Electronic Supplementary Material (ESI) for Polymer Chemistry

Supporting Information

to

Protected N-Heterocyclic Carbenes as Latent Pre-Catalysts for the Polymerization of ε-Caprolactone

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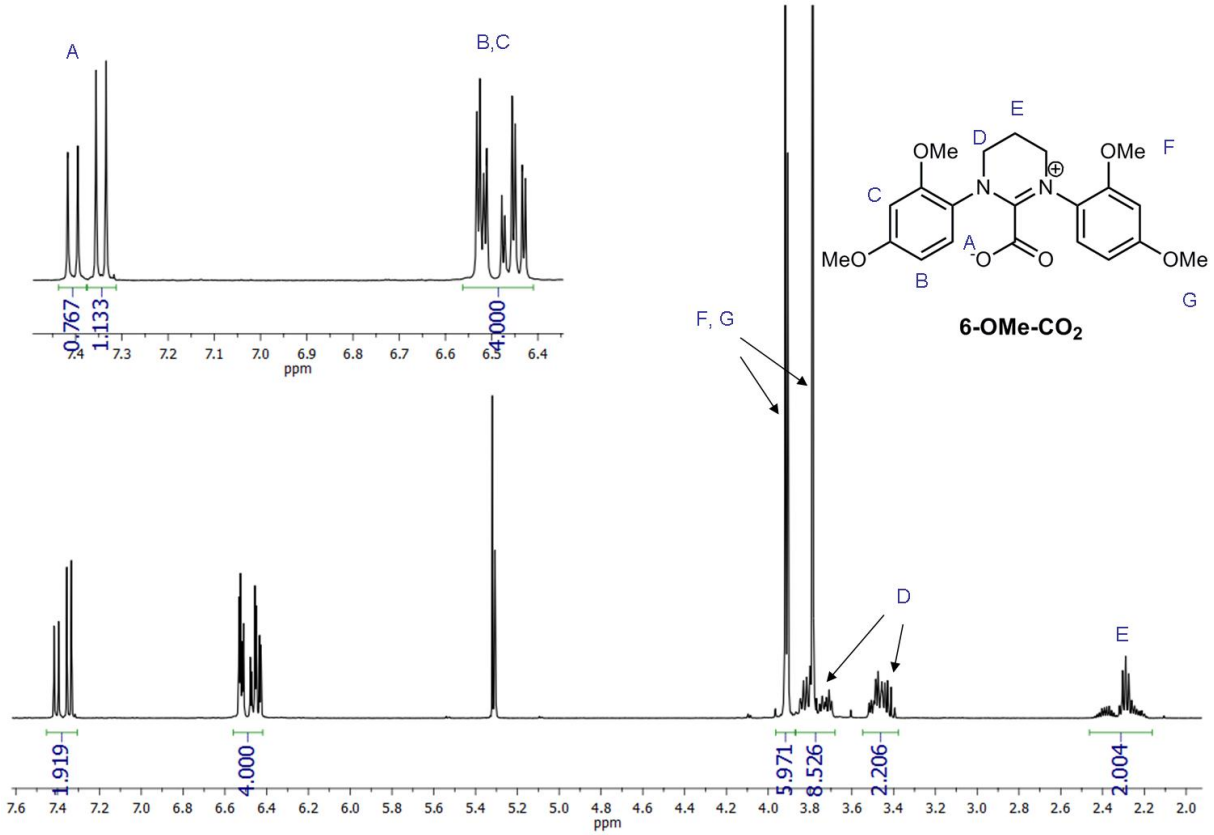

Figure S1. ^{1}H-NMR of **6-OMe-CO$_2$** (CD_2Cl_2, RT).

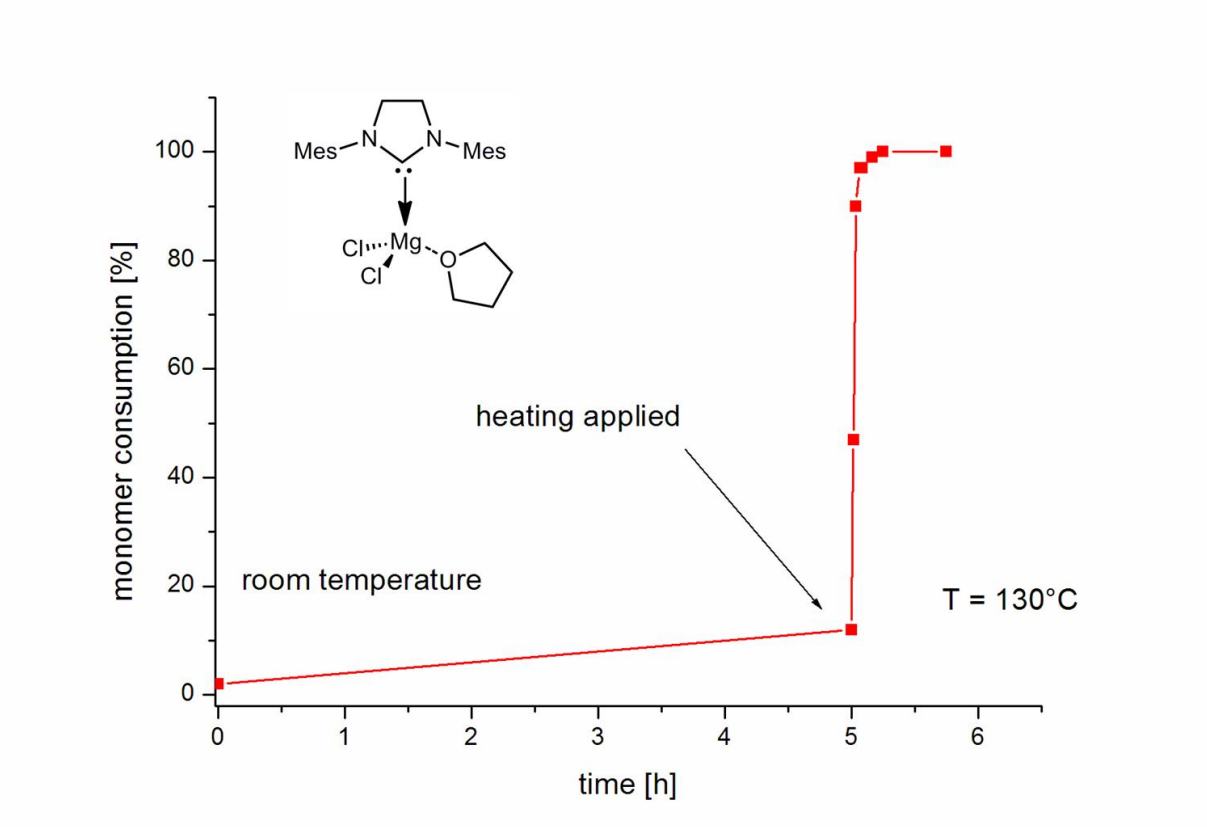

Figure S2: Latent behavior of **5s-Mes-MgCl$_2$** at room temperature and following treatment at 130°C.

[NHC]:[Bn-OH]:[ε-CL] = 1:2:280.

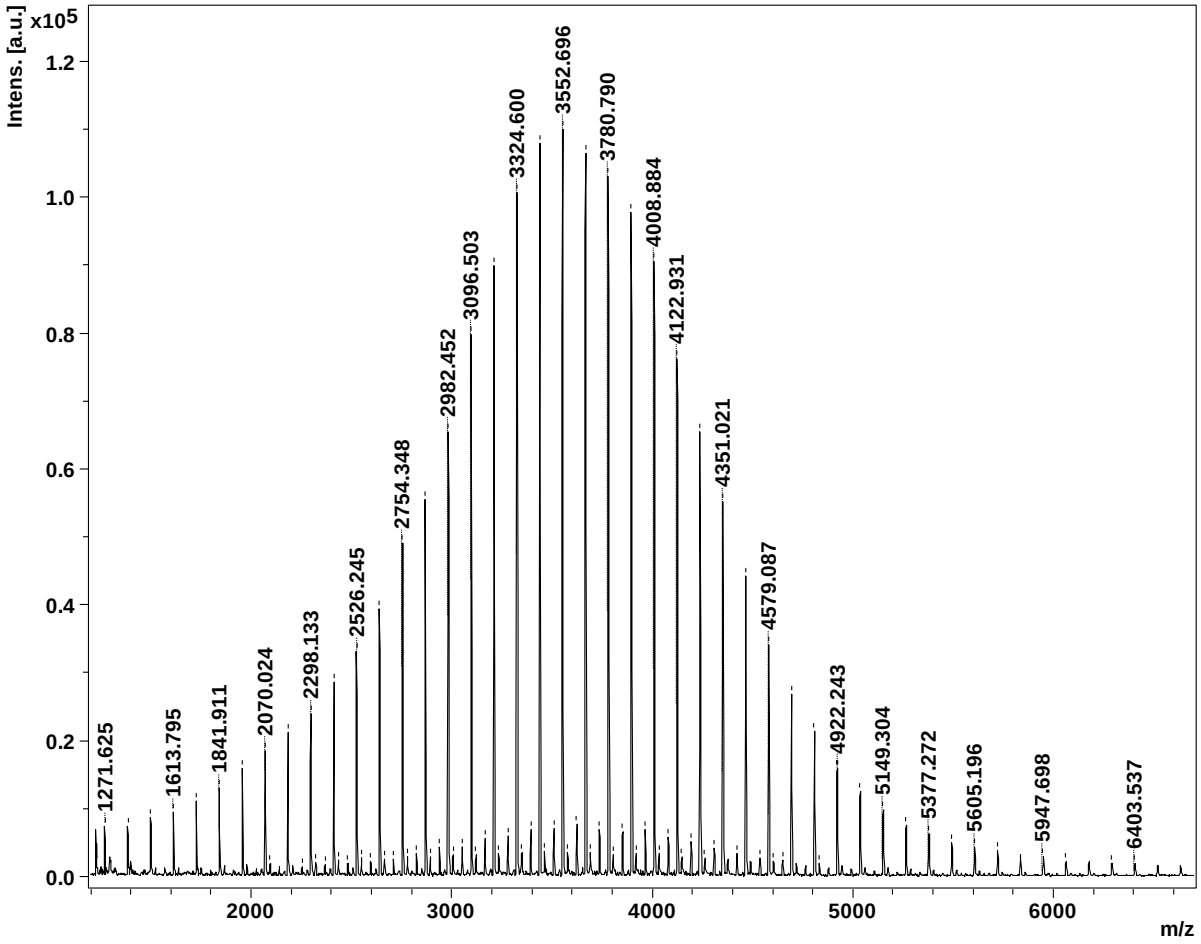

Figure S3. MALDI-TOF of PCL by the action of **5s-tBu-CO_2**/Bn-OH at 70°C. Found: Rep. unit 114.068, end1 107.050, end2 1.00783, cation 22.9898, M_n 3396.86, M_w 3561.55, pd 1.04848, DP 29.78, resid. -0.31296.

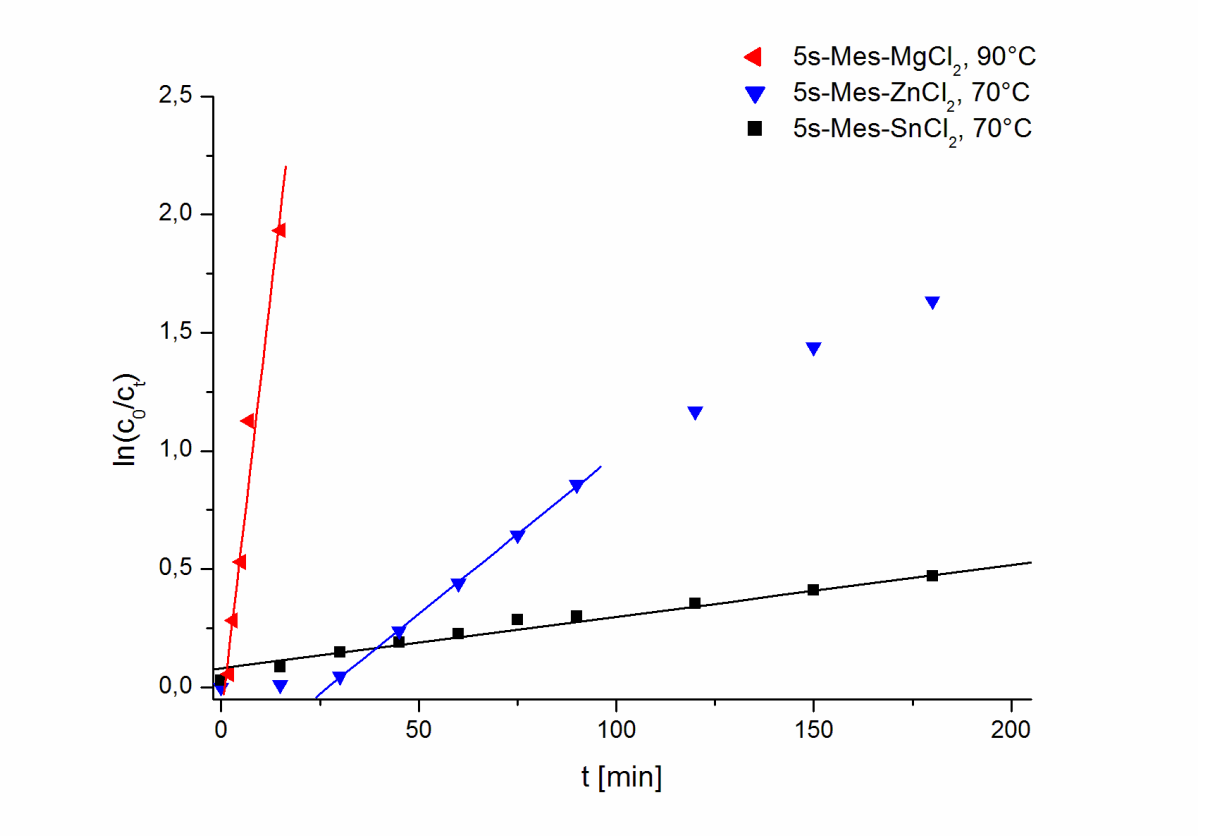

Figure S4: Plot of $\ln(c_0/c_t)$ vs. time. At high conversions, deviations from the linear behavior occur (blue triangles; omitted for the red triangles). **5s-Mes-ZnCl$_2$** shows a distinct induction period. [NHC]:[Bn-OH]:[ε-CL] = 1:2:280.

Table S1. Crystal data and structure refinement for **5s-Mes-$ZnCl_2$**.

Empirical formula	C_{27} H_{38} Cl_2 N_2 $O_{1.50}$ Zn
Formula weight	550.86
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C 2/c
Unit cell dimensions	a = 29.535(4) A alpha = 90 °. b = 11.9480(14) A beta = 96.899(7) °. c = 15.3350(17) A gamma = 90 °.
Volume	5372.3(11) A^3
Z, Calculated density	8, 1.362 g/cm^3
Absorption coefficient	1.137 mm^{-1}
F(000)	2320
Crystal size	0.36 x 0.11 x 0.06 mm
Θ range for data collection	1.84 to 26.43 °.
Limiting indices	-36<=h<=25, -14<=k<=13, -19<=l<=19
Reflections collected / unique	19082 / 5360 [R(int) = 0.0733]
Completeness to **Θ** = 26.43	97.2 %
Absorption correction	Numerical
Max. and min. transmission	0.9859 and 0.8765
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5360 / 0 / 309
Goodness-of-fit on F^2	1.014
Final R indices [I>2σ(I)]	R1 = 0.0481, wR2 = 0.0639
R indices (all data)	R1 = 0.1076, wR2 = 0.0710
Largest diff. peak and hole	0.421 and -0.385 e.A^{-3}

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5s-Mes-ZnCl$_2$**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Zn(1)	1460(1)	3523(1)	875(1)	14(1)
Cl(1)	2021(1)	4425(1)	298(1)	24(1)
Cl(2)	887(1)	3050(1)	-148(1)	21(1)
N(1)	1287(1)	3590(2)	2807(1)	12(1)
C(1)	1269(1)	4112(2)	2024(2)	12(1)
N(2)	1117(1)	5145(2)	2123(1)	12(1)
C(2)	1098(1)	4275(2)	3482(2)	16(1)
C(3)	1045(1)	5415(2)	3038(2)	16(1)
C(4)	1347(1)	2401(2)	2921(2)	11(1)
C(5)	1016(1)	1685(2)	2509(2)	13(1)
C(6)	1095(1)	540(3)	2591(2)	17(1)
C(7)	1474(1)	105(2)	3091(2)	16(1)
C(8)	1785(1)	846(2)	3536(2)	16(1)
C(9)	1725(1)	2002(2)	3455(2)	13(1)
C(10)	581(1)	2102(2)	1997(2)	20(1)
C(11)	1545(1)	-1145(2)	3163(2)	23(1)
C(12)	2070(1)	2791(2)	3929(2)	21(1)
C(13)	1009(1)	5967(2)	1437(2)	12(1)
C(14)	1334(1)	6752(2)	1264(2)	13(1)
C(15)	1200(1)	7588(2)	656(2)	15(1)
C(16)	761(1)	7666(2)	240(2)	15(1)
C(17)	447(1)	6855(2)	420(2)	14(1)
C(18)	564(1)	5995(2)	1016(2)	12(1)
C(19)	1812(1)	6704(2)	1725(2)	20(1)
C(20)	617(1)	8628(2)	-374(2)	24(1)
C(21)	219(1)	5125(2)	1191(2)	17(1)
O(1)	1790(1)	1990(2)	1154(1)	14(1)
C(22)	2267(1)	1948(2)	1490(2)	21(1)
C(23)	2382(1)	717(2)	1614(2)	18(1)
C(24)	1999(1)	113(2)	1034(2)	20(1)
C(25)	1720(1)	1042(2)	576(2)	28(1)
O(1S)	0	-298(2)	2500	30(1)
C(1S)	-168(1)	-993(3)	1772(2)	28(1)
C(2S)	-200(1)	-2159(2)	2144(2)	18(1)

Table S3. Bond lengths [A] and angles [°] for **5s-Mes-ZnCl$_2$**.

Zn(1)-C(1)	2.040(3)
Zn(1)-O(1)	2.0955(19)
Zn(1)-Cl(2)	2.2381(9)
Zn(1)-Cl(1)	2.2451(9)
N(1)-C(1)	1.347(3)
N(1)-C(4)	1.440(4)
N(1)-C(2)	1.481(3)
C(1)-N(2)	1.328(3)
N(2)-C(13)	1.447(3)
N(2)-C(3)	1.480(3)
C(2)-C(3)	1.522(4)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(9)	1.389(4)
C(4)-C(5)	1.392(4)
C(5)-C(6)	1.391(4)
C(5)-C(10)	1.506(4)
C(6)-C(7)	1.378(4)
C(6)-H(6)	0.9500
C(7)-C(8)	1.394(4)
C(7)-C(11)	1.511(4)
C(8)-C(9)	1.396(4)
C(8)-H(8)	0.9500
C(9)-C(12)	1.509(4)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.390(4)
C(13)-C(18)	1.392(4)
C(14)-C(15)	1.391(4)
C(14)-C(19)	1.503(4)
C(15)-C(16)	1.377(4)
C(15)-H(15)	0.9500
C(16)-C(17)	1.392(4)
C(16)-C(20)	1.514(4)
C(17)-C(18)	1.390(4)
C(17)-H(17)	0.9500
C(18)-C(21)	1.502(4)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800

C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
O(1)-C(25)	1.437(3)
O(1)-C(22)	1.440(3)
C(22)-C(23)	1.517(4)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-C(24)	1.532(4)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-C(25)	1.506(4)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
O(1S)-C(1S)	1.432(3)
O(1S)-C(1S)#1	1.432(3)
C(1S)-C(2S)	1.512(4)
C(1S)-H(1S1)	0.9900
C(1S)-H(1S2)	0.9900
C(2S)-C(2S)#1	1.511(6)
C(2S)-H(2S1)	0.9900
C(2S)-H(2S2)	0.9900

C(1)-Zn(1)-O(1)	107.18(9)
C(1)-Zn(1)-Cl(2)	115.36(9)
O(1)-Zn(1)-Cl(2)	102.52(6)
C(1)-Zn(1)-Cl(1)	117.99(8)
O(1)-Zn(1)-Cl(1)	98.80(6)
Cl(2)-Zn(1)-Cl(1)	112.10(3)
C(1)-N(1)-C(4)	123.8(2)
C(1)-N(1)-C(2)	112.9(2)
C(4)-N(1)-C(2)	120.7(2)
N(2)-C(1)-N(1)	107.8(2)
N(2)-C(1)-Zn(1)	123.47(19)
N(1)-C(1)-Zn(1)	128.6(2)
C(1)-N(2)-C(13)	126.6(2)
C(1)-N(2)-C(3)	113.6(2)
C(13)-N(2)-C(3)	119.8(2)
N(1)-C(2)-C(3)	102.1(2)
N(1)-C(2)-H(2A)	111.4
C(3)-C(2)-H(2A)	111.4
N(1)-C(2)-H(2B)	111.4
C(3)-C(2)-H(2B)	111.4
H(2A)-C(2)-H(2B)	109.2
N(2)-C(3)-C(2)	102.1(2)
N(2)-C(3)-H(3A)	111.3
C(2)-C(3)-H(3A)	111.3
N(2)-C(3)-H(3B)	111.3
C(2)-C(3)-H(3B)	111.3
H(3A)-C(3)-H(3B)	109.2
C(9)-C(4)-C(5)	121.9(3)
C(9)-C(4)-N(1)	119.2(3)
C(5)-C(4)-N(1)	118.9(3)
C(6)-C(5)-C(4)	117.5(3)
C(6)-C(5)-C(10)	119.8(3)

C(4)-C(5)-C(10)	122.7(3)
C(7)-C(6)-C(5)	122.5(3)
C(7)-C(6)-H(6)	118.7
C(5)-C(6)-H(6)	118.7
C(6)-C(7)-C(8)	118.4(3)
C(6)-C(7)-C(11)	120.6(3)
C(8)-C(7)-C(11)	121.0(3)
C(7)-C(8)-C(9)	121.1(3)
C(7)-C(8)-H(8)	119.4
C(9)-C(8)-H(8)	119.4
C(4)-C(9)-C(8)	118.4(3)
C(4)-C(9)-C(12)	121.3(3)
C(8)-C(9)-C(12)	120.3(3)
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(7)-C(11)-H(11A)	109.5
C(7)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(7)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(9)-C(12)-H(12A)	109.5
C(9)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(9)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(18)	121.9(3)
C(14)-C(13)-N(2)	120.0(3)
C(18)-C(13)-N(2)	117.9(3)
C(13)-C(14)-C(15)	117.8(3)
C(13)-C(14)-C(19)	121.0(3)
C(15)-C(14)-C(19)	121.2(3)
C(16)-C(15)-C(14)	122.3(3)
C(16)-C(15)-H(15)	118.8
C(14)-C(15)-H(15)	118.8
C(15)-C(16)-C(17)	118.3(3)
C(15)-C(16)-C(20)	121.2(3)
C(17)-C(16)-C(20)	120.4(3)
C(18)-C(17)-C(16)	121.7(3)
C(18)-C(17)-H(17)	119.2
C(16)-C(17)-H(17)	119.2
C(17)-C(18)-C(13)	118.0(3)
C(17)-C(18)-C(21)	120.5(3)
C(13)-C(18)-C(21)	121.5(3)
C(14)-C(19)-H(19A)	109.5
C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-H(20A)	109.5

C(16)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(16)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(25)-O(1)-C(22)	104.9(2)
C(25)-O(1)-Zn(1)	122.21(17)
C(22)-O(1)-Zn(1)	120.92(16)
O(1)-C(22)-C(23)	105.8(2)
O(1)-C(22)-H(22A)	110.6
C(23)-C(22)-H(22A)	110.6
O(1)-C(22)-H(22B)	110.6
C(23)-C(22)-H(22B)	110.6
H(22A)-C(22)-H(22B)	108.7
C(22)-C(23)-C(24)	104.2(2)
C(22)-C(23)-H(23A)	110.9
C(24)-C(23)-H(23A)	110.9
C(22)-C(23)-H(23B)	110.9
C(24)-C(23)-H(23B)	110.9
H(23A)-C(23)-H(23B)	108.9
C(25)-C(24)-C(23)	104.3(2)
C(25)-C(24)-H(24A)	110.9
C(23)-C(24)-H(24A)	110.9
C(25)-C(24)-H(24B)	110.9
C(23)-C(24)-H(24B)	110.9
H(24A)-C(24)-H(24B)	108.9
O(1)-C(25)-C(24)	105.2(2)
O(1)-C(25)-H(25A)	110.7
C(24)-C(25)-H(25A)	110.7
O(1)-C(25)-H(25B)	110.7
C(24)-C(25)-H(25B)	110.7
H(25A)-C(25)-H(25B)	108.8
C(1S)-O(1S)-C(1S)#1	109.0(3)
O(1S)-C(1S)-C(2S)	105.8(2)
O(1S)-C(1S)-H(1S1)	110.6
C(2S)-C(1S)-H(1S1)	110.6
O(1S)-C(1S)-H(1S2)	110.6
C(2S)-C(1S)-H(1S2)	110.6
H(1S1)-C(1S)-H(1S2)	108.7
C(2S)#1-C(2S)-C(1S)	101.1(2)
C(2S)#1-C(2S)-H(2S1)	111.5
C(1S)-C(2S)-H(2S1)	111.5
C(2S)#1-C(2S)-H(2S2)	111.5
C(1S)-C(2S)-H(2S2)	111.5
H(2S1)-C(2S)-H(2S2)	109.4

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,-z+1/2

Table S4. Anisotropic displacement parameters ($A^2 \times 10^3$) for **5s-Mes-ZnCl$_2$**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Zn(1)	16(1)	15(1)	11(1)	0(1)	3(1)	2(1)
Cl(1)	29(1)	20(1)	26(1)	2(1)	14(1)	-2(1)
Cl(2)	21(1)	29(1)	13(1)	0(1)	-1(1)	2(1)
N(1)	15(2)	10(2)	10(1)	-1(1)	3(1)	2(1)
C(1)	7(2)	13(2)	15(2)	4(1)	-1(1)	-3(1)
N(2)	16(2)	12(2)	7(1)	1(1)	3(1)	4(1)
C(2)	21(2)	17(2)	12(2)	1(1)	6(1)	8(2)
C(3)	21(2)	17(2)	12(2)	-2(1)	5(1)	4(2)
C(4)	15(2)	10(2)	10(1)	2(1)	6(1)	4(2)
C(5)	14(2)	15(2)	11(1)	4(1)	5(1)	1(2)
C(6)	22(2)	18(2)	12(2)	0(1)	6(2)	-4(2)
C(7)	23(2)	16(2)	11(2)	1(1)	11(2)	-1(2)
C(8)	17(2)	20(2)	11(2)	4(1)	4(1)	9(2)
C(9)	14(2)	15(2)	9(2)	-1(1)	3(1)	2(2)
C(10)	17(2)	21(2)	21(2)	5(1)	-1(2)	-5(2)
C(11)	37(2)	13(2)	20(2)	-1(1)	5(2)	6(2)
C(12)	17(2)	25(2)	19(2)	-1(1)	-2(2)	5(2)
C(13)	18(2)	9(2)	8(1)	1(1)	3(1)	3(2)
C(14)	14(2)	10(2)	15(2)	-5(1)	3(1)	2(2)
C(15)	21(2)	12(2)	14(2)	-1(1)	7(2)	-3(2)
C(16)	21(2)	12(2)	12(2)	-1(1)	4(2)	2(2)
C(17)	14(2)	16(2)	12(2)	-4(1)	-1(1)	3(2)
C(18)	17(2)	8(2)	13(2)	-2(1)	9(1)	0(2)
C(19)	17(2)	18(2)	26(2)	-3(1)	4(2)	3(2)
C(20)	27(2)	20(2)	23(2)	8(2)	2(2)	2(2)
C(21)	17(2)	17(2)	19(2)	1(1)	5(1)	1(2)
O(1)	12(1)	13(1)	18(1)	-3(1)	1(1)	1(1)
C(22)	12(2)	19(2)	30(2)	-2(2)	-1(2)	0(2)
C(23)	16(2)	20(2)	17(2)	-1(1)	5(1)	3(2)
C(24)	23(2)	17(2)	21(2)	-3(2)	2(2)	1(2)
C(25)	36(2)	20(2)	25(2)	-11(2)	-9(2)	2(2)
O(1S)	29(2)	10(2)	51(2)	0	5(2)	0
C(1S)	26(2)	33(2)	26(2)	8(2)	10(2)	6(2)
C(2S)	20(2)	17(2)	17(2)	-3(1)	2(2)	3(2)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **5s-Mes-$ZnCl_2$**.

	x	y	z	U(eq)
H(2A)	1310	4310	4032	20
H(2B)	800	3980	3613	20
H(3A)	737	5729	3068	19
H(3B)	1277	5951	3307	19
H(6)	881	38	2291	20
H(8)	2041	560	3900	19
H(10A)	481	2782	2274	29
H(10B)	345	1525	1992	29
H(10C)	636	2269	1393	29
H(11A)	1362	-1450	3599	35
H(11B)	1868	-1304	3344	35
H(11C)	1451	-1494	2591	35
H(12A)	2165	3341	3512	31
H(12B)	2337	2365	4186	31
H(12C)	1934	3179	4395	31
H(15)	1419	8125	524	18
H(17)	145	6889	128	17
H(19A)	1802	6596	2356	30
H(19B)	1970	7406	1628	30
H(19C)	1975	6078	1492	30
H(20A)	473	9211	-51	35
H(20B)	398	8357	-860	35
H(20C)	885	8938	-607	35
H(21A)	-81	5342	900	26
H(21B)	208	5066	1825	26
H(21C)	307	4401	962	26
H(22A)	2323	2352	2056	25
H(22B)	2454	2293	1068	25
H(23A)	2386	495	2237	21
H(23B)	2683	547	1422	21
H(24A)	2126	-379	603	25
H(24B)	1813	-345	1394	25
H(25A)	1823	1210	0	33
H(25B)	1393	835	483	33
H(1S1)	43	-982	1318	33
H(1S2)	-472	-732	1506	33
H(2S1)	-492	-2273	2389	22
H(2S2)	-167	-2739	1695	22

Table S6. Torsion angles [°] for **5s-Mes-ZnCl$_2$**.

C(4)-N(1)-C(1)-N(2)	167.0(2)
C(2)-N(1)-C(1)-N(2)	5.2(3)
C(4)-N(1)-C(1)-Zn(1)	-15.7(4)
C(2)-N(1)-C(1)-Zn(1)	-177.5(2)
O(1)-Zn(1)-C(1)-N(2)	168.7(2)
Cl(2)-Zn(1)-C(1)-N(2)	-77.9(2)
Cl(1)-Zn(1)-C(1)-N(2)	58.5(3)
O(1)-Zn(1)-C(1)-N(1)	-8.1(3)
Cl(2)-Zn(1)-C(1)-N(1)	105.3(3)
Cl(1)-Zn(1)-C(1)-N(1)	-118.4(2)
N(1)-C(1)-N(2)-C(13)	-174.4(3)
Zn(1)-C(1)-N(2)-C(13)	8.1(4)
N(1)-C(1)-N(2)-C(3)	3.4(3)
Zn(1)-C(1)-N(2)-C(3)	-174.0(2)
C(1)-N(1)-C(2)-C(3)	-11.0(3)
C(4)-N(1)-C(2)-C(3)	-173.4(2)
C(1)-N(2)-C(3)-C(2)	-10.0(3)
C(13)-N(2)-C(3)-C(2)	168.0(3)
N(1)-C(2)-C(3)-N(2)	11.6(3)
C(1)-N(1)-C(4)-C(9)	119.3(3)
C(2)-N(1)-C(4)-C(9)	-80.2(3)
C(1)-N(1)-C(4)-C(5)	-62.2(4)
C(2)-N(1)-C(4)-C(5)	98.2(3)
C(9)-C(4)-C(5)-C(6)	-5.1(4)
N(1)-C(4)-C(5)-C(6)	176.5(2)
C(9)-C(4)-C(5)-C(10)	174.1(3)
N(1)-C(4)-C(5)-C(10)	-4.3(4)
C(4)-C(5)-C(6)-C(7)	3.0(4)
C(10)-C(5)-C(6)-C(7)	-176.2(3)
C(5)-C(6)-C(7)-C(8)	0.6(4)
C(5)-C(6)-C(7)-C(11)	179.9(2)
C(6)-C(7)-C(8)-C(9)	-2.2(4)
C(11)-C(7)-C(8)-C(9)	178.5(3)
C(5)-C(4)-C(9)-C(8)	3.6(4)
N(1)-C(4)-C(9)-C(8)	-178.0(2)
C(5)-C(4)-C(9)-C(12)	-177.3(3)
N(1)-C(4)-C(9)-C(12)	1.1(4)
C(7)-C(8)-C(9)-C(4)	0.2(4)
C(7)-C(8)-C(9)-C(12)	-178.9(3)
C(1)-N(2)-C(13)-C(14)	-94.8(3)
C(3)-N(2)-C(13)-C(14)	87.5(3)
C(1)-N(2)-C(13)-C(18)	90.2(4)
C(3)-N(2)-C(13)-C(18)	-87.5(3)
C(18)-C(13)-C(14)-C(15)	0.7(4)
N(2)-C(13)-C(14)-C(15)	-174.1(2)
C(18)-C(13)-C(14)-C(19)	-179.8(3)
N(2)-C(13)-C(14)-C(19)	5.4(4)
C(13)-C(14)-C(15)-C(16)	0.9(4)
C(19)-C(14)-C(15)-C(16)	-178.5(3)
C(14)-C(15)-C(16)-C(17)	-1.9(4)
C(14)-C(15)-C(16)-C(20)	175.9(3)
C(15)-C(16)-C(17)-C(18)	1.3(4)
C(20)-C(16)-C(17)-C(18)	-176.6(3)

C(16)-C(17)-C(18)-C(13)	0.3(4)
C(16)-C(17)-C(18)-C(21)	-179.4(2)
C(14)-C(13)-C(18)-C(17)	-1.3(4)
N(2)-C(13)-C(18)-C(17)	173.6(2)
C(14)-C(13)-C(18)-C(21)	178.4(2)
N(2)-C(13)-C(18)-C(21)	-6.7(4)
C(1)-Zn(1)-O(1)-C(25)	139.2(2)
Cl(2)-Zn(1)-O(1)-C(25)	17.4(2)
Cl(1)-Zn(1)-O(1)-C(25)	-97.8(2)
C(1)-Zn(1)-O(1)-C(22)	-83.8(2)
Cl(2)-Zn(1)-O(1)-C(22)	154.33(18)
Cl(1)-Zn(1)-O(1)-C(22)	39.21(19)
C(25)-O(1)-C(22)-C(23)	-37.0(3)
Zn(1)-O(1)-C(22)-C(23)	179.70(16)
O(1)-C(22)-C(23)-C(24)	19.5(3)
C(22)-C(23)-C(24)-C(25)	4.2(3)
C(22)-O(1)-C(25)-C(24)	39.8(3)
Zn(1)-O(1)-C(25)-C(24)	-177.52(18)
C(23)-C(24)-C(25)-O(1)	-26.5(3)
C(1S)#1-O(1S)-C(1S)-C(2S)	13.16(15)
O(1S)-C(1S)-C(2S)-C(2S)#1	-33.8(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,-z+1/2