Supporting Information for:

Reactions of Zirconacyclopentadienes with Nitrosobenzene. Characterization of Zirconacycle Intermediates and Formation of *N*-Phenylpyrroles.

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Experimental Section

General. All reactions involving air-sensitive compounds were carried out under nitrogen using standard Schlenk techniques and dry, oxygen-free solvents. Pentane, ether, benzene, and tetrahydrofuran were distilled under nitrogen from sodium benzophenone ketyl. Toluene and benzene-d_6 were distilled under nitrogen from Na/K. Butyllithium (1.6 M solution in hexane) and nitrosobenzene were purchased from Aldrich. Zirconacyclopentadienes (**1a**, **1b** and **1c**) were prepared according to reported methods. ^{1}H and ^{13}C NMR spectra were recorded on Bruker AMX (300 MHz and 400 MHz) spectrometers. Chemical shifts are referenced to the residual proton or carbon resonance of the deuterated solvent. All mass spectra were obtained at the Mass Spectrometry Facility of the University of California, Berkeley. Elemental analyses were provided by the Elemental Analysis Facility of the University of California, Berkeley.

2a. To a solution of **1a** (10 mmol) in toluene, prepared from $Cp_2Zr(n\text{-}Bu)_2$ and 2-butyne, was added nitrosobenzene (11 mmol) in toluene at -78 °C. The mixture was allowed to warm to room temperature, and was then stirred for 2 hours. After removal of all volatile material, the resulting solid was purified by short pass column chromatography (Al_2O_3, hexane/ether) and then recrystallization from acetonitrile at -30 °C to give the insertion product **2a** as light yellow crystals in 75% yield. mp. 143 °C (decomp.); ^{1}H NMR (400 MHz, C_6D_6) δ 1.58 (s, 3 H), 1.64 (s, 3 H), 1.97 (s, 3 H), 2.02 (s, 3 H), 5.60 (s, 5 H), 5.81 (s, 5 H), 6.92 (t, J = 7.2 Hz, 1 H), 7.14 (bs, 2 H), 7.35 (bs, 1 H), 7.74 (bs, 1 H). ^{13}C NMR (100 MHz, C_6D_6) δ 11.7, 17.0, 17.2, 25.8, 109.3, 109.8, 119(bs), 121(bs) 125.0, 133.5, 134.4, 136.7, 152.2, 173.5. Anal Calcd for $C_{24}H_{27}NOZr$: C, 66.06; H, 6.23; N, 3.21. Found: C, 66.03; H, 6.29; N, 3.01.

2b. To a solution of zirconacyclopentadiene **1b** (2 mmol) in toluene was added nitrosobenzene (2.1 mmol) in toluene at -78 °C. The mixture was allowed to warm to room temperature, and was then stirred overnight. After removal of all volatiles, the solid was purified by short pass column chromatography (Al_2O_3, hexane/ether) and then recrystallization from acetonitrile to give insertion product **2b** as yellow crystals in 45% yield. mp. 128-129 °C (decomp); ^{1}H NMR (300

MHz, C_6D_6) δ 1.49-1.65 (m, 3 H), 1.66 (s, 3 H), 1.71-1.84 (m, 2 H), 2.05 (s, 3 H), 2.09-2.20 (m, 1 H), 2.30 (dt, J = 15 Hz, 5 Hz, 1 H), 2.99 (dt, J = 12 Hz, 5 Hz, 1 H), 5.58 (s, 5 H), 5.82 (s, 5 H), 6.93 (t, J = 7.2 Hz, 1 H), 7.15 (bs, 2 H), 7.39 (bs, 1 H), 7.75 (bs, 1 H). ^{13}C NMR (100 MHz, C_6D_6) δ 10.9, 24.5, 24.9, 25.0, 28.7, 28.8 109.0, 109.5, 119(bs), 121(bs) 124.7, 133.4, 136.1, 138.2, 152.0, 171.2. Anal Calcd for $C_{26}H_{29}NOZr$: C, 67.45; H, 6.32; N, 3.03. Found: C, 67.42; H,6.51; N, 2.97.

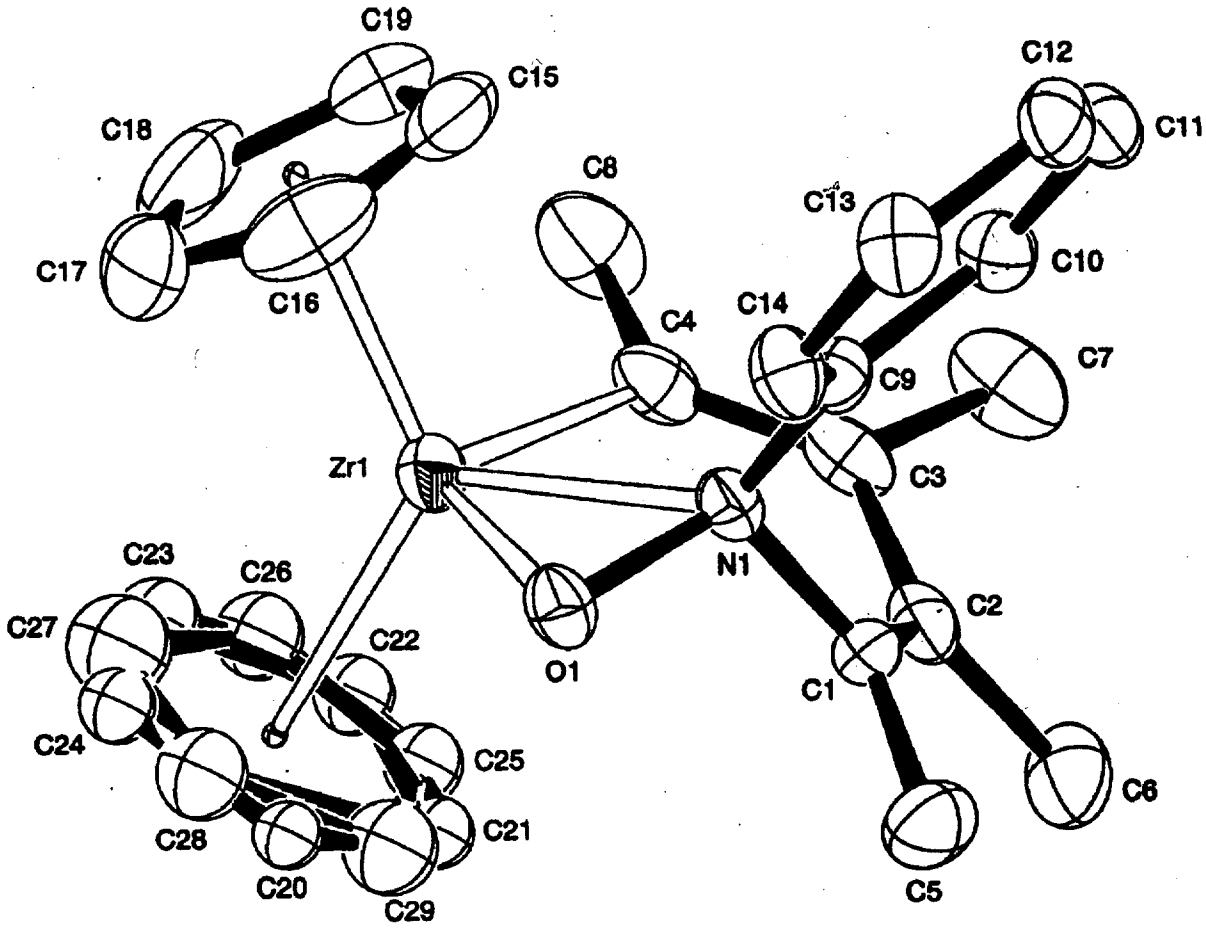
3a. A C_6D_6 solution of **2a** (0.1 mmol) in a sealed NMR tube was placed in a silicone oil bath (70-80 °C). After 2 weeks of heating, ^{1}H NMR spectroscopy revealed the clean formation of **3a** in >90% yield. Alternatively, **3a** can be prepared from a mixture of **2a** (2.0 mmol) and $AlCl_3$ (2.0 mmol) in toluene at 0 °C, which was allowed to react for 1 hour. Column chromatography on Al_2O_3 provided **3a** as a red-orange oil in 95 % yield based on **2a**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.96 (s, 6 H), 2.01 (s, 6 H), 7.18 (d, J = 6.8 Hz, 2 H), 7.36 (t, J = 7.2 Hz, 1 H), 7.43 (t, J = 7.2 Hz, 2 H). ^{13}C NMR (100 MHz, C_6D_6) δ 9.9, 10.9, 114.3, 123.3, 127.1, 128.8, 129.4, 140.4.

3b. Starting from **2b** (0.32 mmol) and $AlCl_3$ (0.4 mmol), the same procedure as that for **3a** was employed. Column chromatography on Al_2O_3 provided **3b** as an orange solid in 92% yield based on **2b**. mp. 59-62 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.82 (quintet, 4 H), 1.99 (s, 6 H), 2.55 (m, 4H), 7.25 (d, J = 8 Hz, 2 H), 7.38 (t, J = 8 Hz, 1 H), 7.47 (t, J = 7 Hz, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 10.4, 21.7, 24.2, 115.6, 122.2, 127.1, 128.3, 128.8, 139.2. Anal Calcd for $C_{16}H_{19}N$: C, 85.28; H, 8.50; N, 6.22. Found: C, 85.42; H, 8.62; N, 6.00.

4. To a solution of zirconacyclopentadiene **1c** (2.5 mmol) in toluene was added nitrosobenzene (3.0 mmol) in toluene at -78 °C. The mixture was allowed to warm to room temperature, and was then stirred overnight. After removal of all volatile material, the crude product was purified by short pass column chromatography (Al_2O_3, ether) and then recrystallization from ether at -30 °C to give **4** as colorless crystals in 45% yield. : ^{1}H NMR (400 MHz, C_6D_6) δ 1.39 (s, 3 H), 1.56-1.60 (m, 1 H), 1.83 (s, 3 H), 1.90-1.99 (m, 2 H), 2.10-2.30 (m, 1H), 2.45-2.55 (m, 1H), 2.62-2.72 (m, 1H), 3.76 (s, 1H), 5.48 (s, 5 H), 5.92 (s, 5 H), 6.55 (d, J = 8 Hz, 1 H), 6.86 (t, J = 7.2 Hz, 1 H), 7.05 (d, J = 7.2 Hz, 1 H), 7.12 (t, J = 8 Hz, 1 H). ^{13}C NMR (100 MHz, C_6D_6) δ 23.2, 23.6, 24.0, 32.0, 38.4, 71.9, 104.4, 109.1, 111.3, 111.6, 118.8, 124.9, 127.0, 139.4, 146.2, 148.7, 173.4. Anal Calcd for $C_{25}H_{27}NOZr$: C, 66.92; H, 6.06; N, 3.12. Found: C, 66.82; H, 6.10; N, 3.35.

5. Starting from **4**, the procedure for **3a** was used. Column chromatography on Al_2O_3 (hexane/ether) provided **5** as a deep red oil in 96% yield based on **4**. ^{1}H NMR (400 MHz, $CDCl_3$) δ, 1.53 (dt, J = 6.8 Hz, 2 Hz, 3 H), 1.91-1.99 (m, 1 H), 2.02-2.15 (m, 3H), 2.22 (s, 3 H), 2.5-2.7 (m, 2 H), 4.67 (qd, J = 6.9, 2.7 Hz 1H), 7.13 (t, J = 7.6 Hz, 1 H), 7.20 (d, J = 6 Hz, 1 H), 7.26 (t, J = 7.6 Hz, 1 H), 7.49 (d, J = 7.6 Hz, 1H). ^{13}C NMR (100 MHz, C_6D_6) δ 14.9, 16.1, 25.0,

29.8, 36.0, 68.6, 117.3, 120.1, 121.6, 125.1, 124.4, 142.9, 148.1, 155.8, 185.4. Anal Calcd for $C_{15}H_{17}N$: C, 85.26; H, 8.11; N, 6.63. Found: C, 84.96; H, 8.32; N, 6.73. EI-MS : 211 (100, m/z), 210 (85, m-1), 196 (65, m-Me).



EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$ZrONC_{24}H_{27}$
Formula Weight	436.70
Crystal Color, Habit	yellow, prism
Crystal Dimensions	0.24 X 0.19 X 0.18 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 9.5019(2) Å
	b = 16.8065(1) Å
	c = 12.9792(3) Å
	β = 97.672(1)°
	V = 2054.14(7) Å^3
Space Group	$P2_1/a$ (#14)
Z value	4
Dcalc	1.412 g/cm^3
F_{000}	904.00
μ(MoKα)	5.48 cm^{-1}

B. Intensity Measurements

Diffractometer	Bruker SMART CCD
Radiation	MoKα (λ = 0.71069 Å)
	graphite monochromated
Detector Position	60.00 mm
Exposure Time	10.0 seconds per frame.
Scan Type	ω (0.3 degrees per frame)
$2\theta_{max}$	49.4°
No. of Reflections Measured	Total: 8963 Unique: 3606 (R_{int} = 0.026)
Corrections	Lorentz-polarization
	Absorption (T_{max} = 0.93 T_{min} = 0.76)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares Function Minimized $\Sigma w (\|Fo\| - \|Fc\|)^2$
Least Squares Weights	$1/\sigma^2(Fo) = 4Fo^2/\sigma^2(Fo^2)$

p-factor	0.0500
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	2263
No. Variables	239
Reflection/Parameter Ratio	9.47
Residuals: R; Rw; Rall	0.032 ; 0.041; 0.054
Goodness of Fit Indicator	1.13
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.36 e-/Å^3
Minimum peak in Final Diff. Map	-0.44 e-/Å^3

Table 1. Atomic coordinates and Biso/Beq and occupancy for **2a**.

Atom	x	y	z	Beq	occ
Zr(1)	0.79446(4)	0.05702(2)	0.80688(3)	2.128(9)	
O(1)	0.8871(3)	-0.0508(2)	0.8577(2)	2.16(6)	
N(1)	0.7916(3)	-0.0741(2)	0.7683(2)	1.79(7)	
C(1)	0.6681(4)	-0.1146(2)	0.8006(3)	1.89(9)	
C(2)	0.5380(4)	-0.0895(3)	0.7619(3)	2.19(9)	
C(3)	0.5056(4)	-0.0200(3)	0.6922(3)	2.38(9)	
C(4)	0.5798(4)	0.0478(2)	0.7004(3)	2.40(9)	
C(5)	0.7045(5)	-0.1812(3)	0.8759(3)	3.0(1)	
C(6)	0.4124(4)	-0.1332(3)	0.7954(3)	3.4(1)	
C(7)	0.3688(5)	-0.0288(3)	0.6150(4)	3.8(1)	
C(8)	0.5162(5)	0.1197(3)	0.6396(3)	4.0(1)	
C(9)	0.8597(4)	-0.1210(2)	0.6959(3)	1.81(9)	
C(10)	0.7815(4)	-0.1403(2)	0.6010(3)	2.15(9)	
C(11)	0.8425(4)	-0.1850(2)	0.5300(3)	2.37(10)	
C(12)	0.9811(4)	-0.2109(2)	0.5526(3)	2.46(10)	
C(13)	1.0584(4)	-0.1914(3)	0.6461(3)	2.62(10)	
C(14)	0.9992(4)	-0.1462(2)	0.7192(3)	2.34(9)	
C(15)	0.9394(6)	0.0586(3)	0.6516(4)	4.4(1)	
C(16)	1.0347(6)	0.0688(4)	0.7399(5)	5.2(2)	
C(17)	1.0040(7)	0.1419(4)	0.7841(4)	5.5(2)	
C(18)	0.8897(7)	0.1754(3)	0.7204(5)	5.1(2)	
C(19)	0.8504(6)	0.1236(3)	0.6389(4)	4.6(1)	
C(20)	0.799(1)	0.0568(7)	1.0050(6)	1.7(1)	1/2
C(21)	0.655(1)	0.0419(6)	0.9609(9)	1.9(2)	1/2
C(22)	0.601(1)	0.1182(10)	0.9044(8)	2.3(2)	1/2
C(23)	0.719(2)	0.1738(6)	0.9163(9)	2.5(2)	1/2
C(24)	0.8418(10)	0.1355(8)	0.9787(8)	2.0(2)	1/2
C(25)	0.601(1)	0.0777(8)	0.9248(8)	2.3(2)	1/2
C(26)	0.644(2)	0.1535(8)	0.8980(7)	2.8(2)	1/2
C(27)	0.782(2)	0.1643(8)	0.943(1)	3.8(3)	1/2
C(28)	0.826(1)	0.094(1)	0.9941(8)	2.9(2)	1/2
C(29)	0.714(2)	0.0402(6)	0.9830(9)	3.2(3)	1/2
C(100)	0.9436	0.1137	0.7070	0.2000	0.000
C(101)	0.7183	0.1056	0.9508	0.2000	0.000
H(1)	0.7919	-0.2043	0.8634	3.7442	
H(2)	0.6318	-0.2212	0.8657	3.7442	

Table 1. Atomic coordinates and Biso/Beq and occupancy for **2a** (continued).

atom	x	y	z	Beq	occ
H(3)	0.7117	-0.1619	0.9445	3.7442	
H(4)	0.4051	-0.1861	0.7675	4.1741	
H(5)	0.3270	-0.1057	0.7751	4.1741	
H(6)	0.4244	-0.1387	0.8710	4.1741	
H(7)	0.3554	-0.0842	0.5955	4.8270	
H(8)	0.2883	-0.0128	0.6469	4.8270	
H(9)	0.3732	0.0014	0.5544	4.8270	
H(10)	0.5261	0.1146	0.5672	4.9997	
H(11)	0.5566	0.1667	0.6664	4.9997	
H(12)	0.4136	0.1214	0.6431	4.9997	
H(13)	0.6853	-0.1233	0.5861	2.7508	
H(14)	0.7886	-0.1991	0.4644	2.8765	
H(15)	1.0225	-0.2423	0.5027	2.8896	
H(16)	1.1553	-0.2087	0.6606	3.2298	
H(17)	1.0523	-0.1332	0.7849	2.9060	
H(18)	0.9328	0.0120	0.6049	5.1910	
H(19)	1.1086	0.0320	0.7668	6.6463	
H(20)	1.0558	0.1645	0.8480	6.5146	
H(21)	0.8434	0.2256	0.7288	6.4028	
H(22)	0.7753	0.1310	0.5822	5.4510	

$Beq = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 2. Anisotropic Displacement Parameters for atoms in **2a**.

Atom	U11	U22	U33	U12	U13	U23
Zr(1)	0.0341(2)	0.0210(2)	0.0256(2)	-0.0012(2)	0.0038(2)	-0.0029(2)
O(1)	0.025(1)	0.030(2)	0.025(1)	0.000(1)	-0.005(1)	-0.003(1)
N(1)	0.024(2)	0.023(2)	0.019(2)	0.000(1)	-0.001(1)	-0.003(1)
C(1)	0.031(2)	0.020(2)	0.021(2)	-0.004(2)	0.006(2)	0.000(2)
C(2)	0.026(2)	0.032(2)	0.025(2)	-0.003(2)	0.004(2)	-0.010(2)
C(3)	0.027(2)	0.041(3)	0.022(2)	0.010(2)	0.001(2)	-0.006(2)
C(4)	0.039(2)	0.029(3)	0.023(2)	0.011(2)	0.001(2)	-0.003(2)
C(5)	0.046(3)	0.029(3)	0.041(3)	0.000(2)	0.009(2)	0.005(2)
C(6)	0.032(3)	0.049(3)	0.050(3)	-0.011(2)	0.014(2)	-0.013(2)
C(7)	0.032(3)	0.071(4)	0.040(3)	0.013(2)	-0.003(2)	-0.007(3)
C(8)	0.073(4)	0.039(3)	0.037(3)	0.019(3)	-0.008(3)	-0.001(2)
C(9)	0.025(2)	0.018(2)	0.026(2)	-0.001(2)	0.004(2)	-0.002(2)
C(10)	0.024(2)	0.029(2)	0.028(2)	0.001(2)	0.000(2)	0.000(2)
C(11)	0.032(3)	0.033(3)	0.025(2)	-0.001(2)	0.002(2)	-0.005(2)
C(12)	0.034(3)	0.027(2)	0.034(2)	-0.002(2)	0.010(2)	-0.008(2)
C(13)	0.022(2)	0.033(3)	0.044(3)	0.002(2)	0.004(2)	-0.008(2)
C(14)	0.023(2)	0.031(3)	0.033(2)	0.002(2)	-0.001(2)	-0.007(2)
C(15)	0.086(4)	0.035(3)	0.053(3)	-0.024(3)	0.040(3)	-0.006(3)
C(16)	0.050(3)	0.071(5)	0.080(4)	-0.009(3)	0.029(3)	0.022(4)
C(17)	0.074(4)	0.085(5)	0.053(4)	-0.054(4)	0.018(3)	-0.017(4)
C(18)	0.090(5)	0.027(3)	0.083(4)	-0.013(3)	0.038(4)	0.005(3)
C(19)	0.083(4)	0.052(4)	0.043(3)	-0.026(3)	0.018(3)	0.011(3)

The general temperature factor expression:

$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 3. Bond Lengths(Å) in complex **2a**.

atom	atom	distance	atom	atom	distance
Zr1	O1	2.083(3)	Zr1	N1	2.259(3)
Zr1	C4	2.311(4)	Zr1	C15	2.589(4)
Zr1	C16	2.556(5)	Zr1	C17	2.500(5)
Zr1	C18	2.511(5)	Zr1	C19	2.568(5)
Zr1	C20	2.566(8)	Zr1	C21	2.552(8)
Zr1	C22	2.580(9)	Zr1	C23	2.579(9)
Zr1	C24	2.578(8)	Zr1	C25	2.571(9)
Zr1	C26	2.556(9)	Zr1	C27	2.54(1)
Zr1	C28	2.486(10)	Zr1	C29	2.52(1)
Zr1	C100	2.2556(4)	Zr1	C101	2.2455(4)
O1	N1	1.429(4)	N1	C1	1.466(5)
N1	C9	1.444(5)	C1	C2	1.339(5)
C1	C5	1.495(6)	C2	C3	1.485(6)
C2	C6	1.513(6)	C3	C4	1.338(6)
C3	C7	1.538(6)	C4	C8	1.522(6)
C9	C10	1.390(5)	C9	C14	1.385(5)
C10	C11	1.375(5)	C11	C12	1.381(5)
C12	C13	1.371(5)	C13	C14	1.392(5)
C15	C16	1.373(8)	C15	C19	1.378(7)
C15	C100	1.170(5)	C16	C17	1.403(8)
C16	C100	1.183(6)	C17	C18	1.393(8)
C17	C100	1.185(5)	C18	C19	1.383(7)
C18	C100	1.180(6)	C19	C100	1.177(6)
C20	C21	1.43(1)	C20	C24	1.44(1)
C20	C28	0.69(1)	C20	C29	0.87(1)
C20	C101	1.270(8)	C21	C22	1.53(1)
C21	C25	0.89(1)	C21	C28	1.84(1)
C21	C29	0.59(1)	C21	C101	1.240(9)
C22	C23	1.45(1)	C22	C25	0.73(1)
C22	C26	0.73(1)	C22	C101	1.212(9)
C23	C24	1.48(1)	C23	C26	0.80(1)
C23	C27	0.67(1)	C23	C101	1.231(10)
C24	C27	0.84(1)	C24	C28	0.75(1)
C24	C101	1.283(9)	C25	C26	1.40(1)
C25	C29	1.38(2)	C25	C101	1.218(9)
C26	C27	1.38(2)	C26	C101	1.222(9)

Table 3. Bond Lengths(Å) in complex **2a** (continued).

atom	atom	distance	atom	atom	distance
C27	C28	1.39(2)	C27	C101	1.17(1)
C28	C29	1.39(2)	C28	C101	1.117(10)
C29	C101	1.18(1)	C19	H22	0.96
C5	H1	0.95	C5	H2	0.96
C5	H3	0.94	C6	H4	0.96
C6	H5	0.94	C6	H6	0.98
C7	H7	0.97	C7	H8	0.96
C7	H9	0.94	C8	H10	0.96
C8	H11	0.93	C8	H12	0.98
C10	H13	0.95	C11	H14	0.96
C12	H15	0.96	C13	H16	0.96
C14	H17	0.96	C15	H18	0.99
C16	H19	0.97	C17	H20	0.98
C18	H21	0.97			

Table 4. Bond Angles(°) in complex **2a**.

atom	atom	atom	angle	atom	atom	atom	angle
O1	Zr1	N1	38.17(10)	O1	Zr1	C4	115.7(1)
O1	Zr1	C100	106.14(7)	O1	Zr1	C101	102.82(7)
N1	Zr1	C4	79.6(1)	N1	Zr1	C100	105.91(8)
N1	Zr1	C101	122.90(8)	C4	Zr1	C100	104.9(1)
C4	Zr1	C101	99.50(10)	C100	Zr1	C101	128.48(2)
Zr1	O1	N1	77.6(2)	Zr1	N1	O1	64.2(2)
Zr1	N1	C1	112.1(2)	Zr1	N1	C9	133.1(2)
O1	N1	C1	109.9(3)	O1	N1	C9	112.8(3)
C1	N1	C9	112.2(3)	N1	C1	C2	118.8(3)
N1	C1	C5	114.2(3)	C2	C1	C5	127.0(4)
C1	C2	C3	125.6(4)	C1	C2	C6	117.6(4)
C3	C2	C6	116.7(4)	C2	C3	C4	123.9(4)
C2	C3	C7	114.2(4)	C4	C3	C7	121.7(4)
Zr1	C4	C3	121.2(3)	Zr1	C4	C8	121.0(3)
C3	C4	C8	117.8(4)	N1	C9	C10	118.1(3)
N1	C9	C14	121.6(3)	C10	C9	C14	120.3(4)
C9	C10	C11	119.9(4)	C10	C11	C12	120.3(4)
C11	C12	C13	119.7(4)	C12	C13	C14	121.1(4)
C9	C14	C13	118.7(4)	C16	C15	C19	109.0(5)
C15	C16	C17	107.6(5)	C16	C17	C18	107.3(5)
C17	C18	C19	108.1(5)	C15	C19	C18	108.0(5)
Zr1	C100	C15	92.7(2)	Zr1	C100	C16	90.5(2)
Zr1	C100	C17	87.4(2)	Zr1	C100	C18	88.1(2)
Zr1	C100	C19	91.3(2)	Zr1	C101	C20	89.3(3)
Zr1	C101	C21	89.3(4)	Zr1	C101	C22	91.5(4)
Zr1	C101	C23	91.0(4)	Zr1	C101	C24	89.6(4)
Zr1	C101	C25	90.9(4)	Zr1	C101	C26	90.0(4)
Zr1	C101	C27	90.5(5)	Zr1	C101	C28	88.8(5)
Zr1	C101	C29	89.2(5)	H8	C7	H9	109.7
C1	C5	H1	109.0	C1	C5	H2	109.6
C1	C5	H3	110.0	H1	C5	H2	108.6
H1	C5	H3	110.3	H2	C5	H3	109.3
C2	C6	H4	111.2	C2	C6	H5	111.4
C2	C6	H6	110.1	H4	C6	H5	109.5
H4	C6	H6	106.5	H5	C6	H6	107.9

Table 4. Bond Angles(°) in complex **2a** (continued).

atom	atom	atom	angle	atom	atom	atom	angle
C3	C7	H7	109.4	C3	C7	H8	110.3
C3	C7	H9	111.3	H7	C7	H8	107.4
H7	C7	H9	108.5	C100	C19	H22	178.7
C4	C8	H10	110.7	C4	C8	H11	111.6
C4	C8	H12	109.1	H10	C8	H11	110.6
H10	C8	H12	106.0	H11	C8	H12	108.8
C9	C10	H13	119.6	C11	C10	H13	120.5
C10	C11	H14	120.3	C12	C11	H14	119.4
C11	C12	H15	119.6	C13	C12	H15	120.7
C12	C13	H16	119.2	C14	C13	H16	119.7
C9	C14	H17	120.1	C13	C14	H17	121.3
Zr1	C15	H18	118.3	C16	C15	H18	126.4
C19	C15	H18	124.6	C100	C15	H18	178.3
Zr1	C16	H19	117.8	C15	C16	H19	126.0
C17	C16	H19	126.4	C100	C16	H19	179.7
Zr1	C17	H20	115.9	C16	C17	H20	125.2
C18	C17	H20	127.5	C100	C17	H20	178.7
Zr1	C18	H21	116.4	C17	C18	H21	128.1
C19	C18	H21	123.9	C100	C18	H21	177.8
Zr1	C19	H22	119.4	C15	C19	H22	125.1
C18	C19	H22	126.9				

Table 5. Torsion Angles(°) in **2a**.

atom	atom	atom	atom	angle
Zr1	O1	N1	C1	-105.6(2)
Zr1	N1	C1	C2	58.7(4)
Zr1	N1	C9	C10	-98.2(4)
Zr1	C4	C3	C2	11.3(6)
O1	Zr1	N1	C1	102.3(3)
O1	Zr1	C4	C3	14.8(4)
O1	Zr1	C100	C15	56.6(3)
O1	Zr1	C100	C17	-87.5(4)
O1	Zr1	C100	C19	128.5(3)
O1	Zr1	C101	C21	-52.7(7)
O1	Zr1	C101	C23	157.2(8)
O1	Zr1	C101	C25	-94.9(7)
O1	Zr1	C101	C27	124.9(10)
O1	Zr1	C101	C29	-24.4(9)
O1	N1	Zr1	C100	96.0(2)
O1	N1	C1	C2	128.1(3)
O1	N1	C9	C10	-173.5(3)
N1	Zr1	C4	C3	27.5(3)
N1	Zr1	C100	C15	16.8(3)
N1	Zr1	C100	C17	-127.2(4)
N1	Zr1	C100	C19	88.8(3)
N1	Zr1	C101	C21	-17.1(7)
N1	Zr1	C101	C23	-167.2(8)
N1	Zr1	C101	C25	-59.3(7)
N1	Zr1	C101	C27	160.5(10)
N1	Zr1	C101	C29	11.2(9)
N1	O1	Zr1	C100	-95.4(2)
N1	C1	C2	C3	-3.7(6)
N1	C9	C10	C11	-179.9(4)
C1	N1	Zr1	C4	-59.1(2)
C1	N1	Zr1	C101	35.6(3)
C1	N1	C9	C14	-118.5(4)
C1	C2	C3	C7	148.7(4)
C2	C3	C4	C8	-167.0(4)
C3	C4	Zr1	C100	131.3(3)
C4	Zr1	N1	C9	100.8(3)

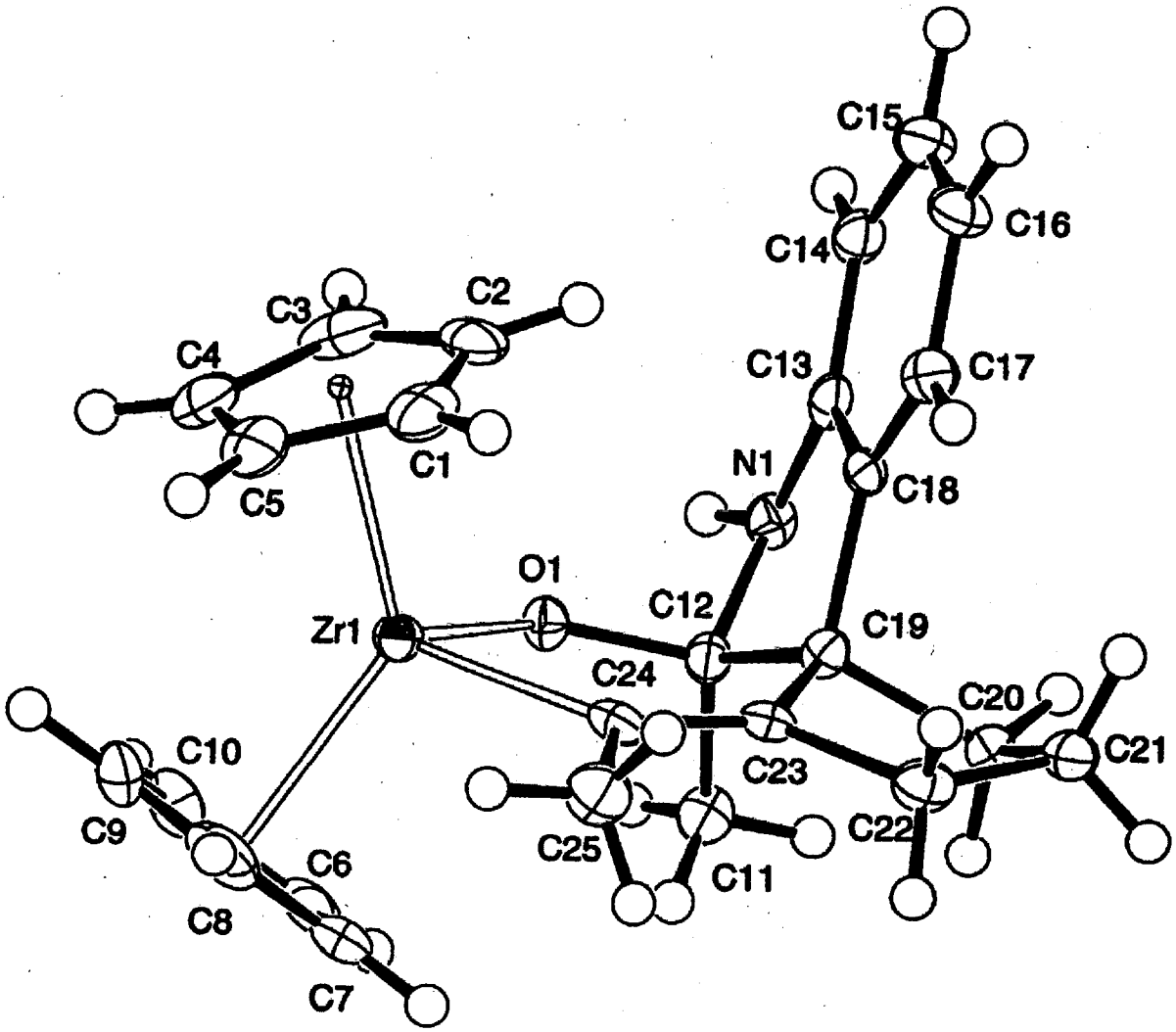
atom	atom	atom	atom	angle
Zr1	O1	N1	C9	128.3(3)
Zr1	N1	C1	C5	-121.0(3)
Zr1	N1	C9	C14	81.6(5)
Zr1	C4	C3	C7	-175.0(3)
O1	Zr1	N1	C9	-97.8(3)
O1	Zr1	C4	C8	-167.0(3)
O1	Zr1	C100	C16	-14.8(3)
O1	Zr1	C100	C18	-159.7(3)
O1	Zr1	C101	C20	16.9(6)
O1	Zr1	C101	C22	-129.9(8)
O1	Zr1	C101	C24	85.4(7)
O1	Zr1	C101	C26	-164.8(8)
O1	Zr1	C101	C28	49.8(9)
O1	N1	Zr1	C4	-161.3(2)
O1	N1	Zr1	C101	-66.7(2)
O1	N1	C1	C5	-51.6(4)
O1	N1	C9	C14	6.3(5)
N1	Zr1	C4	C8	-154.3(3)
N1	Zr1	C100	C16	-54.6(4)
N1	Zr1	C100	C18	160.6(4)
N1	Zr1	C101	C20	52.5(6)
N1	Zr1	C101	C22	-94.3(8)
N1	Zr1	C101	C24	121.0(7)
N1	Zr1	C101	C26	-129.2(8)
N1	Zr1	C101	C28	85.4(9)
N1	O1	Zr1	C4	20.4(2)
N1	O1	Zr1	C101	127.7()
N1	C1	C2	C6	179.1(3)
N1	C9	C14	C13	179.8(4)
C1	N1	Zr1	C100	-161.7(2)
C1	N1	C9	C10	61.7(4)
C1	C2	C3	C4	-37.2(6)
C2	C1	N1	C9	-105.5(4)
C3	C2	C1	C5	176.0(4)
C3	C4	Zr1	C101	-94.5(3)
C4	Zr1	C100	C15	-66.3(3)

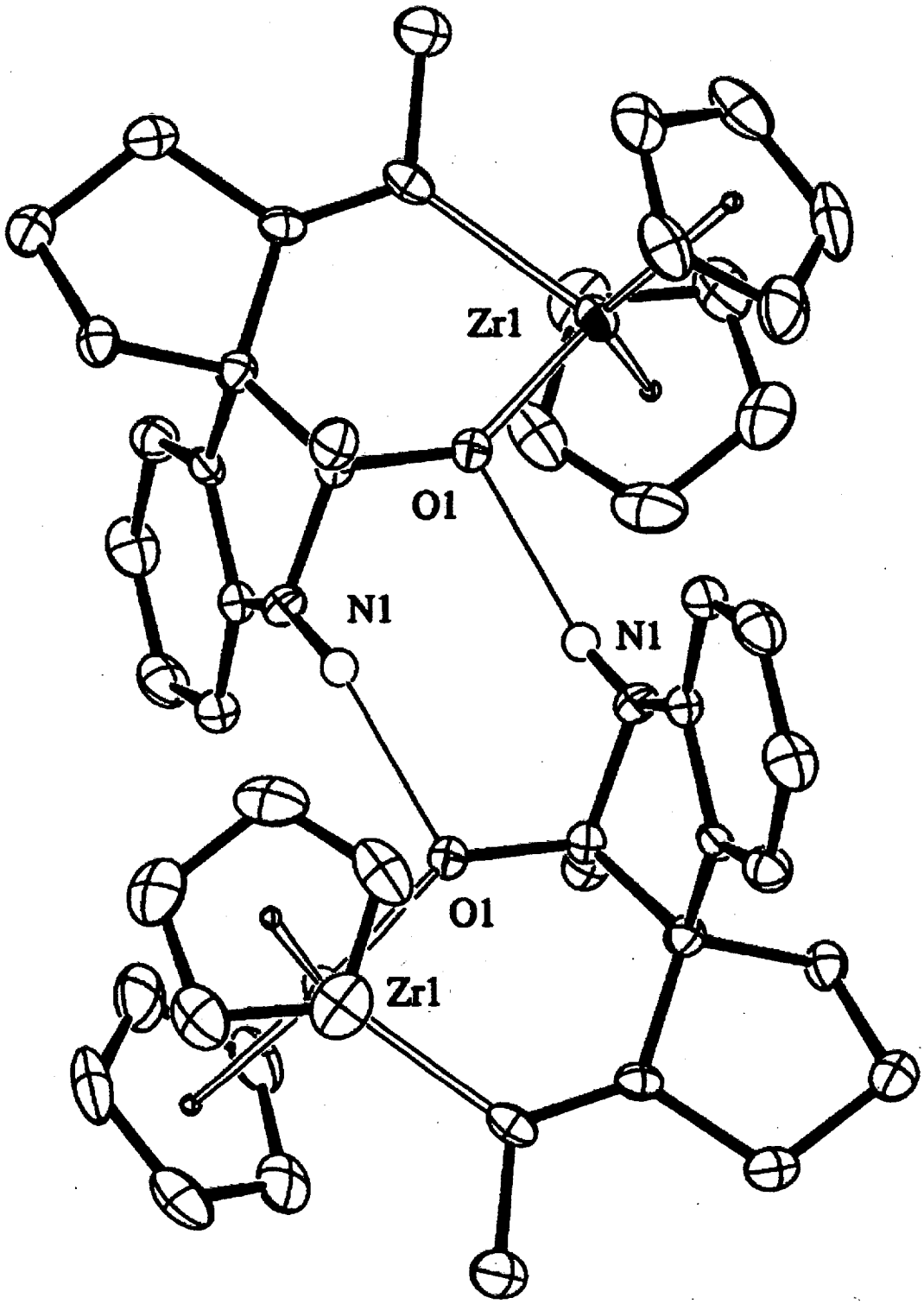
Table 5. Torsion Angles(°) in **2a** (continued).

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C4	Zr1	C100	C16	-137.8(4)	C4	Zr1	C100	C17	149.6(4)
C4	Zr1	C100	C18	77.4(4)	C4	Zr1	C100	C19	5.6(3)
C4	Zr1	C101	C20	136.1(6)	C4	Zr1	C101	C21	66.6(7)
C4	Zr1	C101	C22	-10.6(8)	C4	Zr1	C101	C23	-83.6(8)
C4	Zr1	C101	C24	-155.4(7)	C4	Zr1	C101	C25	24.3(7)
C4	Zr1	C101	C26	-45.5(8)	C4	Zr1	C101	C27	-115.8(10)
C4	Zr1	C101	C28	169.1(9)	C4	Zr1	C101	C29	94.9(9)
C4	C3	C2	C6	139.9(4)	C5	C1	N1	C9	74.7(4)
C5	C1	C2	C6	-1.1(6)	C6	C2	C3	C7	-34.2(5)
C7	C3	C4	C8	6.7(6)	C8	C4	Zr1	C100	-50.4(3)
C8	C4	Zr1	C101	83.8(3)	C9	N1	Zr1	C100	-1.8(3)
C9	N1	Zr1	C101	-164.5(3)	C9	C10	C11	C12	0.2(6)
C9	C14	C13	C12	0.0(6)	C10	C9	C14	C13	-0.4(6)
C10	C11	C12	C13	-0.6(6)	C11	C10	C9	C14	0.3(6)
C11	C12	C13	C14	0.5(7)	C15	C16	C17	C18	-0.5(6)
C15	C19	C18	C17	-0.1(6)	C15	C100	Zr1	C101	178.3(3)
C16	C15	C19	C18	-0.2(6)	C16	C100	Zr1	C101	106.8(3)
C17	C16	C15	C19	0.4(6)	C17	C100	Zr1	C101	34.2(4)
C18	C100	Zr1	C101	-38.0(3)	C19	C100	Zr1	C101	-109.8(3)

Table 6. Non-bonded Contacts out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
O1	C28	3.20(1)	75703	O1	C20	3.26(1)	75703
O1	C24	3.42(1)	75703	C5	C27	3.49(1)	64702
C12	C19	3.458(6)	75603	C21	C21	3.54(2)	65703





EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$ZrONC_{25}H_{27}$
Formula Weight	448.71
Crystal Color, Habit	cololess, rhombohedral
Crystal Dimensions	0.10 X 0.13 X 0.21 mm
Crystal System	triclinic
Lattice Type	Primitive
Lattice Parameters	a = 8.9298(8) Å
	b = 9.9455(9) Å
	c = 12.915(1) Å
	α = 96.503(2)°
	β = 91.808(1)°
	γ = 115.417(1)°
	V = 1025.2(2) Å^3
Space Group	P-1(#2)
Z value	2
D_{calc}	1.453 g/cm^3
F_{000}	464.00

μ(MoKα)	40.19 cm^{-1}

B. Intensity Measurements

Diffractometer	Bruker SMART CCD
Radiation	MoKα (λ = 0.71069 Å)
	graphite monochromated
Detector Position	60.00 mm
Exposure Time	10.0 seconds per frame.
Scan Type	ω (0.3 degrees per frame)
2θmax	49.5°
No. of Reflections Measured	Total: 5181 Unique: 2664 (Rint = 0.032)
Corrections	Lorentz-polarization
	Absorption (T_{max} = 0.96 T_{min} = 0.55)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR97)
Refinement	Full-matrix least-squares Function Minimized $\Sigma w (\|Fo\| - \|Fc\|)^2$
Least Squares Weights	$1/\sigma^2(Fo) = 4Fo^2/\sigma^2 (Fo^2)$

p-factor	0.0300
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	2681
No. Variables	253
Reflection/Parameter Ratio	10.60
Residuals: R; Rw; Rall	0.043 ; 0.050; 0.053
Goodness of Fit Indicator	1.87
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.72 e-/Å^3
Minimum peak in Final Diff. Map	-0.76 e-/Å^3

Table 7. Atomic coordinates and Biso/Beq and occupancy for **4**.

atom	x	y	z	Beq	occ
Zr1	0.25408(5)	0.14937(5)	0.27336(3)	1.43(1)	
O1	0.1244(3)	0.0087(3)	0.3669(2)	1.40(6)	
N1	-0.1172(4)	-0.1829(4)	0.4197(3)	1.43(8)	
C1	0.0909(6)	0.1809(5)	0.1198(4)	2.4(1)	
C2	-0.0187(6)	0.1404(6)	0.1976(4)	2.5(1)	
C3	0.0403(7)	0.2547(6)	0.2823(4)	2.8(1)	
C4	0.1904(6)	0.3696(5)	0.2564(4)	2.6(1)	
C5	0.2203(6)	0.3246(5)	0.1563(4)	2.4(1)	
C6	0.5083(6)	0.1697(5)	0.3807(4)	2.4(1)	
C7	0.5388(6)	0.1454(5)	0.2764(4)	2.5(1)	
C8	0.5573(6)	0.2723(6)	0.2302(4)	3.1(1)	
C9	0.5388(6)	0.3742(5)	0.3059(4)	2.9(1)	
C10	0.5052(6)	0.3102(5)	0.3994(4)	2.7(1)	
C11	0.1590(6)	-0.1796(5)	0.4498(3)	1.74(10)	
C12	0.0455(5)	-0.1469(4)	0.3769(3)	1.32(9)	
C13	-0.2329(5)	-0.2073(4)	0.3365(3)	1.44(9)	
C14	-0.3859(6)	-0.2027(5)	0.3378(4)	1.8(1)	
C15	-0.4826(6)	-0.2365(5)	0.2429(4)	2.1(1)	
C16	-0.4274(6)	-0.2723(5)	0.1506(4)	2.1(1)	
C17	-0.2730(5)	-0.2755(5)	0.1496(3)	1.63(10)	
C18	-0.1759(5)	-0.2438(4)	0.2429(3)	1.20(9)	
C19	-0.0078(5)	-0.2425(4)	0.2662(3)	1.28(9)	
C20	-0.0345(5)	-0.4077(5)	0.2696(3)	1.51(9)	
C21	-0.0530(5)	-0.4704(5)	0.1548(3)	1.7(1)	
C22	0.0759(6)	-0.3410(5)	0.1057(3)	1.76(10)	
C23	0.1060(5)	-0.1959(5)	0.1768(3)	1.30(9)	
C24	0.2088(5)	-0.0571(5)	0.1590(3)	1.48(9)	
C25	0.3025(6)	-0.0448(5)	0.0605(4)	2.2(1)	
C101	0.1046	0.2540	0.2024	0.3000	0.000
C102	0.5297	0.2543	0.3185	0.3000	0.000
H1	0.0805	0.1225	0.0541	2.8727	
H2	-0.1177	0.0494	0.1934	3.0439	
H3	-0.0104	0.2556	0.3457	3.3404	
H4	0.2586	0.4612	0.2999	3.1632	
H5	0.3116	0.3807	0.1190	2.9042	
H6	0.4924	0.1025	0.4305	2.8396	

Table 7. Atomic coordinates and Biso/Beq and occupancy for complex **4** (continued).

atom	x	y	z	Beq	occ
H7	0.5458	0.0585	0.2427	2.9842	
H8	0.5787	0.2862	0.1596	3.7184	
H9	0.5474	0.4704	0.2962	3.5224	
H10	0.4843	0.3540	0.4632	3.2383	
H11	0.2596	-0.1623	0.4188	2.0890	
H12	0.1833	-0.1154	0.5145	2.0890	
H13	0.1051	-0.2814	0.4616	2.0890	
H14	-0.0961	-0.1282	0.4848	3.1131	
H15	-0.4240	-0.1773	0.4015	2.1497	
H16	-0.5881	-0.2347	0.2422	2.5463	
H17	-0.4950	-0.2950	0.0869	2.5042	
H18	-0.2347	-0.2993	0.0854	1.9554	
H19	0.0588	-0.4100	0.3055	1.8061	
H20	-0.1321	-0.4622	0.3025	1.8061	
H21	-0.0300	-0.5556	0.1464	2.0869	
H22	-0.1621	-0.4975	0.1244	2.0869	
H23	0.1766	-0.3515	0.1022	2.1154	
H24	0.0345	-0.3398	0.0373	2.1154	
H25	0.3695	-0.0972	0.0638	2.6816	
H26	0.2247	-0.0876	0.0004	2.6816	
H27	0.3713	0.0580	0.0562	2.6816	

$Beq = 8/3\ \pi^2(U_{11}(aa^*)^2 + U^{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 8. Anisotropic Displacement Parameters for atoms in **4**.

atom	U11	U22	U33	U12	U13	U23
Zr1	0.0154(3)	0.0168(3)	0.0229(3)	0.0067(2)	0.0028(2)	0.0067(2)
O1	0.018(2)	0.015(2)	0.017(2)	0.005(1)	0.003(1)	0.001(1)
N1	0.020(2)	0.018(2)	0.014(2)	0.008(2)	0.002(2)	-0.001(2)
C1	0.038(3)	0.034(3)	0.027(3)	0.023(3)	-0.007(2)	0.006(2)
C2	0.017(3)	0.032(3)	0.053(3)	0.012(2)	0.001(2)	0.023(3)
C3	0.040(3)	0.046(3)	0.042(3)	0.034(3)	0.019(3)	0.023(3)
C4	0.037(3)	0.027(3)	0.044(3)	0.023(3)	-0.004(3)	0.004(2)
C5	0.031(3)	0.027(3)	0.040(3)	0.015(2)	0.005(2)	0.020(2)
C6	0.014(3)	0.030(3)	0.039(3)	0.003(2)	-0.007(2)	0.009(2)
C7	0.012(3)	0.028(3)	0.052(3)	0.007(2)	-0.001(2)	0.002(3)
C8	0.015(3)	0.042(3)	0.053(4)	0.004(2)	0.007(2)	0.013(3)
C9	0.022(3)	0.016(3)	0.066(4)	0.001(2)	-0.005(3)	0.008(3)
C10	0.023(3)	0.027(3)	0.042(3)	0.004(2)	-0.008(2)	-0.004(2)
C11	0.026(3)	0.021(2)	0.019(2)	0.011(2)	0.000(2)	0.002(2)
C12	0.017(2)	0.014(2)	0.019(2)	0.006(2)	0.002(2)	0.002(2)
C13	0.019(3)	0.012(2)	0.022(2)	0.005(2)	0.007(2)	0.002(2)
C14	0.021(3)	0.018(2)	0.030(3)	0.008(2)	0.009(2)	0.003(2)
C15	0.017(3)	0.025(3)	0.040(3)	0.010(2)	0.004(2)	0.009(2)
C16	0.018(3)	0.027(3)	0.033(3)	0.009(2)	-0.005(2)	0.006(2)
C17	0.021(3)	0.021(2)	0.021(2)	0.009(2)	0.003(2)	0.005(2)
C18	0.012(2)	0.012(2)	0.020(2)	0.004(2)	0.005(2)	0.004(2)
C19	0.018(2)	0.015(2)	0.017(2)	0.008(2)	0.003(2)	0.002(2)
C20	0.017(2)	0.016(2)	0.024(2)	0.008(2)	-0.001(2)	0.003(2)
C21	0.019(3)	0.022(3)	0.025(3)	0.011(2)	-0.002(2)	-0.001(2)
C22	0.022(3)	0.027(3)	0.020(2)	0.013(2)	0.003(2)	0.001(2)
C23	0.012(2)	0.022(2)	0.017(2)	0.009(2)	0.001(2)	0.003(2)
C24	0.011(2)	0.025(2)	0.020(2)	0.007(2)	0.002(2)	0.008(2)
C25	0.027(3)	0.030(3)	0.029(3)	0.013(2)	0.009(2)	0.006(2)

The general temperature factor expression:

$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 9. Bond Lengths(Å) in complex **4**.

atom	atom	distance	atom	atom	distance
Zr1	O1	1.959(3)	Zr1	C1	2.551(4)
Zr1	C2	2.558(4)	Zr1	C3	2.541(5)
Zr1	C4	2.517(4)	Zr1	C5	2.537(4)
Zr1	C6	2.542(4)	Zr1	C7	2.559(5)
Zr1	C8	2.559(5)	Zr1	C9	2.546(5)
Zr1	C10	2.517(5)	Zr1	C24	2.264(4)
Zr1	C101	2.2440(4)	Zr1	C102	2.2480(5)
O1	C12	1.423(4)	N1	C12	1.481(5)
N1	C13	1.392(5)	C1	C2	1.395(7)
C1	C5	1.412(7)	C2	C3	1.391(7)
C3	C4	1.419(7)	C4	C5	1.392(7)
C6	C7	1.398(7)	C6	C10	1.402(7)
C7	C8	1.406(7)	C8	C9	1.393(7)
C9	C10	1.409(7)	C11	C12	1.520(6)
C12	C19	1.561(6)	C13	C14	1.387(6)
C13	C18	1.397(6)	C14	C15	1.397(6)
C15	C16	1.371(6)	C16	C17	1.393(6)
C17	C18	1.385(6)	C18	C19	1.516(6)
C19	C20	1.562(6)	C19	C23	1.540(6)
C20	C21	1.517(6)	C21	C22	1.531(6)
C22	C23	1.533(6)	C23	C24	1.340(6)
C24	C25	1.532(6)	C25	H26	0.95
N1	H14	0.91	C1	H1	0.95
C2	H2	0.95	C3	H3	0.95
C4	H4	0.95	C5	H5	0.95
C6	H6	0.95	C7	H7	0.95
C8	H8	0.95	C9	H9	0.95
C10	H10	0.95	C11	H11	0.95
C11	H12	0.95	C11	H13	0.95
C14	H15	0.95	C15	H16	0.95
C16	H17	0.95	C17	H18	0.95
C20	H19	0.95	C20	H20	0.95
C21	H21	0.95	C21	H22	0.95
C22	H23	0.95	C22	H24	0.95
C25	H25	0.95	C25	H27	0.95

Table 10. Bond Angles(°) in complex **4**.

atom	atom	atom	angle	atom	atom	atom	angle
O1	Zr1	C24	86.1(1)	O1	Zr1	C101	110.95(8)
O1	Zr1	C102	113.16(8)	C24	Zr1	C101	105.4(1)
C24	Zr1	C102	103.8(1)	C101	Zr1	C102	127.92(2)
Zr1	O1	C12	142.4(2)	C12	N1	C13	107.7(3)
C2	C1	C5	107.6(4)	C1	C2	C3	109.0(4)
C2	C3	C4	107.4(4)	C3	C4	C5	108.1(4)
C1	C5	C4	107.9(4)	C7	C6	C10	108.5(4)
C6	C7	C8	107.8(4)	C7	C8	C9	108.0(5)
C8	C9	C10	108.4(4)	C6	C10	C9	107.3(4)
O1	C12	N1	109.3(3)	O1	C12	C11	108.1(3)
O1	C12	C19	109.8(3)	N1	C12	C11	110.8(3)
N1	C12	C19	102.0(3)	C11	C12	C19	116.7(3)
N1	C13	C14	129.2(4)	N1	C13	C18	109.7(4)
C14	C13	C18	121.1(4)	C13	C14	C15	118.3(4)
C14	C15	C16	121.0(4)	C15	C16	C17	120.6(4)
C16	C17	C18	119.4(4)	C13	C18	C17	119.7(4)
C13	C18	C19	109.1(3)	C17	C18	C19	131.2(4)
C12	C19	C18	100.6(3)	C12	C19	C20	111.9(3)
C12	C19	C23	120.4(3)	C18	C19	C20	108.5(3)
C18	C19	C23	112.9(3)	C20	C19	C23	102.5(3)
C19	C20	C21	103.0(3)	C20	C21	C22	104.2(3)
C21	C22	C23	106.4(3)	C19	C23	C22	106.7(3)
C19	C23	C24	128.6(4)	C22	C23	C24	124.6(4)
Zr1	C24	C23	121.8(3)	Zr1	C24	C25	121.2(3)
C23	C24	C25	116.9(4)	H12	C11	H13	109.5
C12	N1	H14	107.2	C13	N1	H14	131.7
C2	C1	H1	126.2	C5	C1	H1	126.2
C1	C2	H2	125.5	C3	C2	H2	125.5
C2	C3	H3	126.3	C4	C3	H3	126.3
C3	C4	H4	126.0	C5	C4	H4	126.0
C1	C5	H5	126.0	C4	C5	H5	126.0
C7	C6	H6	125.8	C10	C6	H6	125.8
C6	C7	H7	126.1	C8	C7	H7	126.1
C7	C8	H8	126.0	C9	C8	H8	126.0
C8	C9	H9	125.8	C10	C9	H9	125.8
C6	C10	H10	126.3	C9	C10	H10	126.3

Table 10. Bond Angles(°) in complex **4** (continued).

atom	atom	atom	angle
C12	C11	H11	109.5
C12	C11	H13	109.5
H11	C11	H13	109.5
C13	C14	H15	120.9
C14	C15	H16	119.5
C15	C16	H17	119.7
C16	C17	H18	120.3
C19	C20	H19	111.1
C21	C20	H19	111.1
H19	C20	H20	109.5
C20	C21	H22	110.8
C22	C21	H22	110.8
C21	C22	H23	110.2
C23	C22	H23	110.2
H23	C22	H24	109.5
C24	C25	H26	109.5
H25	C25	H26	109.5

atom	atom	atom	angle
C12	C11	H12	109.5
H11	C11	H12	109.5
H26	C25	H27	109.5
C15	C14	H15	120.9
C16	C15	H16	119.5
C17	C16	H17	119.7
C18	C17	H18	120.3
C19	C20	H20	111.1
C21	C20	H20	111.1
C20	C21	H21	110.8
C22	C21	H21	110.8
H21	C21	H22	109.5
C21	C22	H24	110.2
C23	C22	H24	110.2
C24	C25	H25	109.5
C24	C25	H27	109.5
H25	C25	H27	109.5

Table 11. Torsion Angles(°) in complex **4**.

atom	atom	atom	atom	angle
Zr1	O1	C12	N1	-138.6(3)
Zr1	O1	C12	C19	-27.5(6)
Zr1	C24	C23	C22	-176.9(3)
O1	Zr1	C101	C2	-35.8(3)
O1	Zr1	C101	C4	108.5(3)
O1	Zr1	C102	C6	9.4(3)
O1	Zr1	C102	C8	153.5(3)
O1	Zr1	C102	C10	-62.6(3)
O1	C12	C19	C18	-85.7(4)
O1	C12	C19	C23	39.0(5)
N1	C12	C19	C20	-84.9(4)
N1	C13	C14	C15	-178.0(4)
N1	C13	C18	C19	-0.3(4)
C11	C12	C19	C18	151.0(4)
C11	C12	C19	C23	-84.4(5)
C12	O1	Zr1	C101	110.8(4)
C12	N1	C13	C14	-160.0(4)
C12	C19	C18	C13	-19.2(4)
C12	C19	C20	C21	-169.9(3)
C12	C19	C23	C24	-32.8(6)
C13	C14	C15	C16	-0.5(7)
C13	C18	C19	C20	98.3(4)
C14	C13	C18	C17	0.2(6)
C14	C15	C16	C17	-0.1(7)
C15	C16	C17	C18	0.7(7)
C17	C18	C19	C20	-80.7(5)
C18	C19	C20	C21	80.0(4)
C18	C19	C23	C24	85.9(5)
C19	C23	C22	C21	-0.6(4)
C20	C19	C23	C22	24.5(4)
C20	C21	C22	C23	-24.5(4)
C21	C22	C23	C24	-178.6(4)
C23	C24	Zr1	C101	-103.3(3)
C25	C24	Zr1	C101	80.2(3)

atom	atom	atom	atom	angle
Zr1	O1	C12	C11	100.7(4)
Zr1	C24	C23	C19	5.7(6)
O1	Zr1	C101	C1	-107.7(3)
O1	Zr1	C101	C3	35.6(3)
O1	Zr1	C101	C5	179.8(3)
O1	Zr1	C102	C7	81.2(3)
O1	Zr1	C102	C9	-134.9(3)
O1	C12	N1	C13	83.6(4)
O1	C12	C19	C20	159.3(3)
N1	C12	C19	C18	30.1(4)
N1	C12	C19	C23	154.8(3)
N1	C13	C18	C17	178.9(4)
C11	C12	N1	C13	-157.3(3)
C11	C12	C19	C20	35.9(5)
C12	O1	Zr1	C24	5.8(4)
C12	O1	Zr1	C102	-97.6(4)
C12	N1	C13	C18	21.5(4)
C12	C19	C18	C17	161.8(4)
C12	C19	C23	C22	149.4(3)
C13	N1	C12	C19	-32.5(4)
C13	C18	C17	C16	-0.7(6)
C13	C18	C19	C23	-148.8(3)
C14	C13	C18	C19	-179.0(4)
C15	C14	C13	C18	0.4(6)
C16	C17	C18	C19	178.2(4)
C17	C18	C19	C23	32.1(6)
C18	C19	C23	C22	-91.9(4)
C19	C20	C21	C22	39.7(4)
C19	C23	C24	C25	-177.7(4)
C20	C19	C23	C24	-157.6(4)
C21	C20	C19	C23	-39.6(4)
C22	C23	C24	C25	-0.2(6)
C23	C24	Zr1	C102	120.3(3)
C25	C24	Zr1	C102	-56.2(3)

Table 12. Non-bonded Contacts out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
O1	N1	3.103(4)	55602	C4	C21	3.499(6)	56501
C4	C20	3.568(6)	56501	C6	C11	3.595(6)	65602
C8	C21	3.569(7)	66501	C9	C20	3.562(7)	66501