Supporting Information

for

Cationic Zirconium Complexes that Contain Mesityl-substituted Diamido/Donor Ligands. Decomposition via CH Activation and Its Influence on 1-Hexene Polymerization.

by

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For compounds **2b** and **3**.

1. Fully labeled ORTEP drawing.
2. Crystal data and structure refinement.
3. Atomic coordinates and equivalent isotropic displacement parameters.
4. Bond lengths and angles.
5. Anisotropic displacement parameters.
6. Hydrogen coordinates and isotropic displacement parameters.

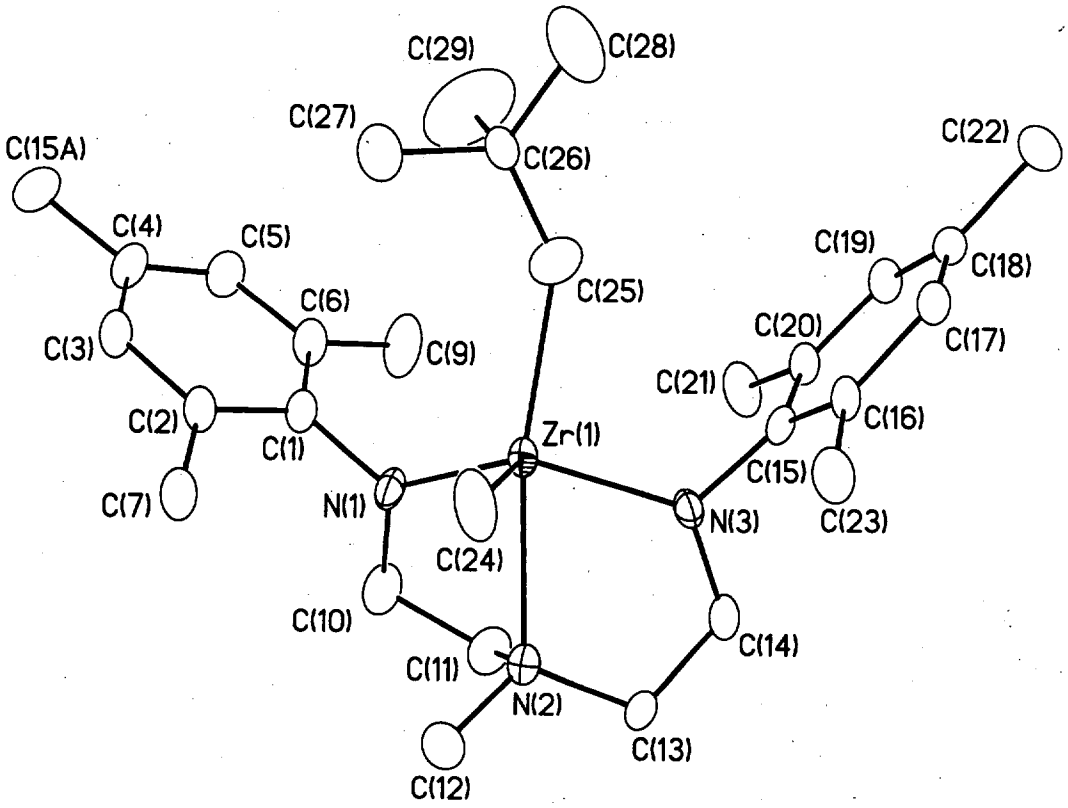


Table 1. Crystal data and structure refinement for **2b**.

Empirical Formula	$C_{29}H_{47}N_3Zr$
Formula weight	528.93
Temperature	183(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 10.152(6) Å α = 90 deg.
	b = 17.044(10) Å β = 90 deg.
	c = 17.052(6) Å γ = 90 deg.
Volume	2950(3) $Å^3$
Z, Calculated density	4, 1.191 g/cm^3
Absorption coefficient	0.392 mm^{-1}
F(000)	1128
Crystal size	0.25 x 0.2 x 0.2 mm
θ range for data collection	2.33 to 23.32 deg.
Limiting indices	-10<=h<=7, -18<=k<=10, -17<=l<=18
Reflections collected / unique	5661 / 3916 [R(int) = 0.0476]
Completeness to θ = 23.32	95.7 %
Absorption correction	Empirical
Max. and min. transmission	0.3264 and 0.1927
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3916 / 0 / 299
Goodness-of-fit on F2	1.016
Final R indices [I>2σ(I)]	R1 = 0.0557, wR2 = 0.1300
R indices (all data)	R1 = 0.0824, wR2 = 0.1443
Extinction coefficient	0.0001(4)
Largest diff. peak and hole	0.590 and -0.634 $e.Å^{-3}$

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

Atom	x	y	z	U(eq)
Zr(1)	10427(1)	9996(1)	8172(1)	44(1)
C(16)	9959(7)	9830(4)	5984(4)	45(2)
N(3)	11420(5)	9938(4)	7119(3)	45(1)
N(1)	11276(7)	9750(3)	9241(3)	51(2)
C(2)	9814(9)	9803(4)	10405(4)	57(2)
C(17)	9312(8)	9372(4)	5398(4)	52(2)
C(1)	10611(8)	9356(5)	9872(4)	52(2)
C(20)	11201(8)	8692(4)	6369(4)	49(2)
C(15)	10882(7)	9489(4)	6479(4)	41(2)
C(18)	9622(9)	8593(4)	5306(4)	52(2)
C(19)	10588(9)	8265(4)	5786(4)	54(2)
C(3)	9194(8)	9417(5)	11003(4)	63(3)
C(10)	12661(8)	9943(9)	9436(4)	77(3)
C(24)	9231(11)	11126(5)	8226(6)	86(3)
N(2)	12514(7)	10754(4)	8283(4)	60(2)
C(25)	8845(16)	9107(8)	7902(8)	185(9)
C(14)	12708(9)	10253(5)	6941(4)	73(3)
C(4)	9312(9)	8613(6)	11113(4)	64(2)
C(7)	9696(12)	10672(5)	10348(5)	81(3)
C(23)	9648(11)	10707(4)	6020(5)	66(2)
C(15A)	8602(9)	8211(5)	11790(5)	79(3)
C(21)	12195(10)	8301(5)	6897(5)	75(3)
C(26)	7631(9)	8781(5)	8190(5)	66(2)
C(11)	13355(9)	10188(6)	8685(5)	80(3)
C(9)	11607(11)	8069(5)	9450(5)	92(4)
C(5)	10105(9)	8201(5)	10599(5)	67(3)
C(22)	8927(10)	8103(5)	4686(5)	80(3)
C(6)	10762(8)	8548(5)	9977(4)	57(2)
C(28)	6660(16)	8482(12)	7633(8)	197(8)
C(12)	12424(11)	11508(6)	8733(6)	91(3)
C(13)	12957(9)	10959(5)	7483(4)	65(2)
C(27)	7091(13)	9175(9)	8901(7)	145(6)
C(29)	8040(20)	7999(9)	8563(12)	233(10)

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

Zr(1)-N(1)	2.060(6)
Zr(1)-N(3)	2.061(5)
Zr(1)-C(25)	2.256(12)
Zr(1)-C(24)	2.279(8)
Zr(1)-N(2)	2.488(6)
C(16)-C(15)	1.388(9)
C(16)-C(17)	1.427(10)
C(16)-C(23)	1.530(10)
N(3)-C(15)	1.440(8)
N(3)-C(14)	1.446(10)
N(1)-C(1)	1.437(9)
N(1)-C(10)	1.481(10)
C(2)-C(3)	1.366(10)
C(2)-C(1)	1.436(10)
C(2)-C(7)	1.489(12)
C(17)-C(18)	1.375(10)
C(1)-C(6)	1.397(11)
C(20)-C(19)	1.381(10)
C(20)-C(15)	1.410(10)
C(20)-C(21)	1.507(10)
C(18)-C(19)	1.395(11)
C(18)-C(22)	1.521(10)
C(3)-C(4)	1.389(11)
C(10)-C(11)	1.520(11)
N(2)-C(11)	1.459(11)
N(2)-C(13)	1.477(9)
N(2)-C(12)	1.500(11)
C(25)-C(26)	1.438(14)
C(14)-C(13)	1.538(11)
C(4)-C(5)	1.382(11)
C(4)-C(15A)	1.524(11)
C(26)-C(28)	1.460(15)
C(26)-C(27)	1.491(13)
C(26)-C(29)	1.534(17)
C(9)-C(6)	1.487(11)
C(5)-C(6)	1.385(11)
N(1)-Zr(1)-N(3)	123.8(2)
N(1)-Zr(1)-C(25)	110.0(5)
N(3)-Zr(1)-C(25)	97.9(3)
N(1)-Zr(1)-C(24)	111.1(3)
N(3)-Zr(1)-C(24)	109.6(3)
C(25)-Zr(1)-C(24)	101.3(6)
N(1)-Zr(1)-N(2)	71.5(2)
N(3)-Zr(1)-N(2)	71.0(2)

C(25)-Zr(1)-N(2)	166.0(4)
C(24)-Zr(1)-N(2)	90.7(3)
C(15)-C(16)-C(17)	120.5(6)
C(15)-C(16)-C(23)	121.6(7)
C(17)-C(16)-C(23)	117.8(7)
C(15)-N(3)-C(14)	112.3(5)
C(15)-N(3)-Zr(1)	120.0(4)
C(14)-N(3)-Zr(1)	127.4(4)
C(1)-N(1)-C(10)	112.4(6)
C(1)-N(1)-Zr(1)	124.1(5)
C(10)-N(1)-Zr(1)	123.4(5)
C(3)-C(2)-C(1)	118.4(7)
C(3)-C(2)-C(7)	119.4(8)
C(1)-C(2)-C(7)	122.1(8)
C(18)-C(17)-C(16)	120.2(7)
C(6)-C(1)-C(2)	120.2(7)
C(6)-C(1)-N(1)	120.3(7)
C(2)-C(1)-N(1)	119.4(7)
C(19)-C(20)-C(15)	120.0(7)
C(19)-C(20)-C(21)	119.9(7)
C(15)-C(20)-C(21)	120.1(7)
C(16)-C(15)-C(20)	118.5(7)
C(16)-C(15)-N(3)	119.7(6)
C(20)-C(15)-N(3)	121.7(7)
C(17)-C(18)-C(19)	118.8(7)
C(17)-C(18)-C(22)	120.3(8)
C(19)-C(18)-C(22)	120.9(7)
C(20)-C(19)-C(18)	121.9(7)
C(2)-C(3)-C(4)	122.5(8)
N(1)-C(10)-C(11)	108.2(6)
C(11)-N(2)-C(13)	114.4(7)
C(11)-N(2)-C(12)	111.1(7)
C(13)-N(2)-C(12)	106.8(6)
C(11)-N(2)-Zr(1)	101.0(5)
C(13)-N(2)-Zr(1)	108.2(4)
C(12)-N(2)-Zr(1)	115.6(6)
C(26)-C(25)-Zr(1)	143.1(7)
N(3)-C(14)-C(13)	108.2(7)
C(5)-C(4)-C(3)	117.7(7)
C(5)-C(4)-C(15A)	121.9(8)
C(3)-C(4)-C(15A)	120.4(8)
C(25)-C(26)-C(28)	119.4(10)
C(25)-C(26)-C(27)	114.7(8)
C(28)-C(26)-C(27)	115.9(10)
C(25)-C(26)-C(29)	104.1(13)
C(28)-C(26)-C(29)	98.8(12)

C(27)-C(26)-C(29)	98.8(11)
N(2)-C(11)-C(10)	107.9(7)
C(4)-C(5)-C(6)	123.3(8)
C(5)-C(6)-C(1)	117.8(8)
C(5)-C(6)-C(9)	120.4(8)
C(1)-C(6)-C(9)	121.8(7)
N(2)-C(13)-C(14)	108.6(6)

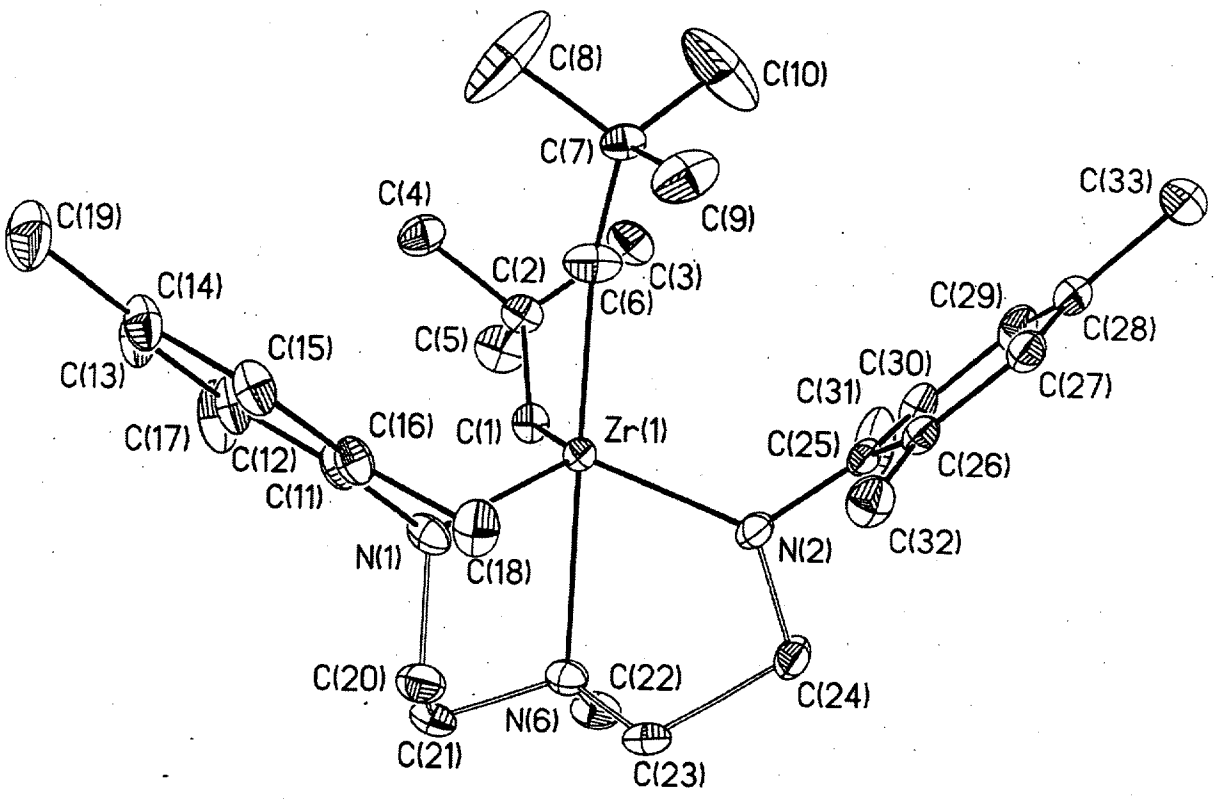
Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for **2b**.
The anisotropic displacement factor exponent takes the form: -2 _2 [h2 a*2 U11 + ... + 2 h k a* b* U12]

Atom	U11	U22	U33	U23	U13	U12
Zr(1)	54(1)	51(1)	27(1)	1(1)	1(1)	-3(1)
C(16)	54(5)	54(6)	26(4)	-2(3)	4(3)	7(4)
N(3)	45(4)	58(3)	32(3)	-13(4)	2(2)	-3(5)
N(1)	47(4)	75(5)	30(3)	9(3)	6(3)	-2(3)
C(2)	63(5)	77(7)	31(4)	-1(4)	-1(4)	-1(5)
C(17)	55(6)	69(5)	32(4)	13(4)	-9(4)	-3(4)
C(1)	43(5)	81(6)	30(4)	3(4)	-2(4)	1(4)
C(20)	60(5)	56(5)	31(4)	4(3)	0(4)	3(4)
C(15)	48(5)	47(4)	29(4)	5(3)	10(3)	-1(3)
C(18)	62(5)	55(5)	37(4)	-4(3)	6(4)	-11(5)
C(19)	78(6)	44(4)	40(4)	-4(3)	6(4)	5(4)
C(3)	71(7)	94(7)	24(4)	4(4)	-3(4)	-7(5)
C(10)	67(6)	121(7)	43(4)	22(6)	-9(4)	-1(8)
C(24)	115(9)	93(6)	50(5)	-12(5)	-9(6)	45(6)
N(2)	73(5)	72(4)	36(4)	0(3)	5(4)	-19(4)
C(25)	223(18)	181(13)	150(13)	-116(11)	134(13)	-138(13)
C(14)	77(6)	109(8)	33(4)	-10(4)	9(4)	-23(5)
C(4)	66(7)	93(6)	35(5)	22(4)	1(4)	-6(5)
C(7)	126(9)	70(6)	47(6)	-7(4)	23(6)	-14(7)
C(23)	99(7)	51(5)	47(5)	8(4)	-14(5)	15(6)
C(15A)	60(6)	115(7)	62(5)	29(6)	-2(5)	-13(5)
C(21)	108(7)	63(5)	52(5)	-3(4)	-19(6)	29(5)
C(26)	81(6)	84(6)	34(4)	-6(5)	-4(5)	-25(5)
C(11)	59(6)	119(10)	63(6)	16(6)	-5(4)	-10(6)
C(9)	134(10)	80(6)	61(6)	21(5)	25(6)	45(7)
C(5)	82(7)	75(5)	43(5)	22(4)	-2(5)	-1(5)
C(22)	97(7)	84(6)	60(6)	1(5)	-19(5)	-25(6)
C(6)	70(6)	65(5)	36(4)	13(4)	-4(4)	14(4)
C(28)	168(17)	310(20)	107(11)	-73(13)	-24(11)	-40(17)
C(12)	115(9)	92(7)	65(6)	-18(5)	12(6)	-35(6)
C(13)	75(6)	86(6)	35(4)	4(4)	10(4)	-29(5)
C(27)	135(11)	201(15)	99(9)	-82(10)	52(9)	-62(11)
C(29)	260(20)	158(15)	280(20)	118(16)	47(19)	-24(15)

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

Atom	x	y	z	U(eq)
H(17A)	8679	9603	5078	62
H(19A)	10825	7743	5712	65
H(3A)	8673	9703	11348	76
H(10A)	13095	9489	9662	92
H(10B)	12689	10366	9816	92
H(24A)	8309	11004	8192	129
H(24B)	9473	11460	7796	129
H(24C)	9406	11391	8712	129
H(25A)	8591	9263	7376	222
H(25B)	9367	8636	7827	222
H(14A)	12745	10417	6397	87
H(14B)	13377	9855	7025	87
H(7A)	9130	10861	10758	122
H(7B)	9330	10810	9847	122
H(7C)	10552	10905	10402	122
H(23A)	10129	10943	6444	98
H(23B)	8720	10780	6104	98
H(23C)	9899	10951	5534	98
H(15A)	8786	7659	11778	118
H(15B)	7670	8294	11741	118
H(15C)	8903	8428	12278	118
H(21A)	12306	7764	6739	112
H(21B)	11889	8319	7429	112
H(21C)	13023	8570	6858	112
H(11A)	14200	10425	8807	96
H(11B)	13505	9735	8354	96
H(9A)	11996	8402	9059	137
H(9B)	11082	7674	9199	137
H(9C)	12291	7823	9752	137
H(5A)	10203	7664	10674	80
H(22A)	9254	7574	4703	120
H(22B)	9091	8322	4177	120
H(22C)	7996	8102	4786	120
H(28A)	7104	8251	7193	295
H(28B)	6115	8907	7454	295
H(28C)	6122	8094	7885	295
H(12A)	13272	11757	8743	136
H(12B)	12145	11399	9260	136
H(12C)	11797	11849	8485	136
H(13A)	13888	11087	7488	78
H(13B)	12475	11413	7294	78
H(27A)	7804	9349	9227	217

H(27B)	6554	8811	9189	217
H(27C)	6567	9617	8746	217
H(29A)	8441	7670	8173	349
H(29B)	7282	7742	8776	349
H(29C)	8666	8097	8976	349


C(8)
C(10)
C(7)
C(9)
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C(27)
C(17)
C(16)
C(1)
Zr(1)
C(25)
C(26)
C(12)
C(11)
C(32)
N(1)
C(18)
N(2)
C(20)
C(22)
C(24)
N(6)
C(21)
C(23)

Table 6. Crystal data and structure refinement for **3**.

Empirical Formula	$C_{33}H_{55}N_3Zr$
Formula weight	585.04
Temperature	183(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, $P\bar{1}$
a = 10.3392(8) Å	α = 84.518(1) deg.
b = 10.7823(8) Å	β = 76.001(1) deg.
c = 15.789(1) Å	γ = 77.137(1) deg.
Volume	1663.4(2) $Å^3$
Z, Calculated density	2, 1.164 g/cm^3
Absorption coefficient	0.354 mm^{-1}
F(000)	624
Crystal size	0.3 x 0.25 x 0.2 mm
θ range for data collection	2.30 to 23.25 deg.
Limiting indices	-11<=h<=11, -11<=k<=7, 17<=l<=17
Reflections collected / unique	6629 / 4642 [R(int) = 0.0245]
Completeness to θ = 23.25	97.3 %
Absorption correction	Empirical
Max. and min. transmission	0.3693 and 0.3234
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4642 / 0 / 380
Goodness-of-fit on F2	1.036
Final R indices [I>2σ(I)]	R1 = 0.0376, wR2 = 0.1009
R indices (all data)	R1 = 0.0416, wR2 = 0.1039
Largest diff. peak and hole	0.425 and -0.342 e $Å^{-3}$

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters for **3** ($Å^2$ x 10^3). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Zr(1)	3715(1)	2668(1)	2486(1)	38(1)
N(3)	6117(3)	1479(3)	1968(2)	57(1)
C(1)	4643(4)	4451(3)	2363(2)	53(1)
N(1)	3911(3)	1969(3)	1264(2)	58(1)
N(2)	4285(3)	1468(3)	3500(2)	59(1)
C(16)	2028(4)	1259(3)	864(2)	51(1)
C(25)	3435(3)	1478(3)	4366(2)	49(1)
C(11)	2852(3)	2165(3)	794(2)	52(1)
C(26)	2505(3)	672(3)	4605(2)	51(1)
C(15)	1029(4)	1478(4)	386(2)	58(1)
C(2)	4011(4)	5840(3)	2599(3)	60(1)
C(7)	25(3)	3505(3)	3249(2)	53(1)
C(27)	1627(4)	764(3)	5414(2)	60(1)
C(4)	3041(5)	6469(4)	2007(3)	79(1)
C(12)	2643(4)	3245(4)	245(2)	65(1)
C(29)	2602(5)	2340(4)	5793(3)	75(1)
C(14)	801(4)	2551(4)	-152(2)	67(1)
C(28)	1637(4)	1608(4)	6011(3)	69(1)
C(9)	-332(5)	2185(4)	3432(4)	97(2)
C(30)	3533(4)	2281(4)	4982(3)	67(1)
C(18)	2199(5)	87(4)	1447(3)	72(1)
C(32)	2447(5)	-300(4)	3996(3)	73(1)
C(3)	3226(5)	5926(4)	3552(3)	80(1)
C(5)	5145(5)	6614(4)	2454(4)	90(1)
C(13)	1626(5)	3418(4)	-218(2)	73(1)
C(33)	607(6)	1714(6)	6881(3)	112(2)
C(6)	1504(4)	3348(4)	2886(3)	77(1)
C(17)	3552(6)	4213(5)	138(3)	97(2)
C(31)	4673(7)	3016(6)	4794(4)	117(2)
C(8)	-778(9)	4256(7)	2648(7)	202(5)
C(19)	-309(5)	2769(6)	-652(3)	97(2)
C(10)	-329(10)	4158(8)	4103(5)	195(5)
C(21)	6395(6)	1503(7)	959(5)	64(2)
C(23)	5996(7)	174(6)	2316(6)	64(2)
C(22)	7229(7)	1890(8)	2178(6)	74(3)
C(24)	5639(10)	650(12)	3526(7)	77(3)
C(20)	5127(12)	882(12)	908(8)	73(3)
C(24A)	5395(11)	230(11)	3282(8)	53(3)
C(20A)	5157(15)	1411(11)	624(8)	51(3)
C(23A)	6676(8)	1196(10)	2809(6)	70(3)
C(21A)	5926(10)	365(10)	1679(8)	74(3)
C(22A)	7070(9)	2159(10)	1365(7)	77(3)

Table 8. Bond lengths [Å] and angles [deg] for **3**.

Zr(1)-N(2)	2.076(3)
Zr(1)-N(1)	2.086(3)
Zr(1)-C(6)	2.191(4)
Zr(1)-C(1)	2.305(3)
Zr(1)-N(3)	2.506(3)
N(3)-C(21A)	1.395(11)
N(3)-C(22)	1.438(7)
N(3)-C(22A)	1.467(9)
N(3)-C(23)	1.481(8)
N(3)-C(21)	1.549(8)
N(3)-C(23A)	1.551(9)
C(1)-C(2)	1.538(5)
N(1)-C(11)	1.434(4)
N(1)-C(20A)	1.478(15)
N(1)-C(20)	1.548(12)
N(2)-C(25)	1.434(4)
N(2)-C(24)	1.487(10)
N(2)-C(24A)	1.559(12)
C(16)-C(15)	1.388(5)
C(16)-C(11)	1.413(4)
C(16)-C(18)	1.494(5)
C(25)-C(30)	1.398(5)
C(25)-C(26)	1.399(5)
C(11)-C(12)	1.393(5)
C(26)-C(27)	1.374(5)
C(26)-C(32)	1.509(5)
C(15)-C(14)	1.379(5)
C(2)-C(3)	1.528(6)
C(2)-C(4)	1.539(6)
C(2)-C(5)	1.546(5)
C(7)-C(6)	1.476(5)
C(7)-C(8)	1.477(6)
C(7)-C(10)	1.508(7)
C(7)-C(9)	1.533(5)
C(27)-C(28)	1.375(6)
C(12)-C(13)	1.390(6)
C(12)-C(17)	1.525(5)
C(29)-C(28)	1.367(6)
C(29)-C(30)	1.400(6)
C(14)-C(13)	1.380(5)
C(14)-C(19)	1.509(6)
C(28)-C(33)	1.517(6)
C(30)-C(31)	1.519(6)
C(21)-C(20)	1.620(14)
C(23)-C(24)	1.953(13)

C(24A)-C(23A)	1.839(15)
N(2)-Zr(1)-N(1)	120.91(13)
N(2)-Zr(1)-C(6)	106.47(15)
N(1)-Zr(1)-C(6)	101.39(15)
N(2)-Zr(1)-C(1)	109.48(12)
N(1)-Zr(1)-C(1)	111.35(12)
C(6)-Zr(1)-C(1)	105.78(14)
N(2)-Zr(1)-N(3)	71.14(10)
N(1)-Zr(1)-N(3)	71.37(10)
C(6)-Zr(1)-N(3)	168.25(12)
C(1)-Zr(1)-N(3)	85.69(11)
C(21A)-N(3)-C(22)	135.8(6)
C(21A)-N(3)-C(22A)	116.8(7)
C(22)-N(3)-C(22A)	54.5(6)
C(21A)-N(3)-C(23)	41.6(5)
C(22)-N(3)-C(23)	113.1(5)
C(22A)-N(3)-C(23)	140.7(5)
C(21A)-N(3)-C(21)	68.6(6)
C(22)-N(3)-C(21)	106.6(5)
C(22A)-N(3)-C(21)	54.6(5)
C(23)-N(3)-C(21)	108.7(5)
C(21A)-N(3)-C(23A)	110.6(7)
C(22)-N(3)-C(23A)	50.8(5)
C(22A)-N(3)-C(23A)	105.0(6)
C(23)-N(3)-C(23A)	70.8(5)
C(21)-N(3)-C(23A)	148.8(4)
C(21A)-N(3)-Zr(1)	102.1(4)
C(22)-N(3)-Zr(1)	120.5(3)
C(22A)-N(3)-Zr(1)	117.6(4)
C(23)-N(3)-Zr(1)	100.9(3)
C(21)-N(3)-Zr(1)	106.4(3)
C(23A)-N(3)-Zr(1)	104.2(3)
C(2)-C(1)-Zr(1)	132.1(2)
C(11)-N(1)-C(20A)	104.3(6)
C(11)-N(1)-C(20)	113.0(5)
C(20A)-N(1)-C(20)	26.3(4)
C(11)-N(1)-Zr(1)	125.4(2)
C(20A)-N(1)-Zr(1)	129.3(6)
C(20)-N(1)-Zr(1)	119.8(5)
C(25)-N(2)-C(24)	108.3(4)
C(25)-N(2)-C(24A)	115.2(5)
C(24)-N(2)-C(24A)	28.0(4)
C(25)-N(2)-Zr(1)	122.5(2)
C(24)-N(2)-Zr(1)	128.5(4)
C(24A)-N(2)-Zr(1)	119.2(5)
C(15)-C(16)-C(11)	118.8(3)

C(15)-C(16)-C(18)	119.7(3)
C(11)-C(16)-C(18)	121.5(3)
C(30)-C(25)-C(26)	119.2(3)
C(30)-C(25)-N(2)	120.7(3)
C(26)-C(25)-N(2)	120.1(3)
C(12)-C(11)-C(16)	119.2(3)
C(12)-C(11)-N(1)	120.1(3)
C(16)-C(11)-N(1)	120.8(3)
C(27)-C(26)-C(25)	119.3(3)
C(27)-C(26)-C(32)	119.2(3)
C(25)-C(26)-C(32)	121.4(3)
C(14)-C(15)-C(16)	122.6(3)
C(3)-C(2)-C(1)	111.3(3)
C(3)-C(2)-C(4)	109.0(4)
C(1)-C(2)-C(4)	110.7(3)
C(3)-C(2)-C(5)	108.6(3)
C(1)-C(2)-C(5)	109.8(3)
C(4)-C(2)-C(5)	107.2(3)
C(6)-C(7)-C(8)	112.1(5)
C(6)-C(7)-C(10)	108.6(5)
C(8)-C(7)-C(10)	109.6(6)
C(6)-C(7)-C(9)	108.8(3)
C(8)-C(7)-C(9)	109.2(4)
C(10)-C(7)-C(9)	108.4(4)
C(26)-C(27)-C(28)	122.6(4)
C(13)-C(12)-C(11)	119.6(3)
C(13)-C(12)-C(17)	120.5(4)
C(11)-C(12)-C(17)	119.9(4)
C(28)-C(29)-C(30)	122.3(4)
C(15)-C(14)-C(13)	117.6(3)
C(15)-C(14)-C(19)	121.2(4)
C(13)-C(14)-C(19)	121.1(4)
C(29)-C(28)-C(27)	117.7(4)
C(29)-C(28)-C(33)	121.6(5)
C(27)-C(28)-C(33)	120.6(5)
C(25)-C(30)-C(29)	118.6(4)
C(25)-C(30)-C(31)	120.5(4)
C(29)-C(30)-C(31)	120.8(4)
C(14)-C(13)-C(12)	122.2(4)
C(7)-C(6)-Zr(1)	166.7(3)
N(3)-C(21)-C(20)	96.5(6)
N(3)-C(23)-C(24)	92.7(5)
N(2)-C(24)-C(23)	93.4(6)
N(1)-C(20)-C(21)	100.7(7)
N(2)-C(24A)-C(23A)	90.1(6)
N(3)-C(23A)-C(24A)	90.5(6)

Table 9. Anisotropic displacement parameters for **3** (Å2 x 103). The anisotropic displacement factor exponent takes the form: -2 _2 [h2 a*2 U11 + ... + 2 h k a* b* U12]

Atom	U11	U22	U33	U23	U13	U12
Zr(1)	40(1)	34(1)	41(1)	-4(1)	-12(1)	-9(1)
N(3)	41(2)	63(2)	64(2)	-11(2)	-9(1)	-6(1)
C(1)	60(2)	46(2)	57(2)	-2(2)	-15(2)	-20(2)
N(1)	50(2)	75(2)	53(2)	-27(2)	-8(1)	-16(1)
N(2)	44(2)	61(2)	63(2)	14(1)	-15(1)	1(1)
C(16)	62(2)	58(2)	41(2)	-8(2)	-8(2)	-27(2)
C(25)	50(2)	47(2)	51(2)	9(2)	-21(2)	-4(2)
C(11)	59(2)	66(2)	37(2)	-11(2)	-6(2)	-28(2)
C(26)	55(2)	40(2)	55(2)	6(2)	-19(2)	-3(2)
C(15)	65(2)	74(2)	46(2)	-8(2)	-8(2)	-38(2)
C(2)	67(2)	43(2)	72(2)	-10(2)	-10(2)	-21(2)
C(7)	40(2)	48(2)	72(2)	-5(2)	-13(2)	-7(1)
C(27)	57(2)	55(2)	63(2)	13(2)	-15(2)	-7(2)
C(4)	82(3)	49(2)	102(3)	4(2)	-24(2)	-7(2)
C(12)	87(3)	81(3)	38(2)	2(2)	-11(2)	-50(2)
C(29)	116(4)	53(2)	59(2)	-3(2)	-41(2)	-2(2)
C(14)	74(2)	94(3)	42(2)	-1(2)	-18(2)	-33(2)
C(28)	74(3)	60(2)	58(2)	5(2)	-14(2)	12(2)
C(9)	66(3)	74(3)	161(5)	17(3)	-40(3)	-29(2)
C(30)	91(3)	55(2)	71(3)	15(2)	-44(2)	-25(2)
C(18)	101(3)	59(2)	65(2)	-2(2)	-28(2)	-28(2)
C(32)	96(3)	53(2)	77(3)	-4(2)	-29(2)	-17(2)
C(3)	96(3)	62(2)	80(3)	-26(2)	-4(2)	-24(2)
C(5)	97(3)	65(3)	119(4)	-20(3)	-18(3)	-41(2)
C(13)	103(3)	84(3)	46(2)	16(2)	-26(2)	-44(3)
C(33)	112(4)	122(4)	66(3)	-4(3)	2(3)	28(3)
C(6)	52(2)	54(2)	117(4)	-15(2)	-3(2)	-9(2)
C(17)	149(5)	111(4)	63(3)	17(2)	-29(3)	-95(4)
C(31)	172(6)	128(5)	104(4)	45(3)	-87(4)	-100(4)
C(8)	209(8)	122(5)	357(13)	115(7)	-229(9)	-77(5)
C(19)	102(4)	140(5)	69(3)	7(3)	-44(3)	-42(3)
C(10)	246(10)	178(8)	132(6)	-83(6)	88(6)	-94(7)
C(21)	43(4)	71(5)	69(4)	-19(3)	4(3)	-8(3)
C(23)	48(4)	54(4)	81(6)	-17(4)	-12(4)	9(3)
C(22)	44(4)	88(5)	95(7)	-26(5)	-16(4)	-10(4)
C(24)	52(5)	97(9)	69(7)	32(6)	-15(4)	-3(5)
C(20)	61(5)	79(8)	74(8)	-30(6)	-19(5)	8(6)
C(24A)	48(5)	50(6)	71(7)	-13(4)	-34(4)	-1(4)
C(20A)	63(6)	41(6)	52(7)	-9(4)	-19(5)	-10(5)
C(23A)	35(4)	102(7)	60(6)	-2(5)	-9(4)	10(4)
C(21A)	63(6)	75(7)	74(7)	-26(6)	-11(5)	12(5)
C(22A)	56(5)	94(7)	71(7)	-4(5)	11(5)	-20(5)

Table 10. Hydrogen coordinates (x 104) and isotropic displacement parameters for **3** ($Å^2$ x 10^3).

Atom	x	y	z	U(eq)
H(1A)	5368	4203	2675	63
H(1B)	5096	4510	1750	63
H(15A)	493	877	430	70
H(27A)	1002	234	5564	72
H(4A)	2321	6011	2081	118
H(4B)	3537	6453	1408	118
H(4C)	2660	7336	2163	118
H(29A)	2642	2896	6197	89
H(9A)	-106	1753	2895	146
H(9B)	-1290	2276	3684	146
H(9C)	175	1699	3832	146
H(18A)	1557	-412	1406	107
H(18B)	2042	325	2040	107
H(18C)	3108	-404	1271	107
H(32A)	1748	-759	4270	110
H(32B)	3311	-884	3863	110
H(32C)	2246	125	3466	110
H(3A)	3826	5539	3926	119
H(3B)	2486	5490	3643	119
H(3C)	2873	6804	3687	119
H(5A)	5769	6248	2817	135
H(5B)	4745	7479	2604	135
H(5C)	5625	6593	1852	135
H(13A)	1496	4141	-583	88
H(33A)	764	2342	7215	168
H(33B)	702	905	7197	168
H(33C)	-297	1963	6781	168
H(6A)	1573	4108	3140	92
H(6B)	1406	3646	2301	92
H(17A)	4204	3940	495	146
H(17B)	3002	5028	316	146
H(17C)	4022	4280	-463	146
H(31A)	5210	2864	4211	176
H(31B)	5240	2738	5204	176
H(31C)	4290	3909	4846	176
H(8A)	-560	5085	2534	303
H(8B)	-1732	4341	2910	303
H(8C)	-564	3830	2109	303
H(19A)	-320	3562	-985	146
H(19B)	-1174	2796	-249	146
H(19C)	-139	2087	-1039	146
H(10A)	-111	4987	4000	293

H(10B)	183	3661	4496	293
H(10C)	-1286	4241	4356	293
H(21A)	7269	979	700	76
H(21B)	6326	2361	699	76
H(23A)	6834	-452	2143	76
H(23B)	5240	-100	2180	76
H(22A)	8071	1329	1932	111
H(22B)	7106	1876	2801	111
H(22C)	7253	2741	1941	111
H(24A)	5584	-69	3943	92
H(24B)	6282	1123	3625	92
H(20A)	5154	704	312	87
H(20B)	5103	108	1273	87
H(24C)	5227	-279	2861	64
H(24D)	5575	-288	3795	64
H(23C)	6572	1948	3131	84
H(23D)	7606	712	2710	84
H(22D)	7950	1603	1217	116
H(22E)	7143	2890	1639	116
H(22F)	6743	2428	844	116