Supplementary Material (ESI) for Chemical Communications

Supporting Information

X-Ray Crystal Structure of a Heterobimetallic Al-Zn-Oxide Complex

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Experimental Section

Manipulations were performed in a glove box under an Ar-atmosphere or with standard Schlenk techniques. Dry solvents were obtained from a solvent purification system (MBraun) and degassed prior to use. MesnacnacZnH,[1] MesnacnacZnMe,[2] DippnacnacAlH$_2$,[3] DippnacnacAl(Me)OH,[4] and Cp*TiMe$_3$[5] were prepared according to literature methods. MeLi, AlMe$_3$, Al(*i*-Bu)$_3$, HAl(*i*-Bu)$_2$ and ZnMe$_2$ were commercially available (Acros Organics; Alfa Aesar) and used as received. A Bruker Avance 500 spectrometer was used for NMR spectroscopy. ^{1}H and ^{13}C{^{1}H} NMR spectra were referenced to internal C$_6$D$_5$H (^{1}H: δ = 7.154; ^{13}C: δ = 128.0). IR spectra were recorded on an Alpha-T FT-IR spectrometer with a single reflection ATR sampling module. Melting points were measured in sealed capillaries and were not corrected. Elemental analyses were performed at the *Elementaranalyse Labor* of the University of Duisburg-Essen.

[MesnacnacZnOH]$_2$ (1)

4 µL (3.0 mmol) of H$_2$O was slowly added via syringe to a stirred solution of 1.25 g (3.0 mmol) MesnacnacZnMe in THF at −78 °C. The solution was warmed to room temperature and stirred for additional 12h. The resulting white precipitate was separated by centrifugation, washed with 2 mL of hexane and dried under vacuum. Yield: 0.79 g (0.95 mmol), 63 %. Crystals suitable for a single crystal X-ray analysis were obtained by slow cooling of a concentrated toluene solution of [MesnacnacZnOH]$_2$ to −30 °C. M.p. 270 °C. – Elemental analysis (%) calcd for C$_{46}$H$_{60}$N$_4$OZn$_2$ (831.78 g/mol): C 66.42, H 7.27 N 6.74; found C 66.20, H 7.26, N 6.49. – IR: ν = 3667, 2911, 2852, 1524, 1454, 1399, 1276, 1203, 1147, 1012, 856, 745, 727, 600, 502, 433 cm^{-1}. – ^{1}H NMR (300 MHz, [C$_6$D$_6$], 20 °C): δ = –0.20 (s, 2H, OH), 1.46 (s, 12H, CH$_3$ backbone), 1.95 (s, 24H, aryl CH$_3$), 2.34 (s, 24H, aryl CH$_3$), 4.73 (s, 2H, H backbone), 6.75 (m, 8H, aryl). – ^{13}C NMR (75 MHz, [C$_6$D$_6$], 20 °C): 17.9 (CH$_3$), 21.0 (CH$_3$ backbone), 22.8 (CH$_3$), 93.8 (backbone), 128.7 (aryl), 131,1 (aryl), 132.1 (aryl), 145.6 (aryl), 167.3 (backbone).

Investigations on the reactivity of [MesnacnacZnOH]$_2$

The reactivity of [MesnacnacZnOH]$_2$ towards MeLi, AlMe$_3$, Al(*i*-Bu)$_3$, HAl(*i*-Bu)$_2$, Cp*TiMe$_3$, ZnMe$_2$ and DippnacnacAlH$_2$ was tested. The experimental procedures for the reactions of [MesnacnacZnOH]$_2$ with Al(*i*-Bu)$_3$ and HAl(*i*-Bu)$_2$ are given exemplary:

a) 30 mg (0.036 mmol) [MesnacnacZnOH]$_2$ was dissolved in an NMR tube in 0.5 mL of benzene-d$_6$. 15 mg 0.076 mmol of Al(*i*-Bu)$_3$ was added to this solution, immediately resulting in a gas evolution and the formation of small amounts of a colourless precipitate. The progress of the reaction was then monitored via ^{1}H NMR spectroscopy. The ^{1}H NMR spectrum after 5 minutes at room temperature showed complete conversion of [MesnacnacZnOH]$_2$ to MesnacnacZn(*i*-Bu), which was identified by its ^{1}H NMR spectrum.

b) 30 mg (0.036 mmol) [MesnacnacZnOH]$_2$ was dissolved in an NMR tube in 0.5 mL of benzene-d$_6$. 8 mg 0.07 mmol of HAl(*i*-Bu)$_2$ was added and the progress of the reaction was monitored via ^{1}H NMR spectroscopy. After 5 minutes at room temperature, the ^{1}H NMR spectrum showed complete conversion of [MesnacnacZnOH]$_2$ to a mixture of MesnacnacZn(*i*-Bu) and MesnacnacZnH (ratio approx. 5:1), which again were unambigously identified by their ^{1}H NMR spectra.

MesnacnacZn(i-Bu): ^{1}H NMR (300 MHz, [benzene-d$_6$], 20 °C): δ = 0.44 (d, ^{3}J(H,H) = 5.7 Hz, 2H, *i*-Bu), 0.66 (d, ^{3}J(H,H) = 6.4 Hz, 6H, *i*-Bu), 1.63 (s, 6H, CH$_3$ backbone), 1.81 (m, 1H, *i*-Bu), 2.14 (s, 12H, aryl CH$_3$), 2.15 (s, 6H, aryl CH$_3$), 4.97 (s, 1H, H backbone), 6.83 (m, 4H, aryl).

MesnacnacZnOAl(Me)Dippnacnac (2)

300 mg (0.63 mmol) DippnacnacAl(Me)OH and 300 mg (0.75 mmol) MesnacnacZnH were dissolved in a sealed pyrex tube in 5 mL of toluene and the solution was stirred at 100 °C for six days. The ^{1}H NMR sprectrum revealed an almost quantitative formation of **2**. The solvent was thereafter removed under reduced pressure and 5 mL of hexane was added to the residue. The insoluble powder (presumably excess MesnacnacZnH) was filtered off and the remaining solution was concentrated to a volume of approximately 1 mL. Slow cooling of this solution to −30 °C afforded colourless crystals of the desired product in low yield. Yield: 100 mg (0.14 mmol), 18 %. M.p. 211 °C. − IR: ν = 2961, 2866, 1527, 1437, 1389, 1318, 1259, 1201, 1099, 1018, 919, 859, 797, 753, 618, 448 cm^{-1}. − Elemental analysis (%) calcd for $C_{53}H_{73}AlN_4OZn$ (874.54 g/mol): C 72.79, H 8.41, N 6.41; found C 71.10, H 8.41 N 5.68. ^{1}H NMR (500 MHz, [toluene-d$_8$], 20 °C): δ = −1.32 (s, 3H, Al-CH$_3$), 1.07 (d, ^{3}J(H,H) = 6.8 Hz, 6H, *i*-Pr), 1.11 (d, ^{3}J(H,H) = 6.8 Hz, 6H, *i*-Pr), 1.12 (d, ^{3}J(H,H) = 6.8 Hz, 6H, *i*-Pr), 1.25 (d, ^{3}J(H,H) = 6.8 Hz, 6H, *i*-Pr), 1.51 (s, 6H, CH$_3$ backbone), 1.53 (s, 6H, CH$_3$ backbone), 2.04 (s, 12H, aryl CH$_3$), 2.14 (s, 6H, aryl CH$_3$), 3.22 (sept, ^{3}J(H,H) = 6.8 Hz, 2H, *i*-Pr), 3.60 (sept, ^{3}J(H,H) = 6.8 Hz, 2H, *i*-Pr),

4.77 (s, 2H, H backbone), 4.84 (s, 2H, H backbone), 6.69 (s, 4H, Aryl), 7.02 – 7-11 (m, 6H, aryl). ^{13}C NMR (75 MHz, [toluene-d_8], 20 °C): −11.8 ($AlCH_3$), 28.7 (CH_3), 20.9 (CH_3), 22.9 (CH_3 backbone), 23.4 (CH_3 backbone), 24.2 (*i*-Pr), 24.9 (*i*-Pr), 25.0 (*i*-Pr), 25.7 (*i*-Pr), 27.7 (*i*-Pr), 28.3 (*i*Pr), 94.8 (backbone), 96.7 (backbone), 124.2 (aryl), 126.5 (aryl), 129.4 (aryl), 131.4 (aryl), 133.4 (aryl), 142,1 (aryl), 143.7 (aryl), 144.7 (aryl), 145.0 (aryl), 167.9 (backbone), 168.6 (aryl).

General procedure for CO_2/CHO copolymerization:

3.93 g (40 mmol) CHO and 35 mg (0.04 mmol) **2** was placed in a glovebox in a 25 mL stainless steel reactor equipped with a magnetic stir bar. The reactor was closed and heated to 50 °C before pressurising the system with 10 bar CO_2. The reaction was then stirred at this temperature for two hours. Thereafter, the pressure (CO_2) was carefully released and the solution diluted with 80 mL of dichloromethane. The solvent was evaporated and the polymer precipitated by addition of 30 mL of methanol, filtered off and dried in vacuo to constant weight. The resulting solid (217 mg) was contamined by small amounts of CD_2Cl_2-insoluble by-products (ZnO, Al_2O_3). The product was characterized by ^{1}H NMR spectroscopy (CD_2Cl_2).

Crystal structure determination

The crystals of **1** und **2** were mounted on nylon loops in inert oil. Data were collected on a Bruker AXS D8 Kappa diffractometer with APEX2 detector (mono-chromated $Mo_{K\alpha}$ radiation, λ = 0.71073 Å) at 108 K (1) and 203 K (2). The structures were solved by Direct Methods (SHELXS-97) [6] and refined anisotropically by full-matrix least-squares on F^2 (SHELXL-97) [7]. Absorption corrections were performed semi-empirically from equivalent reflections on basis of multi-scans (Buker AXS APEX2). Hydrogen atoms were refined using a riding model or rigid methyl groups. The position of H(1) in **1** was taken from the fourier map and refined by riding model all other non-methyl H were placed on idealialised positions.

CCDC 804558 (**1**) and 804557 (**2**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

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

Empirical formula	$C_{46}\ H_{60}\ N_4\ O_2\ Zn_2$	
Formula weight	831.72 Da	
Density (calculated)	1.302 g cm^{-3}	
F(000)	440	
Temperature	108(1) K	
Crystal size	0.25 x 0.22 x 0.17 mm	
Crystal color	colourless	
Crystal description	block	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	$P\ \bar{1}$	
Unit cell dimensions	a = 8.4102(2) Å	α = 69.2140(10)°
	b = 10.1431(3) Å	β = 82.6750(10)°
	c = 13.5329(3) Å	γ = 80.1370(10)°
Volume	1060.55(5) $Å^3$	
Z	1	
Cell measurement reflections used	8618	
Cell measurement theta min/max	2.17° to 26.98°	
Diffractometer control software	Bruker AXS APEX 2 Vers.3.0/2009	
Diffractometer measurement device	Bruker D8 KAPPA series II with	
	APEX II area detector system	
Diffractometer measurement method	Data collection strategy APEX 2/COSMO	
Theta range for data collection	1.61° to 27.00°	
Completeness to theta = 27.00°	98.3 %	
Index ranges	-10<=*h*<=8, -12<=*k*<=12, -17<=*l*<=16	
Computing data reduction	Bruker AXS APEX 2 Vers.3/2009	
Absorption coefficient	1.172 mm^{-1}	
Absorption correction	Semi-empirical from equivalents	
Empirical absorption correction	Bruker AXS APEX 2 Vers.3/2009	
Max. / min. transmission	0.75 / 0.67	
$R_{(merg)}$ before/after correction	0.0360 / 0.0319	
Computing structure solution	Bruker AXS SHELXTL Vers. 2008/4/(c) 2008	
Computing structure refinement	Bruker AXS SHELXTL Vers. 2008/4/(c) 2008	
Refinement method	Full-matrix least-squares on F^2	
Reflections collected	14027	

Independent reflections	4555 [$R_{(int)}$ = 0.0225]
Data / restraints / parameters	4167 / 0 / 244
Goodness-of-fit on F^2	1.057
Weighting details	$w = 1/[\sigma^2 (Fo^2)+ (0.0341*P)^2+0.4985*P]$ where $P = (Fo^2+2Fc^2)/3$
Final R indices [I>2sigma(I)]	R_1 = 0.0245, wR_2 = 0.0647
R indices (all data)	R_1 = 0.0284, wR_2 = 0.0669
Largest diff. peak and hole	0.383 and -0.256 eÅ^{-3}
Treatment of hydrogen atoms	Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent Uij of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent Uij of the corresponding carbon atom. Hydrogen atom position H(1) taken from a Fourier-map and also refined as riding group with the 1.5 fold isotropic displacement parameters of the equivalent Uij of the corresponding oxygen atom.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **1**. *U*(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	*U*(eq)
Zn(1)	4071(1)	6182(1)	5279(1)	14(1)
N(1)	3279(2)	6578(1)	6586(1)	16(1)
N(2)	3350(2)	8062(1)	4252(1)	15(1)
O(1)	3615(1)	4576(1)	4924(1)	17(1)
C(1)	2904(2)	7927(2)	6545(1)	17(1)
C(2)	2943(2)	9117(2)	5615(1)	19(1)
C(3)	3029(2)	9188(2)	4558(1)	18(1)
C(4)	2358(2)	8228(2)	7562(1)	26(1)
C(5)	2661(2)	10653(2)	3742(1)	27(1)
C(6)	2988(2)	5497(2)	7597(1)	16(1)
C(7)	1481(2)	5001(2)	7845(1)	19(1)
C(8)	1160(2)	4046(2)	8858(1)	22(1)
C(9)	2296(2)	3561(2)	9615(1)	21(1)
C(10)	3804(2)	4026(2)	9326(1)	22(1)
C(11)	4182(2)	4971(2)	8320(1)	19(1)
C(12)	237(2)	5505(2)	7039(2)	29(1)
C(13)	1913(2)	2553(2)	10718(1)	31(1)
C(14)	5856(2)	5390(2)	8022(1)	29(1)
C(15)	3075(2)	8220(2)	3190(1)	16(1)
C(16)	4358(2)	8386(2)	2408(1)	19(1)
C(17)	4031(2)	8576(2)	1382(1)	22(1)
C(18)	2492(2)	8552(2)	1123(1)	25(1)
C(19)	1257(2)	8320(2)	1925(1)	24(1)
C(20)	1523(2)	8145(2)	2963(1)	19(1)
C(21)	6046(2)	8347(2)	2682(1)	25(1)
C(22)	2195(3)	8731(2)	6(2)	38(1)
C(23)	179(2)	7868(2)	3832(1)	28(1)

Table 3. Bond lengths [Å] and angles [°] for **1**.

Zn(1)-N(1)	1.9612(13)	O(1)-Zn(1)-N(2)	114.13(5)
Zn(1)-O(1)	1.9623(10)	N(1)-Zn(1)-O(1)#1	119.62(5)
Zn(1)-N(2)	1.9681(12)	O(1)-Zn(1)-O(1)#1	85.17(4)
Zn(1)-O(1)#1	1.9890(11)	N(2)-Zn(1)-O(1)#1	115.39(5)
Zn(1)-Zn(1)#1	2.9094(3)	N(1)-Zn(1)-Zn(1)#1	136.72(4)
N(1)-C(1)	1.3336(19)	O(1)-Zn(1)-Zn(1)#1	42.94(3)
N(1)-C(6)	1.4400(18)	N(2)-Zn(1)-Zn(1)#1	124.67(4)
N(2)-C(3)	1.323(2)	O(1)#1-Zn(1)-Zn(1)#1	42.23(3)
N(2)-C(15)	1.4320(19)	C(1)-N(1)-C(6)	116.78(13)
C(1)-C(2)	1.403(2)	C(1)-N(1)-Zn(1)	118.99(10)
C(1)-C(4)	1.511(2)	C(6)-N(1)-Zn(1)	124.15(10)
C(2)-C(3)	1.400(2)	C(3)-N(2)-C(15)	119.18(12)
C(3)-C(5)	1.513(2)	C(3)-N(2)-Zn(1)	119.71(10)
C(6)-C(11)	1.396(2)	C(15)-N(2)-Zn(1)	121.00(9)
C(6)-C(7)	1.400(2)	Zn(1)-O(1)-Zn(1)#1	94.83(4)
C(7)-C(8)	1.394(2)	N(1)-C(1)-C(2)	124.87(14)
C(7)-C(12)	1.503(2)	N(1)-C(1)-C(4)	118.82(14)
C(8)-C(9)	1.391(2)	C(2)-C(1)-C(4)	116.30(13)
C(9)-C(10)	1.389(2)	C(3)-C(2)-C(1)	129.27(14)
C(9)-C(13)	1.511(2)	N(2)-C(3)-C(2)	124.01(14)
C(10)-C(11)	1.393(2)	N(2)-C(3)-C(5)	119.52(14)
C(11)-C(14)	1.505(2)	C(2)-C(3)-C(5)	116.42(14)
C(15)-C(20)	1.398(2)	C(11)-C(6)-C(7)	120.74(14)
C(15)-C(16)	1.399(2)	C(11)-C(6)-N(1)	120.35(13)
C(16)-C(17)	1.390(2)	C(7)-C(6)-N(1)	118.90(14)
C(16)-C(21)	1.503(2)	C(8)-C(7)-C(6)	118.48(15)
C(17)-C(18)	1.390(2)	C(8)-C(7)-C(12)	121.04(15)
C(18)-C(19)	1.389(2)	C(6)-C(7)-C(12)	120.48(14)
C(18)-C(22)	1.504(2)	C(9)-C(8)-C(7)	122.00(15)
C(19)-C(20)	1.394(2)	C(10)-C(9)-C(8)	117.97(15)
C(20)-C(23)	1.508(2)	C(10)-C(9)-C(13)	120.74(16)
		C(8)-C(9)-C(13)	121.29(15)
N(1)-Zn(1)-O(1)	125.34(5)	C(9)-C(10)-C(11)	121.98(16)
N(1)-Zn(1)-N(2)	98.50(5)	C(10)-C(11)-C(6)	118.65(14)

C(10)-C(11)-C(14)	120.23(15)
C(6)-C(11)-C(14)	121.12(14)
C(20)-C(15)-C(16)	120.84(14)
C(20)-C(15)-N(2)	118.93(14)
C(16)-C(15)-N(2)	120.18(14)
C(17)-C(16)-C(15)	118.36(15)
C(17)-C(16)-C(21)	121.25(15)
C(15)-C(16)-C(21)	120.39(14)
C(18)-C(17)-C(16)	122.11(15)
C(19)-C(18)-C(17)	118.21(15)
C(19)-C(18)-C(22)	121.29(17)
C(17)-C(18)-C(22)	120.48(17)
C(18)-C(19)-C(20)	121.69(16)
C(19)-C(20)-C(15)	118.65(15)
C(19)-C(20)-C(23)	121.18(15)
C(15)-C(20)-C(23)	120.17(15)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zn(1)	16(1)	13(1)	13(1)	-5(1)	-1(1)	1(1)
N(1)	17(1)	16(1)	13(1)	-5(1)	1(1)	-2(1)
N(2)	17(1)	15(1)	12(1)	-5(1)	-3(1)	0(1)
O(1)	15(1)	18(1)	20(1)	-10(1)	-2(1)	-1(1)
C(1)	16(1)	20(1)	17(1)	-9(1)	1(1)	-4(1)
C(2)	24(1)	15(1)	19(1)	-9(1)	-1(1)	-1(1)
C(3)	18(1)	15(1)	19(1)	-5(1)	-3(1)	0(1)
C(4)	40(1)	20(1)	19(1)	-11(1)	6(1)	-6(1)
C(5)	43(1)	15(1)	20(1)	-5(1)	-6(1)	3(1)
C(6)	18(1)	16(1)	14(1)	-7(1)	2(1)	-2(1)
C(7)	18(1)	19(1)	20(1)	-9(1)	1(1)	-2(1)
C(8)	20(1)	22(1)	24(1)	-8(1)	6(1)	-8(1)
C(9)	28(1)	18(1)	18(1)	-6(1)	4(1)	-4(1)
C(10)	24(1)	24(1)	16(1)	-6(1)	-2(1)	-1(1)
C(11)	20(1)	22(1)	17(1)	-8(1)	1(1)	-4(1)
C(12)	19(1)	35(1)	29(1)	-5(1)	-4(1)	-7(1)
C(13)	40(1)	28(1)	21(1)	-3(1)	6(1)	-10(1)
C(14)	20(1)	43(1)	20(1)	-5(1)	-1(1)	-11(1)
C(15)	22(1)	13(1)	14(1)	-5(1)	-4(1)	2(1)
C(16)	23(1)	15(1)	17(1)	-5(1)	-1(1)	-3(1)
C(17)	30(1)	20(1)	14(1)	-5(1)	1(1)	-4(1)
C(18)	36(1)	22(1)	17(1)	-7(1)	-8(1)	-1(1)
C(19)	25(1)	24(1)	23(1)	-8(1)	-10(1)	1(1)
C(20)	20(1)	19(1)	19(1)	-7(1)	-4(1)	2(1)
C(21)	22(1)	30(1)	21(1)	-7(1)	1(1)	-9(1)
C(22)	48(1)	50(1)	19(1)	-11(1)	-10(1)	-7(1)
C(23)	17(1)	41(1)	26(1)	-13(1)	-3(1)	0(1)

Table 5. Hydrogen coordinates (x 10^4) and i displacement parameters (Å^2 x 10^3) for **1**.

	x	*y*	*z*	*U*(eq)
H(1)	2856	4659	4520	25
H(2)	2907	10002	5717	22
H(4A)	1431	7727	7911	39
H(4B)	2041	9254	7400	39
H(4C)	3246	7897	8033	39
H(5A)	3436	10750	3122	40
H(5B)	2751	11378	4048	40
H(5C)	1561	10781	3525	40
H(8)	134	3718	9037	26
H(10)	4601	3688	9829	26
H(12A)	-723	5030	7339	43
H(12B)	687	5278	6405	43
H(12C)	-65	6537	6848	43
H(13A)	2917	1999	11022	47
H(13B)	1196	1906	10683	47
H(13C)	1375	3101	11164	47
H(14A)	6485	5010	8649	43
H(14B)	5782	6430	7746	43
H(14C)	6391	5004	7477	43
H(17)	4886	8728	839	26
H(19)	205	8278	1763	28
H(21A)	6792	8447	2049	37
H(21B)	6369	7437	3234	37
H(21C)	6078	9130	2940	37
H(22A)	2098	7803	-35	57
H(22B)	3102	9126	-476	57
H(22C)	1192	9379	-197	57
H(23A)	-798	7782	3546	42
H(23B)	-44	8660	4105	42
H(23C)	504	6983	4406	42

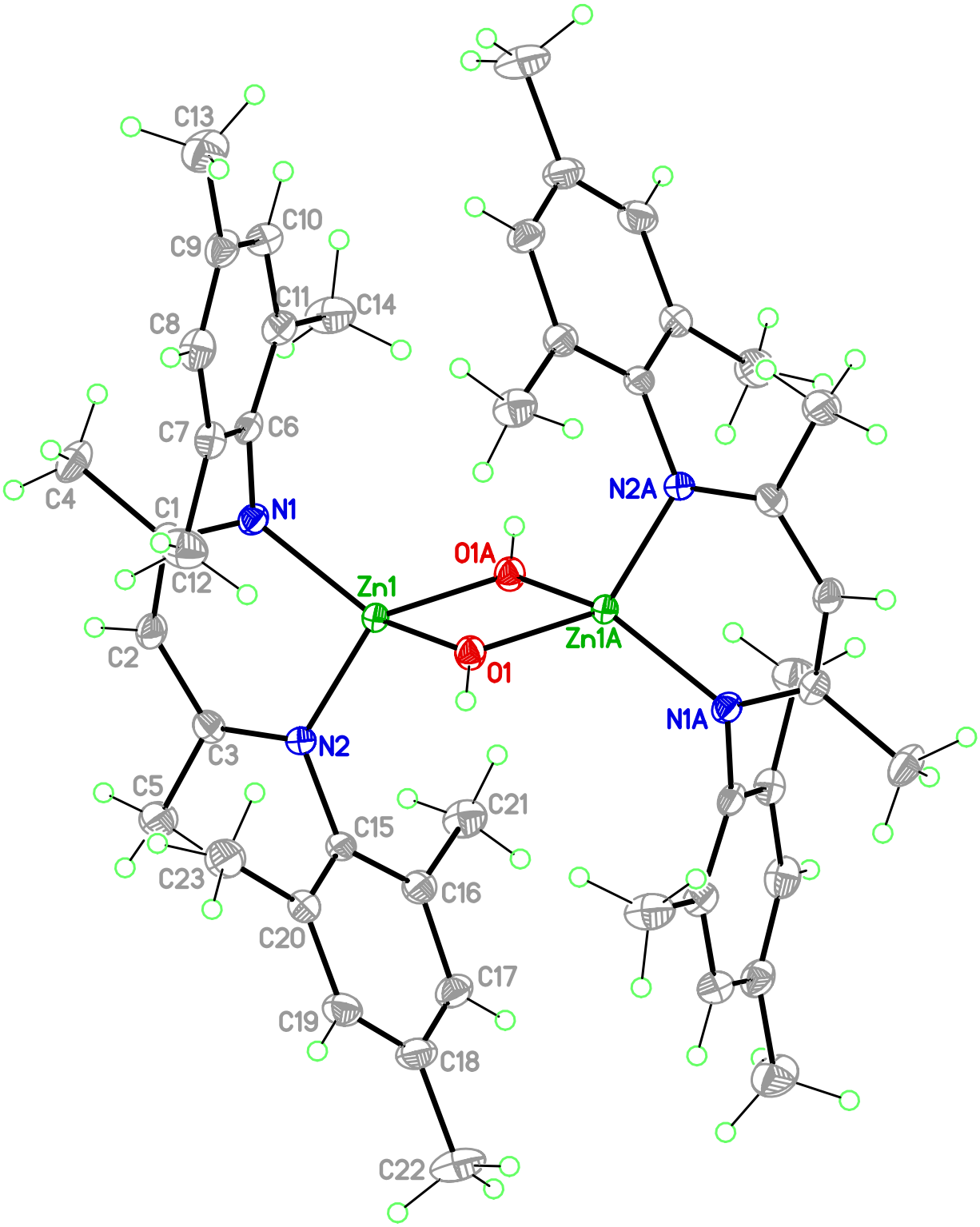


Table 1. Crystal data and structure refinement for **2**.

Empirical formula	$C_{53}\ H_{73}\ Al\ N_4\ O\ Zn$	
Formula weight	874.50 Da	
Density (calculated)	1.122 g cm^{-3}	
F(000)	1880	
Temperature	203(2) K	
Crystal size	0.27 x 0.24 x 0.21 mm	
Crystal color	colourless	
Crystal description	block	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P\ 2_1/n$	
Unit cell dimensions	a = 12.4832(10) Å	α = 90°
	b = 22.036(2) Å	β = 98.078(4)°
	c = 19.0101(16) Å	γ = 90°
Volume	5177.3(8) $Å^3$	
Z	4	
Cell measurement reflections used	9766	
Cell measurement theta min/max	2.79° to 25.61°	
Diffractometer control software	Bruker AXS APEX 2 Vers.3.0/2009	
Diffractometer measurement device	Bruker D8 KAPPA series II with	
	APEX II area detector system	
Diffractometer measurement method	Data collection strategy APEX 2/COSMO	
Theta range for data collection	1.42° to 26.41°	
Completeness to theta = 26.41°	97.2 %	
Index ranges	-15<=*h*<=15, -21<=*k*<=27, -23<=*l*<=22	
Computing data reduction	Bruker AXS APEX 2 Vers.3/2009	
Absorption coefficient	0.530 mm^{-1}	
Absorption correction	Semi-empirical from equivalents	
Empirical absorption correction	Bruker AXS APEX 2 Vers.3/2009	
Max. / min. transmission	0.75 / 0.63	
$R_{(merg)}$ before/after correction	0.0603 / 0.0509	
Computing structure solution	Bruker AXS SHELXTL Vers. 2008/4/(c) 2008	
Computing structure refinement	Bruker AXS SHELXTL Vers. 2008/4/(c) 2008	
Refinement method	Full-matrix least-squares on F^2	
Reflections collected	27572	

Independent reflections	10341 [$R_{(int)}$ = 0.0344]
Data / restraints / parameters	6562 / 0 / 541
Goodness-of-fit on F^2	1.014
Weighting details	$w = 1/[\sigma^2 (Fo^2)+ (0.0725*P)^2+2.9445*P]$ where $P = (Fo^2+2Fc^2)/3$
Final R indices [I>2sigma(I)]	R_1 = 0.0547, wR_2 = 0.1406
R indices (all data)	R_1 = 0.0946, wR_2 = 0.1614
Largest diff. peak and hole	0.434 and -0.284 eÅ^{-3}
Treatment of hydrogen atoms	Riding model on idealized geometries with the 1.2 fold isotropic displacement parameters of the equivalent Uij of the corresponding carbon atom. The methyl groups are idealized with tetrahedral angles in a combined rotating and rigid group refinement with the 1.5 fold isotropic displacement parameters of the equivalent Uij of the corresponding carbon atom.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **2**. *U*(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	*U*(eq)
Zn(1)	9224(1)	2271(1)	155(1)	51(1)
Al(1)	6990(1)	2771(1)	-812(1)	45(1)
O(1)	7850(2)	2470(1)	-139(1)	58(1)
N(1)	6080(2)	3408(1)	-516(1)	45(1)
N(2)	5824(2)	2215(1)	-1086(1)	44(1)
N(3)	9898(2)	1626(1)	775(2)	56(1)
N(4)	10532(2)	2684(1)	-41(2)	60(1)
C(1)	4353(3)	3963(2)	-539(2)	68(1)
C(2)	5023(3)	3427(1)	-719(2)	48(1)
C(3)	4438(3)	2965(1)	-1097(2)	50(1)
C(4)	4801(3)	2386(1)	-1236(2)	48(1)
C(5)	3951(3)	1937(2)	-1560(2)	74(1)
C(6)	6046(3)	1564(1)	-1081(2)	50(1)
C(7)	6428(3)	1295(2)	-1670(2)	62(1)
C(8)	6603(4)	671(2)	-1642(2)	78(1)
C(9)	6405(4)	332(2)	-1071(2)	82(1)
C(10)	6044(3)	604(2)	-500(2)	72(1)
C(11)	5857(3)	1228(1)	-488(2)	54(1)
C(12)	6636(4)	1649(2)	-2311(2)	81(1)
C(13)	5859(6)	1463(3)	-2977(3)	136(2)
C(14)	7792(5)	1576(3)	-2459(3)	133(2)
C(16)	5468(3)	1518(2)	157(2)	61(1)
C(17)	4427(4)	1235(3)	339(3)	108(2)
C(18)	6334(4)	1500(2)	796(2)	87(1)
C(19)	6592(3)	3904(1)	-99(2)	53(1)
C(20)	6843(3)	3824(2)	637(2)	61(1)
C(21)	7334(3)	4305(2)	1037(2)	80(1)
C(22)	7577(3)	4836(2)	724(3)	90(2)
C(23)	7332(3)	4909(2)	3(3)	84(1)
C(24)	6825(3)	4451(2)	-436(2)	63(1)
C(25)	6570(3)	3244(2)	1004(2)	67(1)

C(26)	5500(4)	3302(3)	1298(3)	112(2)
C(28)	6545(4)	4558(2)	-1225(2)	78(1)
C(27)	7445(4)	3042(2)	1586(3)	104(2)
C(29)	5779(5)	5107(2)	-1393(3)	111(2)
C(30)	7553(4)	4664(2)	-1591(3)	107(2)
C(31)	12469(3)	2929(2)	226(3)	96(1)
C(32)	11483(3)	2559(2)	337(2)	67(1)
C(33)	11653(3)	2087(2)	822(2)	77(1)
C(34)	10963(3)	1629(2)	991(2)	67(1)
C(35)	11482(4)	1104(2)	1434(3)	96(2)
C(36)	9278(3)	1114(2)	960(2)	56(1)
C(37)	8949(3)	673(2)	449(2)	66(1)
C(38)	8383(4)	171(2)	651(3)	85(1)
C(39)	8126(4)	99(2)	1323(3)	94(1)
C(40)	8426(4)	548(2)	1803(2)	88(1)
C(41)	8978(3)	1065(2)	1641(2)	71(1)
C(42)	9198(4)	748(2)	-299(2)	92(1)
C(43)	7504(6)	-462(3)	1512(4)	153(3)
C(44)	9237(4)	1555(2)	2184(2)	99(2)
C(45)	10490(3)	3100(2)	-626(2)	62(1)
C(46)	10675(3)	2875(2)	-1286(2)	79(1)
C(47)	10628(4)	3277(3)	-1854(2)	101(2)
C(48)	10416(4)	3889(3)	-1786(2)	95(2)
C(49)	10223(3)	4095(2)	-1130(2)	80(1)
C(50)	10246(3)	3707(2)	-549(2)	66(1)
C(51)	10876(5)	2206(2)	-1384(3)	111(2)
C(52)	10354(6)	4316(3)	-2409(3)	147(3)
C(53)	10005(4)	3950(2)	153(2)	83(1)
C(54)	7543(3)	3063(1)	-1599(2)	60(1)

Table 3. Bond lengths [Å] and angles [°] for **2**.

Zn(1)-O(1)	1.782(2)	C(20)-C(25)	1.517(5)
Zn(1)-N(4)	1.950(3)	C(21)-C(22)	1.366(6)
Zn(1)-N(3)	1.960(3)	C(22)-C(23)	1.372(7)
Al(1)-O(1)	1.686(2)	C(23)-C(24)	1.403(5)
Al(1)-C(54)	1.848(3)	C(24)-C(28)	1.510(6)
Al(1)-N(2)	1.918(2)	C(25)-C(27)	1.508(6)
Al(1)-N(1)	1.938(3)	C(25)-C(26)	1.525(6)
N(1)-C(2)	1.321(4)	C(28)-C(30)	1.539(6)
N(1)-C(19)	1.447(4)	C(28)-C(29)	1.548(6)
N(2)-C(4)	1.324(4)	C(31)-C(32)	1.516(5)
N(2)-C(6)	1.460(4)	C(32)-C(33)	1.386(6)
N(3)-C(34)	1.335(4)	C(33)-C(34)	1.393(6)
N(3)-C(36)	1.438(4)	C(34)-C(35)	1.522(5)
N(4)-C(32)	1.328(5)	C(36)-C(37)	1.396(5)
N(4)-C(45)	1.437(5)	C(36)-C(41)	1.401(5)
C(1)-C(2)	1.515(4)	C(37)-C(38)	1.395(6)
C(2)-C(3)	1.391(4)	C(37)-C(42)	1.507(6)
C(3)-C(4)	1.392(4)	C(38)-C(39)	1.371(6)
C(4)-C(5)	1.518(5)	C(39)-C(40)	1.362(7)
C(6)-C(11)	1.398(4)	C(39)-C(43)	1.528(7)
C(6)-C(7)	1.406(4)	C(40)-C(41)	1.389(6)
C(7)-C(8)	1.393(5)	C(41)-C(44)	1.498(6)
C(7)-C(12)	1.501(5)	C(45)-C(50)	1.384(5)
C(8)-C(9)	1.368(6)	C(45)-C(46)	1.398(5)
C(9)-C(10)	1.371(6)	C(46)-C(47)	1.391(7)
C(10)-C(11)	1.396(5)	C(46)-C(51)	1.513(6)
C(11)-C(16)	1.521(5)	C(47)-C(48)	1.385(7)
C(12)-C(14)	1.517(7)	C(48)-C(49)	1.381(6)
C(12)-C(13)	1.538(7)	C(48)-C(52)	1.506(7)
C(16)-C(18)	1.509(6)	C(49)-C(50)	1.394(5)
C(16)-C(17)	1.524(5)	C(50)-C(53)	1.508(5)
C(19)-C(20)	1.401(5)		
C(19)-C(24)	1.414(5)	O(1)-Zn(1)-N(4)	128.28(12)
C(20)-C(21)	1.395(5)	O(1)-Zn(1)-N(3)	132.88(11)

N(4)-Zn(1)-N(3)	98.80(12)	C(10)-C(11)-C(6)	117.5(3)
O(1)-Al(1)-C(54)	118.70(15)	C(10)-C(11)-C(16)	120.0(3)
O(1)-Al(1)-N(2)	109.41(12)	C(6)-C(11)-C(16)	122.5(3)
C(54)-Al(1)-N(2)	110.98(14)	C(7)-C(12)-C(14)	111.9(4)
O(1)-Al(1)-N(1)	113.67(12)	C(7)-C(12)-C(13)	111.7(4)
C(54)-Al(1)-N(1)	106.50(14)	C(14)-C(12)-C(13)	109.0(4)
N(2)-Al(1)-N(1)	95.05(11)	C(18)-C(16)-C(11)	111.3(3)
Al(1)-O(1)-Zn(1)	144.78(15)	C(18)-C(16)-C(17)	110.1(3)
C(2)-N(1)-C(19)	118.8(3)	C(11)-C(16)-C(17)	113.0(3)
C(2)-N(1)-Al(1)	122.7(2)	C(20)-C(19)-C(24)	122.0(3)
C(19)-N(1)-Al(1)	118.3(2)	C(20)-C(19)-N(1)	118.2(3)
C(4)-N(2)-C(6)	117.3(2)	C(24)-C(19)-N(1)	119.9(3)
C(4)-N(2)-Al(1)	123.2(2)	C(21)-C(20)-C(19)	117.9(4)
C(6)-N(2)-Al(1)	119.3(2)	C(21)-C(20)-C(25)	120.0(4)
C(34)-N(3)-C(36)	118.4(3)	C(19)-C(20)-C(25)	122.1(3)
C(34)-N(3)-Zn(1)	120.4(3)	C(22)-C(21)-C(20)	121.4(4)
C(36)-N(3)-Zn(1)	121.0(2)	C(21)-C(22)-C(23)	120.2(4)
C(32)-N(4)-C(45)	118.9(3)	C(22)-C(23)-C(24)	121.9(4)
C(32)-N(4)-Zn(1)	120.6(3)	C(23)-C(24)-C(19)	116.6(4)
C(45)-N(4)-Zn(1)	120.4(2)	C(23)-C(24)-C(28)	120.0(4)
N(1)-C(2)-C(3)	123.9(3)	C(19)-C(24)-C(28)	123.4(3)
N(1)-C(2)-C(1)	121.3(3)	C(27)-C(25)-C(20)	113.5(4)
C(3)-C(2)-C(1)	114.8(3)	C(27)-C(25)-C(26)	109.7(4)
C(2)-C(3)-C(4)	127.4(3)	C(20)-C(25)-C(26)	111.2(3)
N(2)-C(4)-C(3)	123.4(3)	C(24)-C(28)-C(30)	112.5(4)
N(2)-C(4)-C(5)	120.0(3)	C(24)-C(28)-C(29)	112.2(4)
C(3)-C(4)-C(5)	116.6(3)	C(30)-C(28)-C(29)	108.0(3)
C(11)-C(6)-C(7)	122.2(3)	N(4)-C(32)-C(33)	123.9(3)
C(11)-C(6)-N(2)	118.2(3)	N(4)-C(32)-C(31)	119.6(4)
C(7)-C(6)-N(2)	119.6(3)	C(33)-C(32)-C(31)	116.5(4)
C(8)-C(7)-C(6)	117.1(3)	C(32)-C(33)-C(34)	130.9(4)
C(8)-C(7)-C(12)	120.0(3)	N(3)-C(34)-C(33)	123.7(4)
C(6)-C(7)-C(12)	122.9(3)	N(3)-C(34)-C(35)	119.6(4)
C(9)-C(8)-C(7)	121.6(4)	C(33)-C(34)-C(35)	116.7(4)
C(8)-C(9)-C(10)	120.4(4)	C(37)-C(36)-C(41)	119.9(3)
C(9)-C(10)-C(11)	121.2(4)	C(37)-C(36)-N(3)	119.4(3)

C(41)-C(36)-N(3)	120.6(3)
C(38)-C(37)-C(36)	118.1(4)
C(38)-C(37)-C(42)	121.7(4)
C(36)-C(37)-C(42)	120.1(3)
C(39)-C(38)-C(37)	122.9(4)
C(40)-C(39)-C(38)	117.4(4)
C(40)-C(39)-C(43)	122.1(5)
C(38)-C(39)-C(43)	120.4(5)
C(39)-C(40)-C(41)	123.1(4)
C(40)-C(41)-C(36)	118.3(4)
C(40)-C(41)-C(44)	120.3(4)
C(36)-C(41)-C(44)	121.4(4)
C(50)-C(45)-C(46)	120.2(4)
C(50)-C(45)-N(4)	121.3(3)
C(46)-C(45)-N(4)	118.4(4)
C(47)-C(46)-C(45)	118.6(4)
C(47)-C(46)-C(51)	120.9(4)
C(45)-C(46)-C(51)	120.5(4)
C(48)-C(47)-C(46)	122.3(4)
C(49)-C(48)-C(47)	117.7(4)
C(49)-C(48)-C(52)	120.6(5)
C(47)-C(48)-C(52)	121.7(5)
C(48)-C(49)-C(50)	121.8(4)
C(45)-C(50)-C(49)	119.3(4)
C(45)-C(50)-C(53)	120.8(3)
C(49)-C(50)-C(53)	119.9(4)

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3) for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zn(1)	43(1)	50(1)	62(1)	-4(1)	9(1)	0(1)
Al(1)	46(1)	39(1)	50(1)	1(1)	10(1)	-6(1)
O(1)	44(1)	59(1)	70(2)	4(1)	9(1)	1(1)
N(1)	50(2)	39(1)	47(1)	0(1)	9(1)	-5(1)
N(2)	51(2)	38(1)	44(1)	-2(1)	8(1)	-7(1)
N(3)	48(2)	50(2)	70(2)	-7(1)	3(1)	6(1)
N(4)	46(2)	62(2)	73(2)	-3(1)	18(1)	-6(1)
C(1)	60(2)	54(2)	90(3)	0(2)	15(2)	8(2)
C(2)	55(2)	43(2)	48(2)	10(1)	11(2)	3(1)
C(3)	45(2)	52(2)	51(2)	7(1)	0(1)	-2(2)
C(4)	48(2)	54(2)	42(2)	4(1)	1(1)	-8(1)
C(5)	58(2)	67(2)	91(3)	-13(2)	-12(2)	-13(2)
C(6)	56(2)	42(2)	52(2)	-6(1)	7(2)	-7(1)
C(7)	72(2)	54(2)	60(2)	-14(2)	12(2)	-6(2)
C(8)	94(3)	61(2)	80(3)	-25(2)	20(2)	3(2)
C(9)	106(3)	42(2)	98(3)	-8(2)	16(3)	2(2)
C(10)	86(3)	45(2)	86(3)	6(2)	17(2)	-4(2)
C(11)	56(2)	43(2)	63(2)	-1(2)	12(2)	-7(2)
C(12)	112(4)	77(3)	57(2)	-15(2)	26(2)	-4(2)
C(13)	200(7)	141(5)	62(3)	-6(3)	5(4)	-23(5)
C(14)	132(5)	152(6)	130(5)	7(4)	76(4)	3(4)
C(16)	76(2)	47(2)	63(2)	10(2)	23(2)	1(2)
C(17)	81(3)	144(5)	107(4)	-9(3)	41(3)	-18(3)
C(18)	94(3)	100(3)	68(3)	-11(2)	17(2)	4(3)
C(19)	48(2)	46(2)	65(2)	-10(2)	10(2)	-2(1)
C(20)	50(2)	63(2)	69(2)	-18(2)	6(2)	-2(2)
C(21)	71(3)	83(3)	84(3)	-36(2)	0(2)	-7(2)
C(22)	66(3)	76(3)	126(4)	-50(3)	7(3)	-13(2)
C(23)	68(3)	46(2)	140(4)	-18(2)	28(3)	-11(2)
C(24)	60(2)	38(2)	94(3)	-10(2)	19(2)	-7(2)
C(25)	69(2)	77(3)	52(2)	-6(2)	-3(2)	0(2)
C(26)	87(3)	122(4)	132(4)	41(3)	31(3)	4(3)
C(28)	92(3)	46(2)	101(3)	10(2)	28(2)	-12(2)
C(27)	102(4)	113(4)	87(3)	4(3)	-19(3)	9(3)

C(29)117(4)	74(3)	144(5)	34(3)	32(4)	14(3)
C(30)125(4)	73(3)	133(4)	17(3)	55(3)	-12(3)
C(31)50(2)	122(4)	116(4)	0(3)	15(2)	-19(2)
C(32)45(2)	72(3)	85(3)	-9(2)	11(2)	-5(2)
C(33)43(2)	84(3)	100(3)	-12(2)	-2(2)	0(2)
C(34)57(2)	63(2)	80(3)	-12(2)	1(2)	15(2)
C(35)71(3)	80(3)	129(4)	4(3)	-12(3)	21(2)
C(36)57(2)	45(2)	66(2)	-2(2)	4(2)	8(2)
C(37)71(2)	51(2)	76(2)	-8(2)	8(2)	8(2)
C(38)85(3)	53(2)	112(4)	-10(2)	-2(3)	-2(2)
C(39)100(4)	69(3)	110(4)	23(3)	9(3)	-8(3)
C(40)92(3)	96(3)	74(3)	30(3)	10(2)	3(3)
C(41)77(3)	70(3)	65(2)	4(2)	3(2)	10(2)
C(42)111(4)	80(3)	85(3)	-29(2)	17(3)	-4(3)
C(43)172(7)	97(4)	185(7)	54(4)	7(5)	-40(4)
C(44)118(4)	107(4)	69(3)	-15(3)	9(3)	9(3)
C(45)48(2)	75(3)	64(2)	-6(2)	18(2)	-13(2)
C(46)68(3)	97(3)	75(3)	-21(2)	25(2)	-13(2)
C(47)101(4)	141(5)	67(3)	-6(3)	36(3)	-15(3)
C(48)98(4)	118(4)	74(3)	11(3)	24(3)	-26(3)
C(49)79(3)	82(3)	80(3)	8(2)	17(2)	-23(2)
C(50)60(2)	74(3)	66(2)	-2(2)	18(2)	-17(2)
C(51)112(4)	119(4)	109(4)	-39(3)	39(3)	5(3)
C(52)172(6)	185(7)	91(4)	45(4)	37(4)	-31(5)
C(53)106(3)	67(3)	80(3)	-6(2)	25(2)	-4(2)
C(54)75(2)	38(2)	66(2)	2(2)	9(2)	-12(2)

Table 5. Hydrogen coordinates (x 10^4) and i displacement parameters (Å^2 x 10^3) for **2**.

	x	*y*	*z*	*U*(eq)
H(1A)	4777	4198	−167	102
H(1B)	3692	3824	−376	102
H(1C)	4169	4214	−959	102
H(3)	3702	3059	−1292	60
H(5A)	4232	1707	−1930	111
H(5B)	3302	2154	−1765	111
H(5C)	3774	1662	−1195	111
H(8)	6871	475	−2034	93
H(9)	6527	−98	−1070	98
H(10)	5911	362	−101	86
H(12)	6512	2070	−2224	97
H(13A)	6139	1099	−3171	203
H(13B)	5812	1784	−3329	203
H(13C)	5143	1383	−2853	203
H(14A)	8296	1636	−2025	199
H(14B)	7934	1874	−2811	199
H(14C)	7883	1172	−2642	199
H(16)	5320	1937	45	73
H(17A)	3848	1274	−58	162
H(17B)	4222	1441	751	162
H(17C)	4554	809	450	162
H(18A)	6489	1080	923	130
H(18B)	6087	1708	1193	130
H(18C)	6987	1694	682	130
H(21)	7514	4259	1543	96
H(22)	7916	5161	1011	108
H(23)	7505	5285	−211	100
H(25)	6485	2929	651	81
H(26A)	5371	2941	1564	168
H(26B)	4911	3355	909	168
H(26C)	5538	3652	1609	168
H(28)	6177	4203	−1429	94
H(27A)	8129	3019	1400	156
H(27B)	7273	2648	1768	156

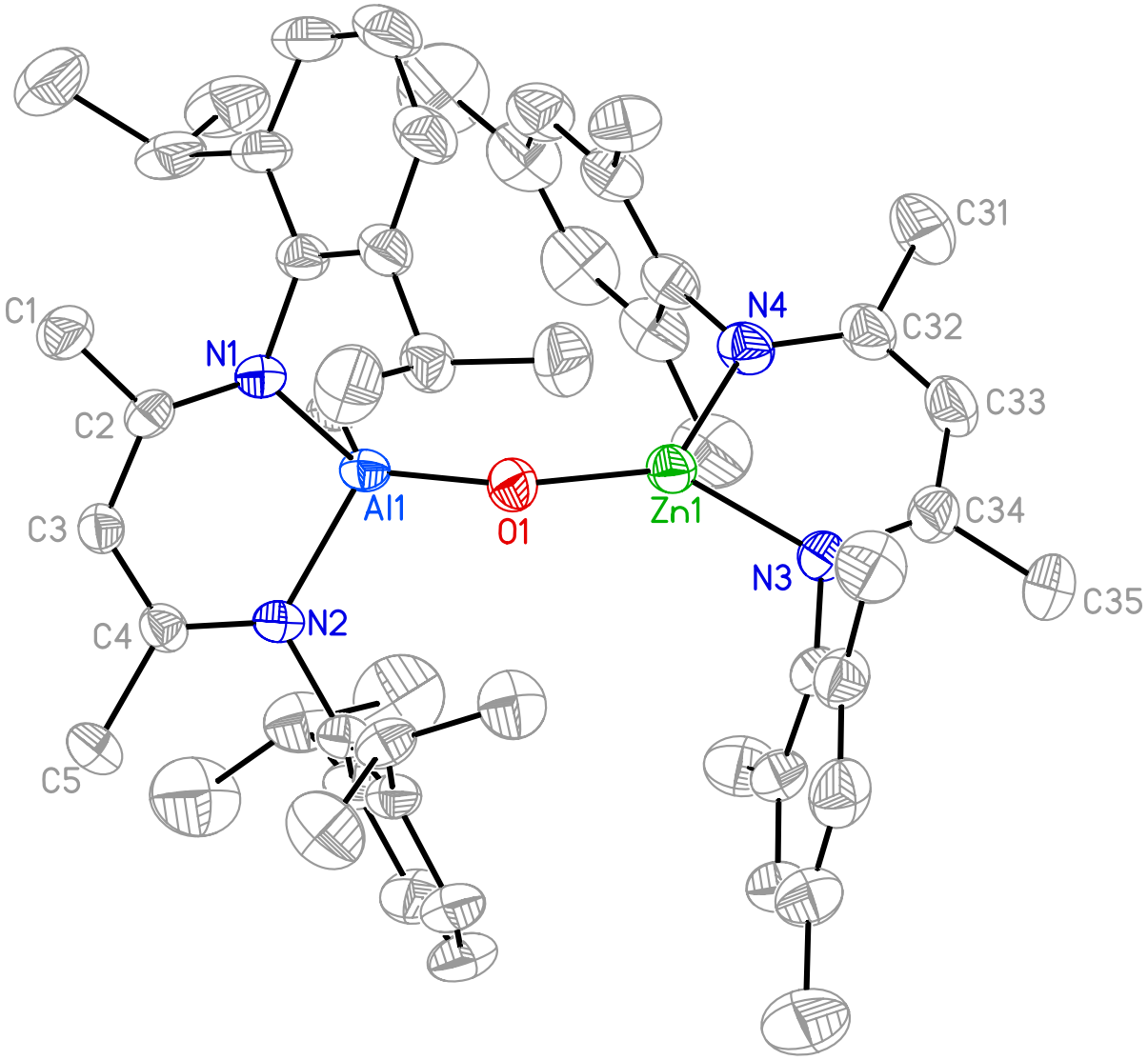
H(27C)	7502	3338	1967	156
H(29A)	5116	5048	-1189	166
H(29B)	5604	5155	-1905	166
H(29C)	6148	5468	-1191	166
H(30A)	7937	5017	-1380	160
H(30B)	7329	4735	-2095	160
H(30C)	8028	4314	-1528	160
H(31A)	12597	2882	-264	143
H(31B)	13099	2789	544	143
H(31C)	12341	3353	320	143
H(33)	12372	2070	1084	92
H(35A)	11598	1218	1933	144
H(35B)	12173	1007	1282	144
H(35C)	11010	752	1370	144
H(38)	8175	-140	304	102
H(40)	8251	503	2276	105
H(42A)	8800	1094	-518	138
H(42B)	8984	386	-574	138
H(42C)	9970	815	-287	138
H(43A)	6736	-366	1451	230
H(43B)	7748	-566	2005	230
H(43C)	7624	-803	1210	230
H(44A)	9858	1431	2521	148
H(44B)	8622	1627	2435	148
H(44C)	9411	1925	1948	148
H(47)	10732	3124	-2313	121
H(49)	10062	4517	-1076	96
H(51A)	11431	2066	-1008	166
H(51B)	11117	2140	-1842	166
H(51C)	10210	1982	-1365	166
H(52A)	10683	4135	-2792	221
H(52B)	10731	4689	-2258	221
H(52C)	9597	4405	-2576	221
H(53A)	9379	3743	288	125
H(53B)	9858	4382	110	125
H(53C)	10625	3883	514	125
H(54A)	7928	3439	-1476	89
H(54B)	6953	3135	-1982	89
H(54C)	8039	2767	-1750	89

Table 6. Torsion angles [°] for **2**.

C(54)-Al(1)-O(1)-Zn(1)	-3.2(3)
N(2)-Al(1)-O(1)-Zn(1)	125.5(2)
N(1)-Al(1)-O(1)-Zn(1)	-129.7(2)
N(4)-Zn(1)-O(1)-Al(1)	34.4(3)
N(3)-Zn(1)-O(1)-Al(1)	-148.4(2)
O(1)-Al(1)-N(1)-C(2)	-132.4(2)
C(54)-Al(1)-N(1)-C(2)	95.0(3)
N(2)-Al(1)-N(1)-C(2)	-18.6(2)
O(1)-Al(1)-N(1)-C(19)	52.1(2)
C(54)-Al(1)-N(1)-C(19)	-80.5(2)
N(2)-Al(1)-N(1)-C(19)	165.9(2)
O(1)-Al(1)-N(2)-C(4)	137.9(2)
C(54)-Al(1)-N(2)-C(4)	-89.2(3)
N(1)-Al(1)-N(2)-C(4)	20.6(2)
O(1)-Al(1)-N(2)-C(6)	-37.4(2)
C(54)-Al(1)-N(2)-C(6)	95.5(2)
N(1)-Al(1)-N(2)-C(6)	-154.6(2)
O(1)-Zn(1)-N(3)-C(34)	-170.5(2)
N(4)-Zn(1)-N(3)-C(34)	7.3(3)
O(1)-Zn(1)-N(3)-C(36)	14.7(3)
N(4)-Zn(1)-N(3)-C(36)	-167.5(2)
O(1)-Zn(1)-N(4)-C(32)	165.3(3)
N(3)-Zn(1)-N(4)-C(32)	-12.7(3)
O(1)-Zn(1)-N(4)-C(45)	-18.6(3)
N(3)-Zn(1)-N(4)-C(45)	163.4(3)
C(19)-N(1)-C(2)-C(3)	-177.3(3)
Al(1)-N(1)-C(2)-C(3)	7.2(4)
C(19)-N(1)-C(2)-C(1)	1.7(4)
Al(1)-N(1)-C(2)-C(1)	-173.7(2)
N(1)-C(2)-C(3)-C(4)	10.0(5)
C(1)-C(2)-C(3)-C(4)	-169.1(3)
C(6)-N(2)-C(4)-C(3)	164.1(3)
Al(1)-N(2)-C(4)-C(3)	-11.3(4)
C(6)-N(2)-C(4)-C(5)	-14.4(4)
Al(1)-N(2)-C(4)-C(5)	170.2(2)
C(2)-C(3)-C(4)-N(2)	-7.8(5)
C(2)-C(3)-C(4)-C(5)	170.7(3)

C(4)-N(2)-C(6)-C(11)	-78.3(4)
Al(1)-N(2)-C(6)-C(11)	97.2(3)
C(4)-N(2)-C(6)-C(7)	100.9(4)
Al(1)-N(2)-C(6)-C(7)	-83.5(3)
N(2)-C(6)-C(7)-C(8)	-178.6(3)
C(11)-C(6)-C(7)-C(12)	-180.0(3)
N(2)-C(6)-C(7)-C(12)	0.8(5)
N(2)-C(6)-C(11)-C(10)	178.2(3)
N(2)-C(6)-C(11)-C(16)	-2.1(5)
Al(1)-N(1)-C(19)-C(20)	-83.8(3)
C(2)-N(1)-C(19)-C(24)	-79.4(4)
Al(1)-N(1)-C(19)-C(24)	96.2(3)
N(1)-C(19)-C(20)-C(21)	-179.8(3)
C(24)-C(19)-C(20)-C(25)	178.5(3)
N(1)-C(19)-C(20)-C(25)	-1.5(5)
N(1)-C(19)-C(24)-C(23)	-179.4(3)
N(1)-C(19)-C(24)-C(28)	1.3(5)
C(45)-N(4)-C(32)-C(33)	-167.5(4)
Zn(1)-N(4)-C(32)-C(33)	8.6(5)
C(45)-N(4)-C(32)-C(31)	10.0(5)
Zn(1)-N(4)-C(32)-C(31)	-173.9(3)
N(4)-C(32)-C(33)-C(34)	5.1(7)
C(31)-C(32)-C(33)-C(34)	-172.5(4)
C(36)-N(3)-C(34)-C(33)	177.4(3)
Zn(1)-N(3)-C(34)-C(33)	2.4(5)
C(36)-N(3)-C(34)-C(35)	-1.2(5)
Zn(1)-N(3)-C(34)-C(35)	-176.2(3)
C(32)-C(33)-C(34)-N(3)	-11.6(7)
C(32)-C(33)-C(34)-C(35)	167.1(4)
C(34)-N(3)-C(36)-C(37)	-102.6(4)
Zn(1)-N(3)-C(36)-C(37)	72.3(4)
C(34)-N(3)-C(36)-C(41)	79.2(4)
Zn(1)-N(3)-C(36)-C(41)	-105.8(3)
N(3)-C(36)-C(37)-C(38)	177.7(3)
N(3)-C(36)-C(37)-C(42)	-2.8(5)
C(37)-C(36)-C(41)-C(40)	5.0(5)
N(3)-C(36)-C(41)-C(40)	-176.9(3)
C(37)-C(36)-C(41)-C(44)	-174.8(4)
N(3)-C(36)-C(41)-C(44)	3.3(6)

C(32)–N(4)–C(45)–C(50)	–96.6(4)
Zn(1)–N(4)–C(45)–C(50)	87.3(4)
C(32)–N(4)–C(45)–C(46)	85.1(4)
Zn(1)–N(4)–C(45)–C(46)	–91.0(4)
C(50)–C(45)–C(46)–C(47)	1.3(6)
N(4)–C(45)–C(46)–C(47)	179.6(4)
C(50)–C(45)–C(46)–C(51)	–176.3(4)
N(4)–C(45)–C(46)–C(51)	2.0(6)
N(4)–C(45)–C(50)–C(49)	179.4(3)
C(46)–C(45)–C(50)–C(53)	177.8(4)
N(4)–C(45)–C(50)–C(53)	–0.5(5)
C(48)–C(49)–C(50)–C(53)	–178.7(4)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C32
N1
C33
C2
Al1
O1
Zn1
C34
C3
N3
C35
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C4
C5