Table 1. Crystal data and structure refinement for $Cp^*_2Zr(Cl)(N=CMePHCy)$ (**1a**).

Identification code	cd385
Empirical formula	C30 H49 Cl N P Zr
Formula weight	581.34
Temperature	220(2) K
Wavelength	0.71073 A
Crystal system	Monoclinic
Space group	P2(1)/n
Unit cell dimensions	a = 10.596(1) A alpha = 90 deg. b = 18.588(1) A beta = 98.46(1)deg. c = 15.553(1) A gamma = 90 deg.
Volume, Z	3029.94(4) A^3, 4
Density (calculated)	1.274 Mg/m^3
Absorption coefficient	0.522 mm^-1
F(000)	1232
Crystal size	0.5 x 0.3 x 0.2 mm
Theta range for data collection	1.72 to 27.92 deg.
Limiting indices	-13<=h<=13, -24<=k<=24, -19<=l<=20
Reflections collected	27729
Independent reflections	6781 [R(int) = 0.0374]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6780 / 0 / 491
Goodness-of-fit on F^2	1.076
Final R indices [I>2sigma(I)]	R1 = 0.0352, wR2 = 0.0782
R indices (all data)	R1 = 0.0498, wR2 = 0.0861
Largest diff. peak and hole	1.457 and -0.797 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for $Cp^*_2Zr(Cl)(N=CMePHCy)$ (**1a**). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Zr(1)	5385(1)	2249(1)	6557(1)	23(1)
Cl(1)	3391(1)	2626(1)	5584(1)	35(1)
P(1)	5134(1)	4527(1)	7732(1)	62(1)
N(1)	5627(2)	3107(1)	7370(1)	30(1)
C(1)	7295(2)	1817(1)	5856(2)	34(1)
C(2)	7720(2)	2422(2)	6373(2)	39(1)
C(3)	7087(2)	3037(1)	5983(2)	39(1)
C(4)	6251(2)	2816(1)	5241(2)	37(1)
C(5)	6355(2)	2060(1)	5168(2)	34(1)
C(6)	7980(3)	1107(2)	5864(2)	54(1)
C(7)	9118(4)	1173(3)	5363(3)	76(1)
C(8)	8803(3)	2425(3)	7119(3)	66(1)
C(9)	7388(5)	3808(2)	6243(3)	67(1)
C(10)	5510(4)	3311(2)	4589(3)	62(1)
C(11)	5691(4)	1609(2)	4432(2)	59(1)
C(12)	4839(2)	1743(1)	7993(1)	31(1)
C(13)	3708(2)	1689(1)	7388(2)	36(1)
C(14)	3917(2)	1174(1)	6747(2)	39(1)
C(15)	5173(3)	911(1)	6958(2)	35(1)
C(16)	5758(2)	1273(1)	7720(2)	31(1)
C(17)	4982(4)	2153(2)	8832(2)	48(1)
C(18)	4481(5)	1725(2)	9554(2)	61(1)
C(19)	2448(3)	2040(2)	7454(3)	64(1)
C(20)	2935(4)	894(2)	6024(2)	70(1)
C(21)	5682(4)	243(2)	6580(3)	62(1)
C(22)	7030(3)	1092(2)	8241(2)	51(1)
C(23)	5895(2)	3623(1)	7892(2)	34(1)
C(24)	6959(3)	3611(2)	8652(2)	54(1)
C(25)	3627(3)	4338(1)	7009(2)	39(1)
C(26)	2518(3)	4163(2)	7489(2)	57(1)
C(27)	1285(3)	4035(2)	6879(3)	62(1)
C(28)	972(3)	4666(2)	6273(3)	61(1)
C(29)	2038(4)	4813(2)	5763(2)	70(1)
C(30)	3295(4)	4962(2)	6380(3)	63(1)

Table 3. Bond lengths [A] and angles [deg] for $Cp^{*}_{2}Zr(Cl)(N=CMePHCy)$ (**1a**).

Zr(1)-N(1)	2.029(2)
Zr(1)-Cl(1)	2.5107(6)
Zr(1)-C(5)	2.549(2)
Zr(1)-C(16)	2.552(2)
Zr(1)-C(2)	2.552(2)
Zr(1)-C(1)	2.564(2)
Zr(1)-C(12)	2.567(2)
Zr(1)-C(13)	2.567(2)
Zr(1)-C(14)	2.577(2)
Zr(1)-C(15)	2.582(2)
Zr(1)-C(3)	2.582(2)
Zr(1)-C(4)	2.586(2)
P(1)-C(25)	1.846(3)
P(1)-C(23)	1.866(3)
P(1)-H(1P)	1.3591(10)
N(1)-C(23)	1.260(3)
C(1)-C(2)	1.416(4)
C(1)-C(5)	1.424(3)
C(1)-C(6)	1.506(4)
C(2)-C(3)	1.417(4)
C(2)-C(8)	1.507(4)
C(3)-C(4)	1.410(4)
C(3)-C(9)	1.510(4)
C(4)-C(5)	1.415(4)
C(4)-C(10)	1.502(4)
C(5)-C(11)	1.507(4)
C(6)-C(7)	1.534(5)
C(6)-H(6A)	1.00(3)
C(6)-H(6B)	0.94(3)
C(7)-H(7A)	0.90(5)
C(7)-H(7B)	0.92(4)
C(7)-H(7C)	1.06(5)
C(8)-H(8A)	0.92(4)
C(8)-H(8B)	0.90(4)
C(8)-H(8C)	1.01(6)
C(9)-H(9A)	0.92(4)
C(9)-H(9B)	0.94(4)
C(9)-H(9C)	0.98(4)
C(10)-H(10A)	0.98(4)
C(10)-H(10B)	0.95(4)
C(10)-H(10C)	0.95(4)
C(11)-H(11A)	0.96(4)
C(11)-H(11B)	0.94(5)
C(11)-H(11C)	0.94(5)
C(12)-C(13)	1.414(3)
C(12)-C(16)	1.419(3)
C(12)-C(17)	1.500(4)
C(13)-C(14)	1.422(4)
C(13)-C(19)	1.503(4)
C(14)-C(15)	1.410(4)
C(14)-C(20)	1.508(4)
C(15)-C(16)	1.423(3)
C(15)-C(21)	1.509(4)
C(16)-C(22)	1.506(4)
C(17)-C(18)	1.532(4)
C(17)-H(17A)	0.97(4)
C(17)-H(17B)	0.89(3)
C(18)-H(18A)	0.92(4)

C(18)-H(18B)	0.90(4)
C(18)-H(18C)	1.00(4)
C(19)-H(19A)	0.95(5)
C(19)-H(19B)	0.95(4)
C(19)-H(19C)	0.97(5)
C(20)-H(20A)	0.96
C(20)-H(20B)	0.96
C(20)-H(20C)	0.96
C(21)-H(21A)	1.01(4)
C(21)-H(21B)	0.95(4)
C(21)-H(21C)	1.03(5)
C(22)-H(22A)	0.96(4)
C(22)-H(22B)	0.92(4)
C(22)-H(22C)	0.97(5)
C(23)-C(24)	1.508(4)
C(24)-H(24A)	1.01(4)
C(24)-H(24B)	0.90(4)
C(24)-H(24C)	0.96(4)
C(25)-C(26)	1.516(4)
C(25)-C(30)	1.525(4)
C(25)-H(25)	0.89(3)
C(26)-C(27)	1.517(5)
C(26)-H(26A)	1.02(4)
C(26)-H(26B)	1.06(4)
C(27)-C(28)	1.511(5)
C(27)-H(27A)	1.00(4)
C(27)-H(27B)	1.00(4)
C(28)-C(29)	1.498(5)
C(28)-H(28A)	0.88(4)
C(28)-H(28B)	0.96(4)
C(29)-C(30)	1.549(6)
C(29)-H(29A)	0.97(4)
C(29)-H(29B)	0.93(4)
C(30)-H(30A)	0.96(4)
C(30)-H(30B)	1.00(5)

N(1)-Zr(1)-Cl(1)	100.07(6)
N(1)-Zr(1)-C(5)	127.40(8)
Cl(1)-Zr(1)-C(5)	86.35(6)
N(1)-Zr(1)-C(16)	97.16(8)
Cl(1)-Zr(1)-C(16)	130.85(6)
C(5)-Zr(1)-C(16)	117.58(8)
N(1)-Zr(1)-C(2)	86.30(8)
Cl(1)-Zr(1)-C(2)	129.90(6)
C(5)-Zr(1)-C(2)	53.43(8)
C(16)-Zr(1)-C(2)	96.73(8)
N(1)-Zr(1)-C(1)	118.44(8)
Cl(1)-Zr(1)-C(1)	118.55(6)
C(5)-Zr(1)-C(1)	32.33(8)
C(16)-Zr(1)-C(1)	91.67(8)
C(2)-Zr(1)-C(1)	32.14(8)
N(1)-Zr(1)-C(12)	76.66(7)
Cl(1)-Zr(1)-C(12)	110.42(6)
C(5)-Zr(1)-C(12)	149.02(8)
C(16)-Zr(1)-C(12)	32.19(7)
C(2)-Zr(1)-C(12)	119.33(8)
C(1)-Zr(1)-C(12)	123.24(8)
N(1)-Zr(1)-C(13)	92.19(8)
Cl(1)-Zr(1)-C(13)	80.37(6)
C(5)-Zr(1)-C(13)	139.98(8)
C(16)-Zr(1)-C(13)	53.19(7)
C(2)-Zr(1)-C(13)	149.50(8)
C(1)-Zr(1)-C(13)	137.30(8)

C(12)-Zr(1)-C(13)	31.98(8)
N(1)-Zr(1)-C(14)	124.15(8)
Cl(1)-Zr(1)-C(14)	79.42(6)
C(5)-Zr(1)-C(14)	108.40(8)
C(16)-Zr(1)-C(14)	53.13(8)
C(2)-Zr(1)-C(14)	136.22(9)
C(1)-Zr(1)-C(14)	109.47(9)
C(12)-Zr(1)-C(14)	53.03(8)
C(13)-Zr(1)-C(14)	32.11(8)
N(1)-Zr(1)-C(15)	127.87(7)
Cl(1)-Zr(1)-C(15)	108.57(6)
C(5)-Zr(1)-C(15)	97.61(8)
C(16)-Zr(1)-C(15)	32.16(8)
C(2)-Zr(1)-C(15)	105.58(9)
C(1)-Zr(1)-C(15)	84.46(8)
C(12)-Zr(1)-C(15)	52.97(7)
C(13)-Zr(1)-C(15)	52.84(8)
C(14)-Zr(1)-C(15)	31.72(8)
N(1)-Zr(1)-C(3)	74.86(8)
Cl(1)-Zr(1)-C(3)	101.68(6)
C(5)-Zr(1)-C(3)	52.88(8)
C(16)-Zr(1)-C(3)	127.25(8)
C(2)-Zr(1)-C(3)	32.03(9)
C(1)-Zr(1)-C(3)	52.85(8)
C(12)-Zr(1)-C(3)	140.07(8)
C(13)-Zr(1)-C(3)	167.05(9)
C(14)-Zr(1)-C(3)	160.73(9)
C(15)-Zr(1)-C(3)	136.07(8)
N(1)-Zr(1)-C(4)	98.42(8)
Cl(1)-Zr(1)-C(4)	76.99(6)
C(5)-Zr(1)-C(4)	31.98(8)
C(16)-Zr(1)-C(4)	144.54(8)
C(2)-Zr(1)-C(4)	52.98(8)
C(1)-Zr(1)-C(4)	52.95(8)
C(12)-Zr(1)-C(4)	171.58(8)
C(13)-Zr(1)-C(4)	156.33(8)
C(14)-Zr(1)-C(4)	134.19(9)
C(15)-Zr(1)-C(4)	129.59(8)
C(3)-Zr(1)-C(4)	31.65(8)
C(25)-P(1)-C(23)	103.20(11)
C(25)-P(1)-H(1P)	105.50(10)
C(23)-P(1)-H(1P)	100.06(9)
C(23)-N(1)-Zr(1)	174.2(2)
C(2)-C(1)-C(5)	107.7(2)
C(2)-C(1)-C(6)	125.3(3)
C(5)-C(1)-C(6)	124.6(3)
C(2)-C(1)-Zr(1)	73.45(13)
C(5)-C(1)-Zr(1)	73.24(13)
C(6)-C(1)-Zr(1)	132.9(2)
C(1)-C(2)-C(3)	107.9(2)
C(1)-C(2)-C(8)	125.6(3)
C(3)-C(2)-C(8)	125.8(3)
C(1)-C(2)-Zr(1)	74.40(13)
C(3)-C(2)-Zr(1)	75.15(14)
C(8)-C(2)-Zr(1)	123.7(2)
C(4)-C(3)-C(2)	108.4(2)
C(4)-C(3)-C(9)	125.4(3)
C(2)-C(3)-C(9)	125.7(3)
C(4)-C(3)-Zr(1)	74.34(13)
C(2)-C(3)-Zr(1)	72.82(13)
C(9)-C(3)-Zr(1)	125.2(2)
C(3)-C(4)-C(5)	108.0(2)
C(3)-C(4)-C(10)	125.2(3)

C(5)-C(4)-C(10)	126.4(3)
C(3)-C(4)-Zr(1)	74.01(13)
C(5)-C(4)-Zr(1)	72.56(13)
C(10)-C(4)-Zr(1)	124.9(2)
C(4)-C(5)-C(1)	108.0(2)
C(4)-C(5)-C(11)	125.4(3)
C(1)-C(5)-C(11)	126.3(3)
C(4)-C(5)-Zr(1)	75.47(13)
C(1)-C(5)-Zr(1)	74.43(13)
C(11)-C(5)-Zr(1)	121.3(2)
C(1)-C(6)-C(7)	109.8(3)
C(1)-C(6)-H(6A)	111(2)
C(7)-C(6)-H(6A)	111(2)
C(1)-C(6)-H(6B)	109(2)
C(7)-C(6)-H(6B)	107(2)
H(6A)-C(6)-H(6B)	109(3)
C(6)-C(7)-H(7A)	108(3)
C(6)-C(7)-H(7B)	111(2)
H(7A)-C(7)-H(7B)	108(4)
C(6)-C(7)-H(7C)	109(3)
H(7A)-C(7)-H(7C)	111(4)
H(7B)-C(7)-H(7C)	110(4)
C(2)-C(8)-H(8A)	110(3)
C(2)-C(8)-H(8B)	110(3)
H(8A)-C(8)-H(8B)	107(4)
C(2)-C(8)-H(8C)	112(3)
H(8A)-C(8)-H(8C)	108(4)
H(8B)-C(8)-H(8C)	109(4)
C(3)-C(9)-H(9A)	109(2)
C(3)-C(9)-H(9B)	111(3)
H(9A)-C(9)-H(9B)	106(3)
C(3)-C(9)-H(9C)	110(3)
H(9A)-C(9)-H(9C)	114(3)
H(9B)-C(9)-H(9C)	108(3)
C(4)-C(10)-H(10A)	107(2)
C(4)-C(10)-H(10B)	108(2)
H(10A)-C(10)-H(10B)	108(3)
C(4)-C(10)-H(10C)	114(2)
H(10A)-C(10)-H(10C)	113(3)
H(10B)-C(10)-H(10C)	108(3)
C(5)-C(11)-H(11A)	110(3)
C(5)-C(11)-H(11B)	113(3)
H(11A)-C(11)-H(11B)	100(4)
C(5)-C(11)-H(11C)	114(3)
H(11A)-C(11)-H(11C)	115(4)
H(11B)-C(11)-H(11C)	104(4)
C(13)-C(12)-C(16)	108.0(2)
C(13)-C(12)-C(17)	125.6(2)
C(16)-C(12)-C(17)	126.0(2)
C(13)-C(12)-Zr(1)	74.02(13)
C(16)-C(12)-Zr(1)	73.33(12)
C(17)-C(12)-Zr(1)	124.4(2)
C(12)-C(13)-C(14)	108.1(2)
C(12)-C(13)-C(19)	126.7(3)
C(14)-C(13)-C(19)	124.9(3)
C(12)-C(13)-Zr(1)	74.00(13)
C(14)-C(13)-Zr(1)	74.32(13)
C(19)-C(13)-Zr(1)	123.1(2)
C(15)-C(14)-C(13)	108.0(2)
C(15)-C(14)-C(20)	125.3(3)
C(13)-C(14)-C(20)	126.4(3)
C(15)-C(14)-Zr(1)	74.36(13)
C(13)-C(14)-Zr(1)	73.57(13)

C(20)-C(14)-Zr(1)	123.0(2)
C(14)-C(15)-C(16)	108.1(2)
C(14)-C(15)-C(21)	125.0(3)
C(16)-C(15)-C(21)	125.2(3)
C(14)-C(15)-Zr(1)	73.92(13)
C(16)-C(15)-Zr(1)	72.74(13)
C(21)-C(15)-Zr(1)	130.5(2)
C(12)-C(16)-C(15)	107.8(2)
C(12)-C(16)-C(22)	125.1(2)
C(15)-C(16)-C(22)	126.1(3)
C(12)-C(16)-Zr(1)	74.48(13)
C(15)-C(16)-Zr(1)	75.10(13)
C(22)-C(16)-Zr(1)	125.0(2)
C(12)-C(17)-C(18)	111.9(3)
C(12)-C(17)-H(17A)	113(2)
C(18)-C(17)-H(17A)	107(2)
C(12)-C(17)-H(17B)	108(2)
C(18)-C(17)-H(17B)	111(2)
H(17A)-C(17)-H(17B)	105(3)
C(17)-C(18)-H(18A)	111(2)
C(17)-C(18)-H(18B)	111(3)
H(18A)-C(18)-H(18B)	103(3)
C(17)-C(18)-H(18C)	109(2)
H(18A)-C(18)-H(18C)	114(3)
H(18B)-C(18)-H(18C)	108(3)
C(13)-C(19)-H(19A)	116(3)
C(13)-C(19)-H(19B)	107(3)
H(19A)-C(19)-H(19B)	108(4)
C(13)-C(19)-H(19C)	114(3)
H(19A)-C(19)-H(19C)	104(4)
H(19B)-C(19)-H(19C)	108(3)
C(14)-C(20)-H(20A)	109.5(2)
C(14)-C(20)-H(20B)	109.5(2)
H(20A)-C(20)-H(20B)	109.5
C(14)-C(20)-H(20C)	109.5(2)
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(15)-C(21)-H(21A)	109(2)
C(15)-C(21)-H(21B)	110(2)
H(21A)-C(21)-H(21B)	111(3)
C(15)-C(21)-H(21C)	114(3)
H(21A)-C(21)-H(21C)	103(3)
H(21B)-C(21)-H(21C)	111(3)
C(16)-C(22)-H(22A)	112(2)
C(16)-C(22)-H(22B)	115(2)
H(22A)-C(22)-H(22B)	107(3)
C(16)-C(22)-H(22C)	112(3)
H(22A)-C(22)-H(22C)	104(3)
H(22B)-C(22)-H(22C)	107(3)
N(1)-C(23)-C(24)	124.4(3)
N(1)-C(23)-P(1)	123.1(2)
C(24)-C(23)-P(1)	112.1(2)
C(23)-C(24)-H(24A)	112(2)
C(23)-C(24)-H(24B)	109(3)
H(24A)-C(24)-H(24B)	108(3)
C(23)-C(24)-H(24C)	112(3)
H(24A)-C(24)-H(24C)	108(3)
H(24B)-C(24)-H(24C)	108(3)
C(26)-C(25)-C(30)	110.9(3)
C(26)-C(25)-P(1)	113.9(2)
C(30)-C(25)-P(1)	110.0(2)
C(26)-C(25)-H(25)	111(2)
C(30)-C(25)-H(25)	105(2)

P(1)-C(25)-H(25)	106(2)
C(25)-C(26)-C(27)	112.6(3)
C(25)-C(26)-H(26A)	108(2)
C(27)-C(26)-H(26A)	110(2)
C(25)-C(26)-H(26B)	109(2)
C(27)-C(26)-H(26B)	113(2)
H(26A)-C(26)-H(26B)	104(3)
C(28)-C(27)-C(26)	110.9(3)
C(28)-C(27)-H(27A)	117(2)
C(26)-C(27)-H(27A)	108(2)
C(28)-C(27)-H(27B)	110(2)
C(26)-C(27)-H(27B)	110(2)
H(27A)-C(27)-H(27B)	101(3)
C(29)-C(28)-C(27)	111.0(3)
C(29)-C(28)-H(28A)	109(3)
C(27)-C(28)-H(28A)	106(2)
C(29)-C(28)-H(28B)	109(2)
C(27)-C(28)-H(28B)	112(2)
H(28A)-C(28)-H(28B)	108(3)
C(28)-C(29)-C(30)	110.5(3)
C(28)-C(29)-H(29A)	120(3)
C(30)-C(29)-H(29A)	99(3)
C(28)-C(29)-H(29B)	111(2)
C(30)-C(29)-H(29B)	113(2)
H(29A)-C(29)-H(29B)	102(3)
C(25)-C(30)-C(29)	111.0(3)
C(25)-C(30)-H(30A)	104(2)
C(29)-C(30)-H(30A)	109(2)
C(25)-C(30)-H(30B)	110(3)
C(29)-C(30)-H(30B)	108(3)
H(30A)-C(30)-H(30B)	115(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for $Cp^*_2Zr(Cl)(N=CMePHCy)$ (**1a**).
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Zr(1)	22(1)	25(1)	22(1)	2(1)	1(1)	-1(1)
Cl(1)	29(1)	40(1)	33(1)	5(1)	-4(1)	1(1)
P(1)	61(1)	39(1)	80(1)	-23(1)	-8(1)	-2(1)
N(1)	30(1)	31(1)	27(1)	2(1)	4(1)	-5(1)
C(1)	28(1)	41(1)	36(1)	6(1)	11(1)	5(1)
C(2)	26(1)	57(2)	33(1)	1(1)	8(1)	-5(1)
C(3)	39(1)	39(1)	45(2)	0(1)	22(1)	-10(1)
C(4)	36(1)	43(1)	36(1)	13(1)	16(1)	6(1)
C(5)	34(1)	43(1)	28(1)	0(1)	9(1)	2(1)
C(6)	53(2)	52(2)	63(2)	18(2)	26(2)	22(2)
C(7)	67(2)	79(3)	92(3)	25(2)	46(2)	37(2)
C(8)	32(2)	111(3)	52(2)	-3(2)	-4(1)	-14(2)
C(9)	81(3)	49(2)	83(3)	-12(2)	49(2)	-28(2)
C(10)	61(2)	70(2)	59(2)	35(2)	24(2)	19(2)
C(11)	58(2)	81(3)	39(2)	-20(2)	10(2)	-8(2)
C(12)	39(1)	27(1)	28(1)	5(1)	10(1)	-1(1)
C(13)	29(1)	37(1)	44(1)	16(1)	11(1)	1(1)
C(14)	41(1)	36(1)	36(1)	9(1)	-2(1)	-15(1)
C(15)	51(2)	24(1)	33(1)	2(1)	12(1)	-2(1)
C(16)	32(1)	31(1)	31(1)	9(1)	6(1)	1(1)
C(17)	75(2)	42(2)	31(1)	-1(1)	21(1)	-7(2)
C(18)	94(3)	57(2)	38(2)	4(2)	31(2)	-7(2)
C(19)	41(2)	75(2)	82(3)	37(2)	29(2)	18(2)
C(20)	76(2)	59(2)	65(2)	14(2)	-22(2)	-36(2)
C(21)	96(3)	31(2)	67(2)	-5(2)	39(2)	-1(2)
C(22)	40(2)	67(2)	45(2)	22(2)	3(1)	10(2)
C(23)	37(1)	35(1)	29(1)	-1(1)	4(1)	-10(1)
C(24)	56(2)	61(2)	40(2)	-1(1)	-10(1)	-20(2)
C(25)	50(2)	28(1)	40(1)	-5(1)	7(1)	3(1)
C(26)	64(2)	59(2)	48(2)	5(2)	11(2)	-15(2)
C(27)	55(2)	59(2)	71(2)	-2(2)	10(2)	-12(2)
C(28)	54(2)	55(2)	70(2)	-14(2)	-1(2)	15(2)
C(29)	87(3)	72(2)	51(2)	20(2)	9(2)	23(2)
C(30)	68(2)	55(2)	70(2)	21(2)	23(2)	3(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for $Cp^*_2Zr(Cl)(N=CMePHCy)$ (**1a**).

	x	y	z	U(eq)
H(1P)	4800	4634	8533	100(13)
H(20A)	2156(4)	1160(2)	6012(2)	149(23)
H(20B)	2777(4)	394(2)	6122(2)	137(19)
H(20C)	3246(4)	949(2)	5478(2)	170(25)
H(6A)	7382(30)	716(18)	5617(20)	55(9)
H(6B)	8317(29)	991(17)	6441(21)	57(9)
H(7A)	9483(41)	739(25)	5356(27)	99(14)
H(7B)	8857(35)	1307(20)	4792(26)	74(12)
H(7C)	9766(46)	1557(27)	5679(31)	121(18)
H(8A)	9551(43)	2563(23)	6925(27)	93(13)
H(8B)	8650(41)	2750(23)	7520(30)	95(16)
H(8C)	8942(52)	1934(33)	7403(37)	152(23)
H(9A)	7950(38)	3988(21)	5897(26)	84(12)
H(9B)	6650(39)	4097(22)	6132(26)	84(14)
H(9C)	7699(39)	3834(22)	6868(30)	96(15)
H(10A)	6090(38)	3467(21)	4193(25)	87(12)
H(10B)	4849(38)	3037(21)	4260(25)	77(13)
H(10C)	5129(37)	3701(22)	4844(25)	84(13)
H(11A)	6107(39)	1664(22)	3926(28)	94(13)
H(11B)	5798(46)	1114(28)	4524(31)	117(18)
H(11C)	4804(52)	1672(28)	4331(32)	132(19)
H(17A)	4538(34)	2613(20)	8784(23)	70(11)
H(17B)	5803(33)	2266(17)	8981(21)	55(10)
H(18A)	4574(35)	1985(21)	10063(26)	79(12)
H(18B)	3628(39)	1657(22)	9433(25)	82(14)
H(18C)	4904(33)	1244(21)	9610(23)	74(11)
H(19A)	1812(45)	1732(26)	7624(30)	114(16)
H(19B)	2612(39)	2412(24)	7875(28)	85(15)
H(19C)	2035(41)	2256(23)	6917(30)	97(14)
H(21A)	5241(36)	-190(23)	6792(25)	88(12)
H(21B)	5537(34)	268(20)	5965(26)	75(11)
H(21C)	6630(48)	143(26)	6803(31)	124(18)
H(22A)	6952(35)	728(23)	8671(26)	89(13)
H(22B)	7641(35)	937(20)	7917(24)	75(11)
H(22C)	7393(44)	1498(26)	8579(29)	112(17)
H(24A)	7436(37)	3139(23)	8693(25)	88(13)
H(24B)	7515(39)	3965(23)	8584(26)	89(13)
H(24C)	6643(38)	3686(23)	9195(29)	98(14)
H(25)	3796(28)	3967(17)	6678(20)	51(8)
H(26A)	2404(33)	4588(20)	7890(23)	75(11)
H(26B)	2779(34)	3728(21)	7917(24)	80(11)
H(27A)	623(40)	3887(22)	7238(27)	97(14)
H(27B)	1361(38)	3589(24)	6535(27)	95(13)
H(28A)	871(35)	5040(21)	6606(24)	76(12)
H(28B)	198(36)	4595(19)	5882(24)	76(11)
H(29A)	2335(41)	4435(24)	5408(28)	100(14)
H(29B)	1823(35)	5177(21)	5360(25)	82(12)
H(30A)	3993(38)	4971(20)	6050(25)	83(12)
H(30B)	3179(41)	5415(25)	6709(28)	105(15)

Table 1. Crystal data and structure refinement for $[Cp^*_2(Cl)Zr(\mu\text{-}N{=}CMe\text{-}CMe{=}N)Zr(Cl)Cp^*_2]$ (**2a**).

Identification code	cd133	
Empirical formula	C48 H74 Cl2 N2 Zr2	
Formula weight	932.44	
Temperature	213(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.750(1) Å	alpha = 73.608(1) deg.
	b = 10.623(1) Å	beta = 77.941(1) deg.
	c = 13.635(1) Å	gamma = 72.720(1) deg.
Volume, Z	1150.0(2) Å^3, 1	
Density (calculated)	1.346 Mg/m^3	
Absorption coefficient	0.603 mm^-1	
F(000)	490	
Crystal size	0.25 x 0.25 x 0.20 mm	
Theta range for data Collection	1.57 to 26.12 deg.	
Index ranges	-10<=h<=10, -10<=k<=13, -13<=l<=16	
Reflections collected	5174	
Independent reflections	3793 [R(int) = 0.0238]	
Absorption correction	SADABS	
Max. and min. transmission	0.8889 and 0.8639	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	3793 / 0 / 325	
Goodness-of-fit on F^2	1.093	
Final R indices [I>2sigma(I)]	R1 = 0.0474, wR2 = 0.1044	
R indices (all data)	R1 = 0.0561, wR2 = 0.1114	
Extinction coefficient	0.0003(7)	
Largest diff. peak and hole	0.811 and -0.739 e.A^-3	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for [Cp^*_2(Cl)Zr(μ-N=CMe-CMe=N)Zr(Cl)Cp^*_2] (**2a**). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Zr(1)	1740(1)	2356(1)	2225(1)	18(1)
Cl	-841(1)	1638(1)	2756(1)	30(1)
N	1164(4)	3843(4)	961(3)	25(1)
C(1)	1572(6)	2528(5)	4078(3)	27(1)
C(2)	3024(5)	2881(5)	3543(3)	28(1)
C(3)	2604(6)	4103(5)	2795(4)	29(1)
C(4)	891(6)	4531(4)	2892(3)	26(1)
C(5)	260(5)	3564(5)	3688(3)	26(1)
C(6)	1450(10)	1331(7)	4983(4)	50(2)
C(7)	4654(7)	2268(9)	3914(6)	52(2)
C(8)	3761(10)	4892(8)	2139(6)	53(2)
C(9)	-74(9)	5876(6)	2337(5)	50(2)
C(10)	-1498(6)	3725(7)	4135(5)	43(1)
C(11)	-1953(8)	4486(8)	4996(5)	51(2)
C(23)	826(5)	4803(4)	180(3)	25(1)
C(24)	1985(7)	5629(6)	-454(4)	39(1)
C(12)	2601(9)	-77(6)	1987(7)	71(3)
C(13)	2455(7)	752(7)	1035(6)	59(2)
C(14)	3641(7)	1416(5)	758(4)	45(2)
C(15)	4524(6)	1060(6)	1579(5)	45(2)
C(16)	3846(9)	100(6)	2356(4)	64(2)
C(17)	1686(14)	-1134(8)	2526(13)	242(11)
C(18)	1265(11)	794(15)	372(11)	216(9)
C(19)	4098(15)	2265(9)	-283(6)	163(7)
C(20)	6076(9)	1401(13)	1534(11)	189(8)
C(21)	4583(18)	-766(11)	3304(6)	219(9)
C(22)	5753(16)	-2102(10)	3093(7)	186(8)

Table 3. Bond lengths [A] and angles [deg] for [Cp^*_2(Cl)Zr(μ-N=CMe-CMe=N)Zr(Cl)Cp^*_2] (**2a**).

Zr(1)-N	2.018(3)
Zr(1)-Cl	2.4969(11)
Zr(1)-C(15)	2.531(5)
Zr(1)-C(13)	2.536(5)
Zr(1)-C(16)	2.539(5)
Zr(1)-C(14)	2.553(5)
Zr(1)-C(3)	2.552(4)
Zr(1)-C(1)	2.555(4)
Zr(1)-C(12)	2.563(6)
Zr(1)-C(2)	2.566(4)
Zr(1)-C(4)	2.570(4)
Zr(1)-C(5)	2.585(4)
N-C(23)	1.266(5)
C(1)-C(5)	1.409(6)
C(1)-C(2)	1.424(6)
C(1)-C(6)	1.513(7)
C(2)-C(3)	1.409(7)
C(2)-C(7)	1.509(7)
C(3)-C(4)	1.420(6)
C(3)-C(8)	1.493(7)
C(4)-C(5)	1.412(6)
C(4)-C(9)	1.506(7)
C(5)-C(10)	1.509(7)
C(10)-C(11)	1.530(8)
C(23)-C(24)	1.510(7)
C(23)-C(23)#1	1.524(8)
C(12)-C(13)	1.355(10)
C(12)-C(16)	1.371(11)
C(12)-C(17)	1.504(9)
C(13)-C(14)	1.356(9)
C(13)-C(18)	1.498(9)
C(14)-C(15)	1.393(8)
C(14)-C(19)	1.497(8)
C(15)-C(16)	1.415(9)
C(15)-C(20)	1.491(8)
C(16)-C(21)	1.503(8)
C(21)-C(22)	1.546(9)
N-Zr(1)-Cl	99.50(11)
N-Zr(1)-C(15)	101.77(19)
Cl-Zr(1)-C(15)	129.57(13)
N-Zr(1)-C(13)	85.7(2)
Cl-Zr(1)-C(13)	84.80(16)
C(15)-Zr(1)-C(13)	52.28(17)
N-Zr(1)-C(16)	129.16(16)
Cl-Zr(1)-C(16)	102.3(2)
C(15)-Zr(1)-C(16)	32.4(2)
C(13)-Zr(1)-C(16)	51.8(2)
N-Zr(1)-C(14)	76.90(15)
Cl-Zr(1)-C(14)	115.35(16)
C(15)-Zr(1)-C(14)	31.81(18)
C(13)-Zr(1)-C(14)	30.9(2)
C(16)-Zr(1)-C(14)	52.27(17)
N-Zr(1)-C(3)	85.76(15)
Cl-Zr(1)-C(3)	129.10(11)
C(15)-Zr(1)-C(3)	97.75(15)
C(13)-Zr(1)-C(3)	145.99(19)

C(16)-Zr(1)-C(3)	113.1(2)
C(14)-Zr(1)-C(3)	115.14(18)
N-Zr(1)-C(1)	129.23(15)
Cl-Zr(1)-C(1)	88.12(11)
C(15)-Zr(1)-C(1)	111.39(17)
C(13)-Zr(1)-C(1)	145.1(2)
C(16)-Zr(1)-C(1)	96.97(16)
C(14)-Zr(1)-C(1)	143.21(17)
C(3)-Zr(1)-C(1)	53.37(15)
N-Zr(1)-C(12)	116.3(2)
Cl-Zr(1)-C(12)	77.29(15)
C(15)-Zr(1)-C(12)	52.29(19)
C(13)-Zr(1)-C(12)	30.8(2)
C(16)-Zr(1)-C(12)	31.2(2)
C(14)-Zr(1)-C(12)	51.14(19)
C(3)-Zr(1)-C(12)	144.3(2)
C(1)-Zr(1)-C(12)	114.4(2)
N-Zr(1)-C(2)	117.60(15)
Cl-Zr(1)-C(2)	120.41(11)
C(15)-Zr(1)-C(2)	88.23(16)
C(13)-Zr(1)-C(2)	138.76(17)
C(16)-Zr(1)-C(2)	89.1(2)
C(14)-Zr(1)-C(2)	117.32(18)
C(3)-Zr(1)-C(2)	31.96(15)
C(1)-Zr(1)-C(2)	32.29(14)
C(12)-Zr(1)-C(2)	117.8(3)
N-Zr(1)-C(4)	76.43(14)
Cl-Zr(1)-C(4)	99.65(11)
C(15)-Zr(1)-C(4)	129.59(16)
C(13)-Zr(1)-C(4)	162.0(2)
C(16)-Zr(1)-C(4)	141.8(2)
C(14)-Zr(1)-C(4)	138.77(17)
C(3)-Zr(1)-C(4)	32.19(15)
C(1)-Zr(1)-C(4)	52.85(14)
C(12)-Zr(1)-C(4)	167.2(2)
C(2)-Zr(1)-C(4)	52.78(14)
N-Zr(1)-C(5)	101.44(15)
Cl-Zr(1)-C(5)	76.42(10)
C(15)-Zr(1)-C(5)	140.71(16)
C(13)-Zr(1)-C(5)	160.74(19)
C(16)-Zr(1)-C(5)	128.10(16)
C(14)-Zr(1)-C(5)	168.23(18)
C(3)-Zr(1)-C(5)	53.12(14)
C(1)-Zr(1)-C(5)	31.82(14)
C(12)-Zr(1)-C(5)	136.8(2)
C(2)-Zr(1)-C(5)	52.84(14)
C(4)-Zr(1)-C(5)	31.80(14)
C(23)-N-Zr(1)	177.9(3)
C(5)-C(1)-C(2)	108.0(4)
C(5)-C(1)-C(6)	125.7(5)
C(2)-C(1)-C(6)	126.0(5)
C(5)-C(1)-Zr(1)	75.2(2)
C(2)-C(1)-Zr(1)	74.3(2)
C(6)-C(1)-Zr(1)	121.3(3)
C(3)-C(2)-C(1)	108.1(4)
C(3)-C(2)-C(7)	125.5(5)
C(1)-C(2)-C(7)	124.5(5)
C(3)-C(2)-Zr(1)	73.5(2)
C(1)-C(2)-Zr(1)	73.4(2)
C(7)-C(2)-Zr(1)	131.6(4)
C(2)-C(3)-C(4)	107.6(4)
C(2)-C(3)-C(8)	125.1(5)
C(4)-C(3)-C(8)	126.7(5)

C(2)-C(3)-Zr(1)	74.6(2)
C(4)-C(3)-Zr(1)	74.6(3)
C(8)-C(3)-Zr(1)	123.7(4)
C(5)-C(4)-C(3)	108.4(4)
C(5)-C(4)-C(9)	125.9(5)
C(3)-C(4)-C(9)	125.3(5)
C(5)-C(4)-Zr(1)	74.7(3)
C(3)-C(4)-Zr(1)	73.2(2)
C(9)-C(4)-Zr(1)	124.2(3)
C(1)-C(5)-C(4)	107.9(4)
C(1)-C(5)-C(10)	126.2(5)
C(4)-C(5)-C(10)	125.4(5)
C(1)-C(5)-Zr(1)	72.9(2)
C(4)-C(5)-Zr(1)	73.5(2)
C(10)-C(5)-Zr(1)	125.9(3)
C(5)-C(10)-C(11)	111.5(5)
N-C(23)-C(24)	123.7(4)
N-C(23)-C(23)#1	120.8(5)
C(24)-C(23)-C(23)#1	115.5(5)
C(13)-C(12)-C(16)	108.9(5)
C(13)-C(12)-C(17)	126.6(11)
C(16)-C(12)-C(17)	124.2(11)
C(13)-C(12)-Zr(1)	73.5(3)
C(16)-C(12)-Zr(1)	73.4(3)
C(17)-C(12)-Zr(1)	124.1(5)
C(14)-C(13)-C(12)	109.1(6)
C(14)-C(13)-C(18)	126.6(10)
C(12)-C(13)-C(18)	124.1(10)
C(14)-C(13)-Zr(1)	75.2(3)
C(12)-C(13)-Zr(1)	75.7(4)
C(18)-C(13)-Zr(1)	120.4(4)
C(13)-C(14)-C(15)	108.6(5)
C(13)-C(14)-C(19)	127.3(8)
C(15)-C(14)-C(19)	123.7(8)
C(13)-C(14)-Zr(1)	73.9(3)
C(15)-C(14)-Zr(1)	73.2(3)
C(19)-C(14)-Zr(1)	124.5(4)
C(14)-C(15)-C(16)	106.0(5)
C(14)-C(15)-C(20)	125.4(8)
C(16)-C(15)-C(20)	127.4(8)
C(14)-C(15)-Zr(1)	75.0(3)
C(16)-C(15)-Zr(1)	74.1(3)
C(20)-C(15)-Zr(1)	126.0(4)
C(12)-C(16)-C(15)	107.4(5)
C(12)-C(16)-C(21)	126.2(10)
C(15)-C(16)-C(21)	125.3(10)
C(12)-C(16)-Zr(1)	75.4(3)
C(15)-C(16)-Zr(1)	73.5(3)
C(21)-C(16)-Zr(1)	126.3(4)
C(16)-C(21)-C(22)	111.1(6)

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+1,-z

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for [Cp^*_2(Cl)Zr(μ-N=CMe-CMe=N)Zr(Cl)Cp^*_2] (**2a**).
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Zr(1)	15(1)	20(1)	18(1)	-3(1)	-2(1)	-4(1)
Cl	22(1)	38(1)	35(1)	-13(1)	2(1)	-14(1)
N	24(2)	26(2)	22(2)	-4(2)	-4(2)	-5(2)
C(1)	36(3)	28(2)	18(2)	-9(2)	-2(2)	-7(2)
C(2)	22(2)	42(3)	23(2)	-17(2)	-7(2)	-4(2)
C(3)	33(3)	35(3)	28(2)	-17(2)	4(2)	-18(2)
C(4)	32(2)	24(2)	23(2)	-9(2)	-9(2)	0(2)
C(5)	26(2)	35(3)	22(2)	-16(2)	0(2)	-9(2)
C(6)	73(5)	49(4)	26(3)	-6(3)	-3(3)	-19(4)
C(7)	30(3)	78(5)	55(4)	-39(4)	-15(3)	5(3)
C(8)	64(5)	66(5)	44(4)	-15(3)	8(3)	-46(4)
C(9)	68(5)	31(3)	48(4)	-13(3)	-17(3)	4(3)
C(10)	26(3)	60(4)	51(4)	-35(3)	7(2)	-12(3)
C(11)	36(3)	69(5)	54(4)	-38(3)	12(3)	-13(3)
C(23)	24(2)	25(2)	23(2)	-3(2)	-5(2)	-4(2)
C(24)	30(3)	42(3)	39(3)	7(3)	-9(2)	-12(2)
C(12)	60(4)	26(3)	108(6)	-29(4)	50(4)	-15(3)
C(13)	31(3)	76(5)	91(5)	-69(4)	-12(3)	7(3)
C(14)	56(4)	33(3)	23(3)	-5(2)	11(2)	12(3)
C(15)	15(2)	58(4)	76(4)	-50(3)	1(2)	-3(2)
C(16)	86(5)	46(4)	22(3)	-9(3)	-10(3)	43(4)
C(17)	169(11)	41(5)	430(2)	-82(9)	217(14)	-57(6)
C(18)	68(6)	347(19)	329(18)	-312(18)	-91(9)	67(9)
C(19)	233(13)	72(6)	50(5)	12(4)	83(6)	63(7)
C(20)	31(4)	293(15)	355(18)	-296(16)	70(7)	-67(7)
C(21)	339(18)	143(9)	56(5)	-59(6)	-100(8)	197(11)
C(22)	282(15)	120(8)	69(6)	-55(6)	-96(8)	161(10)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for [Cp°$_2$(Cl)Zr(μ-N=CMe-CMe=N)Zr(Cl)Cp°$_2$] (**2a**).

	x	y	z	U(eq)
H(17A)	2076	-1641	3271	150
H(17B)	1919	-1867	2067	150
H(17C)	408	-654	2626	150
H(18A)	1392	1539	-346	150
H(18B)	54	1065	769	150
H(18C)	1492	-191	215	150
H(19A)	5099	2648	-257	150
H(19B)	3079	3105	-498	150
H(19C)	4446	1654	-845	150
H(20A)	6482	1009	2283	150
H(20B)	5893	2489	1315	150
H(20C)	6976	952	972	150
H(21A)	3635	-997	3920	150
H(21B)	5230	-212	3549	150
H(22A)	6277	-2695	3783	150
H(22B)	6701	-1872	2477	150
H(22C)	5099	-2672	2871	150
H(6A)	2380(12)	660(10)	5000(7)	120(4)
H(6B)	500(11)	1110(9)	5020(7)	110(3)
H(6C)	1370(9)	1740(7)	5580(6)	90(2)
H(7A)	4790(10)	1420(9)	4270(7)	100(3)
H(7B)	4670(9)	2870(8)	4410(6)	100(3)
H(7C)	5530(8)	2500(6)	3360(5)	55(18)
H(8A)	3410(7)	5410(6)	1600(5)	45(18)
H(8B)	4810(13)	4390(11)	2170(8)	140(4)
H(8C)	3950(9)	5490(8)	2560(6)	80(2)
H(9A)	520(7)	6250(6)	1690(5)	57(19)
H(9B)	-340(7)	6500(6)	2810(5)	60(18)
H(9C)	-1060(8)	5790(7)	2250(5)	60(2)
H(10A)	-1690(7)	2870(6)	4360(5)	54(18)
H(10B)	-2210(8)	4190(6)	3620(5)	60(19)
H(11A)	-3100(7)	4540(6)	5310(4)	48(16)
H(11B)	-1760(8)	5420(7)	4730(5)	70(2)
H(11C)	-1340(8)	4020(7)	5590(5)	70(2)
H(24A)	1630(7)	6510(6)	-420(4)	43(16)
H(24B)	2990(7)	5310(5)	-180(4)	43(15)
H(24C)	2150(7)	5580(6)	-1210(5)	58(18)

The methyl and ethyl groups of one of the Cp° rings (atoms C12 - C22) have large thermal parameters. While the programme SHELX97 gives splitting positions for the methyl and ethyl groups (C17 - C21), no splitting positions are given for the cyclopentadienyl ring C atoms C12 - C16 as the anisotropic displacement parameters are not large enough.
Although refinement of the atoms C17 - C21 only in splitting positions results in a lower R value (wR2 decreases from 0.11 to 0.08), this approach results in meaningless bond angles.