Supporting Information

Organozinc Catalyst on Phenalenyl Scaffold for Intramolecular Hydroamination of Aminoalkenes

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Complete Reference of 27 from the main text:

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Vreven, Jr. T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03, Revision C.02*, Gaussian, Inc., Wallingford CT, **2004**.

(1) ^{1}H NMR of [PhNMe$_2$H][B(C$_6$F$_5$)$_4$]:

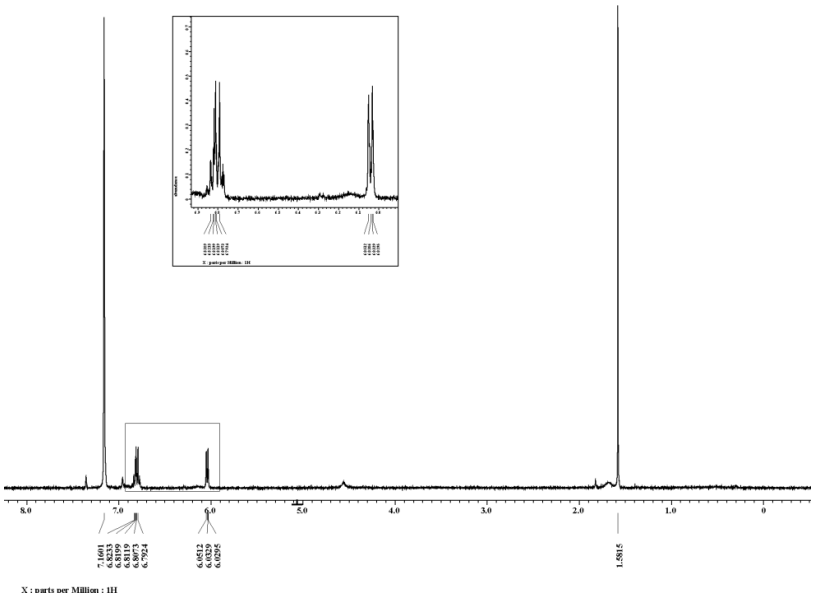


Figure S1. ^{1}H NMR spectrum of [PhNMe$_2$H][B(C$_6$F$_5$)$_4$] in C$_6$D$_6$.

(2) ^{1}H NMR spectrum of the reaction mixture containing of [N(Cy),N(Cy)-PLY-ZnMe] (2) and 1 equivalent of [PhNMe$_2$H][B(C$_6$F$_5$)$_4$]:

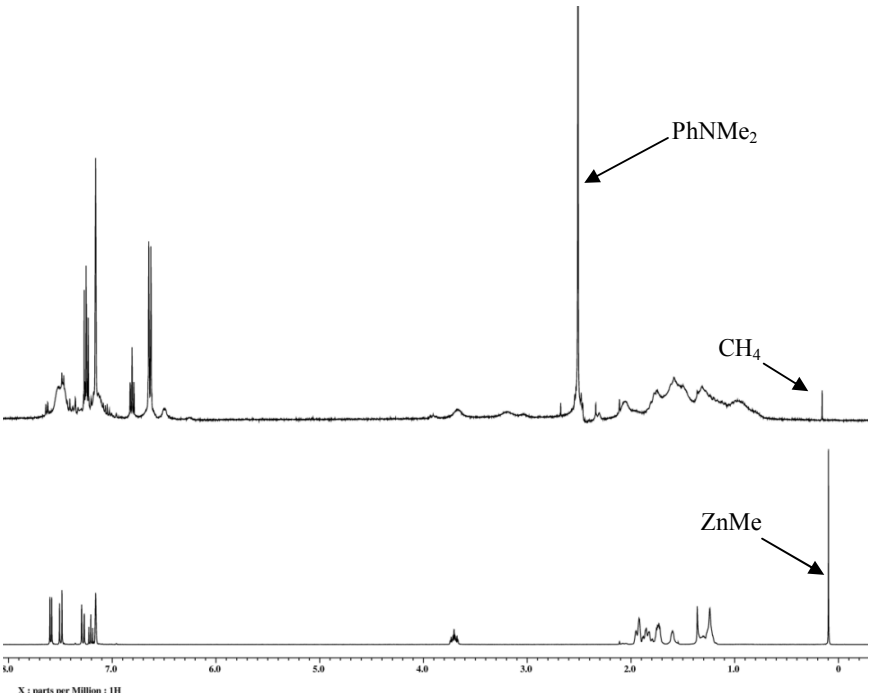
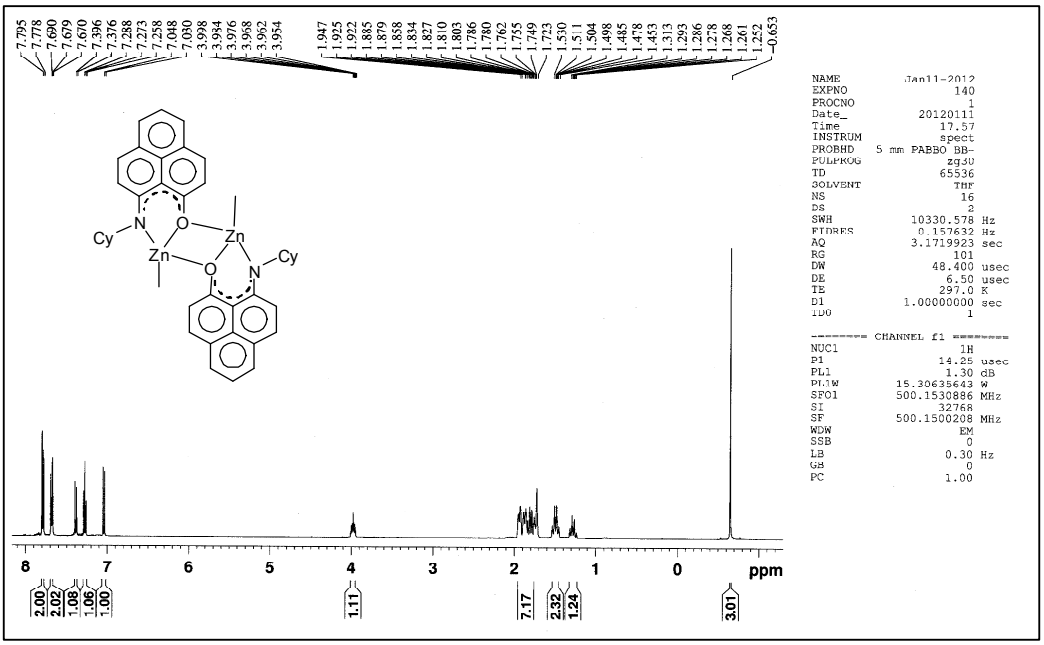
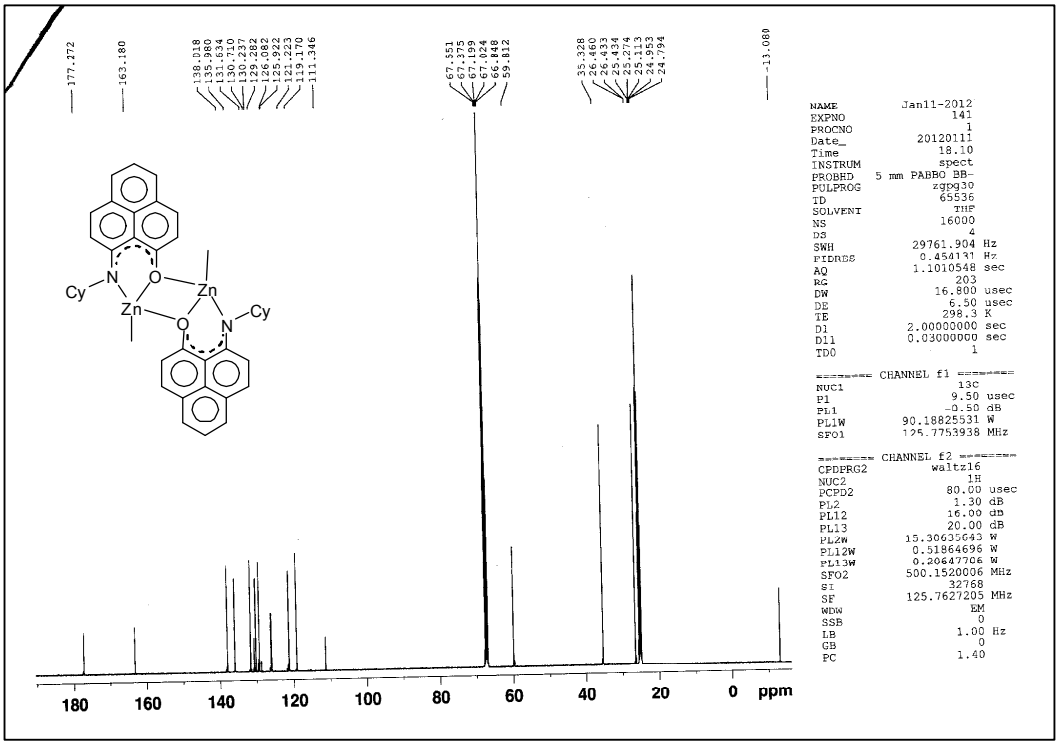


Figure S2. ^{1}H NMR spectrum of [N(Cy),N(Cy)-PLY-ZnMe] (**2**) and 1 equivalent of [PhNMe$_2$H][B(C$_6$F$_5$)$_4$] in C$_6$D$_6$.

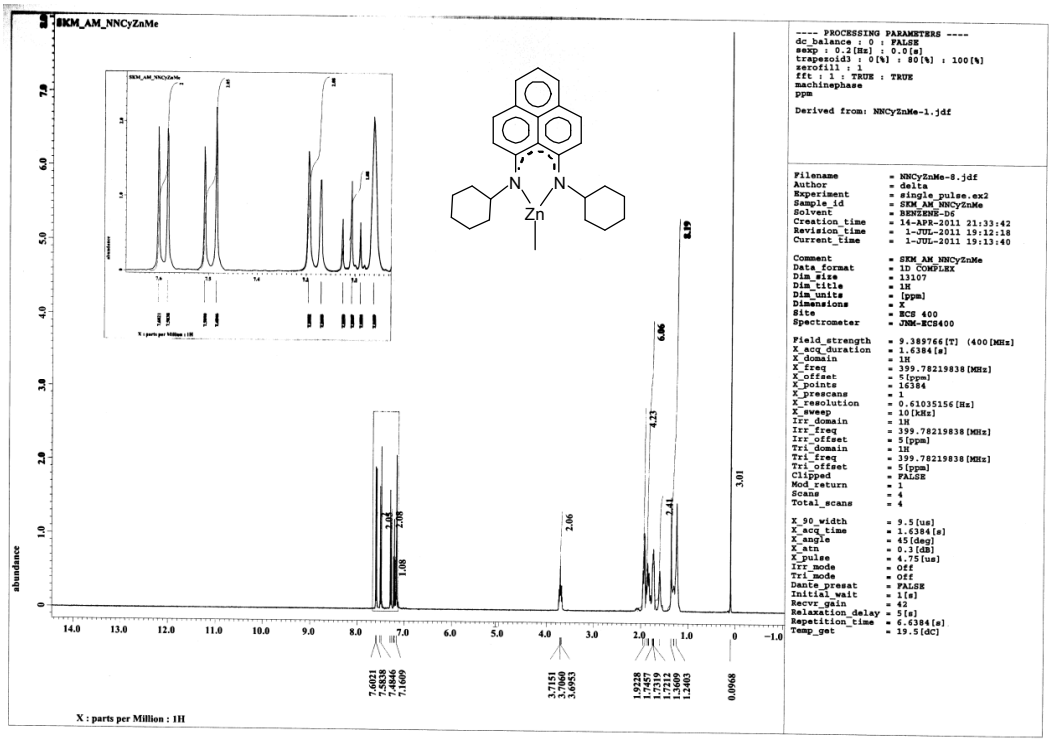
(3) ^{1}H NMR Spectra of [N(Cy),O-PLY-ZnMe]$_2$ (1):



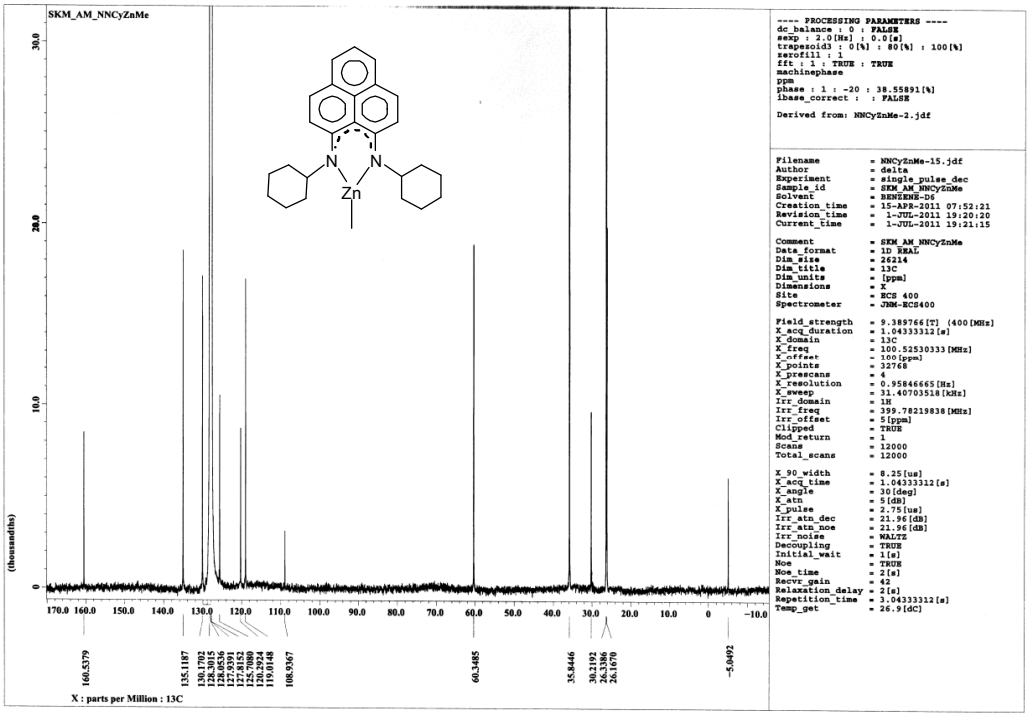
(4) ^{13}C NMR Spectra of [N(Cy),O-PLY-ZnMe]$_2$ (1):



(5) ^{1}H NMR Spectra of [N(Cy),N(Cy)-PLY-ZnMe] (2) :



(6) ^{13}C NMR Spectra of [N(Cy),N(Cy)-PLY-ZnMe] (2) :



X-ray Crystallographic Details of 1:

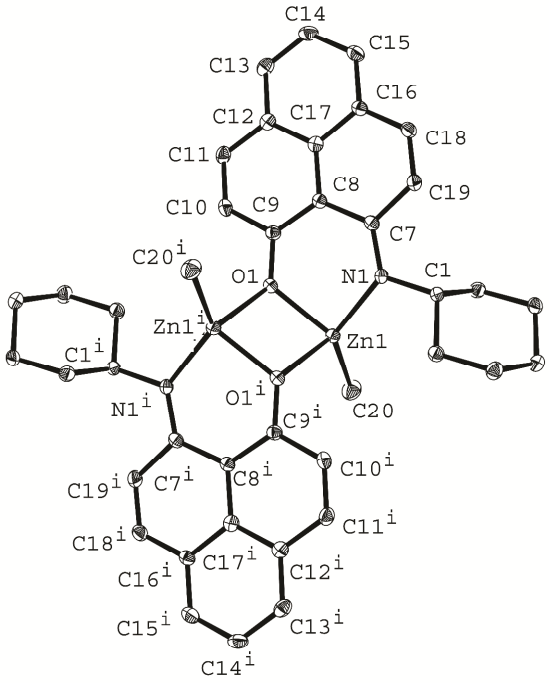


Figure S3. Molecular structure of the organozinc complex **1**. Thermal ellipsoids are drawn with 50% probability level. Hydrogen atoms are omitted for the sake of clarity.

Table S1. Crystal data and structure refinement for **1**

Empirical formula	$C_{40}H_{42}N_2O_2Zn_2$
CCDC No.	911744
Formula weight	713.54
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	monoclinic, $P2_1/n$
Unit cell dimensions	a = 9.035(2) Å
	b = 12.178(3) Å
	c = 14.405(3) Å
	α = 90.00°
	β = 99.573(4)°
	γ = 90.00°

Volume	1562.8(6) $Å^3$
Z, Calculated density	2, 1.521 g/mm^3
Absorption coefficient	1.576 mm^{-1}
F(000)	744
Crystal size	0.21 x 0.13 x 0.11 mm^3
Theta range for data collection	2.20–27.0°
Limiting indices	–11<=h<=11, –15<=k<=15, –10<=l<=18
Reflections collected / unique	3404 / 2863 (R_{int} = 0.0368)
Refinement method	Full-matrix least-squares on F^2
Goodness-of-fit on F^2	1.059
Final R indices [I>2σ(I)]	$R1$ = 0.0318, $wR2$ = 0.0756
R indices (all data)	$R1$ = 0.0418, $wR2$ = 0.0796
Largest diff. peak and hole	0.474 and –0.360e. $Å^{-3}$

Table S2 - Final Coordinates and Equivalent Isotropic Displacement

Parameters of the non-Hydrogen atoms for **1:**

Atom	x	y	z	U(eq) [Ang^2]
Zn1	0.38192(3)	0.57112(2)	0.04954(2)	0.0146(1)
O1	0.48718(17)	0.42797(13)	0.06642(11)	0.0159(5)
N1	0.4880(2)	0.61924(15)	0.17844(14)	0.0136(5)
C1	0.4750(2)	0.73776(17)	0.19980(16)	0.0136(6)
C2	0.3399(2)	0.76128(18)	0.24853(17)	0.0165(7)
C3	0.3370(2)	0.88297(19)	0.27469(17)	0.0173(7)
C4	0.3304(3)	0.95550(19)	0.18807(18)	0.0188(7)
C5	0.4584(3)	0.92840(19)	0.13472(18)	0.0192(7)
C6	0.4623(3)	0.80645(18)	0.11036(17)	0.0162(7)
C7	0.5445(2)	0.55240(18)	0.24776(16)	0.0135(6)
C8	0.5606(2)	0.43348(18)	0.23558(16)	0.0129(6)

C9	0.5320(2)	0.37930(18)	0.14741(16)	0.0140(6)
C10	0.5522(3)	0.26306(19)	0.14323(18)	0.0182(7)
C11	0.5921(3)	0.20161(18)	0.22129(17)	0.0174(7)
C12	0.6185(2)	0.25020(19)	0.31127(17)	0.0156(7)
C13	0.6575(2)	0.18574(19)	0.39254(18)	0.0181(7)
C14	0.6851(3)	0.2326(2)	0.48030(18)	0.0201(7)
C15	0.6769(3)	0.3462(2)	0.48824(17)	0.0183(7)
C16	0.6382(2)	0.41209(19)	0.40944(16)	0.0145(6)
C17	0.6050(2)	0.36610(18)	0.31789(17)	0.0141(6)
C18	0.6336(2)	0.5293(2)	0.41715(18)	0.0171(7)
C19	0.5929(2)	0.59471(19)	0.34270(17)	0.0171(7)
C20	0.1782(3)	0.6083(2)	-0.0121(2)	0.0252(8)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters for **1:**

Atom	x	y	z	U(iso) [Ang^2]
H1	0.56620	0.76010	0.24230	0.0160
H2A	0.24790	0.74220	0.20680	0.0200
H2B	0.34640	0.71670	0.30490	0.0200
H3A	0.25010	0.89740	0.30440	0.0210
H3B	0.42620	0.90060	0.31960	0.0210
H4A	0.33720	1.03200	0.20720	0.0230
H4B	0.23510	0.94480	0.14690	0.0230
H5A	0.55310	0.94900	0.17290	0.0230
H5B	0.44650	0.97120	0.07710	0.0230
H6A	0.37160	0.78670	0.06770	0.0190
H6B	0.54740	0.79170	0.07910	0.0190
H10	0.53740	0.22870	0.08480	0.0220

H11	0.60230	0.12600	0.21560	0.0210
H13	0.66470	0.11000	0.38670	0.0220
H14	0.70890	0.18910	0.53370	0.0240
H15	0.69780	0.37850	0.54750	0.0220
H18	0.66000	0.56110	0.47630	0.0200
H19	0.59560	0.67030	0.35180	0.0210
H20A	0.17710	0.61790	-0.07840	0.0380
H20B	0.14690	0.67510	0.01420	0.0380
H20C	0.11090	0.55000	-0.00240	0.0380

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S4 - (An)isotropic Displacement Parameters for **1**:

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Zn1	0.0154(1)	0.0142(1)	0.0133(2)	-0.0005(1)	0.0001(1)	0.0010(1)
O1	0.0207(8)	0.0148(8)	0.0119(8)	-0.0006(7)	0.0022(6)	0.0016(6)
N1	0.0158(9)	0.0113(9)	0.0135(10)	-0.0013(8)	0.0018(7)	0.0001(7)
C1	0.0155(10)	0.0123(10)	0.0124(12)	-0.0010(9)	0.0009(9)	0.0003(8)
C2	0.0181(10)	0.0160(11)	0.0161(13)	0.0019(9)	0.0046(9)	0.0006(9)
C3	0.0168(10)	0.0204(12)	0.0151(13)	-0.0020(10)	0.0036(9)	0.0057(9)
C4	0.0217(11)	0.0157(11)	0.0192(13)	0.0000(10)	0.0038(10)	0.0043(9)
C5	0.0230(11)	0.0152(11)	0.0208(13)	0.0017(10)	0.0075(10)	0.0006(9)
C6	0.0175(11)	0.0167(11)	0.0155(12)	0.0007(9)	0.0060(9)	0.0000(8)
C7	0.0124(10)	0.0166(11)	0.0124(12)	0.0002(9)	0.0043(8)	-0.0014(8)
C8	0.0111(9)	0.0154(10)	0.0124(12)	0.0002(9)	0.0030(8)	-0.0004(8)
C9	0.0141(10)	0.0149(11)	0.0134(12)	0.0012(9)	0.0031(9)	-0.0003(8)
C10	0.0236(11)	0.0156(11)	0.0154(13)	-0.0037(10)	0.0031(10)	0.0003(9)
C11	0.0208(11)	0.0120(11)	0.0202(13)	-0.0009(10)	0.0056(10)	-0.0007(8)
C12	0.0130(10)	0.0163(11)	0.0182(13)	0.0009(9)	0.0049(9)	-0.0008(8)

C13 0.0186(11) 0.0131(11 0.0234(14) 0.0038(10) 0.0060(10)-0.0005(8)

C14 0.0221(11) 0.0223(12) 0.0162(13) 0.0073(10) 0.0042(10)0.0014(9)

C15 0.0189(11) 0.0236(12) 0.0126(12) 0.0006(10) 0.0031(9)0.0005(9)

C16 0.0116(9) 0.0196(12) 0.0126(12) 0.0008(9) 0.0030(8)0.0006(8)

C17 0.0101(9) 0.0159(11) 0.0169(13) -0.0001(9) 0.0039(8)-0.0013(8)

C18 0.0163(10) 0.0206(12) 0.0136(12)-0.0025(10) 0.0006(9) 0.0023(9)

C19 0.0190(11) 0.0156(11) 0.0162(13) -0.0031(9) 0.0014(9) 0.0014(8)

C20 0.0197(11) 0.0247(13)0.0293(16)-0.0011(11)-0.0011(11)0.0029(10)

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for
Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and
h(i) are the Reflection Indices.

Table S5 - Bond Distances (Angstrom) for **1:**

Zn1	-O1	1.9813(17)	C16	-C17	1.418(3)
Zn1	-N1	2.029(2)	C16	-C18	1.433(3)
Zn1	-C20	1.959(3)	C18	-C19	1.337(3)
Zn1	-O1^{i}	2.2014(17)	C1	-H1	0.9800
O1	-C9	1.311(3)	C2	-H2A	0.9700
N1	-C1	1.485(3)	C2	-H2B	0.9700
N1	-C7	1.323(3)	C3	-H3A	0.9700
C1	-C2	1.533(3)	C3	-H3B	0.9700
C1	-C6	1.524(3)	C4	-H4A	0.9700
C2	-C3	1.530(3)	C4	-H4B	0.9700
C3	-C4	1.522(3)	C5	-H5A	0.9700
C4	-C5	1.527(4)	C5	-H5B	0.9700
C5	-C6	1.528(3)	C6	-H6A	0.9700
C7	-C8	1.469(3)	C6	-H6B	0.9700
C7	-C19	1.459(3)	C10	-H10	0.9300

C8	-C9	1.416(3)	C11	-H11	0.9300
C8	-C17	1.443(3)	C13	-H13	0.9300
C9	-C10	1.430(3)	C14	-H14	0.9300
C10	-C11	1.349(3)	C15	-H15	0.9300
C11	-C12	1.409(3)	C18	-H18	0.9300
C12	-C13	1.405(3)	C19	-H19	0.9300
C12	-C17	1.421(3)	C20	-H20A	0.9600
C13	-C14	1.372(4)	C20	-H20B	0.9600
C14	-C15	1.391(3)	C20	-H20C	0.9600

Table S6 - Bond Angles (Degrees) For **1**:

O1-Zn1-N1	89.87(7)	C8-C9-C10	119.6(2)
O1-Zn1-C20	130.89(9)	C9-C10-C11	122.2(2)
O1-Zn1-O1^{i}	77.88(6)	C10-C11-C12	121.0(2)
N1-Zn1-C20	127.82(10)	C11-C12-C13	120.8(2)
O1^{i}-Zn1-N1	117.47(7)	C11-C12-C17	118.4(2)
O1^{i} -Zn1-C20	103.75(9)	C13-C12-C17	120.8(2)
Zn1-O1-C9	125.30(14)	C12-C13-C14	121.2(2)
Zn1-O1-Zn1^{i}	102.12(7)	C13-C14-C15	119.1(2)
Zn1^{i} -O1-C9	123.51(13)	C14-C15-C16	121.2(2)
Zn1-N1-C1	115.39(14)	C15-C16-C17	121.2(2)
Zn1-N1-C7	125.25(15)	C15-C16-C18	121.3(2)
C1-N1-C7	118.40(19)	C17-C16-C18	117.5(2)
N1-C1-C2	111.91(17)	C8-C17-C12	121.7(2)
N1-C1-C6	110.84(18)	C8-C17-C16	121.8(2)
C2-C1-C6	109.32(18)	C12-C17-C16	116.6(2)
C1-C2-C3	109.95(16)	C16-C18-C19	122.6(2)
C2-C3-C4	111.1(2)	C7-C19-C18	122.8(2)

C3-C4-C5	110.9(2)	N1-C1-H1	108.00
C4-C5-C6	112.0(2)	C2-C1-H1	108.00
C1-C6-C5	109.92(19)	C6-C1-H1	108.00
N1-C7-C8	123.4(2)	C1-C2-H2A	110.00
N1-C7-C19	120.5(2)	C1-C2-H2B	110.00
C8-C7-C19	116.10(19)	C3-C2-H2A	110.00
C7-C8-C9	124.0(2)	C3-C2-H2B	110.00
C7-C8-C17	118.8(2)	H2A-C2-H2B	108.00
C9-C8-C17	117.2(2)	C2-C3-H3A	109.00
O1-C9-C8	124.8(2)	C2-C3-H3B	109.00
O1-C9-C10	115.6(2)	C4-C3-H3A	109.00

Table S7 - Torsion Angles (Degrees) for **1**:

N1-Zn1-O1-C9	29.36(16)
N1-Zn1-O1-Zn1^{i}	-118.18(7)
C20-Zn1-O1-C9	-114.66(18)
C20-Zn1-O1-Zn1^{i}	97.80(13)
O1^{i} -Zn1-O1-C9	147.54(17)
O1^{i} -Zn1-O1-Zn1^{i}	0.00(4)
O1-Zn1-N1-C1	168.08(14)
O1-Zn1-N1-C7	-23.37(18)
C20-Zn1-N1-C1	-46.14(19)
C20-Zn1-N1-C7	122.42(18)
O1^{i} -Zn1-N1-C1	91.83(14)
O1^{i} -Zn1-N1-C7	-99.61(17)
O1-Zn1-O1^{i} -Zn1^{i}	0.00(7)
O1-Zn1-O1^{i} -C9^{i}	148.31(17)
N1-Zn1-O1^{i} -Zn1^{i}	83.44(9)

N1-Zn1-O1^{i} -C9^{i}	-128.25(16)
C20-Zn1-O1^{i} -Zn1^{i}	-129.55(9)
C20-Zn1-O1^{i} -C9^{i}	18.76(18)
Zn1^{i} -O1-C9-C8	118.07(18)
Zn1^{i} -O1-C9-C10	-61.9(2)
Zn1-O1-C9-C10	157.12(16)
Zn1-O1-C9-C8	-22.9(3)
Zn1-N1-C1-C6	-30.8(2)
C7-N1-C1-C2	-77.9(2)
Zn1-N1-C7-C8	10.7(3)
Zn1-N1-C7-C19	-168.35(14)
C7-N1-C1-C6	159.81(19)
Zn1-N1-C1-C2	91.51(19)

X-ray Crystallographic Details of 2:

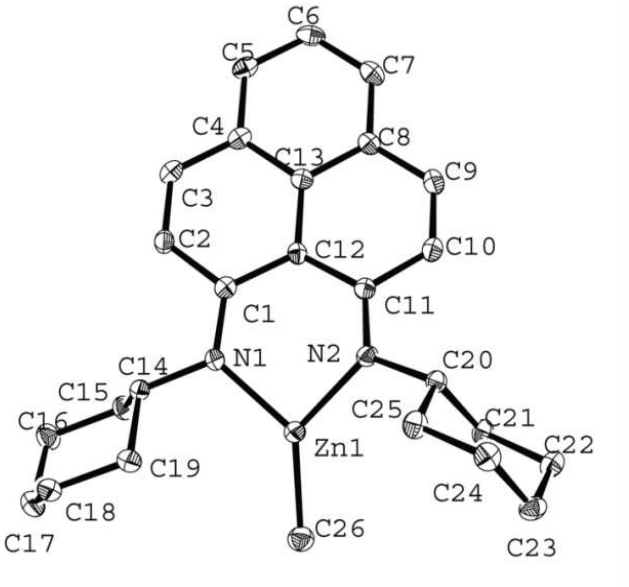


Figure S4. Molecular structure of the organozinc complex **2**. Thermal ellipsoids are drawn with 50% probability level. Hydrogen atoms are omitted for the sake of clarity.

Table S8. Crystal data and structure refinement for **2**

Empirical formula	$C_{26}H_{32}N_2Zn$
CCDC No.	805581
Formula weight	437.91
Temperature	100 (2) K
Wavelength	0.71073 Å
Crystal system, space group	monoclinic, *C*2/*c*
Unit cell dimensions	a = 21.5916(6) Å
	b = 12.3044(4) Å
	c = 16.4599(4) Å
	α = 90.00°
	β = 105.688(2) °
	γ = 90.00°
Volume	4210.0(2) $Å^3$
Z, Calculated density	8, 1.382 g/mm^3
Absorption coefficient	1.182 mm^{-1}
F(000)	1856
Crystal size	0.10 x 0.06 x 0.04 mm^3
Theta range for data collection	2.1605–27.130°
Limiting indices	–27<=h<=27, –14<=k<=15, –21<=l<=21
Reflections collected / unique	4590 / 3539 (R_{int} = 0.0515)
Refinement method	Full-matrix least-squares on F^2
Goodness-of-fit on F^2	1.041
Final R indices [I>2σ(I)]	$R1$ = 0.0404, $wR2$ = 0.0927
R indices (all data)	$R1$ = 0.0605, $wR2$ = 0.1023

Largest diff. peak and hole 0.169 and –0.200 e. Å $^{-3}$

Table S9 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for 2:

Atom	x	y	z	U(eq) [Ang^2]
Zn1	0.07601(1)	0.73344(3)	0.09678(2)	0.0174(1)
N1	0.14690(10)	0.63895(18)	0.15707(12)	0.0153(6)
N2	0.08090(10)	0.68463(18)	-0.01425(12)	0.0160(6)
C1	0.19374(12)	0.6037(2)	0.12364(15)	0.0151(8)
C2	0.24956(12)	0.5485(2)	0.17694(15)	0.0175(8)
C3	0.30004(12)	0.5167(2)	0.14932(16)	0.0181(8)
C4	0.30248(12)	0.5366(2)	0.06529(15)	0.0162(8)
C5	0.35628(12)	0.5053(2)	0.03866(16)	0.0189(8)
C6	0.36020(12)	0.5273(2)	-0.04239(16)	0.0200(8)
C7	0.30946(13)	0.5804(2)	-0.09772(16)	0.0194(8)
C8	0.25416(12)	0.6102(2)	-0.07382(15)	0.0154(7)
C9	0.20188(13)	0.6624(2)	-0.13196(15)	0.0186(8)
C10	0.14711(13)	0.6863(2)	-0.11141(15)	0.0174(8)
C11	0.13800(12)	0.6643(2)	-0.02863(14)	0.0150(7)
C12	0.19275(12)	0.6210(2)	0.03569(14)	0.0141(7)
C13	0.24889(12)	0.5899(2)	0.00937(14)	0.0146(8)
C14	0.15473(12)	0.6232(2)	0.24866(14)	0.0157(7)
C15	0.19655(13)	0.7128(2)	0.29922(15)	0.0185(8)

C16	0.20733(13)	0.6985(3)	0.39387(16)	0.0235(9)
C17	0.14332(13)	0.6899(3)	0.41677(16)	0.0250(9)
C18	0.10005(13)	0.6034(2)	0.36450(15)	0.0216(8)
C19	0.08951(12)	0.6213(2)	0.26918(15)	0.0187(8)
C20	0.02326(12)	0.7007(2)	-0.08621(14)	0.0155(8)
C21	0.00777(12)	0.8208(2)	-0.10507(15)	0.0175(8)
C22	-0.05483(12)	0.8367(2)	-0.17461(16)	0.0201(8)

Table S10 - Hydrogen Atom Positions and Isotropic Displacement Parameters For **2**:

Atom	x	y	z	U(iso) [Ang^2]
H2	0.25050	0.53420	0.23400	0.0210
H3	0.33490	0.48000	0.18700	0.0220
H5	0.39070	0.46820	0.07690	0.0230
H6	0.39710	0.50640	-0.05970	0.0240
H7	0.31210	0.59690	-0.15310	0.0230
H9	0.20560	0.68080	-0.18650	0.0220
H10	0.11290	0.71890	-0.15290	0.0210
H14	0.17660	0.55190	0.26580	0.0190
H15A	0.23870	0.71310	0.28610	0.0220
H15B	0.17570	0.78400	0.28200	0.0220
H16A	0.23200	0.76120	0.42380	0.0280
H16B	0.23300	0.63190	0.41260	0.0280
H17A	0.15180	0.67190	0.47740	0.0300
H17B	0.12110	0.76100	0.40710	0.0300
H18A	0.05790	0.60430	0.37760	0.0260
H18B	0.11970	0.53100	0.38010	0.0260

H19A	0.06250	0.56210	0.23730	0.0220
H19B	0.06680	0.69100	0.25210	0.0220
H20	0.03130	0.66620	-0.13740	0.0190
H21A	0.00410	0.85750	-0.05300	0.0210
H21B	0.04350	0.85540	-0.12260	0.0210
H22A	-0.04930	0.80870	-0.22860	0.0240
H22B	-0.06470	0.91520	-0.18170	0.0240
H23A	-0.12000	0.81130	-0.10370	0.0250
H23B	-0.15010	0.78580	-0.20200	0.0250

Table S11 - (An)isotropic Displacement Parameters For **2**:

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Zn1	0.0162(2)	0.0200(2)	0.0156(2)	-0.0003(1)	0.0035(1)	0.0033(1)
N1	0.0165(11)	0.0168(12)	0.0124(10)	-0.0001(8)	0.0034(8)	0.0008(9)
N2	0.0146(11)	0.0170(12)	0.0153(10)	-0.0013(9)	0.0022(9)	0.0020(9)
C1	0.0145(13)	0.0134(14)	0.0165(12)	-0.0014(10)	0.0025(10)	-0.0015(11)
C2	0.0195(14)	0.0177(15)	0.0146(11)	0.0019(10)	0.0032(10)	0.0012(11)
C3	0.0152(14)	0.0157(15)	0.0222(13)	0.0019(11)	0.0028(11)	0.0015(11)
C4	0.0137(13)	0.0129(14)	0.0207(12)	-0.0014(10)	0.0027(10)	-0.0019(11)
C5	0.0156(14)	0.0150(15)	0.0249(13)	-0.0022(11)	0.0032(11)	0.0006(11)
C6	0.0164(14)	0.0195(15)	0.0271(13)	-0.0062(11)	0.0111(11)	-0.0030(11)
C7	0.0223(14)	0.0196(15)	0.0179(12)	-0.0036(11)	0.0083(11)	-0.0058(12)
C8	0.0174(13)	0.0133(14)	0.0153(11)	-0.0036(10)	0.0041(10)	-0.0042(11)
C9	0.0237(15)	0.0172(15)	0.0145(11)	0.0001(10)	0.0045(11)	-0.0021(12)
C10	0.0182(14)	0.0157(14)	0.0163(12)	0.0008(10)	0.0015(10)	0.0001(11)

C11 0.0169(13) 0.0124(14) 0.0148(11)-0.0015(10) 0.0030(10)-0.0008(11)

C12 0.0167(13) 0.0121(14) 0.0125(11) -0.0011(9) 0.0025(10)-0.0018(11)

C13 0.0162(13) 0.0112(14) 0.0161(12) -0.0032(9) 0.0039(10)-0.0025(10)

C14 0.0169(13) 0.0160(14) 0.0136(11) 0.0003(10) 0.0033(10) 0.0027(11)

C15 0.0180(14) 0.0214(16) 0.0155(12)-0.0008(10) 0.0034(10)-0.0015(11)

C16 0.0243(15) 0.0287(17) 0.0167(12)-0.0023(11) 0.0044(11)-0.0006(13)

C17 0.0270(16) 0.0315(18) 0.0176(13)-0.0001(12) 0.0077(12) 0.0030(13)

C18 0.0230(15) 0.0233(16) 0.0213(13) 0.0022(11) 0.0106(11) 0.0042(12)

C19 0.0195(14) 0.0187(15) 0.0190(12)-0.0015(11) 0.0070(11)-0.0002(11)

C20 0.0122(13) 0.0193(15) 0.0135(11)-0.0016(10) 0.0011(10) 0.0002(11)

C21 0.0148(13) 0.0190(15) 0.0160(12)-0.0001(10)-0.0006(10)-0.0012(11)

C22 0.0189(14) 0.0173(15) 0.0213(13) 0.0000(11) 0.0006(11) 0.0008(12)

C23 0.0139(13) 0.0237(16) 0.0237(13)-0.0035(11) 0.0024(11) 0.0012(12)

Table S12 - Bond Distances (Angstrom) for **2**:

Zn1	-N1	1.964(2)	C20	-C21	1.528(3)
Zn1	-N2	1.954(2)	C20	-C25	1.538(4)
Zn1	-C26	1.966(3)	C21	-C22	1.529(4)
N1	-C1	1.347(3)	C22	-C23	1.530(4)
N1	-C14	1.484(3)	C23	-C24	1.518(4)
N2	-C11	1.340(3)	C24	-C25	1.533(4)
N2	-C20	1.481(3)	C2	-H2	0.9500
C1	-C2	1.453(4)	C3	-H3	0.9500
C1	-C12	1.458(3)	C5	-H5	0.9500
C2	-C3	1.348(4)	C6	-H6	0.9500
C3	-C4	1.420(4)	C7	-H7	0.9500
C4	-C5	1.402(4)	C9	-H9	0.9500
C4	-C13	1.428(4)	C10	-H10	0.9500
C5	-C6	1.386(4)	C14	-H14	1.0000
C6	-C7	1.385(4)	C15	-H15A	0.9900
C7	-C8	1.403(4)	C15	-H15B	0.9900
C8	-C9	1.421(4)	C16	-H16A	0.9900
C8	-C13	1.426(3)	C16	-H16B	0.9900
C9	-C10	1.348(4)	C17	-H17A	0.9900
C10	-C11	1.454(3)	C17	-H17B	0.9900
C11	-C12	1.458(3)	C18	-H18A	0.9900
C12	-C13	1.445(4)	C18	-H18B	0.9900
C14	-C15	1.522(4)	C19	-H19A	0.9900

C14	-C19	1.535(4)	C19	-H19B	0.9900
C15	-C16	1.522(4)	C20	-H20	1.0000
C16	-C17	1.531(4)	C21	-H21A	0.9900
C17	-C18	1.520(4)	C21	-H21B	0.9900

Table S13 - Bond Angles(Degrees)for **2**:

N1-Zn1-N2	93.37(9)	C1-C12-C11	124.5(2)
N1-Zn1-C26	132.90(10)	C1-C12-C13	118.1(2)
N2-Zn1-C26	133.66(10)	C11-C12-C13	117.4(2)
Zn1-N1-C1	123.56(16)	C4-C13-C8	116.0(2)
Zn1-N1-C14	116.73(16)	C4-C13-C12	121.8(2)
C1-N1-C14	118.8(2)	C8-C13-C12	122.2(2)
Zn1-N2-C11	120.50(16)	N1-C14-C15	110.4(2)
Zn1-N2-C20	117.44(16)	N1-C14-C19	111.5(2)
C11-N2-C20	119.86(19)	C15-C14-C19	109.6(2)
N1-C1-C2	119.7(2)	C14-C15-C16	112.3(2)
N1-C1-C12	123.2(2)	C15-C16-C17	111.2(2)
C2-C1-C12	117.1(2)	C16-C17-C18	111.5(2)
C1-C2-C3	123.1(2)	C17-C18-C19	112.1(2)
C2-C3-C4	121.7(2)	C14-C19-C18	109.6(2)
C3-C4-C5	120.6(2)	N2-C20-C21	112.5(2)
C3-C4-C13	118.0(2)	N2-C20-C25	108.60(19)
C5-C4-C13	121.3(2)	C21-C20-C25	110.2(2)
C4-C5-C6	121.3(2)	C20-C21-C22	112.1(2)
C5-C6-C7	118.8(2)	C21-C22-C23	111.6(2)

C6-C7-C8	121.4(2)	C22-C23-C24	110.8(2)
C7-C8-C9	120.7(2)	C23-C24-C25	110.8(2)
C7-C8-C13	121.2(2)	C20-C25-C24	111.7(2)
C9-C8-C13	118.1(2)	C1-C2-H2	118.00
C8-C9-C10	121.4(2)	C3-C2-H2	118.00
C9-C10-C11	123.0(2)	C2-C3-H3	119.00
N2-C11-C10	119.7(2)	C4-C3-H3	119.00
N2-C11-C12	123.0(2)	C4-C5-H5	119.00

Table S14 - Torsion Angles (Degrees) For **2**:

N2-Zn1-N1-C1	25.6(2)
N2-Zn1-N1-C14	-165.69(18)
C26-Zn1-N1-C1	-151.4(2)
C26-Zn1-N1-C14	17.3(2)
N1-Zn1-N2-C11	-37.8(2)
N1-Zn1-N2-C20	159.06(18)
C26-Zn1-N2-C11	139.2(2)
C26-Zn1-N2-C20	-23.9(2)
Zn1-N1-C14-C15	-87.0(2)
Zn1-N1-C1-C2	170.34(18)
Zn1-N1-C1-C12	-7.6(3)
C14-N1-C1-C2	1.9(3)
C14-N1-C1-C12	-176.1(2)
C1-N1-C14-C19	-155.8(2)
Zn1-N1-C14-C19	35.0(2)

C1-N1-C14-C15	82.2(3)
C20-N2-C11-C12	-164.1(2)
Zn1-N2-C20-C21	64.9(2)
Zn1-N2-C20-C25	-57.3(2)
C11-N2-C20-C21	-98.3(3)
Zn1-N2-C11-C10	-146.40(19)
Zn1-N2-C11-C12	33.2(3)
C20-N2-C11-C10	16.3(3)
C11-N2-C20-C25	139.4(2)
N1-C1-C12-C11	-8.8(4)
C12-C1-C2-C3	2.1(4)
C2-C1-C12-C13	-4.6(3)