	42(2)	75(3)	54(3)	-7(2)	-4(2)	4(2)
B(1)	45(4)	45(4)	40(3)	5(3)	1(3)	-4(3)
C(1)	63(4)	72(5)	56(4)	-6(3)	4(3)	-26(4)
C(2)	78(6)	115(8)	95(6)	31(6)	12(5)	-44(5)
C(3)	51(4)	71(5)	52(4)	-6(3)	21(3)	4(3)
C(4)	49(4)	76(5)	104(6)	-9(5)	17(4)	11(4)
C(5)	60(4)	37(3)	74(4)	-12(3)	-4(3)	-8(3)
C(6)	86(15)	58(17)	130(30)	-34(17)	54(17)	-24(11)
C(6')	90(15)	31(10)	110(20)	-25(13)	54(15)	-7(8)
C(7)	100(6)	44(4)	65(4)	11(3)	-10(4)	14(4)
C(8)	277(17)	98(8)	70(6)	19(6)	-12(8)	81(10)
C(10)	78(6)	103(7)	109(7)	0(6)	-11(5)	18(5)
C(11)	62(4)	72(5)	57(4)	15(3)	8(3)	-23(4)
C(12)	43(3)	38(3)	35(3)	7(2)	-3(2)	-3(2)
C(13)	35(3)	38(3)	28(2)	1(2)	-1(2)	0(2)
C(14)	29(3)	39(3)	33(2)	2(2)	-2(2)	-2(2)
C(15)	42(3)	45(3)	35(3)	-2(2)	1(2)	11(3)
C(16)	50(3)	32(3)	46(3)	0(2)	-8(3)	7(3)
C(17)	46(4)	68(5)	60(4)	23(3)	-7(3)	-17(3)
C(18)	40(3)	62(4)	38(3)	-12(3)	0(2)	1(3)
C(19)	34(3)	63(4)	49(3)	11(3)	-7(3)	-11(3)
C(20)	52(4)	72(5)	53(4)	-8(3)	7(3)	23(3)
C(21)	82(5)	35(3)	82(5)	-12(3)	-18(4)	7(3)
C(22)	68(4)	43(3)	34(3)	-7(2)	0(3)	18(3)
C(23)	63(4)	46(3)	36(3)	-2(2)	12(3)	4(3)
C(24)	61(4)	66(4)	27(3)	-9(3)	1(3)	9(3)
C(25)	80(5)	76(5)	45(3)	-37(3)	17(3)	-34(4)
C(26)	127(7)	39(3)	26(3)	-10(2)	12(3)	-6(4)
C(27)	89(6)	111(7)	57(4)	-24(4)	-11(4)	56(5)
C(28)	99(6)	82(6)	68(5)	5(4)	43(5)	-3(5)
C(29)	119(8)	131(9)	39(4)	-15(4)	-16(4)	56(6)
C(30)	106(7)	179(11)	91(6)	-91(7)	42(5)	-81(7)
C(31)	279(15)	37(4)	49(4)	0(3)	35(6)	-9(6)

B(2)	45(4)	38(3)	36(3)	3(3)	-7(3)	2(3)
C(32)	40(3)	38(3)	55(3)	2(3)	-8(3)	0(3)
C(33)	50(4)	37(3)	59(4)	1(3)	-16(3)	-8(3)
C(34)	59(4)	30(3)	71(4)	5(3)	-20(3)	-15(3)
C(35)	46(4)	26(3)	98(5)	6(3)	-27(4)	-1(3)
C(36)	45(4)	41(4)	90(5)	-2(3)	-6(3)	7(3)
C(37)	50(4)	45(4)	67(4)	9(3)	-5(3)	2(3)
C(38)	37(3)	37(3)	39(3)	0(2)	1(2)	-2(2)
C(39)	43(3)	41(3)	50(3)	-2(3)	3(3)	3(3)
C(40)	50(4)	45(3)	51(3)	-4(3)	1(3)	-13(3)
C(41)	32(3)	59(4)	40(3)	13(3)	0(2)	0(3)
C(42)	49(3)	40(3)	35(3)	14(2)	11(2)	10(3)
C(43)	44(3)	32(3)	40(3)	6(2)	1(2)	-1(2)
C(44)	35(3)	39(3)	50(3)	6(2)	-5(2)	6(2)
C(45)	37(3)	57(4)	55(4)	7(3)	-3(3)	0(3)
C(46)	41(4)	78(5)	54(4)	17(3)	8(3)	9(3)
C(47)	49(4)	47(4)	73(4)	15(3)	26(3)	5(3)
C(48)	37(3)	38(3)	89(5)	-8(3)	11(3)	4(3)
C(49)	35(3)	42(3)	51(3)	-3(3)	0(2)	14(2)
F(2)	71(3)	50(2)	56(2)	9(2)	3(2)	-3(2)
F(3)	90(3)	43(2)	73(3)	17(2)	-22(2)	-12(2)
F(4)	70(3)	43(2)	131(4)	16(2)	-33(3)	6(2)
F(5)	65(3)	69(3)	126(4)	0(3)	9(3)	22(2)
F(6)	71(3)	70(3)	81(3)	11(2)	20(2)	19(2)
F(7)	54(2)	46(2)	94(3)	-21(2)	-8(2)	13(2)
F(8)	63(3)	55(2)	109(3)	-23(2)	-16(2)	-10(2)
F(9)	38(2)	80(3)	76(3)	15(2)	-6(2)	-8(2)
F(10)	50(2)	54(2)	73(2)	17(2)	14(2)	20(2)
F(11)	63(2)	29(2)	57(2)	2(1)	0(2)	2(2)
F(12)	55(2)	87(3)	48(2)	-6(2)	-5(2)	-21(2)
F(13)	74(3)	114(4)	55(2)	15(2)	10(2)	-1(3)
F(14)	85(3)	69(3)	96(3)	21(2)	41(3)	-4(2)
F(15)	63(3)	55(3)	126(4)	-27(3)	29(2)	-18(2)
F(16)	49(2)	54(2)	65(2)	-15(2)	-3(2)	0(2)

Table S19. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for [(μ_3-O)(μ_2-OC_2H_5)$_3${(Cp*Zr(OC_2H_5))$_2$(BCH_3)}][$HB(C_6F_5)_3$].

	x	y	z	U(eq)
H(1A)	-1425	6558	1684	76
H(1B)	-1387	5907	1316	76
H(2A)	-511	4976	1779	144
H(2B)	-1852	5291	1919	144
H(2C)	-570	5628	2146	144
H(3A)	-256	8210	2647	69
H(3B)	-924	7338	2647	69
H(4A)	-1536	8587	2069	114
H(4B)	-2388	8316	2440	114
H(4C)	-2191	7712	2060	114
H(5A)	2363	9447	1574	69
H(5B)	3104	9071	1977	69
H(5'A)	2752	9380	1606	69
H(5'B)	2823	9042	2074	69
H(6A)	1503	9925	2173	133
H(6B)	1216	9016	2314	133
H(6C)	474	9391	1911	133
H(6'A)	1287	10050	1994	111
H(6'B)	636	9203	2098	111
H(6'C)	563	9539	1630	111
H(7A)	1472	9339	893	84
H(7B)	54	9029	941	84
H(8A)	1372	9007	211	223
H(8B)	145	9536	295	223
H(8C)	31	8572	248	223
H(9A)	-2670	7830	1083	134
H(9B)	-2944	7214	699	134
H(10A)	-3105	8543	439	146
H(10B)	-1872	8135	264	146
H(10C)	-1732	8759	645	146
H(11A)	4356	8250	1318	95
H(11B)	3615	8949	1058	95
H(11C)	3930	8108	838	95
H(17A)	1671	5769	3076	88
H(17B)	1055	5305	2677	88
H(17C)	549	6184	2797	88
H(18A)	3057	7403	3194	70
H(18B)	1638	7499	2999	70
H(18C)	2716	8111	2866	70
H(19A)	5504	7627	2426	74
H(19B)	4359	8257	2449	74

H(19C)	4796	7957	2006	74
H(20A)	4451	5744	1573	89
H(20B)	5544	6186	1854	89
H(20C)	4677	6698	1524	89
H(21A)	2555	5044	1708	101
H(21B)	1826	4813	2113	101
H(21C)	3321	4671	2107	101
H(27A)	3747	5532	409	129
H(27B)	3414	5573	888	129
H(27C)	3786	6383	649	129
H(28A)	3075	7355	180	122
H(28B)	1848	7683	-83	122
H(28C)	2650	6948	-258	122
H(29A)	-342	7580	-152	146
H(29B)	-1515	7025	-39	146
H(29C)	-689	6788	-422	146
H(30A)	-1646	5151	141	186
H(30B)	-2115	5964	357	186
H(30C)	-1611	5217	638	186
H(31A)	1189	4305	694	181
H(31B)	183	4695	988	181
H(31C)	1667	4836	1089	181
H(2)	3140(50)	2690(40)	1833(19)	48

Table S20. Bond lengths [Å] and angles [°] for $[(\mu_3\text{-O})(\mu_2\text{-OC}_2\text{H}_5)_3\{(\text{Cp*Zr(OC}_2\text{H}_5))_2(\text{BCH}_3)\}][\text{HB}(\text{C}_6\text{F}_5)_3]$.

Zr(1)-O(3)	1.908(4)	C(15)-C(16)	1.413(8)
Zr(1)-O(1)	2.147(3)	C(15)-C(20)	1.497(8)
Zr(1)-O(2)	2.177(3)	C(16)-C(21)	1.495(8)
Zr(1)-O(4)	2.178(4)	C(22)-C(23)	1.383(8)
Zr(1)-C(12)	2.496(5)	C(22)-C(26)	1.384(10)
Zr(1)-C(13)	2.506(5)	C(22)-C(27)	1.525(10)
Zr(1)-C(16)	2.514(5)	C(23)-C(24)	1.410(9)
Zr(1)-C(15)	2.539(5)	C(23)-C(28)	1.518(9)
Zr(1)-C(14)	2.541(5)	C(24)-C(25)	1.418(10)
Zr(1)-B(1)	2.813(6)	C(24)-C(29)	1.506(10)
Zr(1)-Zr(2)	3.3680(7)	C(25)-C(26)	1.438(11)
Zr(2)-O(6)	1.914(4)	C(25)-C(30)	1.507(10)
Zr(2)-O(1)	2.121(3)	C(26)-C(31)	1.517(10)
Zr(2)-O(2)	2.144(3)	B(2)-C(44)	1.638(9)
Zr(2)-O(5)	2.174(4)	B(2)-C(38)	1.645(8)
Zr(2)-C(25)	2.493(6)	B(2)-C(32)	1.647(9)
Zr(2)-C(26)	2.497(6)	C(32)-C(37)	1.380(9)
Zr(2)-C(24)	2.501(5)	C(32)-C(33)	1.383(8)
Zr(2)-C(22)	2.516(6)	C(33)-F(2)	1.354(7)
Zr(2)-C(23)	2.517(5)	C(33)-C(34)	1.380(9)
Zr(2)-B(1)	2.803(7)	C(34)-F(3)	1.348(8)
O(1)-B(1)	1.460(7)	C(34)-C(35)	1.359(10)
O(2)-C(1)	1.474(7)	C(35)-F(4)	1.351(7)
O(3)-C(3)	1.428(7)	C(35)-C(36)	1.361(10)
O(4)-C(5)	1.433(7)	C(36)-F(5)	1.346(8)
O(4)-B(1)	1.532(8)	C(36)-C(37)	1.383(9)
O(5)-C(7)	1.427(7)	C(37)-F(6)	1.344(8)
O(5)-B(1)	1.523(8)	C(38)-C(43)	1.374(8)
O(6)-C(9)	1.419(8)	C(38)-C(39)	1.385(8)
B(1)-C(11)	1.578(9)	C(39)-F(7)	1.359(7)
C(1)-C(2)	1.438(10)	C(39)-C(40)	1.382(8)
C(3)-C(4)	1.472(10)	C(40)-F(8)	1.350(7)
C(5)-C(6)	1.477(10)	C(40)-C(41)	1.375(9)
C(5)-C(6')	1.479(10)	C(41)-F(9)	1.348(6)
C(7)-C(8)	1.449(11)	C(41)-C(42)	1.363(8)
C(9)-C(10)	1.503(8)	C(42)-F(10)	1.349(6)
C(12)-C(13)	1.414(7)	C(42)-C(43)	1.367(8)
C(12)-C(16)	1.426(8)	C(43)-F(11)	1.358(6)
C(12)-C(17)	1.522(8)	C(44)-C(45)	1.373(8)
C(13)-C(14)	1.415(7)	C(44)-C(49)	1.392(8)
C(13)-C(18)	1.495(7)	C(45)-F(12)	1.350(7)
C(14)-C(15)	1.412(7)	C(45)-C(46)	1.373(9)
C(14)-C(19)	1.501(7)	C(46)-F(13)	1.357(8)

C(46)-C(47)	1.363(10)	C(48)-F(15)	1.343(7)
C(47)-F(14)	1.362(7)	C(48)-C(49)	1.382(9)
C(47)-C(48)	1.370(10)	C(49)-F(16)	1.347(7)

O(3)-Zr(1)-O(1)	136.34(15)	C(16)-Zr(1)-B(1)	122.8(2)
O(3)-Zr(1)-O(2)	90.82(15)	C(15)-Zr(1)-B(1)	94.69(19)
O(1)-Zr(1)-O(2)	70.91(13)	C(14)-Zr(1)-B(1)	95.14(18)
O(3)-Zr(1)-O(4)	90.78(16)	O(3)-Zr(1)-Zr(2)	106.08(12)
O(1)-Zr(1)-O(4)	63.35(13)	O(1)-Zr(1)-Zr(2)	37.64(9)
O(2)-Zr(1)-O(4)	113.20(13)	O(2)-Zr(1)-Zr(2)	38.43(9)
O(3)-Zr(1)-C(12)	89.50(18)	O(4)-Zr(1)-Zr(2)	77.72(10)
O(1)-Zr(1)-C(12)	133.51(16)	C(12)-Zr(1)-Zr(2)	141.53(13)
O(2)-Zr(1)-C(12)	108.55(16)	C(13)-Zr(1)-Zr(2)	166.45(12)
O(4)-Zr(1)-C(12)	138.24(16)	C(16)-Zr(1)-Zr(2)	114.38(13)
O(3)-Zr(1)-C(13)	87.16(16)	C(15)-Zr(1)-Zr(2)	112.55(12)
O(1)-Zr(1)-C(13)	131.73(15)	C(14)-Zr(1)-Zr(2)	136.30(12)
O(2)-Zr(1)-C(13)	141.29(15)	B(1)-Zr(1)-Zr(2)	53.02(14)
O(4)-Zr(1)-C(13)	105.48(15)	O(6)-Zr(2)-O(1)	134.39(16)
C(12)-Zr(1)-C(13)	32.84(17)	O(6)-Zr(2)-O(2)	91.83(17)
O(3)-Zr(1)-C(16)	120.35(18)	O(1)-Zr(2)-O(2)	72.05(13)
O(1)-Zr(1)-C(16)	100.93(16)	O(6)-Zr(2)-O(5)	89.00(19)
O(2)-Zr(1)-C(16)	94.79(16)	O(1)-Zr(2)-O(5)	63.23(14)
O(4)-Zr(1)-C(16)	138.25(17)	O(2)-Zr(2)-O(5)	116.06(14)
C(12)-Zr(1)-C(16)	33.06(18)	O(6)-Zr(2)-C(25)	88.3(2)
C(13)-Zr(1)-C(16)	54.45(17)	O(1)-Zr(2)-C(25)	136.6(2)
O(3)-Zr(1)-C(15)	140.26(17)	O(2)-Zr(2)-C(25)	104.5(2)
O(1)-Zr(1)-C(15)	82.73(15)	O(5)-Zr(2)-C(25)	139.4(2)
O(2)-Zr(1)-C(15)	113.80(17)	O(6)-Zr(2)-C(26)	119.1(2)
O(4)-Zr(1)-C(15)	105.86(17)	O(1)-Zr(2)-C(26)	103.6(2)
C(12)-Zr(1)-C(15)	54.09(18)	O(2)-Zr(2)-C(26)	89.70(17)
C(13)-Zr(1)-C(15)	53.92(17)	O(5)-Zr(2)-C(26)	142.1(2)
C(16)-Zr(1)-C(15)	32.47(19)	C(25)-Zr(2)-C(26)	33.5(3)
O(3)-Zr(1)-C(14)	115.63(16)	O(6)-Zr(2)-C(24)	87.7(2)
O(1)-Zr(1)-C(14)	99.30(15)	O(1)-Zr(2)-C(24)	132.91(18)
O(2)-Zr(1)-C(14)	145.83(16)	O(2)-Zr(2)-C(24)	137.49(19)
O(4)-Zr(1)-C(14)	88.91(15)	O(5)-Zr(2)-C(24)	106.4(2)
C(12)-Zr(1)-C(14)	54.06(17)	C(25)-Zr(2)-C(24)	33.0(2)
C(13)-Zr(1)-C(14)	32.55(16)	C(26)-Zr(2)-C(24)	54.7(2)
C(16)-Zr(1)-C(14)	53.93(18)	O(6)-Zr(2)-C(22)	140.08(19)
C(15)-Zr(1)-C(14)	32.29(17)	O(1)-Zr(2)-C(22)	85.18(17)
O(3)-Zr(1)-B(1)	116.33(19)	O(2)-Zr(2)-C(22)	108.85(17)
O(1)-Zr(1)-B(1)	30.65(16)	O(5)-Zr(2)-C(22)	110.2(2)
O(2)-Zr(1)-B(1)	91.44(16)	C(25)-Zr(2)-C(22)	54.1(2)
O(4)-Zr(1)-B(1)	32.70(17)	C(26)-Zr(2)-C(22)	32.0(2)
C(12)-Zr(1)-B(1)	147.46(19)	C(24)-Zr(2)-C(22)	53.9(2)
C(13)-Zr(1)-B(1)	123.82(18)	O(6)-Zr(2)-C(23)	117.2(2)

O(1)-Zr(2)-C(23)	100.28(18)	O(1)-B(1)-Zr(2)	47.9(2)
O(2)-Zr(2)-C(23)	140.36(18)	O(5)-B(1)-Zr(2)	50.3(2)
O(5)-Zr(2)-C(23)	92.21(19)	O(4)-B(1)-Zr(2)	108.8(4)
C(25)-Zr(2)-C(23)	54.1(2)	C(11)-B(1)-Zr(2)	136.9(5)
C(26)-Zr(2)-C(23)	53.5(2)	O(1)-B(1)-Zr(1)	48.6(2)
C(24)-Zr(2)-C(23)	32.6(2)	O(5)-B(1)-Zr(1)	111.6(4)
C(22)-Zr(2)-C(23)	31.90(19)	O(4)-B(1)-Zr(1)	50.2(2)
O(6)-Zr(2)-B(1)	113.1(2)	C(11)-B(1)-Zr(1)	134.9(4)
O(1)-Zr(2)-B(1)	30.69(16)	Zr(2)-B(1)-Zr(1)	73.69(16)
O(2)-Zr(2)-B(1)	92.41(16)	C(2)-C(1)-O(2)	114.2(7)
O(5)-Zr(2)-B(1)	32.64(17)	O(3)-C(3)-C(4)	112.0(6)
C(25)-Zr(2)-B(1)	152.5(2)	O(4)-C(5)-C(6)	111.9(18)
C(26)-Zr(2)-B(1)	127.7(3)	O(4)-C(5)-C(6')	110.1(16)
C(24)-Zr(2)-B(1)	126.6(2)	C(6)-C(5)-C(6')	25.4(19)
C(22)-Zr(2)-B(1)	100.1(2)	O(5)-C(7)-C(8)	112.1(7)
C(23)-Zr(2)-B(1)	99.3(2)	O(6)-C(9)-C(10)	104.0(7)
O(6)-Zr(2)-Zr(1)	105.23(13)	C(13)-C(12)-C(16)	108.0(5)
O(1)-Zr(2)-Zr(1)	38.18(9)	C(13)-C(12)-C(17)	125.3(5)
O(2)-Zr(2)-Zr(1)	39.13(9)	C(16)-C(12)-C(17)	126.5(5)
O(5)-Zr(2)-Zr(1)	79.43(11)	C(13)-C(12)-Zr(1)	74.0(3)
C(25)-Zr(2)-Zr(1)	139.9(2)	C(16)-C(12)-Zr(1)	74.2(3)
C(26)-Zr(2)-Zr(1)	113.01(16)	C(17)-C(12)-Zr(1)	122.2(4)
C(24)-Zr(2)-Zr(1)	166.06(15)	C(12)-C(13)-C(14)	108.1(5)
C(22)-Zr(2)-Zr(1)	112.38(13)	C(12)-C(13)-C(18)	124.5(5)
C(23)-Zr(2)-Zr(1)	136.63(15)	C(14)-C(13)-C(18)	127.3(5)
B(1)-Zr(2)-Zr(1)	53.29(13)	C(12)-C(13)-Zr(1)	73.2(3)
B(1)-O(1)-Zr(2)	101.4(3)	C(14)-C(13)-Zr(1)	75.1(3)
B(1)-O(1)-Zr(1)	100.8(3)	C(18)-C(13)-Zr(1)	121.3(4)
Zr(2)-O(1)-Zr(1)	104.18(15)	C(15)-C(14)-C(13)	108.0(5)
C(1)-O(2)-Zr(2)	117.4(3)	C(15)-C(14)-C(19)	125.8(5)
C(1)-O(2)-Zr(1)	126.7(3)	C(13)-C(14)-C(19)	125.9(5)
Zr(2)-O(2)-Zr(1)	102.44(14)	C(15)-C(14)-Zr(1)	73.8(3)
C(3)-O(3)-Zr(1)	170.5(4)	C(13)-C(14)-Zr(1)	72.4(3)
C(5)-O(4)-B(1)	121.5(5)	C(19)-C(14)-Zr(1)	124.6(4)
C(5)-O(4)-Zr(1)	138.9(4)	C(14)-C(15)-C(16)	108.5(5)
B(1)-O(4)-Zr(1)	97.1(3)	C(14)-C(15)-C(20)	125.3(6)
C(7)-O(5)-B(1)	122.6(5)	C(16)-C(15)-C(20)	126.0(5)
C(7)-O(5)-Zr(2)	136.9(4)	C(14)-C(15)-Zr(1)	73.9(3)
B(1)-O(5)-Zr(2)	97.1(3)	C(16)-C(15)-Zr(1)	72.8(3)
C(9)-O(6)-Zr(2)	175.1(6)	C(20)-C(15)-Zr(1)	123.9(4)
O(1)-B(1)-O(5)	98.0(4)	C(15)-C(16)-C(12)	107.5(5)
O(1)-B(1)-O(4)	98.8(4)	C(15)-C(16)-C(21)	125.3(6)
O(5)-B(1)-O(4)	110.3(5)	C(12)-C(16)-C(21)	126.9(6)
O(1)-B(1)-C(11)	120.2(6)	C(15)-C(16)-Zr(1)	74.7(3)
O(5)-B(1)-C(11)	113.4(5)	C(12)-C(16)-Zr(1)	72.8(3)
O(4)-B(1)-C(11)	114.2(5)	C(21)-C(16)-Zr(1)	122.2(4)

C(23)-C(22)-C(26)	109.2(6)	C(34)-C(35)-C(36)	120.1(6)
C(23)-C(22)-C(27)	124.3(7)	F(5)-C(36)-C(35)	119.8(6)
C(26)-C(22)-C(27)	126.5(7)	F(5)-C(36)-C(37)	120.7(7)
C(23)-C(22)-Zr(2)	74.1(3)	C(35)-C(36)-C(37)	119.4(7)
C(26)-C(22)-Zr(2)	73.2(4)	F(6)-C(37)-C(32)	120.9(6)
C(27)-C(22)-Zr(2)	121.6(4)	F(6)-C(37)-C(36)	115.7(6)
C(22)-C(23)-C(24)	108.9(6)	C(32)-C(37)-C(36)	123.4(6)
C(22)-C(23)-C(28)	126.0(7)	C(43)-C(38)-C(39)	113.0(5)
C(24)-C(23)-C(28)	125.0(6)	C(43)-C(38)-B(2)	120.0(5)
C(22)-C(23)-Zr(2)	74.0(3)	C(39)-C(38)-B(2)	126.9(5)
C(24)-C(23)-Zr(2)	73.1(3)	F(7)-C(39)-C(40)	115.5(5)
C(28)-C(23)-Zr(2)	123.0(5)	F(7)-C(39)-C(38)	120.4(5)
C(23)-C(24)-C(25)	107.3(6)	C(40)-C(39)-C(38)	124.1(5)
C(23)-C(24)-C(29)	127.6(7)	F(8)-C(40)-C(41)	120.2(5)
C(25)-C(24)-C(29)	125.0(7)	F(8)-C(40)-C(39)	120.6(6)
C(23)-C(24)-Zr(2)	74.3(3)	C(41)-C(40)-C(39)	119.2(6)
C(25)-C(24)-Zr(2)	73.2(3)	F(9)-C(41)-C(42)	120.7(5)
C(29)-C(24)-Zr(2)	120.7(4)	F(9)-C(41)-C(40)	120.0(6)
C(24)-C(25)-C(26)	106.9(6)	C(42)-C(41)-C(40)	119.2(5)
C(24)-C(25)-C(30)	125.3(9)	F(10)-C(42)-C(41)	119.6(5)
C(26)-C(25)-C(30)	127.6(9)	F(10)-C(42)-C(43)	121.4(5)
C(24)-C(25)-Zr(2)	73.8(3)	C(41)-C(42)-C(43)	119.0(5)
C(26)-C(25)-Zr(2)	73.4(3)	F(11)-C(43)-C(42)	115.6(5)
C(30)-C(25)-Zr(2)	121.6(5)	F(11)-C(43)-C(38)	118.9(5)
C(22)-C(26)-C(25)	107.7(6)	C(42)-C(43)-C(38)	125.5(5)
C(22)-C(26)-C(31)	126.8(9)	C(45)-C(44)-C(49)	113.9(5)
C(25)-C(26)-C(31)	125.3(9)	C(45)-C(44)-B(2)	124.4(5)
C(22)-C(26)-Zr(2)	74.7(3)	C(49)-C(44)-B(2)	121.7(5)
C(25)-C(26)-Zr(2)	73.1(4)	F(12)-C(45)-C(44)	119.8(5)
C(31)-C(26)-Zr(2)	122.1(4)	F(12)-C(45)-C(46)	115.8(6)
C(44)-B(2)-C(38)	111.2(4)	C(44)-C(45)-C(46)	124.4(6)
C(44)-B(2)-C(32)	112.8(5)	F(13)-C(46)-C(47)	119.5(6)
C(38)-B(2)-C(32)	112.6(5)	F(13)-C(46)-C(45)	121.1(7)
C(37)-C(32)-C(33)	114.2(6)	C(47)-C(46)-C(45)	119.4(6)
C(37)-C(32)-B(2)	126.0(5)	F(14)-C(47)-C(46)	119.8(7)
C(33)-C(32)-B(2)	119.7(6)	F(14)-C(47)-C(48)	120.6(6)
F(2)-C(33)-C(34)	116.1(6)	C(46)-C(47)-C(48)	119.6(6)
F(2)-C(33)-C(32)	119.9(5)	F(15)-C(48)-C(47)	119.8(6)
C(34)-C(33)-C(32)	123.9(7)	F(15)-C(48)-C(49)	121.1(7)
F(3)-C(34)-C(35)	120.7(6)	C(47)-C(48)-C(49)	119.1(6)
F(3)-C(34)-C(33)	120.3(7)	F(16)-C(49)-C(48)	115.8(5)
C(35)-C(34)-C(33)	118.9(6)	F(16)-C(49)-C(44)	120.6(5)
F(4)-C(35)-C(34)	119.6(7)	C(48)-C(49)-C(44)	123.6(6)
F(4)-C(35)-C(36)	120.3(7)		

Symmetry transformations used to generate equivalent atoms:

Table S21. Crystal data and structure refinement for $[(\mu_3\text{-O})(\mu_2\text{-OC}_2\text{H}_5)_3\{(\text{Cp*Zr}(\text{OC}_2\text{H}_5))_2(\text{BOC}_2\text{H}_5)\}][\text{HB}(\text{C}_6\text{F}_5)_3]$.

Empirical formula	$C_{50}H_{60}B_2F_{15}O_7Zr_2$	
Formula weight	1262.04	
Temperature	295(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 14.6566(5) Å	α = 90°.
	b = 18.0175(6) Å	β = 90°.
	c = 20.3699(7) Å	γ = 90°.
Volume	5379.2(3) $Å^3$	
Z	4	
Density (calculated)	1.558 Mg/m^3	
Absorption coefficient	0.488 mm^{-1}	
F(000)	2564	
Crystal size	0.36 x 0.30 x 0.25 mm^3	
Theta range for data collection	1.51 to 27.50°.	
Index ranges	-18<=h<=19, -23<=k<=23, -26<=l<=26	
Reflections collected	54149	
Independent reflections	12348 [R(int) = 0.0591]	
Completeness to theta = 27.50°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8877 and 0.8438	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12348 / 2 / 704	
Goodness-of-fit on F^2	1.030	
Final R indices [I>2sigma(I)]	R1 = 0.0412, wR2 = 0.0868	
R indices (all data)	R1 = 0.0481, wR2 = 0.0899	
Absolute structure parameter	-0.02(2)	
Largest diff. peak and hole	0.590 and -0.294 $e.Å^{-3}$	

Table S22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for [(μ_3-O)(μ_2-OC_2H_5)$_3${(Cp*Zr(OC_2H_5))$_2$(BOC_2H_5)}][$HB(C_6F_5)_3$]. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Zr(1)	6515(1)	9184(1)	1384(1)	21(1)
Zr(2)	8066(1)	10513(1)	1691(1)	21(1)
O(1)	7721(1)	9382(1)	1932(1)	20(1)
O(2)	7306(2)	10021(1)	893(1)	25(1)
O(3)	5441(2)	9777(1)	1329(1)	30(1)
O(4)	6379(1)	9183(1)	2457(1)	26(1)
O(5)	7356(2)	10319(1)	2627(1)	26(1)
O(6)	7448(2)	11429(1)	1540(1)	34(1)
O(7)	7769(2)	9185(1)	3139(1)	27(1)
B(1)	7334(3)	9482(2)	2583(2)	24(1)
C(1)	6910(3)	10407(2)	338(2)	38(1)
C(2)	7636(3)	10697(3)	-112(2)	63(2)
C(3)	4578(3)	10099(3)	1227(2)	56(1)
C(4)	4405(3)	10745(2)	1656(3)	56(1)
C(5)	5627(3)	9337(2)	2885(2)	45(1)
C(6)	5591(4)	8914(4)	3494(3)	45(2)
C(6')	4892(7)	8818(6)	2865(6)	47(3)
C(7)	7221(3)	10715(2)	3239(2)	39(1)
C(8)	6916(3)	11487(2)	3111(2)	49(1)
C(9)	7239(3)	12187(2)	1433(3)	60(1)
C(10)	6295(3)	12333(3)	1302(3)	78(2)
C(11)	7881(3)	8396(2)	3164(2)	37(1)
C(12)	8732(3)	8189(2)	3519(2)	50(1)
C(13)	6942(3)	8334(2)	464(2)	28(1)
C(14)	5980(3)	8404(2)	442(2)	29(1)
C(15)	5629(2)	8075(2)	1024(2)	28(1)
C(16)	6375(2)	7794(2)	1395(2)	27(1)
C(17)	7186(2)	7953(2)	1049(2)	25(1)
C(18)	7598(3)	8547(2)	-71(2)	41(1)
C(19)	5412(3)	8722(2)	-104(2)	41(1)
C(20)	4637(3)	8000(2)	1195(2)	39(1)
C(21)	6302(3)	7351(2)	2018(2)	33(1)
C(22)	8149(3)	7722(2)	1226(2)	36(1)
C(23)	9630(2)	10373(2)	1220(2)	33(1)
C(24)	9655(2)	9999(2)	1836(2)	36(1)
C(25)	9537(2)	10531(3)	2335(2)	37(1)
C(26)	9448(3)	11242(2)	2033(2)	33(1)
C(27)	9509(2)	11137(2)	1349(2)	30(1)
C(28)	9817(3)	10031(3)	563(2)	55(1)
C(29)	9857(3)	9189(2)	1933(3)	63(2)

C(30)	9577(3)	10370(3)	3060(2)	60(1)
C(31)	9388(3)	11969(3)	2384(2)	52(1)
C(32)	9551(3)	11748(2)	843(2)	44(1)
B(2)	2989(3)	9766(2)	8956(2)	29(1)
C(33)	2138(2)	9280(2)	9262(2)	26(1)
C(34)	2267(2)	8850(2)	9813(2)	30(1)
C(35)	1590(3)	8442(2)	10124(2)	33(1)
C(36)	722(3)	8470(2)	9869(2)	33(1)
C(37)	553(3)	8885(2)	9326(2)	36(1)
C(38)	1244(2)	9272(2)	9040(2)	29(1)
C(39)	3121(3)	10534(2)	9390(2)	31(1)
C(40)	2420(3)	10949(2)	9668(2)	36(1)
C(41)	2548(3)	11568(2)	10061(2)	41(1)
C(42)	3417(3)	11806(2)	10179(2)	39(1)
C(43)	4137(3)	11431(2)	9902(2)	40(1)
C(44)	3972(3)	10812(2)	9525(2)	33(1)
C(45)	2880(2)	9922(2)	8164(2)	29(1)
C(46)	2601(3)	10573(2)	7865(2)	36(1)
C(47)	2573(3)	10686(2)	7195(2)	41(1)
C(48)	2816(3)	10126(3)	6786(2)	40(1)
C(49)	3081(3)	9454(2)	7043(2)	35(1)
C(50)	3113(2)	9371(2)	7720(2)	30(1)
F(1)	3108(2)	8807(1)	10091(1)	42(1)
F(2)	1765(2)	8040(1)	10664(1)	49(1)
F(3)	40(2)	8102(1)	10178(1)	49(1)
F(4)	-304(2)	8927(2)	9091(1)	54(1)
F(5)	1012(2)	9676(1)	8505(1)	45(1)
F(6)	1536(2)	10759(1)	9554(1)	51(1)
F(7)	1833(2)	11936(1)	10310(1)	63(1)
F(8)	3567(2)	12407(1)	10555(1)	60(1)
F(9)	4995(2)	11660(1)	10021(1)	57(1)
F(10)	4727(1)	10469(1)	9289(1)	43(1)
F(11)	2334(2)	11154(1)	8241(1)	56(1)
F(12)	2305(2)	11343(2)	6951(1)	64(1)
F(13)	2797(2)	10218(2)	6129(1)	59(1)
F(14)	3305(2)	8894(1)	6643(1)	55(1)
F(15)	3392(2)	8704(1)	7935(1)	44(1)

Table S23. Anisotropic displacement parameters ($Å^2$ x 10^3) for $[(\mu_3\text{-O})(\mu_2\text{-OC}_2\text{H}_5)_3\{(\text{Cp*Zr(OC}_2\text{H}_5))_2(\text{BOC}_2\text{H}_5)\}][\text{HB}(\text{C}_6\text{F}_5)_3]$. The anisotropic displacement factor exponent takes the form: $-2p^2[\, h^2 a^{*2} U^{11} + \ldots + 2\, h\, k\, a^*\, b^*\, U^{12}\,]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zr(1)	21(1)	20(1)	21(1)	1(1)	-1(1)	-2(1)
Zr(2)	23(1)	20(1)	21(1)	1(1)	-2(1)	-2(1)
O(1)	17(1)	22(1)	20(1)	-1(1)	0(1)	0(1)
O(2)	30(1)	26(1)	20(1)	5(1)	-5(1)	-4(1)
O(3)	24(1)	32(1)	35(1)	2(1)	-6(1)	3(1)
O(4)	20(1)	34(1)	25(1)	4(1)	4(1)	2(1)
O(5)	34(1)	24(1)	20(1)	-5(1)	-1(1)	4(1)
O(6)	39(2)	23(1)	39(2)	4(1)	-4(1)	2(1)
O(7)	31(1)	30(1)	20(1)	5(1)	-2(1)	3(1)
B(1)	22(2)	26(2)	23(2)	1(2)	1(2)	2(2)
C(1)	49(2)	36(2)	28(2)	12(2)	-16(2)	-10(2)
C(2)	73(3)	79(4)	39(2)	32(3)	-14(2)	-24(3)
C(3)	41(3)	60(3)	66(3)	3(3)	-15(2)	16(2)
C(4)	39(2)	42(2)	87(3)	5(3)	8(2)	13(2)
C(5)	38(2)	51(3)	46(2)	9(2)	22(2)	12(2)
C(6)	38(3)	65(4)	33(3)	8(3)	7(3)	-2(3)
C(7)	54(2)	36(2)	26(2)	-9(2)	-2(2)	12(2)
C(8)	76(3)	34(2)	37(2)	-8(2)	10(2)	14(2)
C(9)	47(3)	24(2)	110(4)	21(3)	-3(3)	0(2)
C(10)	55(3)	34(2)	145(6)	8(3)	-31(4)	10(2)
C(11)	46(2)	34(2)	30(2)	7(2)	-4(2)	-1(2)
C(12)	49(3)	45(2)	57(3)	12(2)	-4(2)	14(2)
C(13)	36(2)	24(2)	23(2)	-4(1)	0(2)	-4(2)
C(14)	33(2)	27(2)	25(2)	-4(2)	-2(2)	-7(2)
C(15)	28(2)	24(2)	32(2)	-5(2)	0(2)	-4(1)
C(16)	32(2)	19(2)	29(2)	-5(1)	-1(2)	-3(1)
C(17)	28(2)	20(2)	26(2)	-5(1)	-3(1)	-1(1)
C(18)	53(3)	40(2)	30(2)	-4(2)	10(2)	-2(2)
C(19)	47(3)	43(2)	33(2)	3(2)	-10(2)	-9(2)
C(20)	30(2)	36(2)	52(3)	-1(2)	0(2)	-12(2)
C(21)	43(2)	28(2)	29(2)	1(2)	1(2)	-5(2)
C(22)	35(2)	32(2)	40(2)	-4(2)	-1(2)	3(2)
C(23)	21(2)	40(2)	38(2)	-3(2)	1(2)	-1(2)
C(24)	22(2)	31(2)	56(3)	10(2)	-9(2)	-3(2)
C(25)	23(2)	55(2)	33(2)	8(2)	-7(2)	-14(2)
C(26)	28(2)	35(2)	35(2)	-4(2)	-1(2)	-12(2)
C(27)	26(2)	32(2)	33(2)	3(2)	0(2)	-9(2)
C(28)	39(3)	67(3)	59(3)	-30(3)	7(2)	-3(2)
C(29)	28(2)	39(2)	122(5)	20(3)	-8(2)	5(2)
C(30)	37(2)	98(4)	47(3)	28(3)	-15(2)	-22(3)

C(31)	46(3)	55(3)	56(3)	-26(2)	3(2)	-15(2)
C(32)	40(2)	45(2)	48(3)	12(2)	0(2)	-12(2)
B(2)	33(2)	26(2)	29(2)	-4(2)	5(2)	-3(2)
C(33)	30(2)	21(2)	26(2)	-2(1)	2(1)	1(1)
C(34)	24(2)	38(2)	29(2)	-9(2)	-4(2)	4(2)
C(35)	49(2)	28(2)	23(2)	0(1)	6(2)	5(2)
C(36)	36(2)	27(2)	36(2)	-11(2)	15(2)	-7(2)
C(37)	27(2)	37(2)	43(2)	-9(2)	1(2)	0(2)
C(38)	30(2)	26(2)	32(2)	0(2)	-3(2)	2(1)
C(39)	34(2)	32(2)	27(2)	4(2)	-1(2)	-3(2)
C(40)	36(2)	34(2)	39(2)	1(2)	5(2)	-6(2)
C(41)	58(3)	30(2)	36(2)	-2(2)	19(2)	2(2)
C(42)	60(3)	26(2)	30(2)	-9(2)	-1(2)	-3(2)
C(43)	45(2)	35(2)	38(2)	4(2)	-9(2)	-12(2)
C(44)	33(2)	32(2)	34(2)	0(2)	4(2)	1(2)
C(45)	26(2)	30(2)	31(2)	-3(2)	3(1)	-3(1)
C(46)	39(2)	32(2)	38(2)	-5(2)	4(2)	3(2)
C(47)	35(2)	40(2)	48(2)	12(2)	1(2)	2(2)
C(48)	29(2)	64(3)	27(2)	7(2)	0(2)	-6(2)
C(49)	30(2)	41(2)	35(2)	-14(2)	4(2)	-5(2)
C(50)	28(2)	23(2)	39(2)	0(1)	-3(2)	-3(2)
F(1)	33(1)	60(2)	34(1)	6(1)	-7(1)	6(1)
F(2)	67(2)	48(1)	32(1)	11(1)	6(1)	2(1)
F(3)	46(1)	46(1)	57(2)	-4(1)	22(1)	-13(1)
F(4)	28(1)	67(2)	66(2)	2(1)	-6(1)	-7(1)
F(5)	34(1)	54(2)	48(1)	13(1)	-9(1)	2(1)
F(6)	37(1)	43(1)	75(2)	-11(1)	9(1)	5(1)
F(7)	70(2)	47(2)	72(2)	-13(1)	34(2)	7(1)
F(8)	98(2)	38(1)	45(1)	-17(1)	7(2)	-16(2)
F(9)	58(2)	51(2)	62(2)	-6(1)	-16(1)	-13(1)
F(10)	28(1)	47(1)	55(1)	-10(1)	2(1)	-5(1)
F(11)	84(2)	34(1)	50(2)	-1(1)	-2(1)	24(1)
F(12)	78(2)	55(2)	59(2)	25(1)	-5(2)	15(2)
F(13)	61(2)	86(2)	29(1)	11(1)	1(1)	-2(2)
F(14)	64(2)	61(2)	40(1)	-21(1)	4(1)	2(1)
F(15)	59(2)	29(1)	45(1)	-1(1)	0(1)	4(1)

Table S24. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for [(μ_3-O)(μ_2-OC_2H_5)$_3${(Cp*Zr(OC_2H_5))$_2$(BOC_2H_5)}][$HB(C_6F_5)_3$].

	x	y	z	U(eq)
H(1A)	6540	10816	494	45
H(1B)	6517	10070	97	45
H(2A)	7951	11100	97	95
H(2B)	7361	10870	-512	95
H(2C)	8061	10308	-210	95
H(3A)	4111	9727	1306	67
H(3B)	4529	10254	772	67
H(4A)	4396	10587	2106	84
H(4B)	3828	10963	1545	84
H(4C)	4880	11106	1596	84
H(5A)	5066	9247	2645	54
H(5B)	5642	9861	2996	54
H(5'A)	5855	9360	3332	54
H(5'B)	5389	9824	2777	54
H(6A)	5066	9062	3743	68
H(6B)	6133	9007	3746	68
H(6C)	5551	8394	3395	68
H(6'A)	4423	8972	3165	70
H(6'B)	5111	8336	2988	70
H(6'C)	4647	8799	2429	70
H(7A)	7788	10723	3484	46
H(7B)	6767	10460	3502	46
H(8A)	7358	11735	2842	73
H(8B)	6853	11746	3521	73
H(8C)	6338	11478	2889	73
H(9A)	7599	12365	1066	72
H(9B)	7421	12468	1818	72
H(10A)	6136	12137	879	117
H(10B)	6190	12859	1306	117
H(10C)	5925	12101	1633	117
H(11A)	7905	8201	2720	44
H(11B)	7360	8176	3383	44
H(12A)	9250	8386	3290	75
H(12B)	8779	7659	3542	75
H(12C)	8714	8390	3956	75
H(18A)	7820	8107	-283	61
H(18B)	8102	8815	116	61
H(18C)	7292	8855	-386	61
H(19A)	5764	9083	-341	61
H(19B)	4880	8956	77	61
H(19C)	5230	8331	-396	61

H(20A)	4389	7572	978	59
H(20B)	4315	8435	1054	59
H(20C)	4573	7944	1661	59
H(21A)	6008	7644	2349	50
H(21B)	6902	7215	2164	50
H(21C)	5951	6911	1937	50
H(22A)	8294	7263	1009	54
H(22B)	8195	7655	1692	54
H(22C)	8569	8099	1088	54
H(28A)	9651	10375	224	83
H(28B)	9465	9585	517	83
H(28C)	10454	9915	528	83
H(29A)	10401	9136	2190	94
H(29B)	9942	8956	1513	94
H(29C)	9355	8959	2157	94
H(30A)	9160	9976	3163	90
H(30B)	9410	10808	3300	90
H(30C)	10185	10224	3177	90
H(31A)	9972	12089	2570	78
H(31B)	8942	11936	2727	78
H(31C)	9213	12350	2079	78
H(32A)	9166	12151	978	66
H(32B)	9345	11562	428	66
H(32C)	10168	11921	803	66

Table S25. Bond lengths [Å] and angles [°] for $[(\mu_3\text{-O})(\mu_2\text{-OC}_2\text{H}_5)_3\{(\text{Cp*Zr}(\text{OC}_2\text{H}_5))_2(\text{BOC}_2\text{H}_5)\}][\text{HB}(\text{C}_6\text{F}_5)_3]$.

Zr(1)-O(3)	1.906(2)	C(15)-C(16)	1.423(5)
Zr(1)-O(1)	2.120(2)	C(15)-C(20)	1.501(5)
Zr(1)-O(2)	2.149(2)	C(16)-C(17)	1.411(5)
Zr(1)-O(4)	2.194(2)	C(16)-C(21)	1.502(5)
Zr(1)-C(15)	2.493(3)	C(17)-C(22)	1.515(5)
Zr(1)-C(13)	2.501(3)	C(23)-C(27)	1.412(5)
Zr(1)-C(14)	2.505(3)	C(23)-C(24)	1.423(5)
Zr(1)-C(16)	2.513(3)	C(23)-C(28)	1.498(5)
Zr(1)-C(17)	2.521(3)	C(24)-C(25)	1.407(6)
Zr(1)-B(1)	2.773(4)	C(24)-C(29)	1.502(5)
Zr(1)-Zr(2)	3.3608(4)	C(25)-C(26)	1.427(6)
Zr(2)-O(6)	1.908(2)	C(25)-C(30)	1.506(6)
Zr(2)-O(1)	2.156(2)	C(26)-C(27)	1.410(5)
Zr(2)-O(2)	2.161(2)	C(26)-C(31)	1.495(6)
Zr(2)-O(5)	2.200(2)	C(27)-C(32)	1.509(5)
Zr(2)-C(27)	2.494(3)	B(2)-C(33)	1.646(5)
Zr(2)-C(23)	2.498(4)	B(2)-C(45)	1.646(5)
Zr(2)-C(26)	2.512(4)	B(2)-C(39)	1.653(5)
Zr(2)-C(24)	2.523(4)	C(33)-C(34)	1.378(5)
Zr(2)-C(25)	2.523(3)	C(33)-C(38)	1.387(5)
Zr(2)-B(1)	2.811(4)	C(34)-F(1)	1.358(4)
O(1)-B(1)	1.454(4)	C(34)-C(35)	1.387(5)
O(2)-C(1)	1.449(4)	C(35)-F(2)	1.342(4)
O(3)-C(3)	1.407(5)	C(35)-C(36)	1.375(6)
O(4)-C(5)	1.433(4)	C(36)-F(3)	1.354(4)
O(4)-B(1)	1.521(4)	C(36)-C(37)	1.358(6)
O(5)-C(7)	1.450(4)	C(37)-F(4)	1.348(4)
O(5)-B(1)	1.510(5)	C(37)-C(38)	1.360(5)
O(6)-C(9)	1.417(4)	C(38)-F(5)	1.354(4)
O(7)-B(1)	1.407(4)	C(39)-C(44)	1.371(5)
O(7)-C(11)	1.431(4)	C(39)-C(40)	1.391(5)
C(1)-C(2)	1.498(6)	C(40)-F(6)	1.361(4)
C(3)-C(4)	1.478(6)	C(40)-C(41)	1.385(6)
C(5)-C(6')	1.427(8)	C(41)-F(7)	1.341(5)
C(5)-C(6)	1.457(6)	C(41)-C(42)	1.366(6)
C(7)-C(8)	1.483(5)	C(42)-F(8)	1.343(4)
C(9)-C(10)	1.434(6)	C(42)-C(43)	1.375(6)
C(11)-C(12)	1.490(5)	C(43)-F(9)	1.346(5)
C(13)-C(14)	1.416(5)	C(43)-C(44)	1.376(5)
C(13)-C(17)	1.422(5)	C(44)-F(10)	1.355(4)
C(13)-C(18)	1.502(5)	C(45)-C(46)	1.385(5)
C(14)-C(15)	1.420(5)	C(45)-C(50)	1.385(5)
C(14)-C(19)	1.503(5)	C(46)-F(11)	1.356(4)

C(46)-C(47)	1.380(5)	C(48)-C(49)	1.374(6)
C(47)-F(12)	1.344(5)	C(49)-F(14)	1.339(4)
C(47)-C(48)	1.357(6)	C(49)-C(50)	1.388(5)
C(48)-F(13)	1.349(4)	C(50)-F(15)	1.343(4)

O(3)-Zr(1)-O(1)	128.71(9)	C(13)-Zr(1)-B(1)	132.12(12)
O(3)-Zr(1)-O(2)	91.40(10)	C(14)-Zr(1)-B(1)	156.75(12)
O(1)-Zr(1)-O(2)	71.16(8)	C(16)-Zr(1)-B(1)	102.78(12)
O(3)-Zr(1)-O(4)	89.10(10)	C(17)-Zr(1)-B(1)	103.91(11)
O(1)-Zr(1)-O(4)	63.38(8)	O(3)-Zr(1)-Zr(2)	99.81(7)
O(2)-Zr(1)-O(4)	120.85(9)	O(1)-Zr(1)-Zr(2)	38.57(6)
O(3)-Zr(1)-C(15)	90.07(11)	O(2)-Zr(1)-Zr(2)	38.89(6)
O(1)-Zr(1)-C(15)	136.40(10)	O(4)-Zr(1)-Zr(2)	82.91(6)
O(2)-Zr(1)-C(15)	134.91(10)	C(15)-Zr(1)-Zr(2)	167.98(8)
O(4)-Zr(1)-C(15)	104.22(11)	C(13)-Zr(1)-Zr(2)	113.99(9)
O(3)-Zr(1)-C(13)	120.36(12)	C(14)-Zr(1)-Zr(2)	138.97(8)
O(1)-Zr(1)-C(13)	106.81(11)	C(16)-Zr(1)-Zr(2)	139.81(8)
O(2)-Zr(1)-C(13)	86.89(10)	C(17)-Zr(1)-Zr(2)	114.45(8)
O(4)-Zr(1)-C(13)	140.29(10)	B(1)-Zr(1)-Zr(2)	53.51(8)
C(15)-Zr(1)-C(13)	54.46(12)	O(6)-Zr(2)-O(1)	137.97(9)
O(3)-Zr(1)-C(14)	90.60(12)	O(6)-Zr(2)-O(2)	89.32(10)
O(1)-Zr(1)-C(14)	139.35(11)	O(1)-Zr(2)-O(2)	70.25(8)
O(2)-Zr(1)-C(14)	101.91(10)	O(6)-Zr(2)-O(5)	93.06(10)
O(4)-Zr(1)-C(14)	137.24(10)	O(1)-Zr(2)-O(5)	62.71(8)
C(15)-Zr(1)-C(14)	33.01(12)	O(2)-Zr(2)-O(5)	110.01(9)
C(13)-Zr(1)-C(14)	32.87(12)	O(6)-Zr(2)-C(27)	88.14(11)
O(3)-Zr(1)-C(16)	119.44(11)	O(1)-Zr(2)-C(27)	133.50(10)
O(1)-Zr(1)-C(16)	103.39(10)	O(2)-Zr(2)-C(27)	114.29(11)
O(2)-Zr(1)-C(16)	138.37(10)	O(5)-Zr(2)-C(27)	135.70(11)
O(4)-Zr(1)-C(16)	89.07(10)	O(6)-Zr(2)-C(23)	117.47(12)
C(15)-Zr(1)-C(16)	33.01(11)	O(1)-Zr(2)-C(23)	101.94(11)
C(13)-Zr(1)-C(16)	54.30(11)	O(2)-Zr(2)-C(23)	98.21(11)
C(14)-Zr(1)-C(16)	54.65(11)	O(5)-Zr(2)-C(23)	138.68(11)
O(3)-Zr(1)-C(17)	143.06(11)	C(27)-Zr(2)-C(23)	32.87(12)
O(1)-Zr(1)-C(17)	88.04(9)	O(6)-Zr(2)-C(26)	88.59(12)
O(2)-Zr(1)-C(17)	106.34(10)	O(1)-Zr(2)-C(26)	128.36(11)
O(4)-Zr(1)-C(17)	107.74(10)	O(2)-Zr(2)-C(26)	146.98(11)
C(15)-Zr(1)-C(17)	54.42(11)	O(5)-Zr(2)-C(26)	103.00(11)
C(13)-Zr(1)-C(17)	32.90(11)	C(27)-Zr(2)-C(26)	32.71(12)
C(14)-Zr(1)-C(17)	54.59(11)	C(23)-Zr(2)-C(26)	54.52(12)
C(16)-Zr(1)-C(17)	32.54(11)	O(6)-Zr(2)-C(24)	140.75(11)
O(3)-Zr(1)-B(1)	107.52(11)	O(1)-Zr(2)-C(24)	81.01(10)
O(1)-Zr(1)-B(1)	31.07(9)	O(2)-Zr(2)-C(24)	114.40(12)
O(2)-Zr(1)-B(1)	92.31(10)	O(5)-Zr(2)-C(24)	106.12(11)
O(4)-Zr(1)-B(1)	33.14(10)	C(27)-Zr(2)-C(24)	54.22(12)
C(15)-Zr(1)-B(1)	129.80(12)	C(23)-Zr(2)-C(24)	32.91(12)

C(26)-Zr(2)-C(24)	54.23(13)	O(7)-B(1)-O(4)	114.7(3)
O(6)-Zr(2)-C(25)	118.61(13)	O(1)-B(1)-O(4)	99.3(3)
O(1)-Zr(2)-C(25)	95.43(11)	O(5)-B(1)-O(4)	112.5(3)
O(2)-Zr(2)-C(25)	146.77(12)	O(7)-B(1)-Zr(1)	146.3(3)
O(5)-Zr(2)-C(25)	87.51(10)	O(1)-B(1)-Zr(1)	48.79(14)
C(27)-Zr(2)-C(25)	54.22(12)	O(5)-B(1)-Zr(1)	104.8(2)
C(23)-Zr(2)-C(25)	54.30(12)	O(4)-B(1)-Zr(1)	52.04(14)
C(26)-Zr(2)-C(25)	32.94(13)	O(7)-B(1)-Zr(2)	126.8(2)
C(24)-Zr(2)-C(25)	32.38(13)	O(1)-B(1)-Zr(2)	48.97(15)
O(6)-Zr(2)-B(1)	119.67(11)	O(5)-B(1)-Zr(2)	51.00(15)
O(1)-Zr(2)-B(1)	30.57(10)	O(4)-B(1)-Zr(2)	118.4(2)
O(2)-Zr(2)-B(1)	91.04(10)	Zr(1)-B(1)-Zr(2)	74.00(9)
O(5)-Zr(2)-B(1)	32.24(10)	O(2)-C(1)-C(2)	111.2(3)
C(27)-Zr(2)-B(1)	143.34(12)	O(3)-C(3)-C(4)	113.0(4)
C(23)-Zr(2)-B(1)	122.11(12)	C(6')-C(5)-O(4)	115.9(6)
C(26)-Zr(2)-B(1)	118.32(12)	C(6')-C(5)-C(6)	69.8(6)
C(24)-Zr(2)-B(1)	91.99(12)	O(4)-C(5)-C(6)	116.4(4)
C(25)-Zr(2)-B(1)	89.95(12)	O(5)-C(7)-C(8)	110.6(3)
O(6)-Zr(2)-Zr(1)	105.38(7)	O(6)-C(9)-C(10)	114.5(4)
O(1)-Zr(2)-Zr(1)	37.80(6)	O(7)-C(11)-C(12)	111.2(3)
O(2)-Zr(2)-Zr(1)	38.64(6)	C(14)-C(13)-C(17)	108.6(3)
O(5)-Zr(2)-Zr(1)	74.19(6)	C(14)-C(13)-C(18)	126.4(3)
C(27)-Zr(2)-Zr(1)	147.38(9)	C(17)-C(13)-C(18)	124.8(4)
C(23)-Zr(2)-Zr(1)	118.49(9)	C(14)-C(13)-Zr(1)	73.7(2)
C(26)-Zr(2)-Zr(1)	165.80(9)	C(17)-C(13)-Zr(1)	74.31(19)
C(24)-Zr(2)-Zr(1)	112.62(9)	C(18)-C(13)-Zr(1)	123.2(2)
C(25)-Zr(2)-Zr(1)	133.13(10)	C(13)-C(14)-C(15)	107.4(3)
B(1)-Zr(2)-Zr(1)	52.49(8)	C(13)-C(14)-C(19)	127.4(3)
B(1)-O(1)-Zr(1)	100.14(18)	C(15)-C(14)-C(19)	125.1(3)
B(1)-O(1)-Zr(2)	100.5(2)	C(13)-C(14)-Zr(1)	73.4(2)
Zr(1)-O(1)-Zr(2)	103.62(9)	C(15)-C(14)-Zr(1)	73.1(2)
C(1)-O(2)-Zr(1)	119.0(2)	C(19)-C(14)-Zr(1)	121.7(3)
C(1)-O(2)-Zr(2)	126.7(2)	C(14)-C(15)-C(16)	108.3(3)
Zr(1)-O(2)-Zr(2)	102.47(9)	C(14)-C(15)-C(20)	125.6(3)
C(3)-O(3)-Zr(1)	169.3(3)	C(16)-C(15)-C(20)	126.1(3)
C(5)-O(4)-B(1)	122.5(3)	C(14)-C(15)-Zr(1)	73.93(19)
C(5)-O(4)-Zr(1)	132.5(2)	C(16)-C(15)-Zr(1)	74.27(18)
B(1)-O(4)-Zr(1)	94.82(17)	C(20)-C(15)-Zr(1)	120.6(2)
C(7)-O(5)-B(1)	122.7(3)	C(17)-C(16)-C(15)	108.1(3)
C(7)-O(5)-Zr(2)	136.9(2)	C(17)-C(16)-C(21)	126.1(3)
B(1)-O(5)-Zr(2)	96.76(18)	C(15)-C(16)-C(21)	125.7(3)
C(9)-O(6)-Zr(2)	164.1(3)	C(17)-C(16)-Zr(1)	74.01(18)
B(1)-O(7)-C(11)	117.3(3)	C(15)-C(16)-Zr(1)	72.72(19)
O(7)-B(1)-O(1)	120.7(3)	C(21)-C(16)-Zr(1)	122.8(2)
O(7)-B(1)-O(5)	108.8(3)	C(16)-C(17)-C(13)	107.8(3)
O(1)-B(1)-O(5)	99.8(3)	C(16)-C(17)-C(22)	127.6(3)

C(13)-C(17)-C(22)	124.5(3)	F(3)-C(36)-C(37)	120.9(4)
C(16)-C(17)-Zr(1)	73.44(19)	F(3)-C(36)-C(35)	119.3(4)
C(13)-C(17)-Zr(1)	72.79(19)	C(37)-C(36)-C(35)	119.7(3)
C(22)-C(17)-Zr(1)	122.7(2)	F(4)-C(37)-C(36)	119.4(4)
C(27)-C(23)-C(24)	107.5(3)	F(4)-C(37)-C(38)	120.8(4)
C(27)-C(23)-C(28)	126.0(4)	C(36)-C(37)-C(38)	119.8(4)
C(24)-C(23)-C(28)	126.1(4)	F(5)-C(38)-C(37)	115.7(3)
C(27)-C(23)-Zr(2)	73.4(2)	F(5)-C(38)-C(33)	119.6(3)
C(24)-C(23)-Zr(2)	74.5(2)	C(37)-C(38)-C(33)	124.7(3)
C(28)-C(23)-Zr(2)	123.5(3)	C(44)-C(39)-C(40)	113.2(3)
C(25)-C(24)-C(23)	108.2(3)	C(44)-C(39)-B(2)	121.3(3)
C(25)-C(24)-C(29)	126.2(4)	C(40)-C(39)-B(2)	125.5(3)
C(23)-C(24)-C(29)	125.5(4)	F(6)-C(40)-C(41)	115.5(4)
C(25)-C(24)-Zr(2)	73.8(2)	F(6)-C(40)-C(39)	120.0(3)
C(23)-C(24)-Zr(2)	72.6(2)	C(41)-C(40)-C(39)	124.6(4)
C(29)-C(24)-Zr(2)	123.6(3)	F(7)-C(41)-C(42)	120.5(4)
C(24)-C(25)-C(26)	108.1(3)	F(7)-C(41)-C(40)	120.7(4)
C(24)-C(25)-C(30)	125.0(4)	C(42)-C(41)-C(40)	118.8(4)
C(26)-C(25)-C(30)	126.7(4)	F(8)-C(42)-C(41)	120.5(4)
C(24)-C(25)-Zr(2)	73.8(2)	F(8)-C(42)-C(43)	120.3(4)
C(26)-C(25)-Zr(2)	73.1(2)	C(41)-C(42)-C(43)	119.2(3)
C(30)-C(25)-Zr(2)	122.6(3)	F(9)-C(43)-C(42)	119.5(4)
C(27)-C(26)-C(25)	107.4(3)	F(9)-C(43)-C(44)	120.9(4)
C(27)-C(26)-C(31)	126.5(4)	C(42)-C(43)-C(44)	119.6(4)
C(25)-C(26)-C(31)	125.9(4)	F(10)-C(44)-C(39)	120.3(3)
C(27)-C(26)-Zr(2)	73.0(2)	F(10)-C(44)-C(43)	115.1(3)
C(25)-C(26)-Zr(2)	74.0(2)	C(39)-C(44)-C(43)	124.6(4)
C(31)-C(26)-Zr(2)	122.9(3)	C(46)-C(45)-C(50)	113.1(3)
C(26)-C(27)-C(23)	108.8(3)	C(46)-C(45)-B(2)	127.2(3)
C(26)-C(27)-C(32)	125.3(4)	C(50)-C(45)-B(2)	119.6(3)
C(23)-C(27)-C(32)	125.5(4)	F(11)-C(46)-C(47)	115.9(3)
C(26)-C(27)-Zr(2)	74.3(2)	F(11)-C(46)-C(45)	119.4(3)
C(23)-C(27)-Zr(2)	73.7(2)	C(47)-C(46)-C(45)	124.7(4)
C(32)-C(27)-Zr(2)	123.7(3)	F(12)-C(47)-C(48)	120.3(4)
C(33)-B(2)-C(45)	112.8(3)	F(12)-C(47)-C(46)	120.3(4)
C(33)-B(2)-C(39)	109.4(3)	C(48)-C(47)-C(46)	119.4(4)
C(45)-B(2)-C(39)	113.1(3)	F(13)-C(48)-C(47)	120.9(4)
C(34)-C(33)-C(38)	112.9(3)	F(13)-C(48)-C(49)	119.5(4)
C(34)-C(33)-B(2)	120.2(3)	C(47)-C(48)-C(49)	119.6(3)
C(38)-C(33)-B(2)	126.8(3)	F(14)-C(49)-C(48)	120.1(3)
F(1)-C(34)-C(33)	119.7(3)	F(14)-C(49)-C(50)	121.0(4)
F(1)-C(34)-C(35)	115.4(3)	C(48)-C(49)-C(50)	118.9(3)
C(33)-C(34)-C(35)	124.9(3)	F(15)-C(50)-C(45)	120.2(3)
F(2)-C(35)-C(36)	120.4(4)	F(15)-C(50)-C(49)	115.5(3)
F(2)-C(35)-C(34)	121.6(4)	C(45)-C(50)-C(49)	124.3(3)
C(36)-C(35)-C(34)	118.1(3)		

Supplementary Material (ESI) for Dalton Transactions

Symmetry transformations used to generate equivalent atoms:

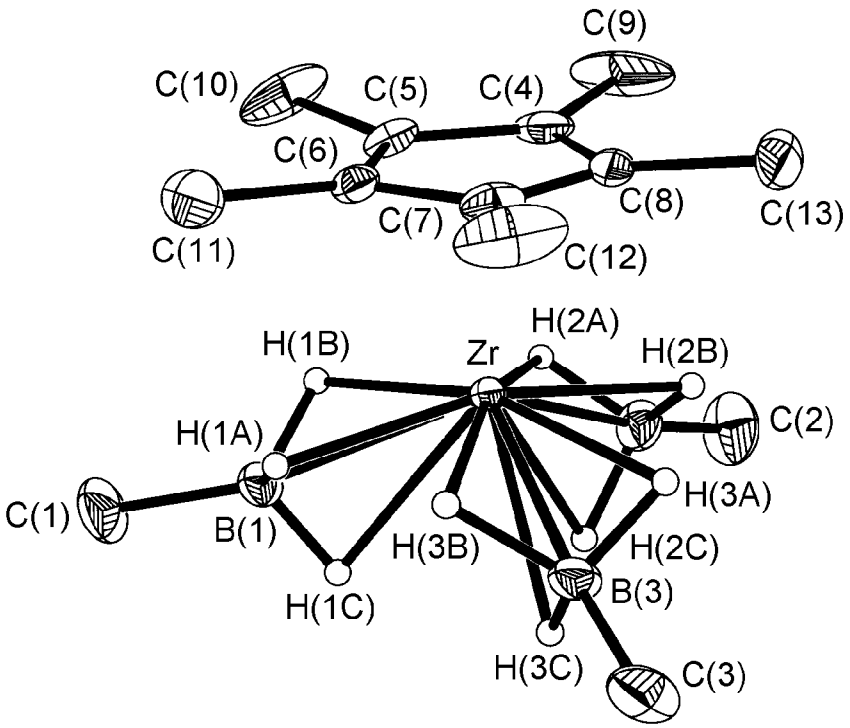

Figure S1. Molecular structure of $Cp^*Zr(BH_3CH_3)_3$, showing 30% probability thermal ellipsoids.

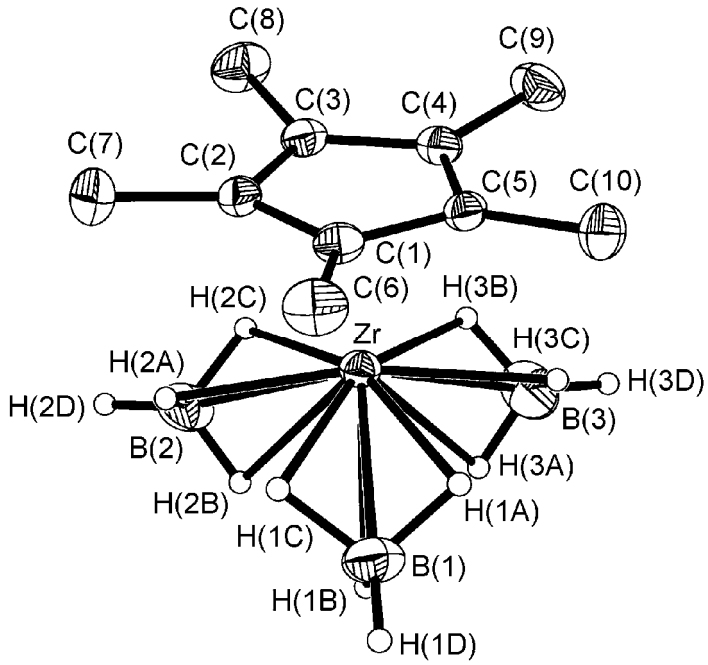

Figure S2. Molecular structure of $Cp^*Zr(BH_4)_3$, showing 50% probability thermal ellipsoids.