Supporting Information

Syntheses and Structures of Zr_4 Tetrahedral Clusters Containing Direct Zr-Zr Bonds: The Missing Cluster in the Series Zr_n (n = 2-6)

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Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $[(\mu_2\text{-H})_8(\mu_2\text{-Cl})_2(Cp^*Zr)_4]\cdot 2(C_7H_8)$.

	x	y	z	U(eq)
Zr(1)	1519(1)	13907(1)	7717(1)	32(1)
Zr(2)	2345(1)	15452(1)	8609(1)	30(1)
Zr(3)	2705(1)	13441(1)	8630(1)	32(1)
Zr(4)	3474(1)	14927(1)	7691(1)	31(1)
Cl(1)	648(1)	15237(1)	8163(1)	40(1)
Cl(2)	4373(1)	13627(1)	8152(1)	39(1)
C(1)	1000(3)	12571(3)	7235(2)	39(1)
C(2)	1159(3)	13261(3)	6894(2)	42(1)
C(3)	427(4)	13925(3)	6975(2)	49(1)
C(4)	-182(3)	13648(4)	7354(2)	46(1)
C(5)	157(3)	12807(3)	7517(2)	41(1)
C(6)	1535(4)	11695(4)	7242(2)	60(2)
C(7)	1885(4)	13211(4)	6482(2)	70(2)
C(8)	257(5)	14735(4)	6669(3)	84(2)
C(9)	-1104(4)	14101(4)	7539(3)	76(2)
C(10)	-343(4)	12201(4)	7872(2)	69(2)
C(11)	2339(4)	17101(3)	8807(2)	42(1)
C(12)	1443(4)	16750(3)	9000(2)	45(1)
C(13)	1691(3)	16155(3)	9380(2)	39(1)
C(14)	2737(3)	16143(3)	9419(2)	37(1)
C(15)	3126(4)	16724(3)	9074(2)	40(1)
C(16)	2405(5)	17830(4)	8436(2)	75(2)
C(17)	422(4)	17065(4)	8862(2)	72(2)
C(18)	935(4)	15716(4)	9710(2)	63(2)
C(19)	3317(4)	15700(4)	9814(2)	58(2)
C(20)	4211(4)	17000(4)	9042(2)	64(2)
C(21)	1957(4)	12200(4)	9129(2)	55(2)
C(22)	2383(4)	12804(4)	9464(2)	49(1)
C(23)	3414(4)	12785(3)	9394(2)	46(1)
C(24)	3616(4)	12167(4)	9025(2)	49(1)
C(25)	2716(5)	11811(3)	8862(2)	54(1)
C(26)	875(5)	11941(5)	9118(3)	107(3)
C(27)	1824(6)	13263(5)	9861(2)	96(3)
C(28)	4199(5)	13235(5)	9701(2)	86(2)
C(29)	4646(5)	11845(5)	8877(3)	98(3)
C(30)	2625(7)	11049(4)	8499(3)	124(4)
C(31)	4829(3)	16016(3)	7456(2)	38(1)
C(32)	5143(4)	15153(3)	7292(2)	45(1)
C(33)	4497(4)	14867(3)	6922(2)	42(1)
C(34)	3785(4)	15541(3)	6845(2)	43(1)
C(35)	3976(3)	16244(3)	7185(2)	37(1)

C(36)	5383(4)	16624(4)	7796(2)	56(2)
C(37)	6078(4)	14675(4)	7450(3)	74(2)
C(38)	4648(5)	14044(4)	6627(2)	77(2)
C(39)	3032(5)	15589(4)	6444(2)	66(2)
C(40)	3461(2)	17121(2)	7185(1)	55(2)
C(41)	2307(2)	16049(2)	11076(1)	165(4)
C(42)	1694(2)	15309(2)	11039(1)	107(3)
C(43)	2098(2)	14458(2)	11047(1)	161(4)
C(44)	3116(2)	14347(2)	11092(1)	117(3)
C(45)	3729(2)	15087(2)	11130(1)	123(3)
C(46)	3324(2)	15938(2)	11122(1)	90(2)
C(47)	1825(4)	16857(4)	11048(2)	164(4)
C(48)	2698(4)	10227(4)	10033(2)	256(8)
C(49)	1689(4)	10231(4)	10131(2)	334(8)
C(50)	1142(4)	9452(4)	10083(2)	334(8)
C(51)	1603(4)	8670(4)	9937(2)	294(9)
C(52)	2612(4)	8665(4)	9838(2)	255(8)
C(53)	3160(4)	9444(4)	9887(2)	296(10)
C(54)	3360(9)	10892(9)	10066(3)	310(10)
H(1)	2340(30)	12970(30)	7949(16)	46
H(2)	1420(30)	13460(30)	8207(15)	46
H(3)	1750(30)	14330(30)	8897(17)	46
H(4)	3260(30)	14580(30)	8862(17)	46
H(5)	3600(30)	15510(30)	8275(17)	46
H(6)	2690(30)	15900(30)	7949(16)	46
H(7)	2130(30)	15030(30)	7419(16)	46
H(8)	2820(30)	13870(30)	7343(16)	46

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

Table S2. Bond lengths [Å] and angles [°] for $[(\mu_2\text{-H})_8(\mu_2\text{-Cl})_2(\text{Cp*Zr})_4]\cdot 2(C_7H_8)$.

Zr(1)-C(1)	2.504(4)	Zr(4)-H(7)	1.96(5)
Zr(1)-C(2)	2.507(5)	Zr(4)-H(8)	2.05(5)
Zr(1)-C(3)	2.515(5)	C(1)-C(2)	1.412(7)
Zr(1)-C(5)	2.533(4)	C(1)-C(5)	1.421(6)
Zr(1)-C(4)	2.536(5)	C(1)-C(6)	1.501(7)
Zr(1)-Cl(1)	2.6206(12)	C(2)-C(3)	1.422(7)
Zr(1)-Zr(3)	3.0539(6)	C(2)-C(7)	1.499(7)
Zr(1)-Zr(4)	3.0541(6)	C(3)-C(4)	1.390(7)
Zr(1)-Zr(2)	3.5514(6)	C(3)-C(8)	1.496(8)
Zr(1)-H(1)	1.90(5)	C(4)-C(5)	1.416(7)
Zr(1)-H(2)	1.51(4)	C(4)-C(9)	1.508(7)
Zr(1)-H(7)	2.06(4)	C(5)-C(10)	1.496(7)
Zr(1)-H(8)	2.04(4)	C(6)-H(6A)	0.9700
Zr(2)-C(14)	2.510(4)	C(6)-H(6B)	0.9700
Zr(2)-C(13)	2.525(4)	C(6)-H(6C)	0.9700
Zr(2)-C(15)	2.527(5)	C(7)-H(7A)	0.9700
Zr(2)-C(11)	2.534(5)	C(7)-H(7B)	0.9700
Zr(2)-C(12)	2.537(5)	C(7)-H(7C)	0.9700
Zr(2)-Cl(1)	2.6176(12)	C(8)-H(8A)	0.9700
Zr(2)-Zr(4)	3.0516(6)	C(8)-H(8B)	0.9700
Zr(2)-Zr(3)	3.0585(6)	C(8)-H(8C)	0.9700
Zr(2)-H(3)	2.03(4)	C(9)-H(9A)	0.9700
Zr(2)-H(4)	1.93(5)	C(9)-H(9B)	0.9700
Zr(2)-H(5)	1.93(4)	C(9)-H(9C)	0.9700
Zr(2)-H(6)	1.99(4)	C(10)-H(10A)	0.9700
Zr(3)-C(23)	2.507(5)	C(10)-H(10B)	0.9700
Zr(3)-C(24)	2.520(5)	C(10)-H(10C)	0.9700
Zr(3)-C(22)	2.520(5)	C(11)-C(15)	1.409(7)
Zr(3)-C(21)	2.524(5)	C(11)-C(12)	1.424(7)
Zr(3)-C(25)	2.530(5)	C(11)-C(16)	1.498(7)
Zr(3)-Cl(2)	2.6239(12)	C(12)-C(13)	1.414(7)
Zr(3)-Zr(4)	3.5643(6)	C(12)-C(17)	1.507(7)
Zr(3)-H(1)	2.06(4)	C(13)-C(14)	1.417(6)
Zr(3)-H(2)	2.09(5)	C(13)-C(18)	1.515(7)
Zr(3)-H(3)	2.00(4)	C(14)-C(15)	1.391(7)
Zr(3)-H(4)	1.97(5)	C(14)-C(19)	1.494(7)
Zr(4)-C(35)	2.511(4)	C(15)-C(20)	1.527(7)
Zr(4)-C(33)	2.524(4)	C(16)-H(16A)	0.9700
Zr(4)-C(32)	2.530(5)	C(16)-H(16B)	0.9700
Zr(4)-C(34)	2.532(5)	C(16)-H(16C)	0.9700
Zr(4)-C(31)	2.539(4)	C(17)-H(17A)	0.9700
Zr(4)-Cl(2)	2.6241(12)	C(17)-H(17B)	0.9700
Zr(4)-H(5)	1.84(5)	C(17)-H(17C)	0.9700
Zr(4)-H(6)	1.95(4)	C(18)-H(18A)	0.9700

C(18)-H(18B)	0.9700	C(36)-H(36B)	0.9700
C(18)-H(18C)	0.9700	C(36)-H(36C)	0.9700
C(19)-H(19A)	0.9700	C(37)-H(37A)	0.9700
C(19)-H(19B)	0.9700	C(37)-H(37B)	0.9700
C(19)-H(19C)	0.9700	C(37)-H(37C)	0.9700
C(20)-H(20A)	0.9700	C(38)-H(38A)	0.9700
C(20)-H(20B)	0.9700	C(38)-H(38B)	0.9700
C(20)-H(20C)	0.9700	C(38)-H(38C)	0.9700
C(21)-C(25)	1.390(8)	C(39)-H(39A)	0.9700
C(21)-C(22)	1.414(8)	C(39)-H(39B)	0.9700
C(21)-C(26)	1.513(8)	C(39)-H(39C)	0.9700
C(22)-C(23)	1.407(7)	C(40)-H(40A)	0.9700
C(22)-C(27)	1.494(7)	C(40)-H(40B)	0.9700
C(23)-C(24)	1.401(7)	C(40)-H(40C)	0.9700
C(23)-C(28)	1.512(8)	C(41)-C(47)	1.379(7)
C(24)-C(25)	1.401(8)	C(41)-C(42)	1.3899
C(24)-C(29)	1.529(7)	C(41)-C(46)	1.3900
C(25)-C(30)	1.520(8)	C(42)-C(43)	1.3900
C(26)-H(26A)	0.9700	C(42)-H(42A)	0.9400
C(26)-H(26B)	0.9700	C(43)-C(44)	1.3900
C(26)-H(26C)	0.9700	C(43)-H(43A)	0.9400
C(27)-H(27A)	0.9700	C(44)-C(45)	1.3899
C(27)-H(27B)	0.9700	C(44)-H(44A)	0.9400
C(27)-H(27C)	0.9700	C(45)-C(46)	1.3900
C(28)-H(28A)	0.9700	C(45)-H(45A)	0.9400
C(28)-H(28B)	0.9700	C(46)-H(46A)	0.9400
C(28)-H(28C)	0.9700	C(47)-H(47A)	0.9700
C(29)-H(29A)	0.9700	C(47)-H(47B)	0.9700
C(29)-H(29B)	0.9700	C(47)-H(47C)	0.9700
C(29)-H(29C)	0.9700	C(48)-C(54)	1.343(11)
C(30)-H(30A)	0.9700	C(48)-C(53)	1.3898
C(30)-H(30B)	0.9700	C(48)-C(49)	1.3901
C(30)-H(30C)	0.9700	C(49)-C(50)	1.3900
C(31)-C(35)	1.414(6)	C(49)-H(49A)	0.9400
C(31)-C(32)	1.436(7)	C(50)-C(51)	1.3900
C(31)-C(36)	1.504(7)	C(50)-H(50A)	0.9400
C(32)-C(33)	1.407(7)	C(51)-C(52)	1.3900
C(32)-C(37)	1.516(7)	C(51)-H(51A)	0.9400
C(33)-C(34)	1.412(7)	C(52)-C(53)	1.3901
C(33)-C(38)	1.491(7)	C(52)-H(52A)	0.9400
C(34)-C(35)	1.432(7)	C(53)-H(53A)	0.9400
C(34)-C(39)	1.501(7)	C(54)-H(54A)	0.9700
C(35)-C(40)	1.489(5)	C(54)-H(54B)	0.9700
C(36)-H(36A)	0.9700	C(54)-H(54C)	0.9700

C(1)-Zr(1)-C(2)	32.74(15)	C(1)-Zr(1)-C(3)	54.27(16)

C(2)-Zr(1)-C(3)	32.90(16)	C(5)-Zr(1)-H(2)	80.7(17)
C(1)-Zr(1)-C(5)	32.76(15)	C(4)-Zr(1)-H(2)	101.6(17)
C(2)-Zr(1)-C(5)	53.89(15)	Cl(1)-Zr(1)-H(2)	83.2(17)
C(3)-Zr(1)-C(5)	53.49(16)	Zr(3)-Zr(1)-H(2)	38.2(17)
C(1)-Zr(1)-C(4)	54.20(15)	Zr(4)-Zr(1)-H(2)	108.8(17)
C(2)-Zr(1)-C(4)	53.86(15)	Zr(2)-Zr(1)-H(2)	72.8(17)
C(3)-Zr(1)-C(4)	31.95(17)	H(1)-Zr(1)-H(2)	55(2)
C(5)-Zr(1)-C(4)	32.44(16)	C(1)-Zr(1)-H(7)	124.2(13)
C(1)-Zr(1)-Cl(1)	137.03(11)	C(2)-Zr(1)-H(7)	92.2(13)
C(2)-Zr(1)-Cl(1)	128.98(12)	C(3)-Zr(1)-H(7)	84.6(13)
C(3)-Zr(1)-Cl(1)	96.15(12)	C(5)-Zr(1)-H(7)	138.1(13)
C(5)-Zr(1)-Cl(1)	105.81(11)	C(4)-Zr(1)-H(7)	109.7(13)
C(4)-Zr(1)-Cl(1)	83.92(11)	Cl(1)-Zr(1)-H(7)	74.9(12)
C(1)-Zr(1)-Zr(3)	113.38(11)	Zr(3)-Zr(1)-H(7)	107.6(13)
C(2)-Zr(1)-Zr(3)	138.76(12)	Zr(4)-Zr(1)-H(7)	39.5(13)
C(3)-Zr(1)-Zr(3)	166.94(12)	Zr(2)-Zr(1)-H(7)	67.0(13)
C(5)-Zr(1)-Zr(3)	114.19(12)	H(1)-Zr(1)-H(7)	120.5(18)
C(4)-Zr(1)-Zr(3)	139.71(13)	H(2)-Zr(1)-H(7)	139(2)
Cl(1)-Zr(1)-Zr(3)	91.55(3)	C(1)-Zr(1)-H(8)	87.3(13)
C(1)-Zr(1)-Zr(4)	129.12(11)	C(2)-Zr(1)-H(8)	72.6(13)
C(2)-Zr(1)-Zr(4)	109.86(11)	C(3)-Zr(1)-H(8)	95.6(13)
C(3)-Zr(1)-Zr(4)	118.83(13)	C(5)-Zr(1)-H(8)	120.0(13)
C(5)-Zr(1)-Zr(4)	161.75(11)	C(4)-Zr(1)-H(8)	125.4(13)
C(4)-Zr(1)-Zr(4)	148.38(14)	Cl(1)-Zr(1)-H(8)	130.0(13)
Cl(1)-Zr(1)-Zr(4)	91.03(3)	Zr(3)-Zr(1)-H(8)	87.5(13)
Zr(3)-Zr(1)-Zr(4)	71.402(15)	Zr(4)-Zr(1)-H(8)	41.8(13)
C(1)-Zr(1)-Zr(2)	167.31(11)	Zr(2)-Zr(1)-H(8)	95.4(13)
C(2)-Zr(1)-Zr(2)	159.22(11)	H(1)-Zr(1)-H(8)	69.3(18)
C(3)-Zr(1)-Zr(2)	137.34(12)	H(2)-Zr(1)-H(8)	121(2)
C(5)-Zr(1)-Zr(2)	143.50(11)	H(7)-Zr(1)-H(8)	58.1(18)
C(4)-Zr(1)-Zr(2)	131.01(11)	C(14)-Zr(2)-C(13)	32.68(14)
Cl(1)-Zr(1)-Zr(2)	47.28(3)	C(14)-Zr(2)-C(15)	32.05(15)
Zr(3)-Zr(1)-Zr(2)	54.538(13)	C(13)-Zr(2)-C(15)	53.63(15)
Zr(4)-Zr(1)-Zr(2)	54.400(12)	C(14)-Zr(2)-C(11)	53.64(15)
C(1)-Zr(1)-H(1)	75.3(14)	C(13)-Zr(2)-C(11)	53.94(16)
C(2)-Zr(1)-H(1)	97.3(13)	C(15)-Zr(2)-C(11)	32.33(15)
C(3)-Zr(1)-H(1)	128.3(14)	C(14)-Zr(2)-C(12)	53.75(15)
C(5)-Zr(1)-H(1)	90.7(14)	C(13)-Zr(2)-C(12)	32.44(16)
C(4)-Zr(1)-H(1)	123.1(14)	C(15)-Zr(2)-C(12)	53.58(16)
Cl(1)-Zr(1)-H(1)	132.1(13)	C(11)-Zr(2)-C(12)	32.61(16)
Zr(3)-Zr(1)-H(1)	41.5(13)	C(14)-Zr(2)-Cl(1)	130.50(11)
Zr(4)-Zr(1)-H(1)	82.8(13)	C(13)-Zr(2)-Cl(1)	97.88(11)
Zr(2)-Zr(1)-H(1)	94.1(14)	C(15)-Zr(2)-Cl(1)	133.99(12)
C(1)-Zr(1)-H(2)	95.2(17)	C(11)-Zr(2)-Cl(1)	102.60(12)
C(2)-Zr(1)-H(2)	127.9(17)	C(12)-Zr(2)-Cl(1)	82.66(12)
C(3)-Zr(1)-H(2)	132.4(17)	C(14)-Zr(2)-Zr(4)	137.17(11)

C(13)-Zr(2)-Zr(4)	167.40(11)	Zr(3)-Zr(2)-H(5)	85.1(13)
C(15)-Zr(2)-Zr(4)	113.81(11)	Zr(1)-Zr(2)-H(5)	88.7(14)
C(11)-Zr(2)-Zr(4)	115.52(11)	H(3)-Zr(2)-H(5)	125.0(18)
C(12)-Zr(2)-Zr(4)	142.06(12)	H(4)-Zr(2)-H(5)	68.9(19)
Cl(1)-Zr(2)-Zr(4)	91.14(3)	C(14)-Zr(2)-H(6)	128.1(14)
C(14)-Zr(2)-Zr(3)	110.99(11)	C(13)-Zr(2)-H(6)	134.6(13)
C(13)-Zr(2)-Zr(3)	116.91(12)	C(15)-Zr(2)-H(6)	96.0(14)
C(15)-Zr(2)-Zr(3)	132.07(11)	C(11)-Zr(2)-H(6)	82.1(13)
C(11)-Zr(2)-Zr(3)	163.88(11)	C(12)-Zr(2)-H(6)	103.6(13)
C(12)-Zr(2)-Zr(3)	145.78(12)	Cl(1)-Zr(2)-H(6)	79.7(13)
Cl(1)-Zr(2)-Zr(3)	91.50(3)	Zr(4)-Zr(2)-H(6)	38.7(13)
Zr(4)-Zr(2)-Zr(3)	71.374(14)	Zr(3)-Zr(2)-H(6)	108.5(13)
C(14)-Zr(2)-Zr(1)	161.20(11)	Zr(1)-Zr(2)-H(6)	70.6(13)
C(13)-Zr(2)-Zr(1)	137.80(11)	H(3)-Zr(2)-H(6)	137.0(19)
C(15)-Zr(2)-Zr(1)	166.51(11)	H(4)-Zr(2)-H(6)	114.2(19)
C(11)-Zr(2)-Zr(1)	141.68(11)	H(5)-Zr(2)-H(6)	49.2(18)
C(12)-Zr(2)-Zr(1)	129.99(11)	C(23)-Zr(3)-C(24)	32.36(17)
Cl(1)-Zr(2)-Zr(1)	47.35(3)	C(23)-Zr(3)-C(22)	32.52(16)
Zr(4)-Zr(2)-Zr(1)	54.466(12)	C(24)-Zr(3)-C(22)	53.49(15)
Zr(3)-Zr(2)-Zr(1)	54.418(13)	C(23)-Zr(3)-C(21)	53.79(17)
C(14)-Zr(2)-H(3)	94.7(13)	C(24)-Zr(3)-C(21)	53.24(17)
C(13)-Zr(2)-H(3)	83.2(13)	C(22)-Zr(3)-C(21)	32.56(18)
C(15)-Zr(2)-H(3)	126.7(13)	C(23)-Zr(3)-C(25)	53.63(17)
C(11)-Zr(2)-H(3)	136.6(13)	C(24)-Zr(3)-C(25)	32.22(18)
C(12)-Zr(2)-H(3)	106.3(13)	C(22)-Zr(3)-C(25)	53.47(17)
Cl(1)-Zr(2)-H(3)	74.4(13)	C(21)-Zr(3)-C(25)	31.93(18)
Zr(4)-Zr(2)-H(3)	107.9(12)	C(23)-Zr(3)-Cl(2)	97.57(12)
Zr(3)-Zr(2)-H(3)	40.2(12)	C(24)-Zr(3)-Cl(2)	82.89(11)
Zr(1)-Zr(2)-H(3)	66.5(13)	C(22)-Zr(3)-Cl(2)	130.06(12)
C(14)-Zr(2)-H(4)	80.2(14)	C(21)-Zr(3)-Cl(2)	133.95(14)
C(13)-Zr(2)-H(4)	102.0(14)	C(25)-Zr(3)-Cl(2)	102.91(15)
C(15)-Zr(2)-H(4)	93.8(14)	C(23)-Zr(3)-Zr(1)	167.50(12)
C(11)-Zr(2)-H(4)	126.1(14)	C(24)-Zr(3)-Zr(1)	141.50(14)
C(12)-Zr(2)-H(4)	132.7(14)	C(22)-Zr(3)-Zr(1)	137.85(13)
Cl(1)-Zr(2)-H(4)	130.0(14)	C(21)-Zr(3)-Zr(1)	113.82(13)
Zr(4)-Zr(2)-H(4)	78.5(13)	C(25)-Zr(3)-Zr(1)	115.53(13)
Zr(3)-Zr(2)-H(4)	38.7(14)	Cl(2)-Zr(3)-Zr(1)	90.92(3)
Zr(1)-Zr(2)-H(4)	90.2(14)	C(23)-Zr(3)-Zr(2)	117.67(13)
H(3)-Zr(2)-H(4)	63.3(18)	C(24)-Zr(3)-Zr(2)	146.65(14)
C(14)-Zr(2)-H(5)	102.5(14)	C(22)-Zr(3)-Zr(2)	111.38(12)
C(13)-Zr(2)-H(5)	133.4(14)	C(21)-Zr(3)-Zr(2)	132.48(14)
C(15)-Zr(2)-H(5)	80.7(14)	C(25)-Zr(3)-Zr(2)	163.94(13)
C(11)-Zr(2)-H(5)	93.4(13)	Cl(2)-Zr(3)-Zr(2)	91.30(3)
C(12)-Zr(2)-H(5)	126.0(13)	Zr(1)-Zr(3)-Zr(2)	71.044(15)
Cl(1)-Zr(2)-H(5)	123.5(14)	C(23)-Zr(3)-Zr(4)	137.69(12)
Zr(4)-Zr(2)-H(5)	34.8(14)	C(24)-Zr(3)-Zr(4)	130.08(11)

C(22)-Zr(3)-Zr(4)	161.02(14)	H(2)-Zr(3)-H(4)	118.9(18)
C(21)-Zr(3)-Zr(4)	166.25(14)	H(3)-Zr(3)-H(4)	63.3(18)
C(25)-Zr(3)-Zr(4)	141.79(13)	C(35)-Zr(4)-C(33)	54.38(15)
Cl(2)-Zr(3)-Zr(4)	47.22(3)	C(35)-Zr(4)-C(32)	54.10(15)
Zr(1)-Zr(3)-Zr(4)	54.302(12)	C(33)-Zr(4)-C(32)	32.33(17)
Zr(2)-Zr(3)-Zr(4)	54.223(12)	C(35)-Zr(4)-C(34)	32.98(15)
C(23)-Zr(3)-H(1)	135.8(13)	C(33)-Zr(4)-C(34)	32.43(16)
C(24)-Zr(3)-H(1)	104.3(13)	C(32)-Zr(4)-C(34)	53.60(16)
C(22)-Zr(3)-H(1)	130.8(13)	C(35)-Zr(4)-C(31)	32.51(15)
C(21)-Zr(3)-H(1)	98.2(13)	C(33)-Zr(4)-C(31)	54.25(15)
C(25)-Zr(3)-H(1)	84.1(13)	C(32)-Zr(4)-C(31)	32.91(16)
Cl(2)-Zr(3)-H(1)	77.8(12)	C(34)-Zr(4)-C(31)	54.04(15)
Zr(1)-Zr(3)-H(1)	37.6(13)	C(35)-Zr(4)-Cl(2)	136.69(11)
Zr(2)-Zr(3)-H(1)	106.5(13)	C(33)-Zr(4)-Cl(2)	97.07(12)
Zr(4)-Zr(3)-H(1)	68.2(12)	C(32)-Zr(4)-Cl(2)	84.03(11)
C(23)-Zr(3)-H(2)	142.0(12)	C(34)-Zr(4)-Cl(2)	129.48(12)
C(24)-Zr(3)-H(2)	131.0(13)	C(31)-Zr(4)-Cl(2)	105.54(11)
C(22)-Zr(3)-H(2)	111.5(12)	C(35)-Zr(4)-Zr(2)	112.88(11)
C(21)-Zr(3)-H(2)	88.8(12)	C(33)-Zr(4)-Zr(2)	166.90(11)
C(25)-Zr(3)-H(2)	99.1(13)	C(32)-Zr(4)-Zr(2)	140.22(13)
Cl(2)-Zr(3)-H(2)	115.8(11)	C(34)-Zr(4)-Zr(2)	138.27(12)
Zr(1)-Zr(3)-H(2)	26.5(12)	C(31)-Zr(4)-Zr(2)	113.82(11)
Zr(2)-Zr(3)-H(2)	80.9(12)	Cl(2)-Zr(4)-Zr(2)	91.45(3)
Zr(4)-Zr(3)-H(2)	80.3(12)	C(35)-Zr(4)-Zr(1)	129.96(11)
H(1)-Zr(3)-H(2)	45.6(16)	C(33)-Zr(4)-Zr(1)	118.45(12)
C(23)-Zr(3)-H(3)	101.7(13)	C(32)-Zr(4)-Zr(1)	148.13(13)
C(24)-Zr(3)-H(3)	131.7(13)	C(34)-Zr(4)-Zr(1)	110.41(11)
C(22)-Zr(3)-H(3)	78.9(13)	C(31)-Zr(4)-Zr(1)	162.38(11)
C(21)-Zr(3)-H(3)	92.0(13)	Cl(2)-Zr(4)-Zr(1)	90.91(3)
C(25)-Zr(3)-H(3)	123.9(13)	Zr(2)-Zr(4)-Zr(1)	71.133(14)
Cl(2)-Zr(3)-H(3)	132.0(13)	C(35)-Zr(4)-Zr(3)	166.44(11)
Zr(1)-Zr(3)-H(3)	78.9(13)	C(33)-Zr(4)-Zr(3)	137.92(11)
Zr(2)-Zr(3)-H(3)	41.0(13)	C(32)-Zr(4)-Zr(3)	131.08(11)
Zr(4)-Zr(3)-H(3)	92.1(13)	C(34)-Zr(4)-Zr(3)	159.94(11)
H(1)-Zr(3)-H(3)	113.9(18)	C(31)-Zr(4)-Zr(3)	142.87(11)
H(2)-Zr(3)-H(3)	69.8(18)	Cl(2)-Zr(4)-Zr(3)	47.22(3)
C(23)-Zr(3)-H(4)	85.7(14)	Zr(2)-Zr(4)-Zr(3)	54.403(12)
C(24)-Zr(3)-H(4)	109.5(14)	Zr(1)-Zr(4)-Zr(3)	54.296(12)
C(22)-Zr(3)-H(4)	95.8(14)	C(35)-Zr(4)-H(5)	94.7(14)
C(21)-Zr(3)-H(4)	128.1(13)	C(33)-Zr(4)-H(5)	134.1(14)
C(25)-Zr(3)-H(4)	139.0(14)	C(32)-Zr(4)-H(5)	103.3(14)
Cl(2)-Zr(3)-H(4)	75.1(13)	C(34)-Zr(4)-H(5)	127.7(14)
Zr(1)-Zr(3)-H(4)	105.5(14)	C(31)-Zr(4)-H(5)	81.2(14)
Zr(2)-Zr(3)-H(4)	38.0(13)	Cl(2)-Zr(4)-H(5)	83.7(14)
Zr(4)-Zr(3)-H(4)	65.2(14)	Zr(2)-Zr(4)-H(5)	37.0(14)
H(1)-Zr(3)-H(4)	133.0(19)	Zr(1)-Zr(4)-H(5)	107.4(14)

Zr(3)-Zr(4)-H(5)	72.2(14)	C(3)-C(2)-Zr(1)	73.9(3)
C(35)-Zr(4)-H(6)	75.9(13)	C(7)-C(2)-Zr(1)	124.9(3)
C(33)-Zr(4)-H(6)	129.1(13)	C(4)-C(3)-C(2)	108.6(5)
C(32)-Zr(4)-H(6)	122.9(13)	C(4)-C(3)-C(8)	124.9(5)
C(34)-Zr(4)-H(6)	98.7(13)	C(2)-C(3)-C(8)	126.1(6)
C(31)-Zr(4)-H(6)	90.1(13)	C(4)-C(3)-Zr(1)	74.9(3)
Cl(2)-Zr(4)-H(6)	129.6(13)	C(2)-C(3)-Zr(1)	73.2(3)
Zr(2)-Zr(4)-H(6)	39.7(13)	C(8)-C(3)-Zr(1)	123.6(4)
Zr(1)-Zr(4)-H(6)	84.0(14)	C(3)-C(4)-C(5)	108.1(4)
Zr(3)-Zr(4)-H(6)	92.8(13)	C(3)-C(4)-C(9)	127.3(5)
H(5)-Zr(4)-H(6)	51.1(19)	C(5)-C(4)-C(9)	124.3(5)
C(35)-Zr(4)-H(7)	88.5(13)	C(3)-C(4)-Zr(1)	73.2(3)
C(33)-Zr(4)-H(7)	101.0(13)	C(5)-C(4)-Zr(1)	73.7(3)
C(32)-Zr(4)-H(7)	130.3(13)	C(9)-C(4)-Zr(1)	123.2(3)
C(34)-Zr(4)-H(7)	77.1(13)	C(4)-C(5)-C(1)	108.1(4)
C(31)-Zr(4)-H(7)	121.0(13)	C(4)-C(5)-C(10)	127.0(5)
Cl(2)-Zr(4)-H(7)	132.1(13)	C(1)-C(5)-C(10)	124.5(5)
Zr(2)-Zr(4)-H(7)	80.2(13)	C(4)-C(5)-Zr(1)	73.9(3)
Zr(1)-Zr(4)-H(7)	41.7(13)	C(1)-C(5)-Zr(1)	72.5(2)
Zr(3)-Zr(4)-H(7)	93.2(13)	C(10)-C(5)-Zr(1)	125.7(3)
H(5)-Zr(4)-H(7)	112.1(19)	C(1)-C(6)-H(6A)	109.5
H(6)-Zr(4)-H(7)	64.7(19)	C(1)-C(6)-H(6B)	109.5
C(35)-Zr(4)-H(8)	117.9(12)	H(6A)-C(6)-H(6B)	109.5
C(33)-Zr(4)-H(8)	79.7(12)	C(1)-C(6)-H(6C)	109.5
C(32)-Zr(4)-H(8)	106.8(12)	H(6A)-C(6)-H(6C)	109.5
C(34)-Zr(4)-H(8)	85.8(12)	H(6B)-C(6)-H(6C)	109.5
C(31)-Zr(4)-H(8)	133.8(12)	C(2)-C(7)-H(7A)	109.5
Cl(2)-Zr(4)-H(8)	81.3(13)	C(2)-C(7)-H(7B)	109.5
Zr(2)-Zr(4)-H(8)	111.6(12)	H(7A)-C(7)-H(7B)	109.5
Zr(1)-Zr(4)-H(8)	41.4(12)	C(2)-C(7)-H(7C)	109.5
Zr(3)-Zr(4)-H(8)	74.1(12)	H(7A)-C(7)-H(7C)	109.5
H(5)-Zr(4)-H(8)	144.6(19)	H(7B)-C(7)-H(7C)	109.5
H(6)-Zr(4)-H(8)	121.1(18)	C(3)-C(8)-H(8A)	109.5
H(7)-Zr(4)-H(8)	59.3(18)	C(3)-C(8)-H(8B)	109.5
Zr(2)-Cl(1)-Zr(1)	85.37(3)	H(8A)-C(8)-H(8B)	109.5
Zr(3)-Cl(2)-Zr(4)	85.56(3)	C(3)-C(8)-H(8C)	109.5
C(2)-C(1)-C(5)	107.5(4)	H(8A)-C(8)-H(8C)	109.5
C(2)-C(1)-C(6)	125.2(5)	H(8B)-C(8)-H(8C)	109.5
C(5)-C(1)-C(6)	126.7(5)	C(4)-C(9)-H(9A)	109.5
C(2)-C(1)-Zr(1)	73.7(3)	C(4)-C(9)-H(9B)	109.5
C(5)-C(1)-Zr(1)	74.8(3)	H(9A)-C(9)-H(9B)	109.5
C(6)-C(1)-Zr(1)	124.1(3)	C(4)-C(9)-H(9C)	109.5
C(1)-C(2)-C(3)	107.7(4)	H(9A)-C(9)-H(9C)	109.5
C(1)-C(2)-C(7)	124.3(5)	H(9B)-C(9)-H(9C)	109.5
C(3)-C(2)-C(7)	127.5(5)	C(5)-C(10)-H(10A)	109.5
C(1)-C(2)-Zr(1)	73.5(3)	C(5)-C(10)-H(10B)	109.5

H(10A)-C(10)-H(10B)	109.5	C(13)-C(18)-H(18A)	109.5
C(5)-C(10)-H(10C)	109.5	C(13)-C(18)-H(18B)	109.5
H(10A)-C(10)-H(10C)	109.5	H(18A)-C(18)-H(18B)	109.5
H(10B)-C(10)-H(10C)	109.5	C(13)-C(18)-H(18C)	109.5
C(15)-C(11)-C(12)	107.4(4)	H(18A)-C(18)-H(18C)	109.5
C(15)-C(11)-C(16)	127.1(5)	H(18B)-C(18)-H(18C)	109.5
C(12)-C(11)-C(16)	125.1(5)	C(14)-C(19)-H(19A)	109.5
C(15)-C(11)-Zr(2)	73.6(3)	C(14)-C(19)-H(19B)	109.5
C(12)-C(11)-Zr(2)	73.8(3)	H(19A)-C(19)-H(19B)	109.5
C(16)-C(11)-Zr(2)	124.6(3)	C(14)-C(19)-H(19C)	109.5
C(13)-C(12)-C(11)	107.9(4)	H(19A)-C(19)-H(19C)	109.5
C(13)-C(12)-C(17)	126.9(5)	H(19B)-C(19)-H(19C)	109.5
C(11)-C(12)-C(17)	124.7(5)	C(15)-C(20)-H(20A)	109.5
C(13)-C(12)-Zr(2)	73.3(3)	C(15)-C(20)-H(20B)	109.5
C(11)-C(12)-Zr(2)	73.6(3)	H(20A)-C(20)-H(20B)	109.5
C(17)-C(12)-Zr(2)	125.1(3)	C(15)-C(20)-H(20C)	109.5
C(12)-C(13)-C(14)	107.4(4)	H(20A)-C(20)-H(20C)	109.5
C(12)-C(13)-C(18)	123.8(5)	H(20B)-C(20)-H(20C)	109.5
C(14)-C(13)-C(18)	128.5(5)	C(25)-C(21)-C(22)	108.2(5)
C(12)-C(13)-Zr(2)	74.2(3)	C(25)-C(21)-C(26)	126.5(6)
C(14)-C(13)-Zr(2)	73.1(2)	C(22)-C(21)-C(26)	124.8(6)
C(18)-C(13)-Zr(2)	123.7(3)	C(25)-C(21)-Zr(3)	74.3(3)
C(15)-C(14)-C(13)	108.6(4)	C(22)-C(21)-Zr(3)	73.5(3)
C(15)-C(14)-C(19)	125.1(5)	C(26)-C(21)-Zr(3)	124.5(4)
C(13)-C(14)-C(19)	125.7(5)	C(23)-C(22)-C(21)	107.5(5)
C(15)-C(14)-Zr(2)	74.6(3)	C(23)-C(22)-C(27)	127.6(6)
C(13)-C(14)-Zr(2)	74.2(3)	C(21)-C(22)-C(27)	124.4(6)
C(19)-C(14)-Zr(2)	124.7(3)	C(23)-C(22)-Zr(3)	73.2(3)
C(14)-C(15)-C(11)	108.8(4)	C(21)-C(22)-Zr(3)	73.9(3)
C(14)-C(15)-C(20)	125.0(5)	C(27)-C(22)-Zr(3)	125.0(4)
C(11)-C(15)-C(20)	125.8(5)	C(24)-C(23)-C(22)	107.7(5)
C(14)-C(15)-Zr(2)	73.3(3)	C(24)-C(23)-C(28)	124.2(5)
C(11)-C(15)-Zr(2)	74.1(3)	C(22)-C(23)-C(28)	127.5(5)
C(20)-C(15)-Zr(2)	125.2(3)	C(24)-C(23)-Zr(3)	74.3(3)
C(11)-C(16)-H(16A)	109.5	C(22)-C(23)-Zr(3)	74.2(3)
C(11)-C(16)-H(16B)	109.5	C(28)-C(23)-Zr(3)	123.9(4)
H(16A)-C(16)-H(16B)	109.5	C(25)-C(24)-C(23)	108.4(5)
C(11)-C(16)-H(16C)	109.5	C(25)-C(24)-C(29)	125.8(6)
H(16A)-C(16)-H(16C)	109.5	C(23)-C(24)-C(29)	125.3(6)
H(16B)-C(16)-H(16C)	109.5	C(25)-C(24)-Zr(3)	74.3(3)
C(12)-C(17)-H(17A)	109.5	C(23)-C(24)-Zr(3)	73.3(3)
C(12)-C(17)-H(17B)	109.5	C(29)-C(24)-Zr(3)	124.8(3)
H(17A)-C(17)-H(17B)	109.5	C(21)-C(25)-C(24)	108.1(5)
C(12)-C(17)-H(17C)	109.5	C(21)-C(25)-C(30)	127.0(7)
H(17A)-C(17)-H(17C)	109.5	C(24)-C(25)-C(30)	124.5(6)
H(17B)-C(17)-H(17C)	109.5	C(21)-C(25)-Zr(3)	73.8(3)

C(24)-C(25)-Zr(3)	73.5(3)	C(34)-C(33)-C(38)	127.3(5)
C(30)-C(25)-Zr(3)	124.3(4)	C(32)-C(33)-Zr(4)	74.1(3)
C(21)-C(26)-H(26A)	109.5	C(34)-C(33)-Zr(4)	74.1(3)
C(21)-C(26)-H(26B)	109.5	C(38)-C(33)-Zr(4)	123.9(3)
H(26A)-C(26)-H(26B)	109.5	C(33)-C(34)-C(35)	108.0(4)
C(21)-C(26)-H(26C)	109.5	C(33)-C(34)-C(39)	127.2(5)
H(26A)-C(26)-H(26C)	109.5	C(35)-C(34)-C(39)	124.4(5)
H(26B)-C(26)-H(26C)	109.5	C(33)-C(34)-Zr(4)	73.4(3)
C(22)-C(27)-H(27A)	109.5	C(35)-C(34)-Zr(4)	72.7(3)
C(22)-C(27)-H(27B)	109.5	C(39)-C(34)-Zr(4)	125.3(3)
H(27A)-C(27)-H(27B)	109.5	C(31)-C(35)-C(34)	108.1(4)
C(22)-C(27)-H(27C)	109.5	C(31)-C(35)-C(40)	126.5(4)
H(27A)-C(27)-H(27C)	109.5	C(34)-C(35)-C(40)	124.6(4)
H(27B)-C(27)-H(27C)	109.5	C(31)-C(35)-Zr(4)	74.8(3)
C(23)-C(28)-H(28A)	109.5	C(34)-C(35)-Zr(4)	74.3(3)
C(23)-C(28)-H(28B)	109.5	C(40)-C(35)-Zr(4)	124.7(3)
H(28A)-C(28)-H(28B)	109.5	C(31)-C(36)-H(36A)	109.5
C(23)-C(28)-H(28C)	109.5	C(31)-C(36)-H(36B)	109.5
H(28A)-C(28)-H(28C)	109.5	H(36A)-C(36)-H(36B)	109.5
H(28B)-C(28)-H(28C)	109.5	C(31)-C(36)-H(36C)	109.5
C(24)-C(29)-H(29A)	109.5	H(36A)-C(36)-H(36C)	109.5
C(24)-C(29)-H(29B)	109.5	H(36B)-C(36)-H(36C)	109.5
H(29A)-C(29)-H(29B)	109.5	C(32)-C(37)-H(37A)	109.5
C(24)-C(29)-H(29C)	109.5	C(32)-C(37)-H(37B)	109.5
H(29A)-C(29)-H(29C)	109.5	H(37A)-C(37)-H(37B)	109.5
H(29B)-C(29)-H(29C)	109.5	C(32)-C(37)-H(37C)	109.5
C(25)-C(30)-H(30A)	109.5	H(37A)-C(37)-H(37C)	109.5
C(25)-C(30)-H(30B)	109.5	H(37B)-C(37)-H(37C)	109.5
H(30A)-C(30)-H(30B)	109.5	C(33)-C(38)-H(38A)	109.5
C(25)-C(30)-H(30C)	109.5	C(33)-C(38)-H(38B)	109.5
H(30A)-C(30)-H(30C)	109.5	H(38A)-C(38)-H(38B)	109.5
H(30B)-C(30)-H(30C)	109.5	C(33)-C(38)-H(38C)	109.5
C(35)-C(31)-C(32)	107.1(4)	H(38A)-C(38)-H(38C)	109.5
C(35)-C(31)-C(36)	125.8(5)	H(38B)-C(38)-H(38C)	109.5
C(32)-C(31)-C(36)	126.5(5)	C(34)-C(39)-H(39A)	109.5
C(35)-C(31)-Zr(4)	72.7(3)	C(34)-C(39)-H(39B)	109.5
C(32)-C(31)-Zr(4)	73.2(3)	H(39A)-C(39)-H(39B)	109.5
C(36)-C(31)-Zr(4)	126.4(3)	C(34)-C(39)-H(39C)	109.5
C(33)-C(32)-C(31)	108.6(4)	H(39A)-C(39)-H(39C)	109.5
C(33)-C(32)-C(37)	125.3(5)	H(39B)-C(39)-H(39C)	109.5
C(31)-C(32)-C(37)	125.8(5)	C(35)-C(40)-H(40A)	109.5
C(33)-C(32)-Zr(4)	73.6(3)	C(35)-C(40)-H(40B)	109.5
C(31)-C(32)-Zr(4)	73.9(3)	H(40A)-C(40)-H(40B)	109.5
C(37)-C(32)-Zr(4)	123.7(3)	C(35)-C(40)-H(40C)	109.5
C(32)-C(33)-C(34)	108.1(4)	H(40A)-C(40)-H(40C)	109.5
C(32)-C(33)-C(38)	124.1(5)	H(40B)-C(40)-H(40C)	109.5

C(47)-C(41)-C(42)	114.7(3)	C(54)-C(48)-C(53)	110.5(7)
C(47)-C(41)-C(46)	125.2(3)	C(54)-C(48)-C(49)	129.5(7)
C(42)-C(41)-C(46)	120.0	C(53)-C(48)-C(49)	120.0
C(41)-C(42)-C(43)	120.0	C(50)-C(49)-C(48)	120.0
C(41)-C(42)-H(42A)	120.0	C(50)-C(49)-H(49A)	120.0
C(43)-C(42)-H(42A)	120.0	C(48)-C(49)-H(49A)	120.0
C(42)-C(43)-C(44)	120.0	C(51)-C(50)-C(49)	120.0
C(42)-C(43)-H(43A)	120.0	C(51)-C(50)-H(50A)	120.0
C(44)-C(43)-H(43A)	120.0	C(49)-C(50)-H(50A)	120.0
C(45)-C(44)-C(43)	120.0	C(52)-C(51)-C(50)	120.0
C(45)-C(44)-H(44A)	120.0	C(52)-C(51)-H(51A)	120.0
C(43)-C(44)-H(44A)	120.0	C(50)-C(51)-H(51A)	120.0
C(44)-C(45)-C(46)	120.0	C(51)-C(52)-C(53)	120.0
C(44)-C(45)-H(45A)	120.0	C(51)-C(52)-H(52A)	120.0
C(46)-C(45)-H(45A)	120.0	C(53)-C(52)-H(52A)	120.0
C(45)-C(46)-C(41)	120.0	C(48)-C(53)-C(52)	120.0
C(45)-C(46)-H(46A)	120.0	C(48)-C(53)-H(53A)	120.0
C(41)-C(46)-H(46A)	120.0	C(52)-C(53)-H(53A)	120.0
C(41)-C(47)-H(47A)	109.5	C(48)-C(54)-H(54A)	109.5
C(41)-C(47)-H(47B)	109.5	C(48)-C(54)-H(54B)	109.5
H(47A)-C(47)-H(47B)	109.5	H(54A)-C(54)-H(54B)	109.5
C(41)-C(47)-H(47C)	109.5	C(48)-C(54)-H(54C)	109.5
H(47A)-C(47)-H(47C)	109.5	H(54A)-C(54)-H(54C)	109.5
H(47B)-C(47)-H(47C)	109.5	H(54B)-C(54)-H(54C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S3. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[(\mu_2\text{-H})_8(\mu_2\text{-Cl})_2(Cp^*Zr)_4]\cdot 2(C_7H_8)$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zr(1)	31(1)	31(1)	36(1)	-3(1)	-5(1)	-2(1)
Zr(2)	30(1)	30(1)	31(1)	-1(1)	-2(1)	1(1)
Zr(3)	31(1)	30(1)	34(1)	2(1)	-1(1)	1(1)
Zr(4)	30(1)	30(1)	33(1)	1(1)	1(1)	-1(1)
Cl(1)	33(1)	39(1)	47(1)	-7(1)	-7(1)	4(1)
Cl(2)	33(1)	39(1)	44(1)	4(1)	3(1)	4(1)
C(1)	37(3)	34(3)	46(3)	-9(2)	-12(2)	-2(2)
C(2)	41(3)	44(3)	41(3)	-8(2)	-5(2)	-11(2)
C(3)	55(3)	32(3)	58(3)	-5(2)	-31(3)	-2(2)
C(4)	30(3)	51(3)	58(3)	-22(3)	-15(2)	4(2)
C(5)	33(3)	43(3)	47(3)	-9(2)	-5(2)	-10(2)
C(6)	62(4)	42(3)	75(4)	-19(3)	-18(3)	8(3)
C(7)	67(4)	86(5)	58(4)	-20(3)	9(3)	-27(4)
C(8)	112(6)	50(4)	91(5)	3(3)	-63(4)	-1(4)
C(9)	40(3)	76(5)	111(5)	-45(4)	-20(3)	16(3)
C(10)	58(4)	81(5)	67(4)	-6(3)	3(3)	-35(3)
C(11)	58(3)	30(3)	37(3)	-3(2)	-4(2)	3(2)
C(12)	48(3)	42(3)	44(3)	-14(2)	-9(2)	13(2)
C(13)	41(3)	41(3)	35(2)	-10(2)	1(2)	1(2)
C(14)	41(3)	38(3)	33(2)	-8(2)	-5(2)	7(2)
C(15)	46(3)	38(3)	36(3)	-9(2)	0(2)	-4(2)
C(16)	136(6)	35(3)	54(4)	3(3)	-4(4)	0(4)
C(17)	55(4)	75(4)	84(4)	-27(4)	-24(3)	27(3)
C(18)	58(4)	66(4)	65(4)	-10(3)	25(3)	-1(3)
C(19)	70(4)	65(4)	38(3)	-4(3)	-11(3)	13(3)
C(20)	55(3)	70(4)	68(4)	-21(3)	-1(3)	-18(3)
C(21)	48(3)	52(3)	64(4)	26(3)	-10(3)	-10(3)
C(22)	56(3)	53(3)	38(3)	15(2)	14(2)	21(3)
C(23)	51(3)	42(3)	46(3)	15(2)	-12(2)	-5(2)
C(24)	55(3)	48(3)	43(3)	20(3)	14(3)	18(3)
C(25)	85(4)	35(3)	42(3)	6(2)	-9(3)	2(3)
C(26)	57(4)	131(7)	131(7)	75(6)	-27(4)	-35(4)
C(27)	156(7)	80(5)	51(4)	22(3)	42(4)	48(5)
C(28)	103(6)	81(5)	75(4)	22(4)	-45(4)	-12(4)
C(29)	80(5)	106(6)	107(6)	56(5)	37(4)	58(4)
C(30)	263(11)	34(4)	75(5)	-2(3)	-52(6)	2(5)
C(31)	35(3)	39(3)	40(3)	3(2)	4(2)	-7(2)
C(32)	40(3)	44(3)	53(3)	16(2)	14(2)	7(2)
C(33)	52(3)	30(3)	45(3)	2(2)	17(3)	-3(2)
C(34)	46(3)	47(3)	37(3)	7(2)	-1(2)	-9(2)
C(35)	29(2)	33(3)	47(3)	6(2)	2(2)	-2(2)

C(36)	48(3)	66(4)	55(3)	-1(3)	1(3)	-22(3)
C(37)	40(3)	87(5)	95(5)	45(4)	23(3)	25(3)
C(38)	105(5)	51(4)	76(4)	-14(3)	43(4)	-9(4)
C(39)	73(4)	82(5)	42(3)	17(3)	-11(3)	-33(3)
C(40)	53(3)	37(3)	75(4)	12(3)	20(3)	5(2)

The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

Table S4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for $[(\mu_2\text{-H})_8(\mu_2\text{-Cl})_2(\text{Cp*Zr})_4]\cdot 2(C_7H_8)$.

	x	y	z	U(eq)
H(6A)	2200	11775	7116	89
H(6B)	1182	11270	7040	89
H(6C)	1569	11475	7573	89
H(7A)	1549	13014	6189	105
H(7B)	2406	12792	6564	105
H(7C)	2172	13795	6428	105
H(8A)	-91	15181	6859	127
H(8B)	-136	14577	6387	127
H(8C)	889	14974	6564	127
H(9A)	-982	14337	7862	114
H(9B)	-1642	13673	7552	114
H(9C)	-1282	14583	7320	114
H(10A)	-763	11785	7697	103
H(10B)	-744	12551	8094	103
H(10C)	152	11875	8055	103
H(16A)	2280	18398	8592	112
H(16B)	1916	17730	8183	112
H(16C)	3061	17833	8293	112
H(17A)	362	17080	8510	107
H(17B)	314	17658	8992	107
H(17C)	-68	16661	8995	107
H(18A)	710	16142	9951	94
H(18B)	1236	15211	9873	94
H(18C)	377	15515	9517	94
H(19A)	2926	15225	9957	87
H(19B)	3481	16133	10064	87
H(19C)	3921	15454	9679	87
H(20A)	4629	16478	9076	96
H(20B)	4361	17419	9300	96
H(20C)	4334	17278	8728	96
H(26A)	661	11780	9443	160
H(26B)	785	11436	8901	160
H(26C)	484	12439	9001	160
H(27A)	1792	12879	10144	143
H(27B)	1158	13395	9749	143
H(27C)	2158	13813	9946	143
H(28A)	4694	13499	9489	130
H(28B)	4510	12799	9911	130
H(28C)	3895	13697	9898	130
H(29A)	4593	11463	8593	147
H(29B)	4939	11513	9144	147

H(29C)	5060	12353	8800	147
H(30A)	2806	10495	8657	186
H(30B)	3063	11156	8226	186
H(30C)	1948	11012	8384	186
H(36A)	5865	16966	7612	85
H(36B)	5719	16273	8041	85
H(36C)	4920	17027	7952	85
H(37A)	6018	14045	7377	111
H(37B)	6173	14753	7798	111
H(37C)	6641	14920	7277	111
H(38A)	4735	13538	6843	116
H(38B)	5233	14112	6426	116
H(38C)	4075	13946	6421	116
H(39A)	3357	15752	6141	99
H(39B)	2537	16032	6524	99
H(39C)	2717	15012	6406	99
H(40A)	2790	17046	7066	83
H(40B)	3813	17532	6975	83
H(40C)	3445	17356	7514	83
H(42A)	1006	15384	11008	128
H(43A)	1684	13957	11021	193
H(44A)	3389	13772	11097	141
H(45A)	4416	15013	11160	148
H(46A)	3739	16439	11147	108
H(47A)	1117	16758	11026	246
H(47B)	2048	17175	10760	246
H(47C)	1972	17207	11336	246
H(49A)	1377	10761	10230	401
H(50A)	459	9455	10149	401
H(51A)	1233	8143	9904	353
H(52A)	2924	8136	9740	306
H(53A)	3842	9441	9820	355
H(54A)	3026	11434	10165	464
H(54B)	3671	10983	9751	464
H(54C)	3861	10738	10305	464

Table S5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for [(μ_2-H)$_6$(Cp*Zr)$_4$]

	x	y	z	U(eq)
Zr(1)	7618(1)	6795(1)	1806(1)	24(1)
Zr(2)	6900(1)	9474(1)	2319(1)	23(1)
Zr(3)	7318(1)	7138(1)	3416(1)	25(1)
Zr(4)	4896(1)	8264(1)	2565(1)	25(1)
C(1)	8900(12)	4591(10)	1389(6)	48(3)
C(2)	9691(11)	5262(12)	1224(7)	50(3)
C(3)	9132(15)	6234(12)	682(7)	61(4)
C(4)	7973(14)	6163(11)	547(6)	54(3)
C(5)	7856(11)	5119(11)	979(6)	45(3)
C(6)	9170(20)	3393(11)	1906(8)	113(7)
C(7)	10974(15)	4930(20)	1509(11)	160(11)
C(8)	9740(20)	7120(16)	284(10)	139(10)
C(9)	7060(20)	7044(16)	4(7)	143(10)
C(10)	6835(14)	4635(16)	956(11)	123(8)
C(11)	6041(10)	11881(9)	1981(7)	40(3)
C(12)	6993(13)	11248(10)	1434(6)	48(3)
C(13)	8178(11)	10695(10)	1706(7)	47(3)
C(14)	8004(11)	10908(10)	2439(7)	44(3)
C(15)	6670(11)	11643(9)	2605(6)	39(3)
C(16)	4614(14)	12710(12)	1893(10)	99(6)
C(17)	6710(20)	11358(15)	656(7)	105(7)
C(18)	9516(14)	10035(13)	1270(10)	102(7)
C(19)	9120(15)	10500(13)	2927(9)	99(7)
C(20)	6028(17)	12192(13)	3323(7)	85(5)
C(21)	9090(11)	5521(12)	4128(6)	47(3)
C(22)	8755(13)	6751(12)	4388(6)	50(3)
C(23)	7483(12)	7181(11)	4717(5)	44(3)
C(24)	7010(12)	6238(12)	4673(5)	45(3)
C(25)	7990(11)	5240(10)	4313(5)	39(3)
C(26)	10424(13)	4666(14)	3785(7)	86(5)
C(27)	9656(17)	7434(17)	4360(9)	110(7)
C(28)	6706(18)	8442(13)	5094(7)	98(6)
C(29)	5682(14)	6267(14)	5002(7)	74(4)
C(30)	7892(15)	3999(12)	4168(7)	73(4)
C(31)	2578(9)	9784(10)	2762(6)	36(2)
C(32)	2692(10)	8657(11)	3215(6)	41(3)
C(33)	3000(11)	7649(10)	2783(7)	45(3)
C(34)	3031(10)	8118(11)	2047(6)	43(3)
C(35)	2785(10)	9436(10)	2042(6)	38(3)
C(36)	2159(11)	11107(10)	3015(7)	52(3)
C(37)	2453(13)	8617(15)	4030(6)	75(4)

C(38)	3212(14)	6254(13)	3036(9)	81(5)
C(39)	3221(13)	7375(15)	1401(7)	75(4)
C(40)	2686(11)	10343(12)	1381(6)	58(4)
H(1)	7630(80)	8450(80)	1540(40)	30
H(2)	8430(80)	5770(80)	2670(40)	30
H(3)	5760(80)	7460(80)	1710(40)	30
H(4)	7500(80)	8990(80)	3430(40)	30
H(5)	5090(80)	9920(80)	2360(40)	30
H(6)	5290(80)	7240(80)	3680(40)	30

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

Table S6. Bond lengths [Å] and angles [°] for $[(\mu_2\text{-H})_6(\text{Cp*Zr})_4]$

Zr(1)-C(2)	2.472(11)	C(3)-C(8)	1.521(17)
Zr(1)-C(1)	2.484(10)	C(4)-C(5)	1.401(16)
Zr(1)-C(4)	2.488(10)	C(4)-C(9)	1.516(17)
Zr(1)-C(3)	2.497(10)	C(5)-C(10)	1.485(16)
Zr(1)-C(5)	2.516(10)	C(6)-H(6A)	0.9800
Zr(1)-Zr(3)	3.0525(13)	C(6)-H(6B)	0.9800
Zr(1)-Zr(2)	3.0603(12)	C(6)-H(6C)	0.9800
Zr(1)-Zr(4)	3.0694(13)	C(7)-H(7A)	0.9800
Zr(1)-H(1)	1.90(8)	C(7)-H(7B)	0.9800
Zr(1)-H(2)	1.98(8)	C(7)-H(7C)	0.9800
Zr(1)-H(3)	1.95(8)	C(8)-H(8A)	0.9800
Zr(2)-C(12)	2.487(10)	C(8)-H(8B)	0.9800
Zr(2)-C(14)	2.488(9)	C(8)-H(8C)	0.9800
Zr(2)-C(13)	2.493(10)	C(9)-H(9A)	0.9800
Zr(2)-C(15)	2.498(9)	C(9)-H(9B)	0.9800
Zr(2)-C(11)	2.532(9)	C(9)-H(9C)	0.9800
Zr(2)-Zr(3)	3.0737(12)	C(10)-H(10A)	0.9800
Zr(2)-Zr(4)	3.0774(12)	C(10)-H(10B)	0.9800
Zr(2)-H(1)	1.87(8)	C(10)-H(10C)	0.9800
Zr(2)-H(4)	2.21(8)	C(11)-C(15)	1.396(15)
Zr(2)-H(5)	1.89(8)	C(11)-C(12)	1.404(16)
Zr(3)-C(23)	2.486(10)	C(11)-C(16)	1.516(16)
Zr(3)-C(25)	2.489(9)	C(12)-C(13)	1.368(16)
Zr(3)-C(22)	2.493(10)	C(12)-C(17)	1.519(16)
Zr(3)-C(24)	2.497(10)	C(13)-C(14)	1.401(16)
Zr(3)-C(21)	2.506(10)	C(13)-C(18)	1.547(16)
Zr(3)-Zr(4)	3.0864(13)	C(14)-C(15)	1.402(15)
Zr(3)-H(2)	2.10(8)	C(14)-C(19)	1.545(14)
Zr(3)-H(4)	2.21(8)	C(15)-C(20)	1.515(15)
Zr(3)-H(6)	2.24(8)	C(16)-H(16A)	0.9800
Zr(4)-C(31)	2.478(10)	C(16)-H(16B)	0.9800
Zr(4)-C(35)	2.479(9)	C(16)-H(16C)	0.9800
Zr(4)-C(33)	2.499(10)	C(17)-H(17A)	0.9800
Zr(4)-C(32)	2.510(10)	C(17)-H(17B)	0.9800
Zr(4)-C(34)	2.522(10)	C(17)-H(17C)	0.9800
Zr(4)-H(3)	1.88(8)	C(18)-H(18A)	0.9800
Zr(4)-H(5)	1.98(8)	C(18)-H(18B)	0.9800
Zr(4)-H(6)	2.28(8)	C(18)-H(18C)	0.9800
C(1)-C(5)	1.379(15)	C(19)-H(19A)	0.9800
C(1)-C(2)	1.389(16)	C(19)-H(19B)	0.9800
C(1)-C(6)	1.521(16)	C(19)-H(19C)	0.9800
C(2)-C(3)	1.408(18)	C(20)-H(20A)	0.9800
C(2)-C(7)	1.503(19)	C(20)-H(20B)	0.9800
C(3)-C(4)	1.409(18)	C(20)-H(20C)	0.9800

C(21)-C(25)	1.404(15)	C(31)-C(35)	1.417(14)
C(21)-C(22)	1.423(16)	C(31)-C(32)	1.421(14)
C(21)-C(26)	1.520(16)	C(31)-C(36)	1.498(14)
C(22)-C(23)	1.393(16)	C(32)-C(33)	1.386(15)
C(22)-C(27)	1.516(16)	C(32)-C(37)	1.517(15)
C(23)-C(24)	1.403(15)	C(33)-C(34)	1.422(15)
C(23)-C(28)	1.540(16)	C(33)-C(38)	1.531(15)
C(24)-C(25)	1.383(15)	C(34)-C(35)	1.410(14)
C(24)-C(29)	1.537(17)	C(34)-C(39)	1.507(16)
C(25)-C(30)	1.527(15)	C(35)-C(40)	1.501(14)
C(26)-H(26A)	0.9800	C(36)-H(36A)	0.9800
C(26)-H(26B)	0.9800	C(36)-H(36B)	0.9800
C(26)-H(26C)	0.9800	C(36)-H(36C)	0.9800
C(27)-H(27A)	0.9800	C(37)-H(37A)	0.9800
C(27)-H(27B)	0.9800	C(37)-H(37B)	0.9800
C(27)-H(27C)	0.9800	C(37)-H(37C)	0.9800
C(28)-H(28A)	0.9800	C(38)-H(38A)	0.9800
C(28)-H(28B)	0.9800	C(38)-H(38B)	0.9800
C(28)-H(28C)	0.9800	C(38)-H(38C)	0.9800
C(29)-H(29A)	0.9800	C(39)-H(39A)	0.9800
C(29)-H(29B)	0.9800	C(39)-H(39B)	0.9800
C(29)-H(29C)	0.9800	C(39)-H(39C)	0.9800
C(30)-H(30A)	0.9800	C(40)-H(40A)	0.9800
C(30)-H(30B)	0.9800	C(40)-H(40B)	0.9800
C(30)-H(30C)	0.9800	C(40)-H(40C)	0.9800

C(2)-Zr(1)-C(1)	32.6(4)	Zr(3)-Zr(1)-Zr(2)	60.37(3)
C(2)-Zr(1)-C(4)	54.5(4)	C(2)-Zr(1)-Zr(4)	169.2(3)
C(1)-Zr(1)-C(4)	53.5(4)	C(1)-Zr(1)-Zr(4)	136.6(3)
C(2)-Zr(1)-C(3)	32.9(4)	C(4)-Zr(1)-Zr(4)	122.8(3)
C(1)-Zr(1)-C(3)	53.7(4)	C(3)-Zr(1)-Zr(4)	150.4(4)
C(4)-Zr(1)-C(3)	32.8(4)	C(5)-Zr(1)-Zr(4)	117.2(3)
C(2)-Zr(1)-C(5)	54.1(4)	Zr(3)-Zr(1)-Zr(4)	60.55(3)
C(1)-Zr(1)-C(5)	32.0(4)	Zr(2)-Zr(1)-Zr(4)	60.27(3)
C(4)-Zr(1)-C(5)	32.5(4)	C(2)-Zr(1)-H(1)	105(3)
C(3)-Zr(1)-C(5)	54.0(4)	C(1)-Zr(1)-H(1)	135(3)
C(2)-Zr(1)-Zr(3)	120.5(3)	C(4)-Zr(1)-H(1)	95(2)
C(1)-Zr(1)-Zr(3)	118.2(3)	C(3)-Zr(1)-H(1)	82(2)
C(4)-Zr(1)-Zr(3)	171.4(3)	C(5)-Zr(1)-H(1)	127(2)
C(3)-Zr(1)-Zr(3)	146.8(4)	Zr(3)-Zr(1)-H(1)	94(2)
C(5)-Zr(1)-Zr(3)	139.3(3)	Zr(2)-Zr(1)-H(1)	35(2)
C(2)-Zr(1)-Zr(2)	130.4(3)	Zr(4)-Zr(1)-H(1)	86(3)
C(1)-Zr(1)-Zr(2)	161.9(3)	C(2)-Zr(1)-H(2)	80(2)
C(4)-Zr(1)-Zr(2)	128.2(3)	C(1)-Zr(1)-H(2)	76(2)
C(3)-Zr(1)-Zr(2)	116.3(2)	C(4)-Zr(1)-H(2)	129(2)
C(5)-Zr(1)-Zr(2)	158.6(3)	C(3)-Zr(1)-H(2)	113(2)

C(5)-Zr(1)-H(2)	104(2)	C(15)-Zr(2)-H(1)	135(3)
Zr(3)-Zr(1)-H(2)	43(2)	C(11)-Zr(2)-H(1)	114(3)
Zr(2)-Zr(1)-H(2)	97(2)	Zr(1)-Zr(2)-H(1)	36(3)
Zr(4)-Zr(1)-H(2)	97(2)	Zr(3)-Zr(2)-H(1)	94(3)
H(1)-Zr(1)-H(2)	121(3)	Zr(4)-Zr(2)-H(1)	86(3)
C(2)-Zr(1)-H(3)	139(2)	C(12)-Zr(2)-H(4)	129(2)
C(1)-Zr(1)-H(3)	114(2)	C(14)-Zr(2)-H(4)	76(2)
C(4)-Zr(1)-H(3)	87(2)	C(13)-Zr(2)-H(4)	105(2)
C(3)-Zr(1)-H(3)	118(2)	C(15)-Zr(2)-H(4)	81(2)
C(5)-Zr(1)-H(3)	86(2)	C(11)-Zr(2)-H(4)	112(2)
Zr(3)-Zr(1)-H(3)	95(2)	Zr(1)-Zr(2)-H(4)	102(2)
Zr(2)-Zr(1)-H(3)	83(2)	Zr(3)-Zr(2)-H(4)	46(2)
Zr(4)-Zr(1)-H(3)	36(2)	Zr(4)-Zr(2)-H(4)	96(2)
H(1)-Zr(1)-H(3)	91(4)	H(1)-Zr(2)-H(4)	127(3)
H(2)-Zr(1)-H(3)	123(3)	C(12)-Zr(2)-H(5)	98(3)
C(12)-Zr(2)-C(14)	53.9(4)	C(14)-Zr(2)-H(5)	128(3)
C(12)-Zr(2)-C(13)	31.9(4)	C(13)-Zr(2)-H(5)	129(3)
C(14)-Zr(2)-C(13)	32.7(4)	C(15)-Zr(2)-H(5)	95(3)
C(12)-Zr(2)-C(15)	53.7(4)	C(11)-Zr(2)-H(5)	79(3)
C(14)-Zr(2)-C(15)	32.7(4)	Zr(1)-Zr(2)-H(5)	93(3)
C(13)-Zr(2)-C(15)	53.6(3)	Zr(3)-Zr(2)-H(5)	93(3)
C(12)-Zr(2)-C(11)	32.5(4)	Zr(4)-Zr(2)-H(5)	38(3)
C(14)-Zr(2)-C(11)	53.8(3)	H(1)-Zr(2)-H(5)	105(4)
C(13)-Zr(2)-C(11)	53.2(4)	H(4)-Zr(2)-H(5)	109(3)
C(15)-Zr(2)-C(11)	32.2(3)	C(23)-Zr(3)-C(25)	53.6(4)
C(12)-Zr(2)-Zr(1)	119.6(3)	C(23)-Zr(3)-C(22)	32.5(4)
C(14)-Zr(2)-Zr(1)	138.1(3)	C(25)-Zr(3)-C(22)	53.9(4)
C(13)-Zr(2)-Zr(1)	116.5(2)	C(23)-Zr(3)-C(24)	32.7(4)
C(15)-Zr(2)-Zr(1)	169.9(2)	C(25)-Zr(3)-C(24)	32.2(4)
C(11)-Zr(2)-Zr(1)	146.1(3)	C(22)-Zr(3)-C(24)	54.1(4)
C(12)-Zr(2)-Zr(3)	169.6(3)	C(23)-Zr(3)-C(21)	54.4(4)
C(14)-Zr(2)-Zr(3)	118.7(3)	C(25)-Zr(3)-C(21)	32.6(3)
C(13)-Zr(2)-Zr(3)	137.8(3)	C(22)-Zr(3)-C(21)	33.1(4)
C(15)-Zr(2)-Zr(3)	125.2(3)	C(24)-Zr(3)-C(21)	54.3(4)
C(11)-Zr(2)-Zr(3)	152.2(3)	C(23)-Zr(3)-Zr(1)	170.1(3)
Zr(1)-Zr(2)-Zr(3)	59.69(3)	C(25)-Zr(3)-Zr(1)	121.3(3)
C(12)-Zr(2)-Zr(4)	129.5(3)	C(22)-Zr(3)-Zr(1)	137.9(3)
C(14)-Zr(2)-Zr(4)	160.7(3)	C(24)-Zr(3)-Zr(1)	147.5(3)
C(13)-Zr(2)-Zr(4)	159.6(3)	C(21)-Zr(3)-Zr(1)	116.4(3)
C(15)-Zr(2)-Zr(4)	129.8(3)	C(23)-Zr(3)-Zr(2)	123.6(3)
C(11)-Zr(2)-Zr(4)	116.9(2)	C(25)-Zr(3)-Zr(2)	171.3(3)
Zr(1)-Zr(2)-Zr(4)	60.01(3)	C(22)-Zr(3)-Zr(2)	118.8(3)
Zr(3)-Zr(2)-Zr(4)	60.23(3)	C(24)-Zr(3)-Zr(2)	150.1(3)
C(12)-Zr(2)-H(1)	84(3)	C(21)-Zr(3)-Zr(2)	138.7(3)
C(14)-Zr(2)-H(1)	113(3)	Zr(1)-Zr(3)-Zr(2)	59.94(3)
C(13)-Zr(2)-H(1)	84(3)	C(23)-Zr(3)-Zr(4)	129.8(3)

C(25)-Zr(3)-Zr(4)	128.6(3)	C(32)-Zr(4)-Zr(1)	159.2(3)
C(22)-Zr(3)-Zr(4)	160.9(3)	C(34)-Zr(4)-Zr(1)	115.8(3)
C(24)-Zr(3)-Zr(4)	116.1(3)	C(31)-Zr(4)-Zr(2)	116.3(2)
C(21)-Zr(3)-Zr(4)	159.0(3)	C(35)-Zr(4)-Zr(2)	118.7(2)
Zr(1)-Zr(3)-Zr(4)	60.00(3)	C(33)-Zr(4)-Zr(2)	170.7(3)
Zr(2)-Zr(3)-Zr(4)	59.94(3)	C(32)-Zr(4)-Zr(2)	140.1(3)
C(23)-Zr(3)-H(2)	131(2)	C(34)-Zr(4)-Zr(2)	144.3(3)
C(25)-Zr(3)-H(2)	84(2)	Zr(1)-Zr(4)-Zr(2)	59.72(3)
C(22)-Zr(3)-H(2)	105(2)	C(31)-Zr(4)-Zr(3)	137.3(2)
C(24)-Zr(3)-H(2)	115(2)	C(35)-Zr(4)-Zr(3)	170.2(3)
C(21)-Zr(3)-H(2)	77(2)	C(33)-Zr(4)-Zr(3)	126.0(3)
Zr(1)-Zr(3)-H(2)	40(2)	C(32)-Zr(4)-Zr(3)	119.6(3)
Zr(2)-Zr(3)-H(2)	94(2)	C(34)-Zr(4)-Zr(3)	153.0(3)
Zr(4)-Zr(3)-H(2)	94(2)	Zr(1)-Zr(4)-Zr(3)	59.45(3)
C(23)-Zr(3)-H(4)	79(2)	Zr(2)-Zr(4)-Zr(3)	59.82(3)
C(25)-Zr(3)-H(4)	128(2)	C(31)-Zr(4)-H(3)	127(3)
C(22)-Zr(3)-H(4)	76(2)	C(35)-Zr(4)-H(3)	94(3)
C(24)-Zr(3)-H(4)	110(2)	C(33)-Zr(4)-H(3)	102(3)
C(21)-Zr(3)-H(4)	105(2)	C(32)-Zr(4)-H(3)	132(3)
Zr(1)-Zr(3)-H(4)	102(2)	C(34)-Zr(4)-H(3)	80(3)
Zr(2)-Zr(3)-H(4)	46(2)	Zr(1)-Zr(4)-H(3)	37(3)
Zr(4)-Zr(3)-H(4)	96(2)	Zr(2)-Zr(4)-H(3)	84(3)
H(2)-Zr(3)-H(4)	123(3)	Zr(3)-Zr(4)-H(3)	96(3)
C(23)-Zr(3)-H(6)	90(2)	C(31)-Zr(4)-H(5)	81(2)
C(25)-Zr(3)-H(6)	86(2)	C(35)-Zr(4)-H(5)	85(2)
C(22)-Zr(3)-H(6)	121(2)	C(33)-Zr(4)-H(5)	135(2)
C(24)-Zr(3)-H(6)	69(2)	C(32)-Zr(4)-H(5)	110(2)
C(21)-Zr(3)-H(6)	118(2)	C(34)-Zr(4)-H(5)	116(2)
Zr(1)-Zr(3)-H(6)	99(2)	Zr(1)-Zr(4)-H(5)	91(2)
Zr(2)-Zr(3)-H(6)	102(2)	Zr(2)-Zr(4)-H(5)	36(2)
Zr(4)-Zr(3)-H(6)	48(2)	Zr(3)-Zr(4)-H(5)	91(2)
H(2)-Zr(3)-H(6)	112(3)	H(3)-Zr(4)-H(5)	100(3)
H(4)-Zr(3)-H(6)	115(3)	C(31)-Zr(4)-H(6)	102(2)
C(31)-Zr(4)-C(35)	33.2(3)	C(35)-Zr(4)-H(6)	129(2)
C(31)-Zr(4)-C(33)	54.4(3)	C(33)-Zr(4)-H(6)	82(2)
C(35)-Zr(4)-C(33)	54.2(4)	C(32)-Zr(4)-H(6)	75(2)
C(31)-Zr(4)-C(32)	33.1(3)	C(34)-Zr(4)-H(6)	114(2)
C(35)-Zr(4)-C(32)	54.4(4)	Zr(1)-Zr(4)-H(6)	97(2)
C(33)-Zr(4)-C(32)	32.1(3)	Zr(2)-Zr(4)-H(6)	101(2)
C(31)-Zr(4)-C(34)	54.8(3)	Zr(3)-Zr(4)-H(6)	46(2)
C(35)-Zr(4)-C(34)	32.7(3)	H(3)-Zr(4)-H(6)	123(3)
C(33)-Zr(4)-C(34)	32.9(4)	H(5)-Zr(4)-H(6)	118(3)
C(32)-Zr(4)-C(34)	54.1(4)	C(5)-C(1)-C(2)	110.0(10)
C(31)-Zr(4)-Zr(1)	160.8(2)	C(5)-C(1)-C(6)	124.2(13)
C(35)-Zr(4)-Zr(1)	129.3(3)	C(2)-C(1)-C(6)	125.7(13)
C(33)-Zr(4)-Zr(1)	128.9(3)	C(5)-C(1)-Zr(1)	75.3(6)

C(2)-C(1)-Zr(1)	73.2(6)	H(9A)-C(9)-H(9B)	109.5
C(6)-C(1)-Zr(1)	121.3(8)	C(4)-C(9)-H(9C)	109.5
C(1)-C(2)-C(3)	107.0(10)	H(9A)-C(9)-H(9C)	109.5
C(1)-C(2)-C(7)	126.6(16)	H(9B)-C(9)-H(9C)	109.5
C(3)-C(2)-C(7)	126.1(15)	C(5)-C(10)-H(10A)	109.5
C(1)-C(2)-Zr(1)	74.2(6)	C(5)-C(10)-H(10B)	109.5
C(3)-C(2)-Zr(1)	74.5(6)	H(10A)-C(10)-H(10B)	109.5
C(7)-C(2)-Zr(1)	121.8(8)	C(5)-C(10)-H(10C)	109.5
C(2)-C(3)-C(4)	107.5(9)	H(10A)-C(10)-H(10C)	109.5
C(2)-C(3)-C(8)	125.3(16)	H(10B)-C(10)-H(10C)	109.5
C(4)-C(3)-C(8)	127.1(16)	C(15)-C(11)-C(12)	107.0(9)
C(2)-C(3)-Zr(1)	72.6(6)	C(15)-C(11)-C(16)	127.1(12)
C(4)-C(3)-Zr(1)	73.2(6)	C(12)-C(11)-C(16)	125.8(12)
C(8)-C(3)-Zr(1)	123.1(8)	C(15)-C(11)-Zr(2)	72.6(5)
C(5)-C(4)-C(3)	108.1(10)	C(12)-C(11)-Zr(2)	72.0(6)
C(5)-C(4)-C(9)	127.0(15)	C(16)-C(11)-Zr(2)	122.7(7)
C(3)-C(4)-C(9)	124.8(15)	C(13)-C(12)-C(11)	108.6(10)
C(5)-C(4)-Zr(1)	74.9(6)	C(13)-C(12)-C(17)	128.0(14)
C(3)-C(4)-Zr(1)	73.9(6)	C(11)-C(12)-C(17)	123.0(13)
C(9)-C(4)-Zr(1)	119.1(8)	C(13)-C(12)-Zr(2)	74.3(6)
C(1)-C(5)-C(4)	107.3(10)	C(11)-C(12)-Zr(2)	75.5(6)
C(1)-C(5)-C(10)	127.1(13)	C(17)-C(12)-Zr(2)	122.8(8)
C(4)-C(5)-C(10)	125.5(14)	C(12)-C(13)-C(14)	109.0(10)
C(1)-C(5)-Zr(1)	72.7(6)	C(12)-C(13)-C(18)	126.0(13)
C(4)-C(5)-Zr(1)	72.6(6)	C(14)-C(13)-C(18)	124.8(13)
C(10)-C(5)-Zr(1)	123.1(8)	C(12)-C(13)-Zr(2)	73.8(6)
C(1)-C(6)-H(6A)	109.5	C(14)-C(13)-Zr(2)	73.4(6)
C(1)-C(6)-H(6B)	109.5	C(18)-C(13)-Zr(2)	122.7(7)
H(6A)-C(6)-H(6B)	109.5	C(13)-C(14)-C(15)	106.7(10)
C(1)-C(6)-H(6C)	109.5	C(13)-C(14)-C(19)	124.7(13)
H(6A)-C(6)-H(6C)	109.5	C(15)-C(14)-C(19)	128.3(13)
H(6B)-C(6)-H(6C)	109.5	C(13)-C(14)-Zr(2)	73.9(6)
C(2)-C(7)-H(7A)	109.5	C(15)-C(14)-Zr(2)	74.1(5)
C(2)-C(7)-H(7B)	109.5	C(19)-C(14)-Zr(2)	121.8(7)
H(7A)-C(7)-H(7B)	109.5	C(11)-C(15)-C(14)	108.6(9)
C(2)-C(7)-H(7C)	109.5	C(11)-C(15)-C(20)	125.3(12)
H(7A)-C(7)-H(7C)	109.5	C(14)-C(15)-C(20)	126.0(12)
H(7B)-C(7)-H(7C)	109.5	C(11)-C(15)-Zr(2)	75.2(6)
C(3)-C(8)-H(8A)	109.5	C(14)-C(15)-Zr(2)	73.3(5)
C(3)-C(8)-H(8B)	109.5	C(20)-C(15)-Zr(2)	121.7(7)
H(8A)-C(8)-H(8B)	109.5	C(11)-C(16)-H(16A)	109.5
C(3)-C(8)-H(8C)	109.5	C(11)-C(16)-H(16B)	109.5
H(8A)-C(8)-H(8C)	109.5	H(16A)-C(16)-H(16B)	109.5
H(8B)-C(8)-H(8C)	109.5	C(11)-C(16)-H(16C)	109.5
C(4)-C(9)-H(9A)	109.5	H(16A)-C(16)-H(16C)	109.5
C(4)-C(9)-H(9B)	109.5	H(16B)-C(16)-H(16C)	109.5

C(12)-C(17)-H(17A)	109.5	C(23)-C(24)-Zr(3)	73.2(6)
C(12)-C(17)-H(17B)	109.5	C(29)-C(24)-Zr(3)	121.5(8)
H(17A)-C(17)-H(17B)	109.5	C(24)-C(25)-C(21)	110.0(10)
C(12)-C(17)-H(17C)	109.5	C(24)-C(25)-C(30)	124.4(11)
H(17A)-C(17)-H(17C)	109.5	C(21)-C(25)-C(30)	125.6(11)
H(17B)-C(17)-H(17C)	109.5	C(24)-C(25)-Zr(3)	74.2(6)
C(13)-C(18)-H(18A)	109.5	C(21)-C(25)-Zr(3)	74.3(6)
C(13)-C(18)-H(18B)	109.5	C(30)-C(25)-Zr(3)	120.0(7)
H(18A)-C(18)-H(18B)	109.5	C(21)-C(26)-H(26A)	109.5
C(13)-C(18)-H(18C)	109.5	C(21)-C(26)-H(26B)	109.5
H(18A)-C(18)-H(18C)	109.5	H(26A)-C(26)-H(26B)	109.5
H(18B)-C(18)-H(18C)	109.5	C(21)-C(26)-H(26C)	109.5
C(14)-C(19)-H(19A)	109.5	H(26A)-C(26)-H(26C)	109.5
C(14)-C(19)-H(19B)	109.5	H(26B)-C(26)-H(26C)	109.5
H(19A)-C(19)-H(19B)	109.5	C(22)-C(27)-H(27A)	109.5
C(14)-C(19)-H(19C)	109.5	C(22)-C(27)-H(27B)	109.5
H(19A)-C(19)-H(19C)	109.5	H(27A)-C(27)-H(27B)	109.5
H(19B)-C(19)-H(19C)	109.5	C(22)-C(27)-H(27C)	109.5
C(15)-C(20)-H(20A)	109.5	H(27A)-C(27)-H(27C)	109.5
C(15)-C(20)-H(20B)	109.5	H(27B)-C(27)-H(27C)	109.5
H(20A)-C(20)-H(20B)	109.5	C(23)-C(28)-H(28A)	109.5
C(15)-C(20)-H(20C)	109.5	C(23)-C(28)-H(28B)	109.5
H(20A)-C(20)-H(20C)	109.5	H(28A)-C(28)-H(28B)	109.5
H(20B)-C(20)-H(20C)	109.5	C(23)-C(28)-H(28C)	109.5
C(25)-C(21)-C(22)	106.0(10)	H(28A)-C(28)-H(28C)	109.5
C(25)-C(21)-C(26)	128.4(12)	H(28B)-C(28)-H(28C)	109.5
C(22)-C(21)-C(26)	125.4(12)	C(24)-C(29)-H(29A)	109.5
C(25)-C(21)-Zr(3)	73.1(6)	C(24)-C(29)-H(29B)	109.5
C(22)-C(21)-Zr(3)	73.0(6)	H(29A)-C(29)-H(29B)	109.5
C(26)-C(21)-Zr(3)	123.1(7)	C(24)-C(29)-H(29C)	109.5
C(23)-C(22)-C(21)	108.2(10)	H(29A)-C(29)-H(29C)	109.5
C(23)-C(22)-C(27)	125.7(13)	H(29B)-C(29)-H(29C)	109.5
C(21)-C(22)-C(27)	125.9(14)	C(25)-C(30)-H(30A)	109.5
C(23)-C(22)-Zr(3)	73.5(6)	C(25)-C(30)-H(30B)	109.5
C(21)-C(22)-Zr(3)	74.0(6)	H(30A)-C(30)-H(30B)	109.5
C(27)-C(22)-Zr(3)	121.9(8)	C(25)-C(30)-H(30C)	109.5
C(22)-C(23)-C(24)	108.5(10)	H(30A)-C(30)-H(30C)	109.5
C(22)-C(23)-C(28)	127.4(13)	H(30B)-C(30)-H(30C)	109.5
C(24)-C(23)-C(28)	124.1(12)	C(35)-C(31)-C(32)	106.8(9)
C(22)-C(23)-Zr(3)	74.0(6)	C(35)-C(31)-C(36)	127.6(10)
C(24)-C(23)-Zr(3)	74.1(6)	C(32)-C(31)-C(36)	125.2(10)
C(28)-C(23)-Zr(3)	119.6(8)	C(35)-C(31)-Zr(4)	73.4(6)
C(25)-C(24)-C(23)	107.3(10)	C(32)-C(31)-Zr(4)	74.7(6)
C(25)-C(24)-C(29)	126.1(11)	C(36)-C(31)-Zr(4)	122.9(7)
C(23)-C(24)-C(29)	126.5(11)	C(33)-C(32)-C(31)	108.3(10)
C(25)-C(24)-Zr(3)	73.6(6)	C(33)-C(32)-C(37)	127.1(11)

C(31)-C(32)-C(37)	124.5(11)	H(36A)-C(36)-H(36C)	109.5
C(33)-C(32)-Zr(4)	73.5(6)	H(36B)-C(36)-H(36C)	109.5
C(31)-C(32)-Zr(4)	72.2(6)	C(32)-C(37)-H(37A)	109.5
C(37)-C(32)-Zr(4)	122.2(8)	C(32)-C(37)-H(37B)	109.5
C(32)-C(33)-C(34)	109.3(9)	H(37A)-C(37)-H(37B)	109.5
C(32)-C(33)-C(38)	126.8(12)	C(32)-C(37)-H(37C)	109.5
C(34)-C(33)-C(38)	123.9(11)	H(37A)-C(37)-H(37C)	109.5
C(32)-C(33)-Zr(4)	74.4(6)	H(37B)-C(37)-H(37C)	109.5
C(34)-C(33)-Zr(4)	74.4(6)	C(33)-C(38)-H(38A)	109.5
C(38)-C(33)-Zr(4)	119.9(8)	C(33)-C(38)-H(38B)	109.5
C(35)-C(34)-C(33)	106.4(9)	H(38A)-C(38)-H(38B)	109.5
C(35)-C(34)-C(39)	126.6(11)	C(33)-C(38)-H(38C)	109.5
C(33)-C(34)-C(39)	126.9(11)	H(38A)-C(38)-H(38C)	109.5
C(35)-C(34)-Zr(4)	72.0(5)	H(38B)-C(38)-H(38C)	109.5
C(33)-C(34)-Zr(4)	72.7(6)	C(34)-C(39)-H(39A)	109.5
C(39)-C(34)-Zr(4)	122.8(8)	C(34)-C(39)-H(39B)	109.5
C(34)-C(35)-C(31)	109.1(9)	H(39A)-C(39)-H(39B)	109.5
C(34)-C(35)-C(40)	125.4(11)	C(34)-C(39)-H(39C)	109.5
C(31)-C(35)-C(40)	125.4(10)	H(39A)-C(39)-H(39C)	109.5
C(34)-C(35)-Zr(4)	75.3(6)	H(39B)-C(39)-H(39C)	109.5
C(31)-C(35)-Zr(4)	73.3(6)	C(35)-C(40)-H(40A)	109.5
C(40)-C(35)-Zr(4)	120.2(7)	C(35)-C(40)-H(40B)	109.5
C(31)-C(36)-H(36A)	109.5	H(40A)-C(40)-H(40B)	109.5
C(31)-C(36)-H(36B)	109.5	C(35)-C(40)-H(40C)	109.5
H(36A)-C(36)-H(36B)	109.5	H(40A)-C(40)-H(40C)	109.5
C(31)-C(36)-H(36C)	109.5	H(40B)-C(40)-H(40C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S7. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for [(μ_2-H)$_6$(Cp*Zr)$_4$]

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zr(1)	28(1)	18(1)	25(1)	0(1)	-3(1)	-10(1)
Zr(2)	23(1)	19(1)	30(1)	0(1)	-5(1)	-11(1)
Zr(3)	26(1)	27(1)	24(1)	2(1)	-4(1)	-13(1)
Zr(4)	23(1)	25(1)	29(1)	3(1)	-6(1)	-12(1)
C(1)	51(7)	21(6)	48(7)	-7(5)	1(6)	7(5)
C(2)	30(6)	59(8)	60(8)	-27(7)	10(6)	-18(6)
C(3)	99(11)	48(8)	51(8)	-32(6)	52(8)	-56(8)
C(4)	82(10)	41(7)	21(6)	-4(5)	-19(6)	-5(7)
C(5)	41(7)	42(7)	62(8)	-22(6)	0(6)	-22(6)
C(6)	210(20)	16(6)	62(10)	-5(6)	11(11)	-3(9)
C(7)	53(10)	250(30)	170(20)	-170(20)	15(12)	-12(13)
C(8)	200(20)	105(14)	137(16)	-84(12)	128(16)	-114(15)
C(9)	220(20)	86(13)	38(9)	-16(8)	-50(12)	31(14)
C(10)	61(10)	122(15)	220(20)	-138(15)	56(12)	-60(10)
C(11)	28(6)	20(5)	77(9)	5(5)	-22(6)	-11(5)
C(12)	80(9)	31(6)	42(7)	12(5)	-13(7)	-33(7)
C(13)	45(7)	35(6)	66(8)	-17(6)	26(6)	-28(6)
C(14)	44(7)	31(6)	77(9)	13(6)	-28(6)	-32(5)
C(15)	58(7)	24(5)	42(6)	-16(5)	12(6)	-25(5)
C(16)	70(10)	38(8)	191(19)	34(10)	-61(12)	-20(7)
C(17)	230(20)	91(12)	53(9)	36(8)	-65(11)	-113(14)
C(18)	86(11)	54(9)	170(17)	-56(10)	78(11)	-47(9)
C(19)	115(13)	71(10)	158(16)	57(10)	-119(12)	-70(10)
C(20)	144(15)	71(10)	59(9)	-30(8)	33(9)	-68(11)
C(21)	44(7)	58(8)	31(6)	15(5)	-13(5)	-14(6)
C(22)	71(9)	64(8)	36(7)	19(6)	-34(6)	-47(7)
C(23)	59(8)	44(7)	20(5)	-8(5)	-3(5)	-11(6)
C(24)	66(8)	64(8)	16(5)	7(5)	-5(5)	-40(7)
C(25)	58(7)	33(6)	32(6)	13(5)	-11(5)	-27(6)
C(26)	63(10)	88(11)	60(9)	21(8)	-3(8)	8(8)
C(27)	135(15)	158(17)	103(13)	64(12)	-77(12)	-125(15)
C(28)	184(19)	62(10)	51(9)	-15(7)	-37(10)	-41(11)
C(29)	92(11)	85(11)	44(8)	13(7)	-4(8)	-41(9)
C(30)	112(12)	44(8)	71(10)	13(7)	-31(9)	-37(8)
C(31)	25(5)	44(6)	41(6)	-12(5)	-1(5)	-14(5)
C(32)	34(6)	47(7)	50(7)	2(5)	3(5)	-26(5)
C(33)	40(7)	37(6)	69(8)	-4(6)	9(6)	-30(6)
C(34)	34(6)	58(8)	50(7)	-10(6)	-10(5)	-30(6)
C(35)	27(6)	42(6)	47(7)	11(5)	-21(5)	-14(5)
C(36)	33(6)	37(7)	87(10)	-21(6)	-4(6)	-10(5)
C(37)	67(9)	119(13)	43(8)	-15(8)	28(7)	-51(9)
C(38)	67(10)	56(9)	123(14)	11(9)	4(9)	-36(8)

C(39)	49(8)	109(12)	69(10)	-20(9)	-17(7)	-28(8)
C(40)	47(7)	76(9)	48(7)	23(6)	-31(6)	-20(7)

The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

Table S8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for [(μ_2-H)$_6$(Cp*Zr)$_4$].

	x	y	z	U(eq)
H(6A)	8356	3308	2077	170
H(6B)	9573	3473	2318	170
H(6C)	9771	2626	1657	170
H(7A)	10996	4460	1983	240
H(7B)	11080	5727	1553	240
H(7C)	11684	4387	1177	240
H(8A)	10120	6821	-196	209
H(8B)	10425	7107	555	209
H(8C)	9069	8004	237	209
H(9A)	7555	7355	-384	214
H(9B)	6380	7782	242	214
H(9C)	6660	6564	-199	214
H(10A)	6578	4360	1445	184
H(10B)	7178	3900	654	184
H(10C)	6074	5327	753	184
H(16A)	4501	13597	1732	148
H(16B)	4096	12708	2355	148
H(16C)	4325	12359	1534	148
H(17A)	7315	10575	423	158
H(17B)	6819	12113	400	158
H(17C)	5813	11456	643	158
H(18A)	9401	9688	845	153
H(18B)	10103	9329	1572	153
H(18C)	9890	10670	1117	153
H(19A)	9511	11131	2848	149
H(19B)	9784	9645	2811	149
H(19C)	8772	10466	3433	149
H(20A)	5954	13080	3314	128
H(20B)	6556	11660	3708	128
H(20C)	5157	12190	3410	128
H(26A)	10952	4088	4159	130
H(26B)	10857	5208	3537	130
H(26C)	10323	4150	3436	130
H(27A)	9147	8328	4486	165
H(27B)	10094	7431	3872	165
H(27C)	10308	6984	4703	165
H(28A)	6726	8258	5617	147
H(28B)	5802	8811	4976	147
H(28C)	7097	9061	4931	147
H(29A)	5344	5903	4675	110
H(29B)	5071	7162	5077	110

H(29C)	5785	5753	5465	110
H(30A)	7864	3489	4625	110
H(30B)	8652	3494	3850	110
H(30C)	7096	4216	3937	110
H(36A)	1215	11477	3146	79
H(36B)	2378	11661	2628	79
H(36C)	2608	11047	3436	79
H(37A)	2770	7715	4228	112
H(37B)	1516	9057	4172	112
H(37C)	2916	9052	4217	112
H(38A)	3448	6068	3533	122
H(38B)	3917	5660	2723	122
H(38C)	2409	6140	3015	122
H(39A)	3655	6446	1532	112
H(39B)	3760	7626	1012	112
H(39C)	2371	7569	1237	112
H(40A)	3473	9976	1049	88
H(40B)	2600	11178	1518	88
H(40C)	1922	10466	1145	88

Table S9. Wiberg bond indices (bond order) obtained by B3LYP with basis LanL2DZ for Zr, and cc-pVDZ for Cl, C, and H.

	bond length(Å)	bond order
1		
Zr(1)-Zr(2)	3.55118	0.246
Zr(1)-Zr(3)	3.05411	0.647
Zr(1)-Zr(4)	3.05384	0.685
Zr(2)-Zr(3)	3.05812	0.654
Zr(2)-Zr(4)	3.05120	0.649
Zr(3)-Zr(4)	3.56439	0.263
2		
Zr(1)-Zr(2)	3.06030	0.781
Zr(1)-Zr(3)	3.05254	0.980
Zr(1)-Zr(4)	3.06946	0.784
Zr(2)-Zr(3)	3.07379	0.745
Zr(2)-Zr(4)	3.07741	0.925
Zr(3)-Zr(4)	3.08625	0.724

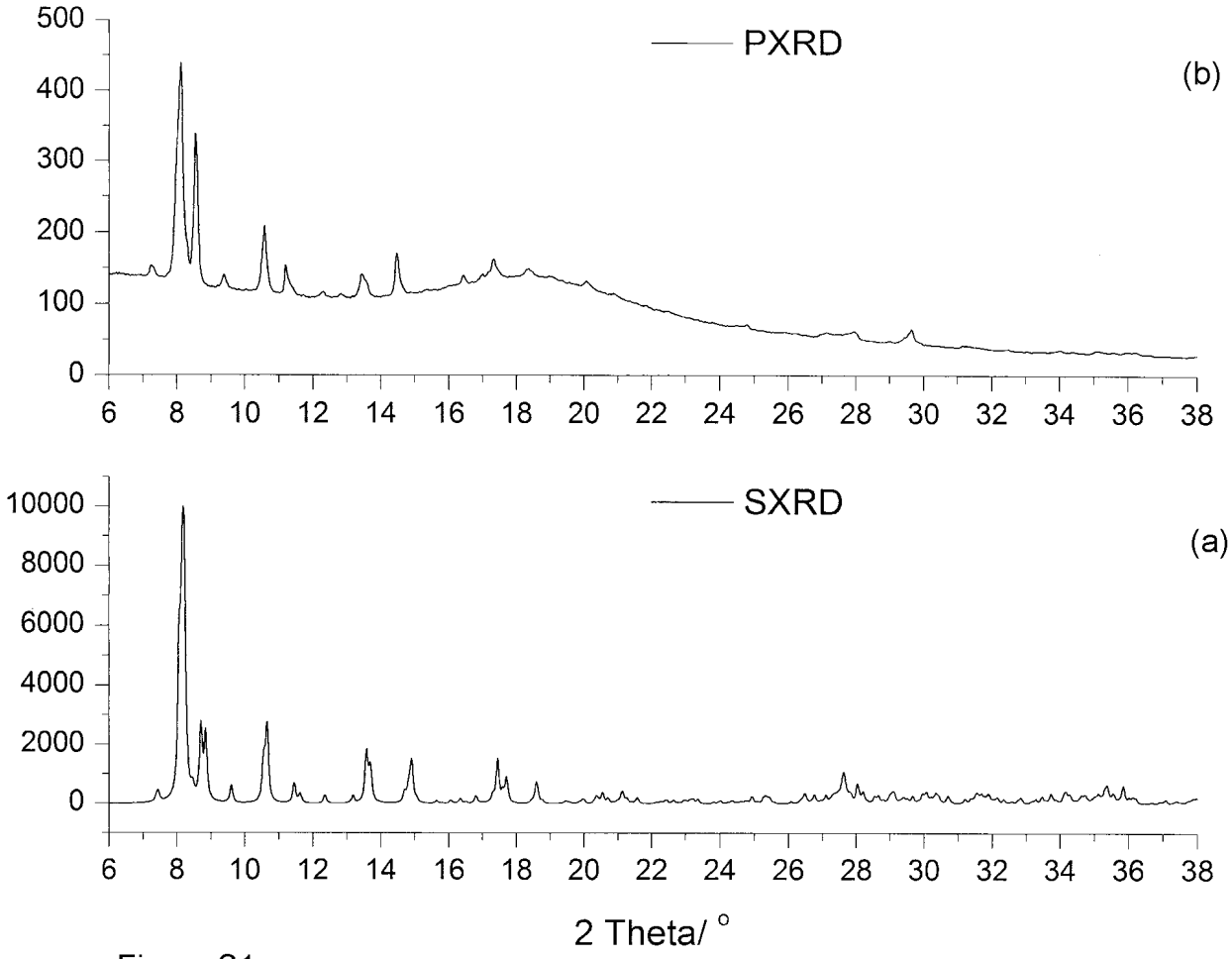

Figure S1