Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Coordination Behavior of Bis-Phenolate Saturated and Unsaturated N-Heterocyclic Carbene Ligands to Zirconium: Reactivity and Activity in the Copolymerization of Cyclohexene Oxide with CO_2

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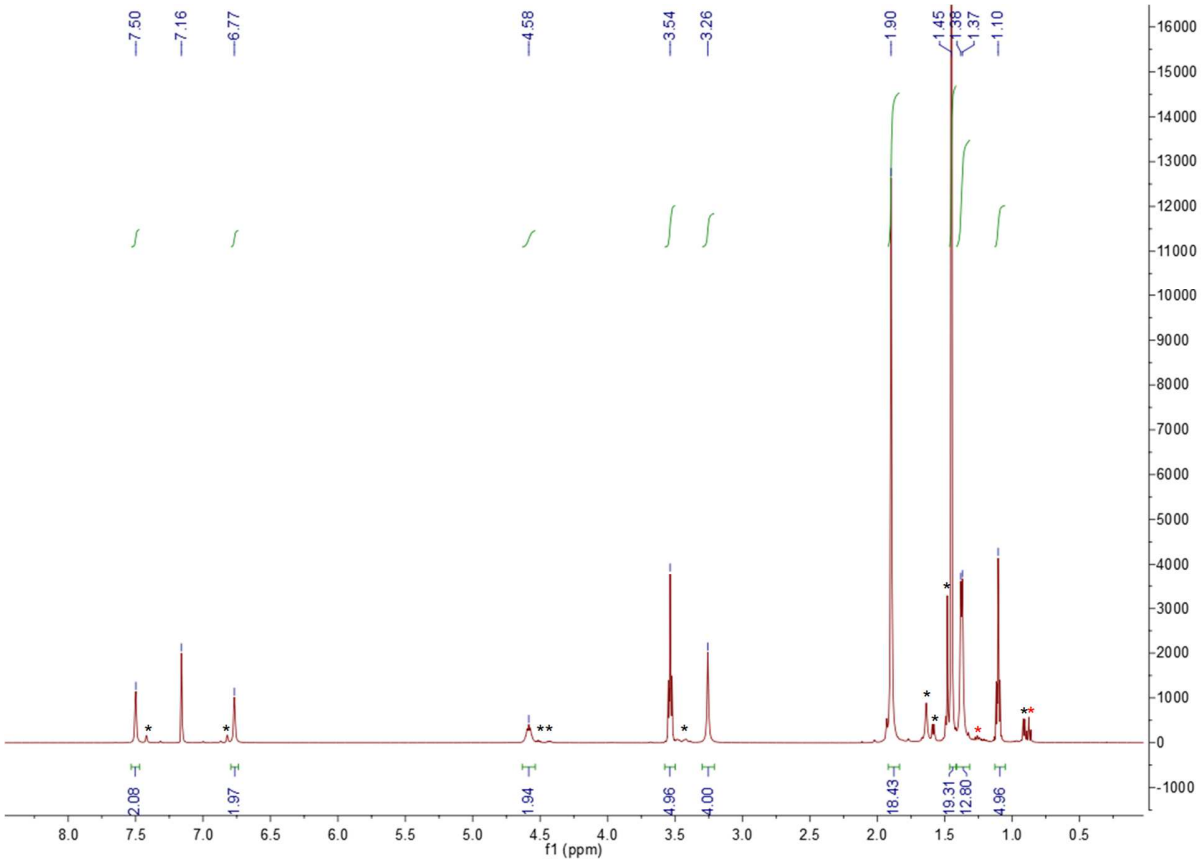

Figure S1. ^{1}H NMR spectrum of complex **3** in benzene-d_6. Traces of residual solvent pentane (*) and dimer (*).

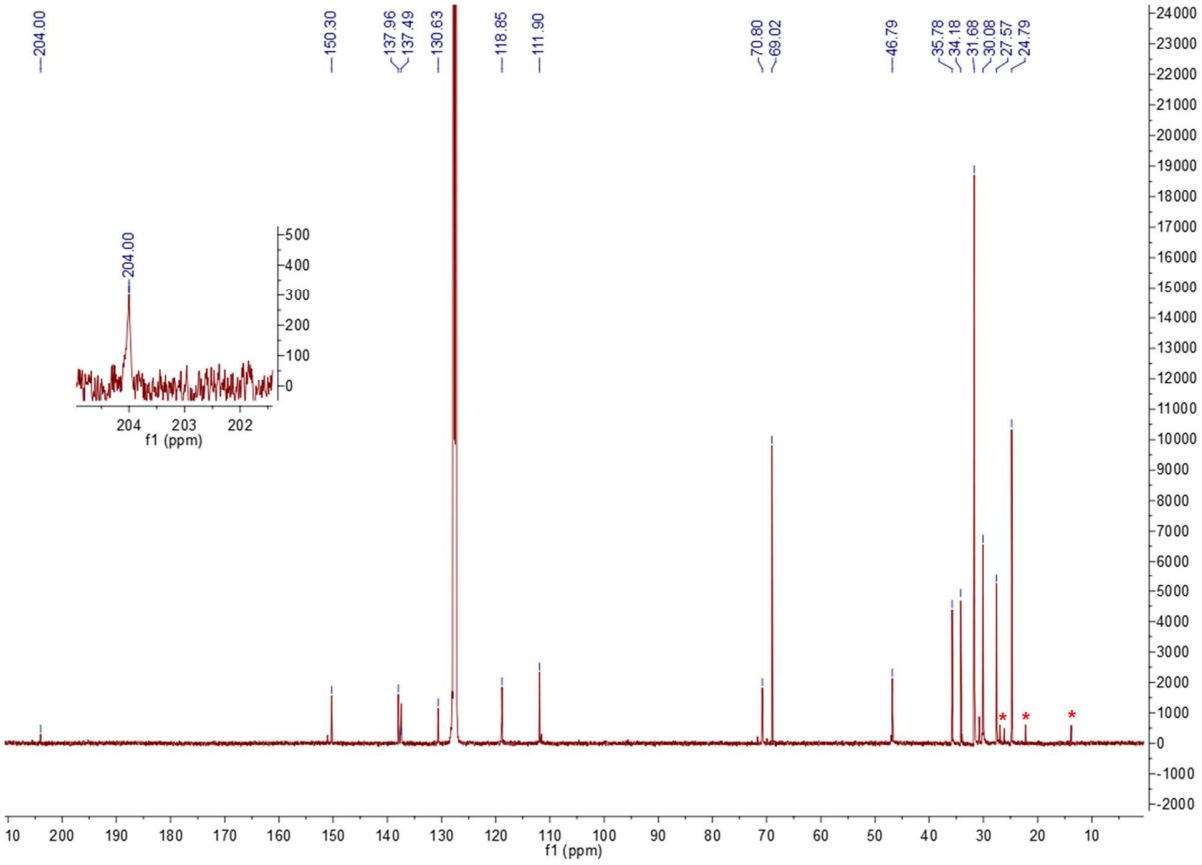

Figure S2. ^{13}C NMR spectrum of complex **3** in benzene-d_6. Trace of residual solvent pentane (*).

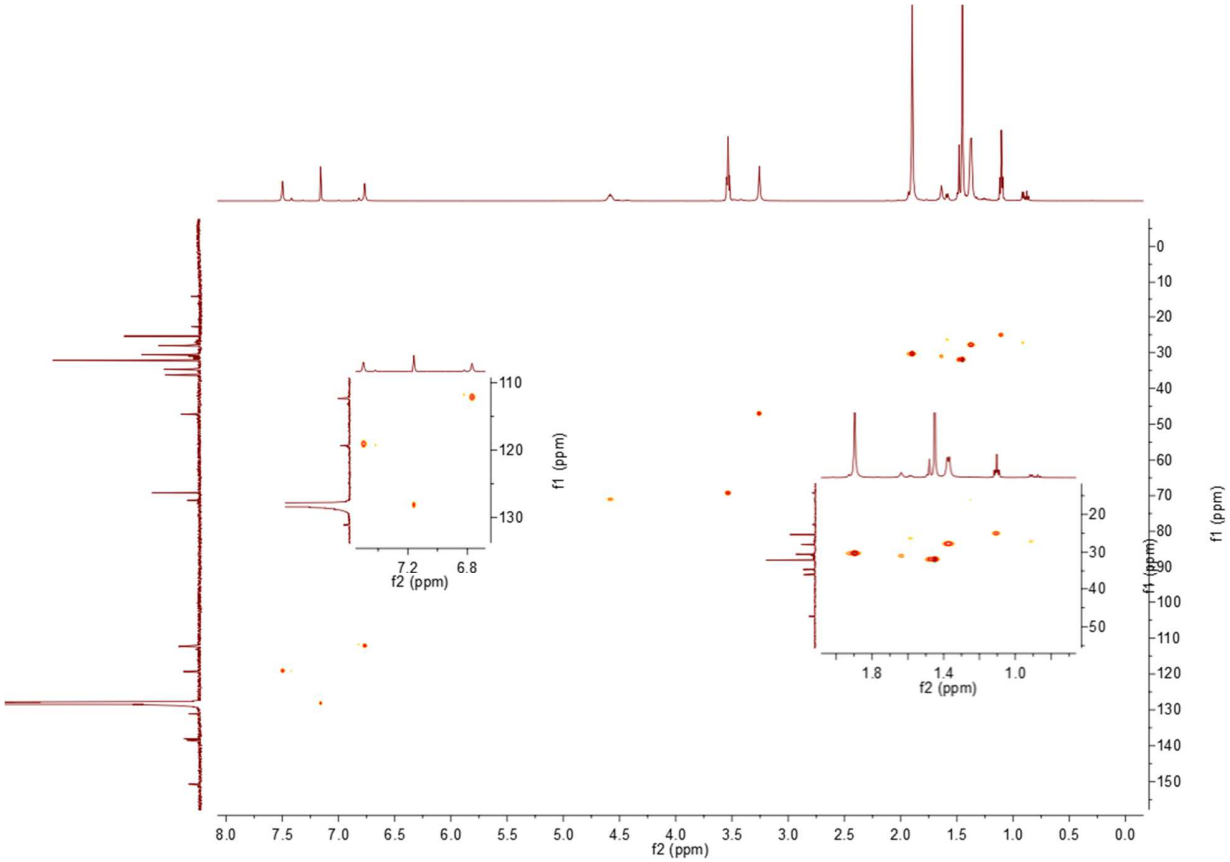

Figure S3. ^{1}H-^{13}C HSQC spectrum of complex **3** in benzene-d_6.

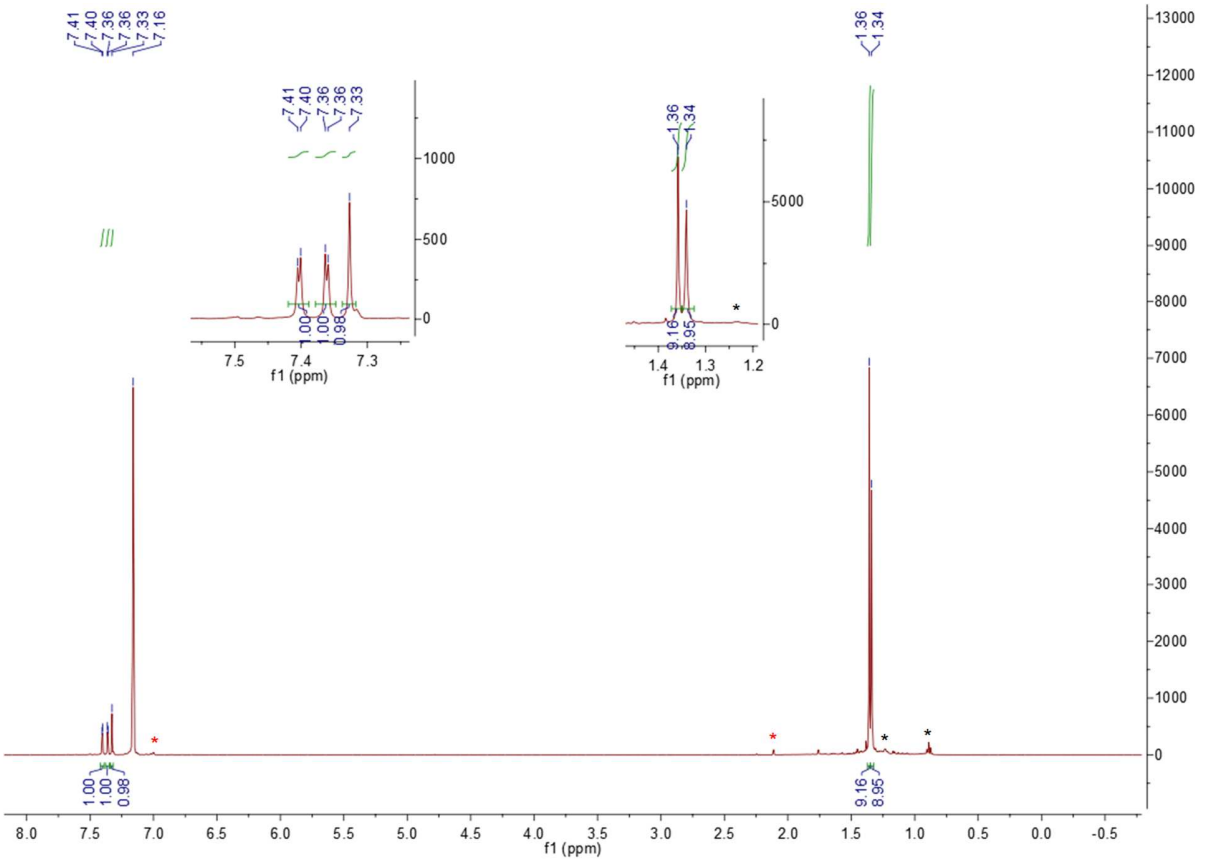

Figure S4. ^{1}H NMR spectrum of complex **4** in benzene-d_6. Traces of residual solvent: hexane (*) and toluene (*).

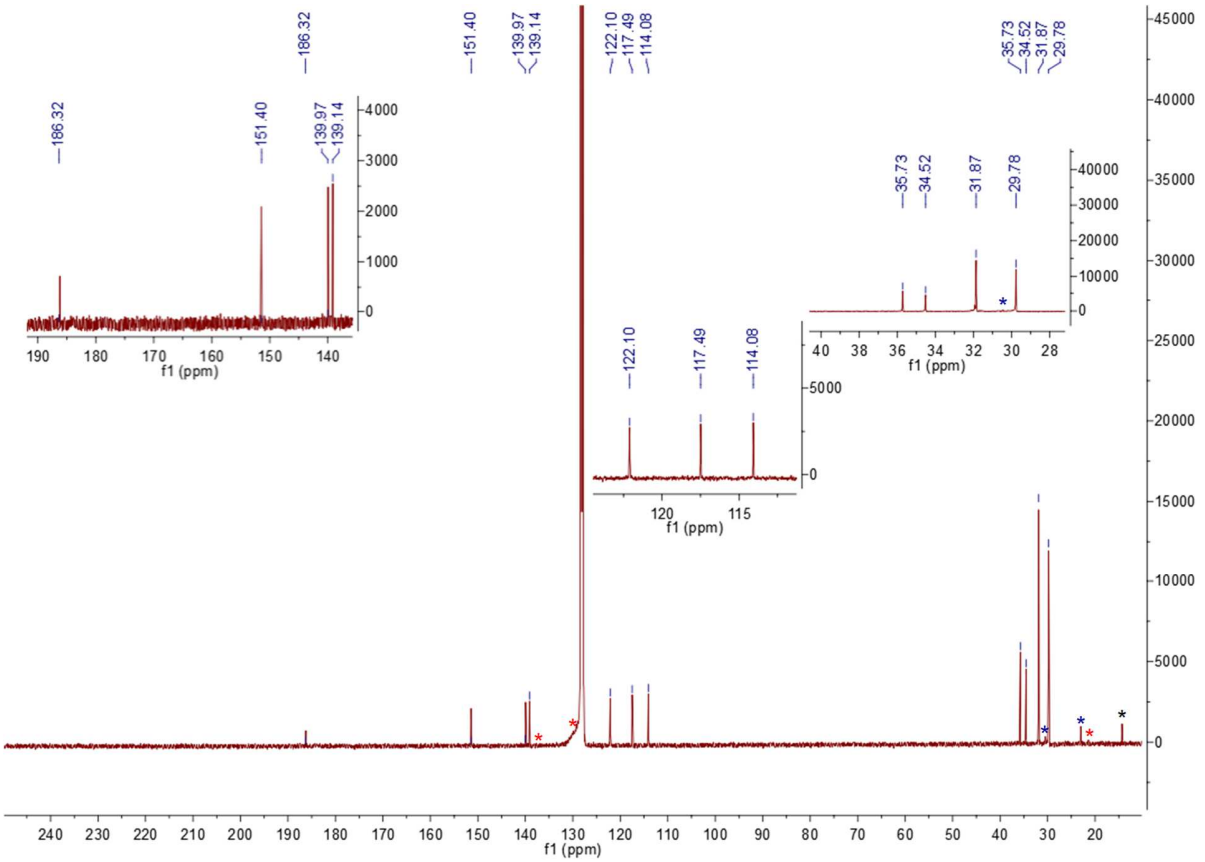

Figure S5. ^{13}C NMR spectrum of complex **4** in benzene-d_6. Traces of residual solvent: hexane (*) and toluene (*).

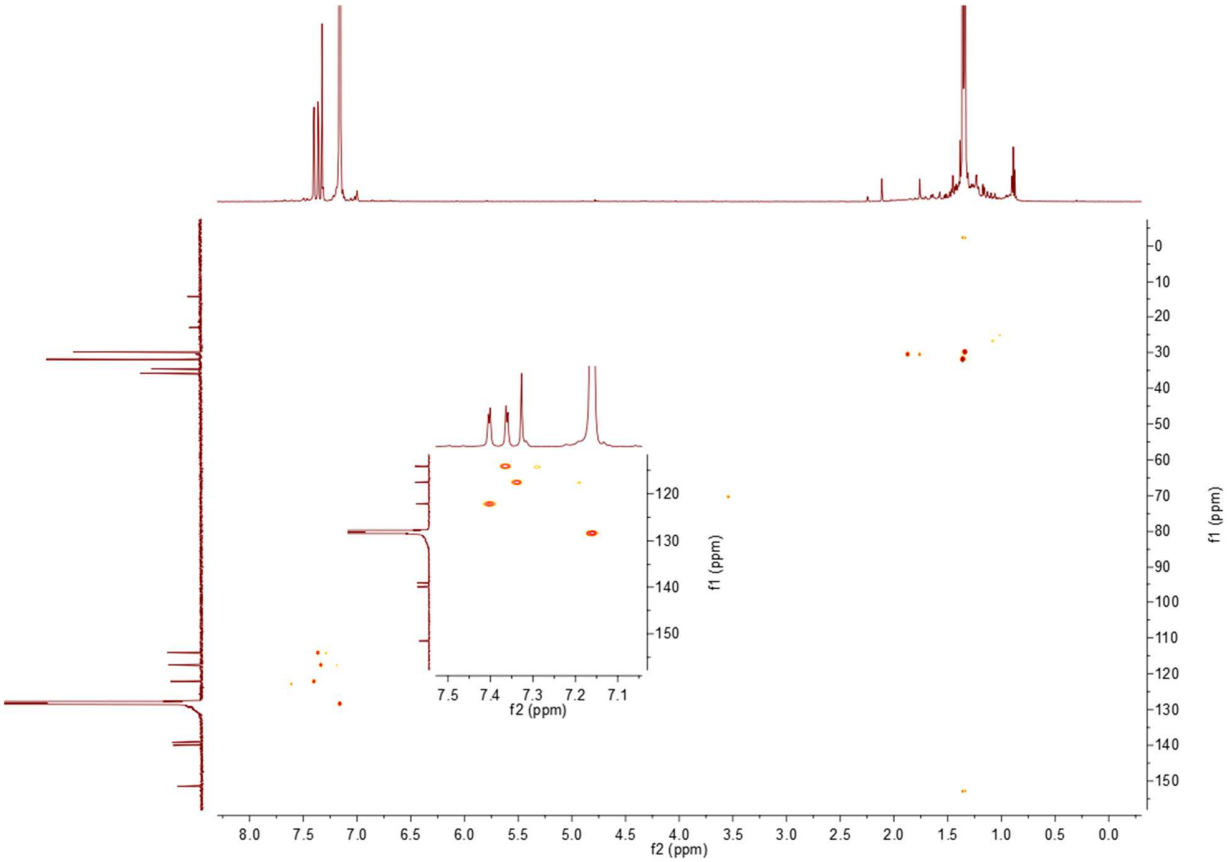

Figure S6. ^{1}H-^{13}C HSQC spectrum of complex **4** in benzene-d_6.

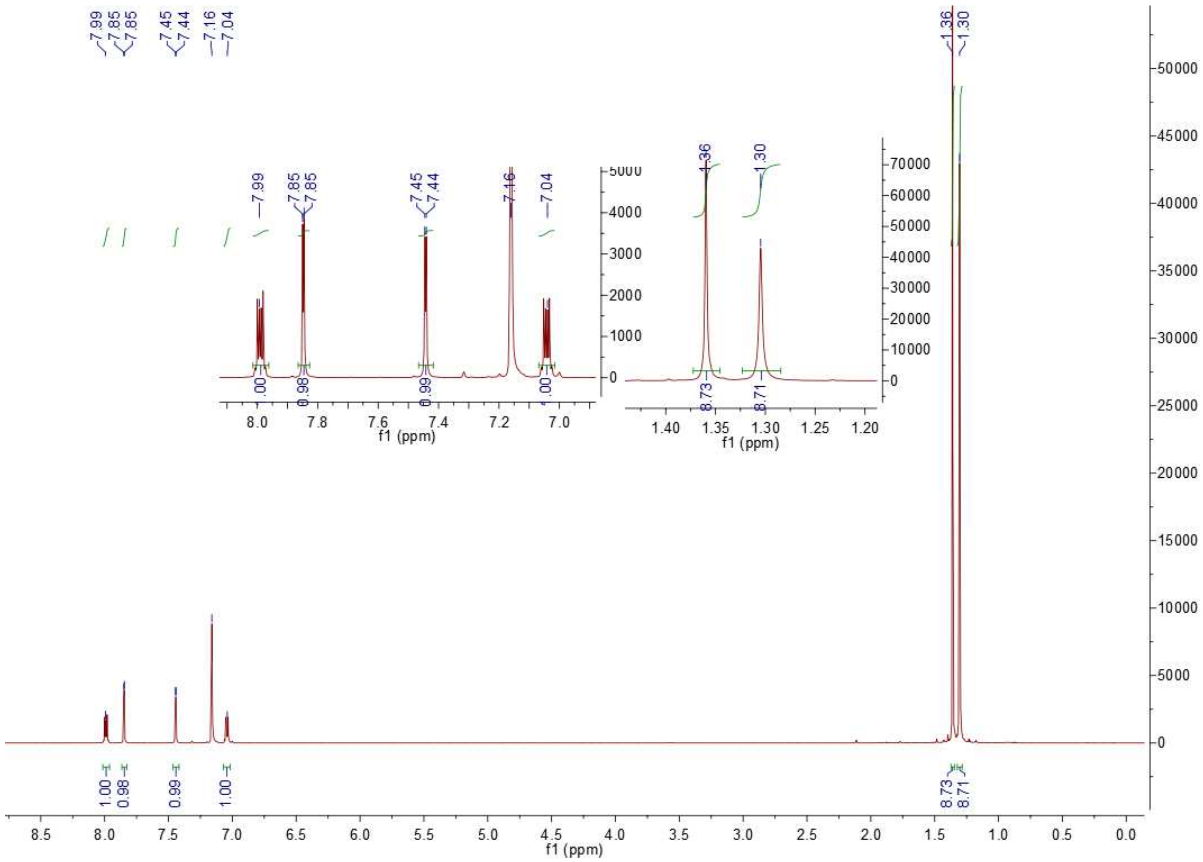

Figure S7. ^{1}H NMR spectrum of complex **5** in benzene-d_6.

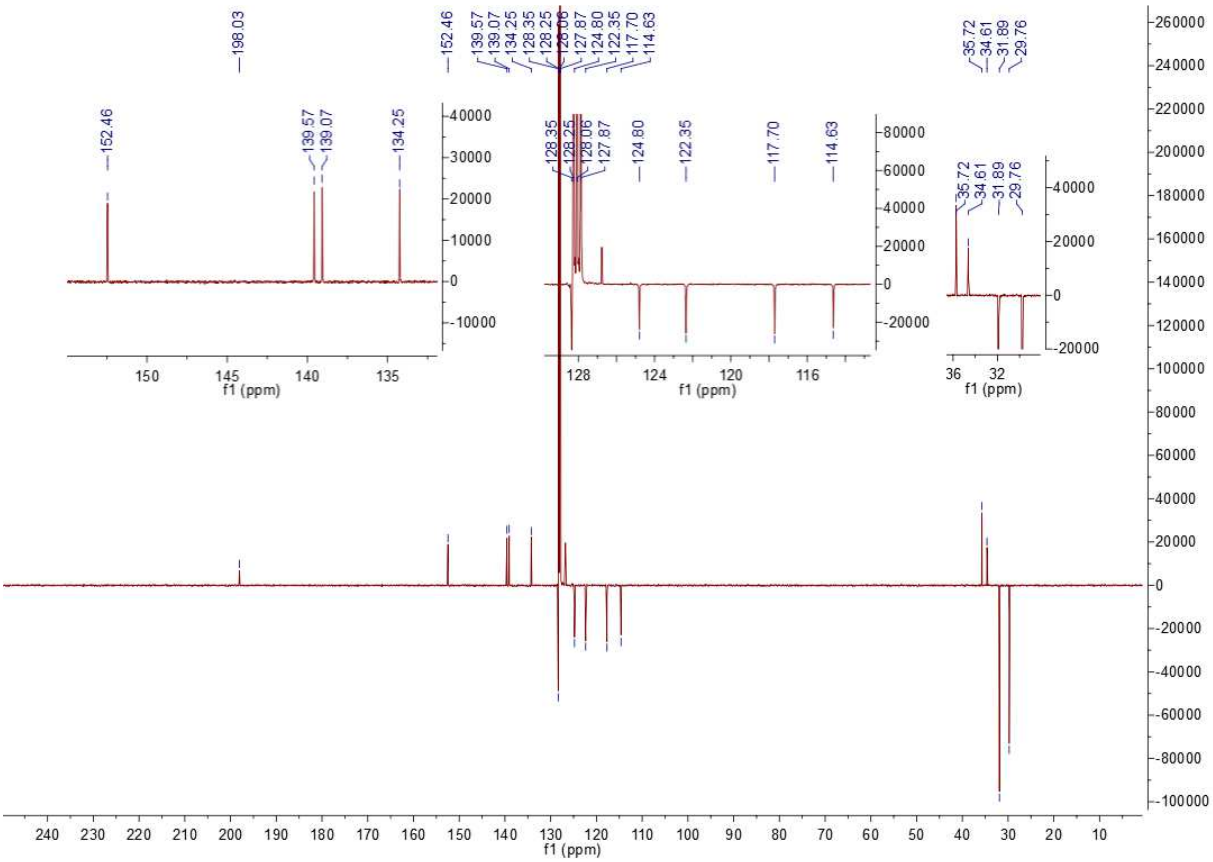

Figure S8. ^{13}C APT NMR spectrum of complex **5** in benzene-d_6.

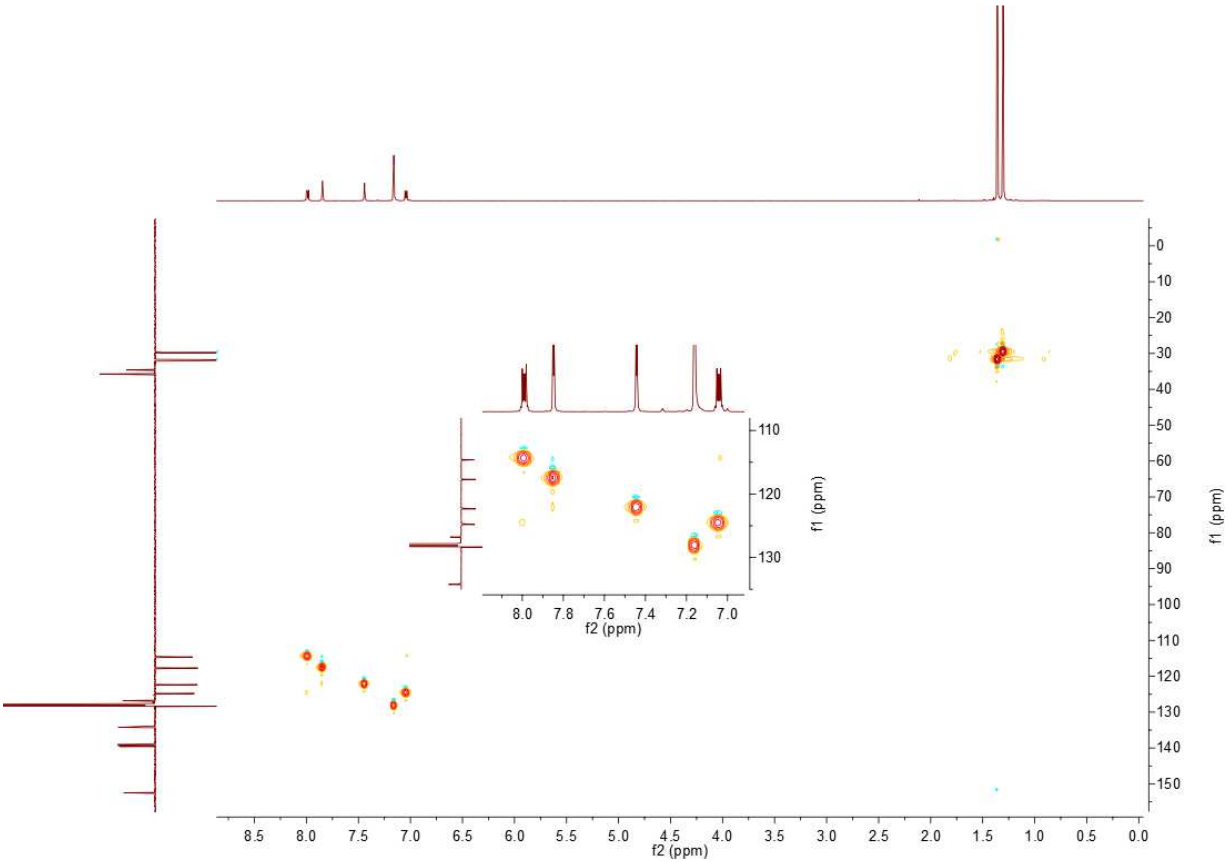

Figure S9. ^{1}H-^{13}C HSQC spectrum of complex **5** in benzene-d_6.

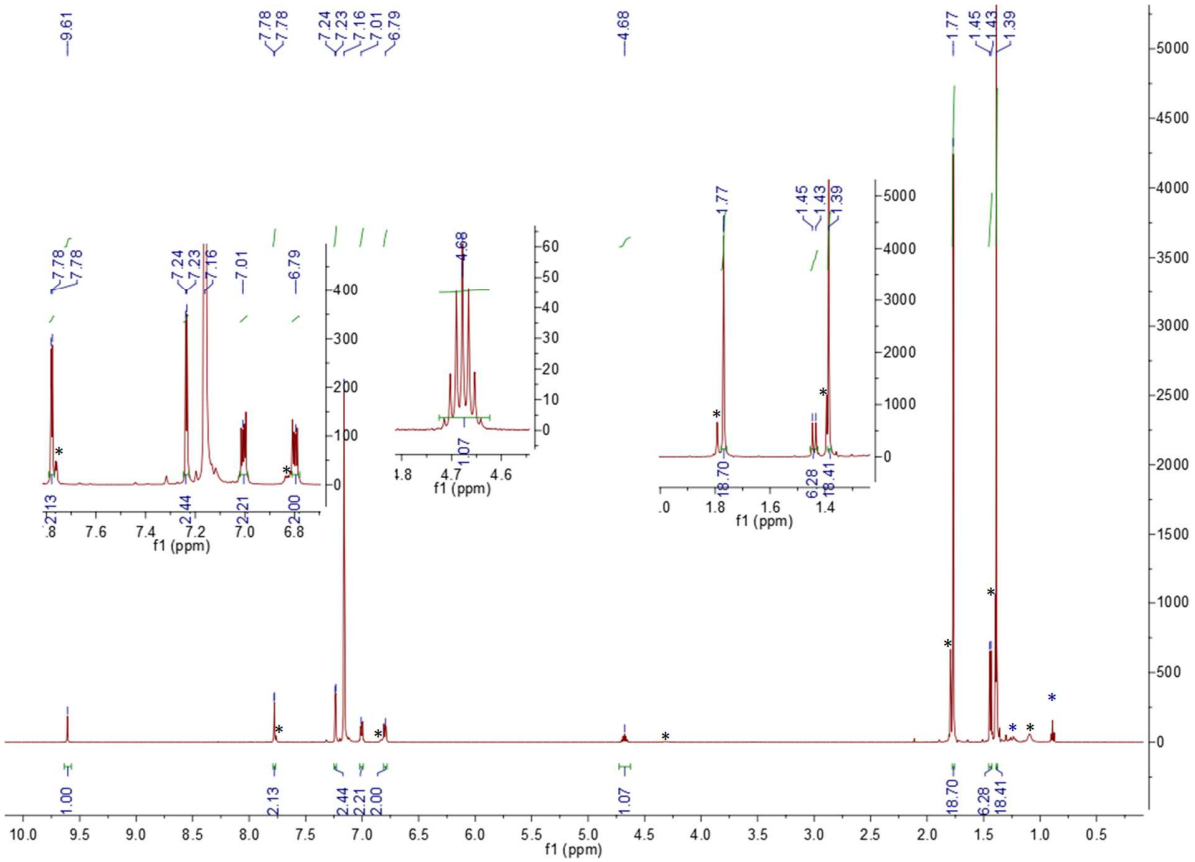

Figure S10. ^{1}H NMR spectrum of complex **5''** in benzene-d_6. Traces of residual solvent hexane (*) and impurities arising from the partial hydrolysis of **5''** (*).

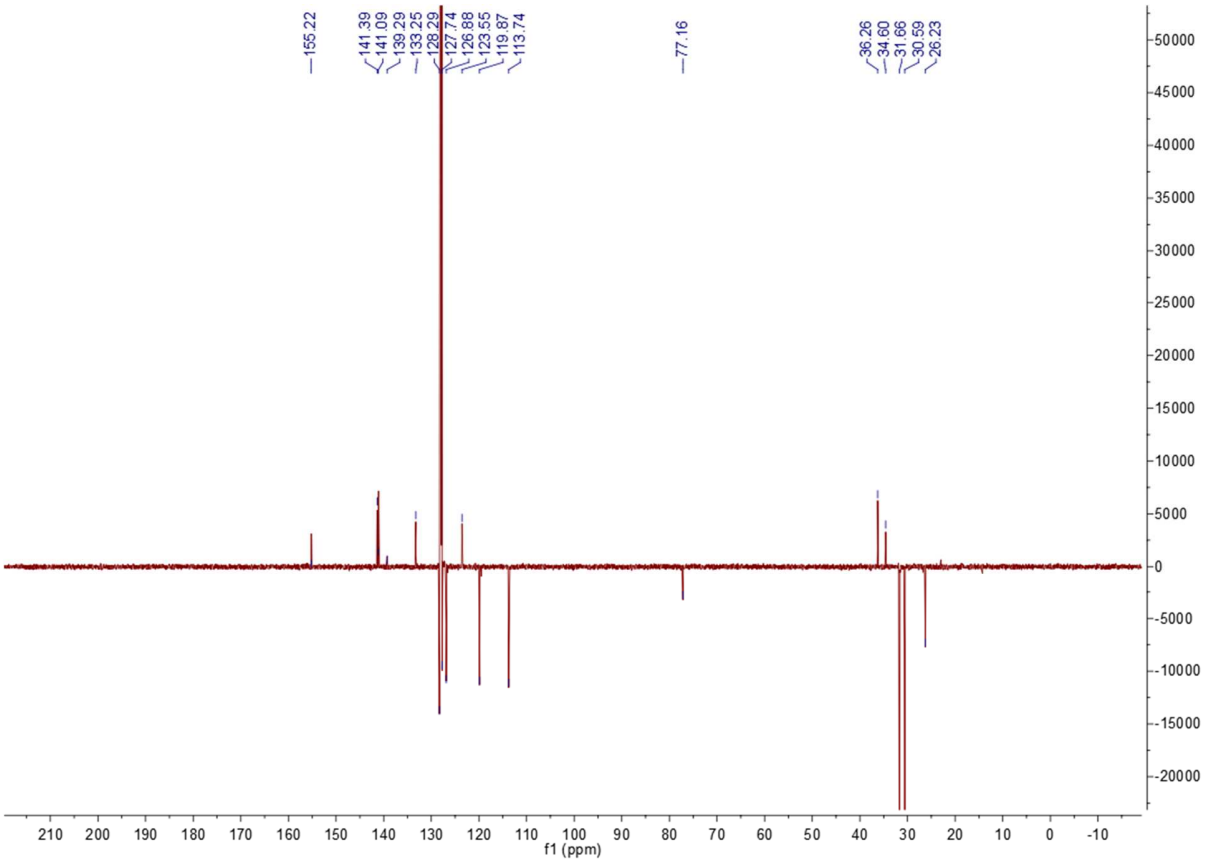

Figure S11. ^{13}C APT NMR spectrum of complex **5''** in benzene-d_6.

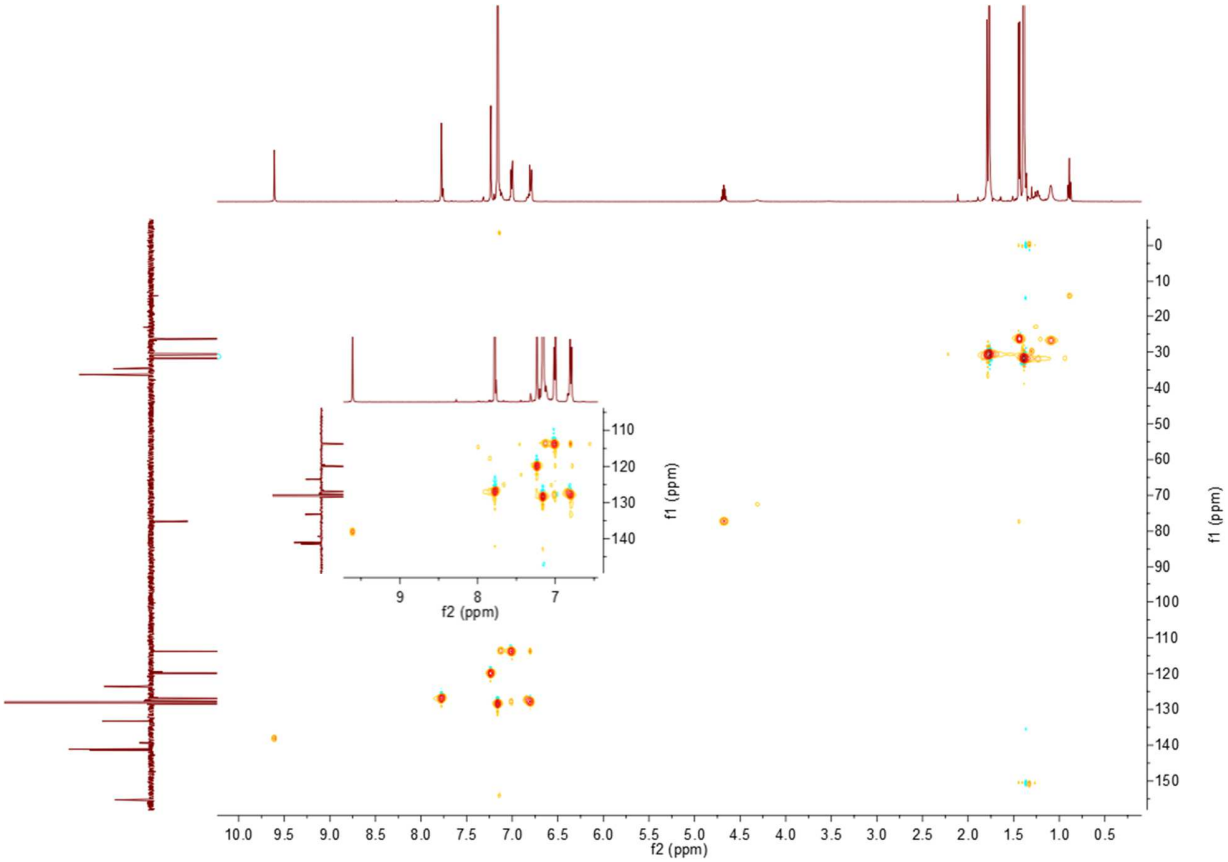

Figure S12. ^{1}H-^{13}C APT HSQC spectrum of complex **5''** in benzene-d_6.

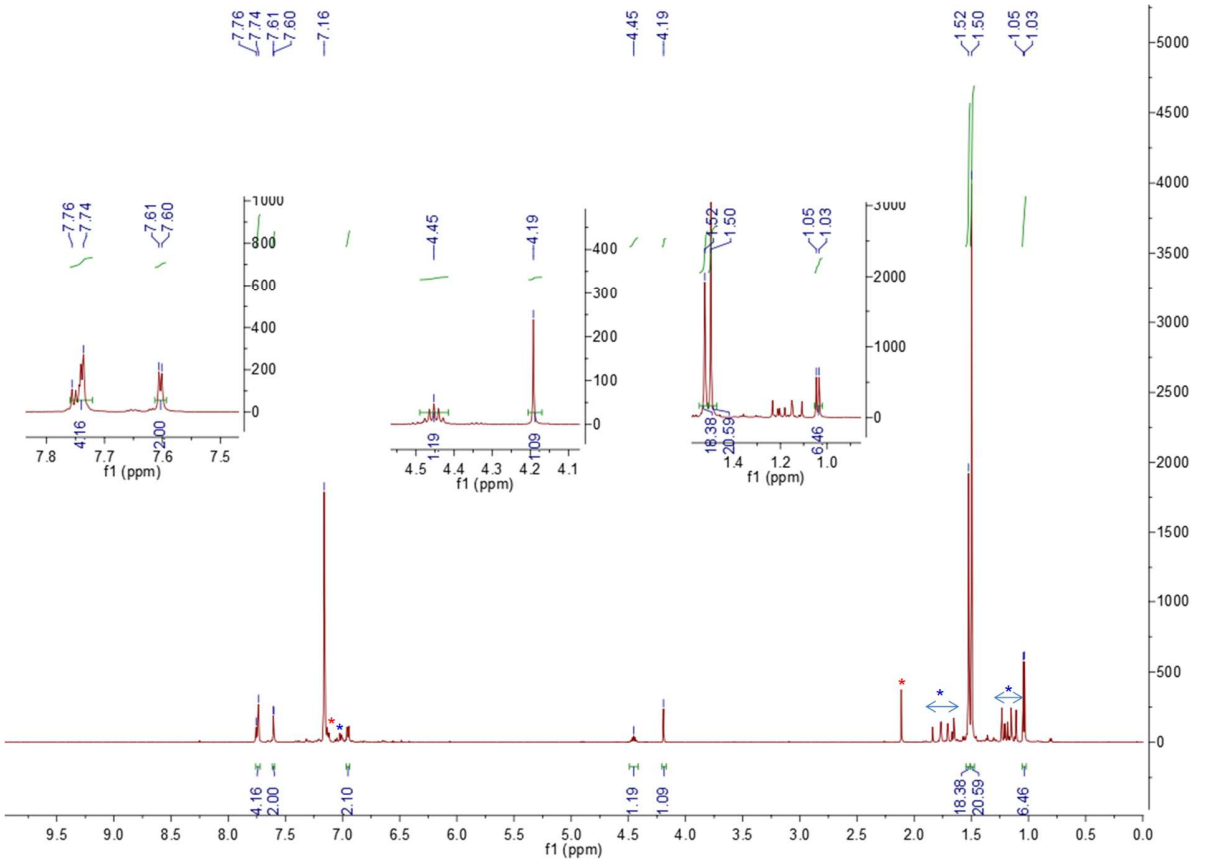

Figure S13. ^{1}H NMR spectrum of complex **6** in benzene-d_6. Traces of residual solvent: toluene (*) and impurities arising from the partial hydrolysis of **6** (*).

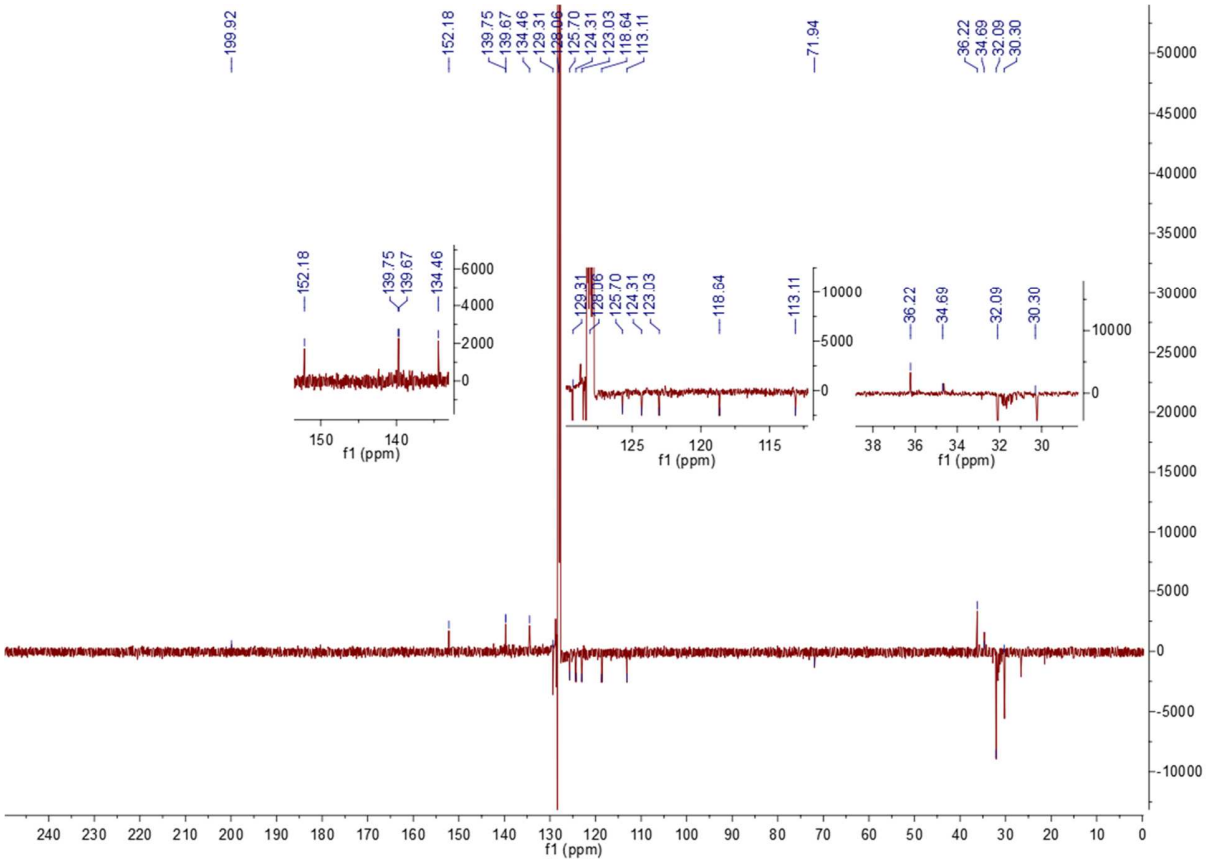

Figure S14. ^{13}C APT NMR spectrum of complex **6** in benzene-d_6.

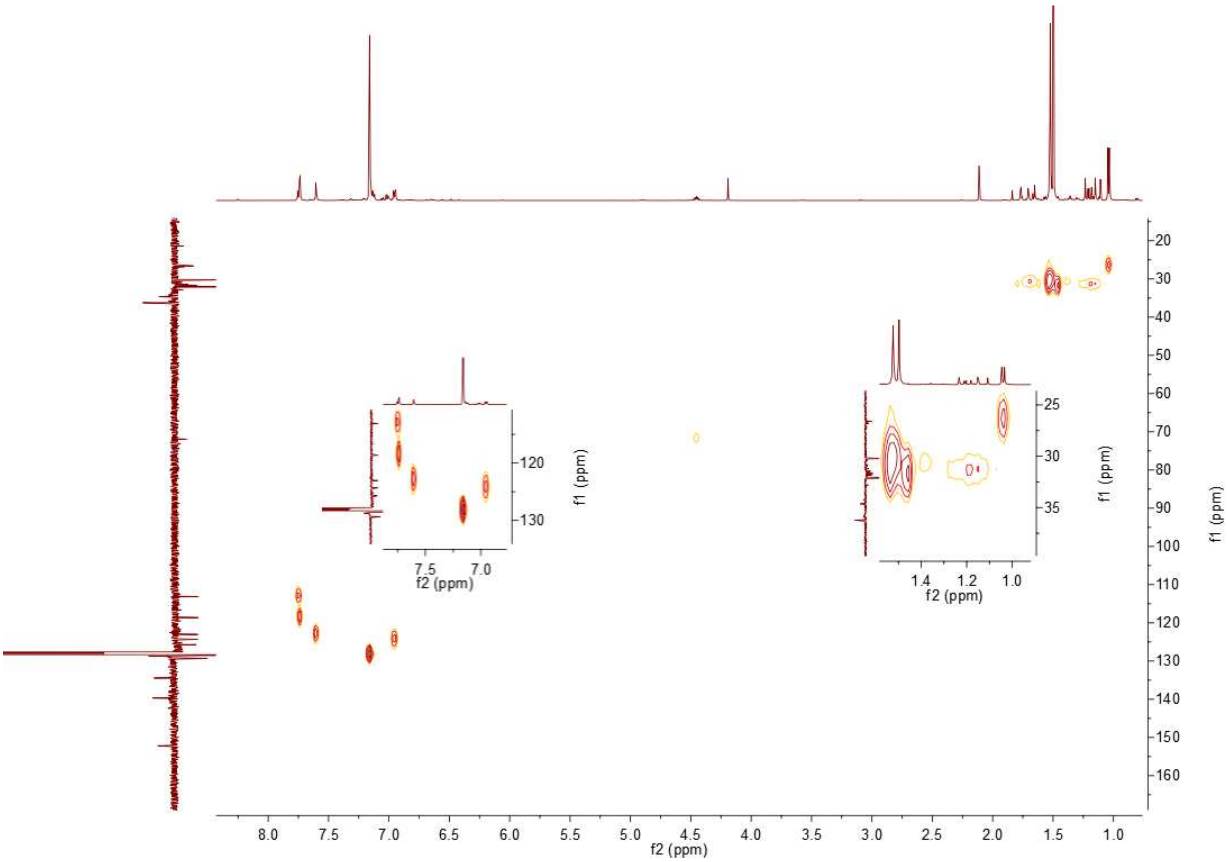

Figure S15. ^{1}H-^{13}C APT HSQC spectrum of complex **6** in benzene-d_6.

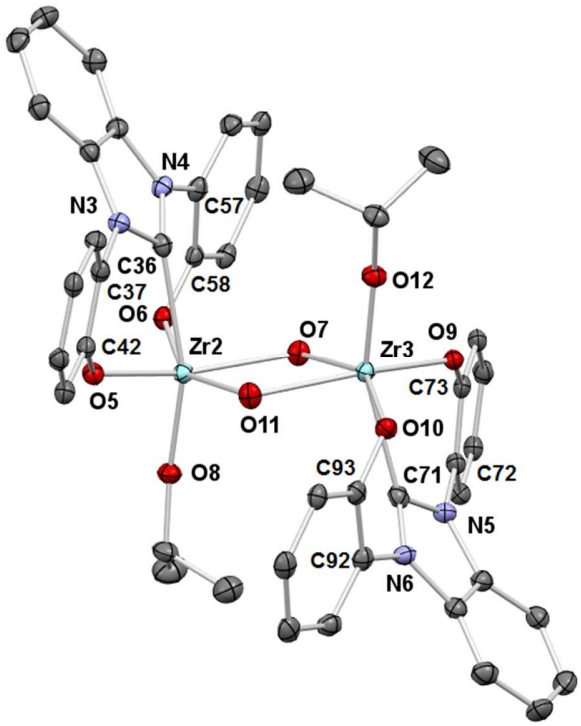

Figure S16. Molecular structure of complex **6** (conformer B, symmetry transformations used to generate equivalent atoms (‘): -*x*+1, -*y*+1, *z*+1) with ADP’s set at the 50% probability level. Hydrogen atoms, *t*Bu groups and co-crystallized toluene molecules were removed for clarity. Selected bond lengths (Å): Zr2-C36 = 2.4415(3), Zr3-C71 = 2.402(3), Zr2-O5 = 2.053(2), Zr2-O6 = 2.041(2), Zr3-O9 = 2.052(2), Zr3-O10 = 2.053(2), Zr2-O7 = 2.127(2), Zr3-O7 = 2.139(2), Zr2-O11 = 2.133(2), Zr3-O11 = 2.133(2), Zr2-O8 = 1.926(2), Zr3-O12 = 1.923(2), C36-N3 = 1.355(3), C36-N4 = 1.361(3), C71-N5 = 1.351(5), C71-N6 = 1.359(3). Selected angle (°): O5-Zr2-O6 = 113.36(8), O9-Zr3-O10 = 116.55(8), C36-Zr2-O11 = 93.31(8), C71-Zr3-O7 = 93.99(8), C36-Zr2-O8 = 163.03(9), C71-Zr3-O12 = 158.56(9), C36-N4-C57-C58 = 37.45, C36-N3-C37-C42 = - 38.13, C71-N5-C72-C73 = 40.94, C71-N6-C92-C93 = - 41.45.

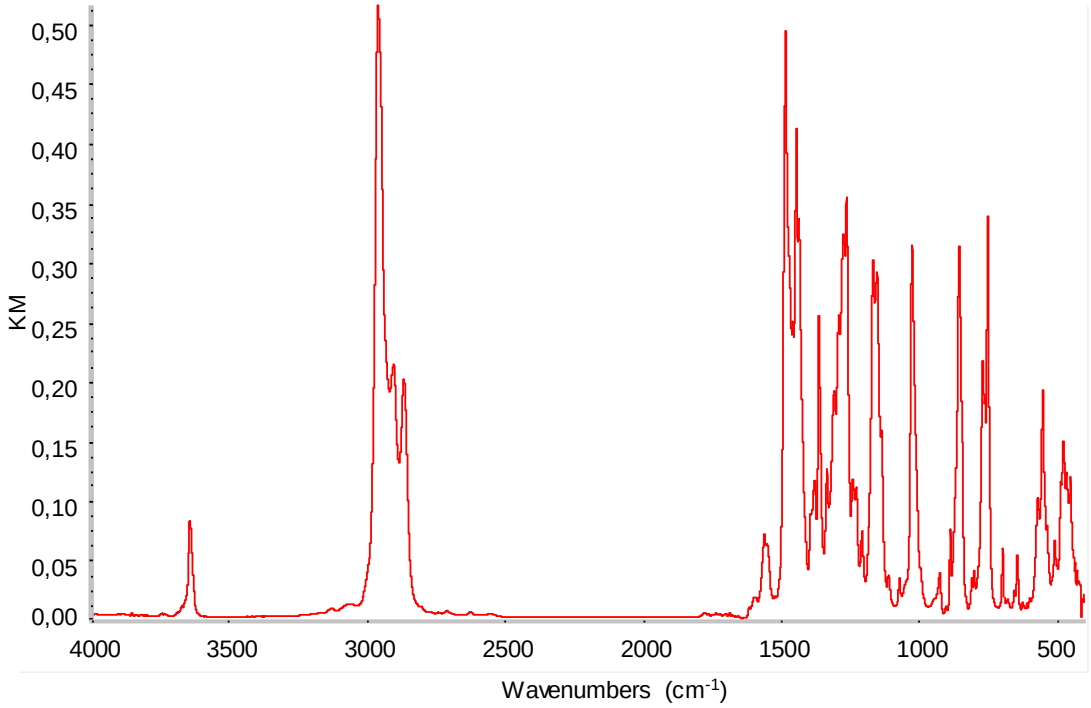

Figure S17. DRIFT spectrum of complex **6**.

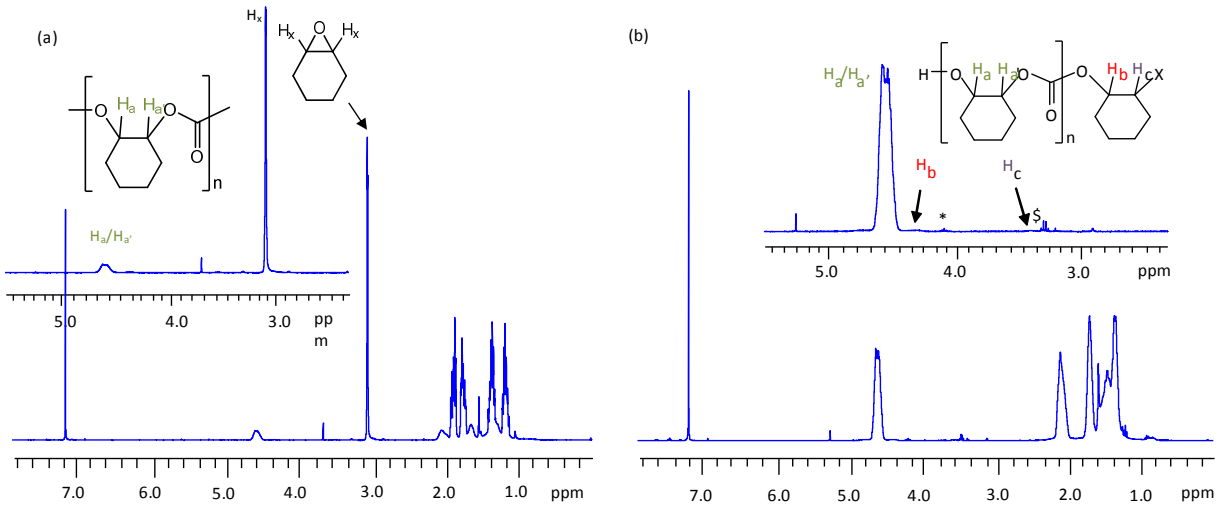

Figure S18. ^{1}H NMR spectra: (a) crude reaction mixture and (b) PCHC after extraction (Table 2, run 3). Traces of cyclohexene carbonate (CHC) at 4.10 ppm (*) and poly(cyclohexene oxide) (PCHO) at 3.55 ppm ($): ≤1%.

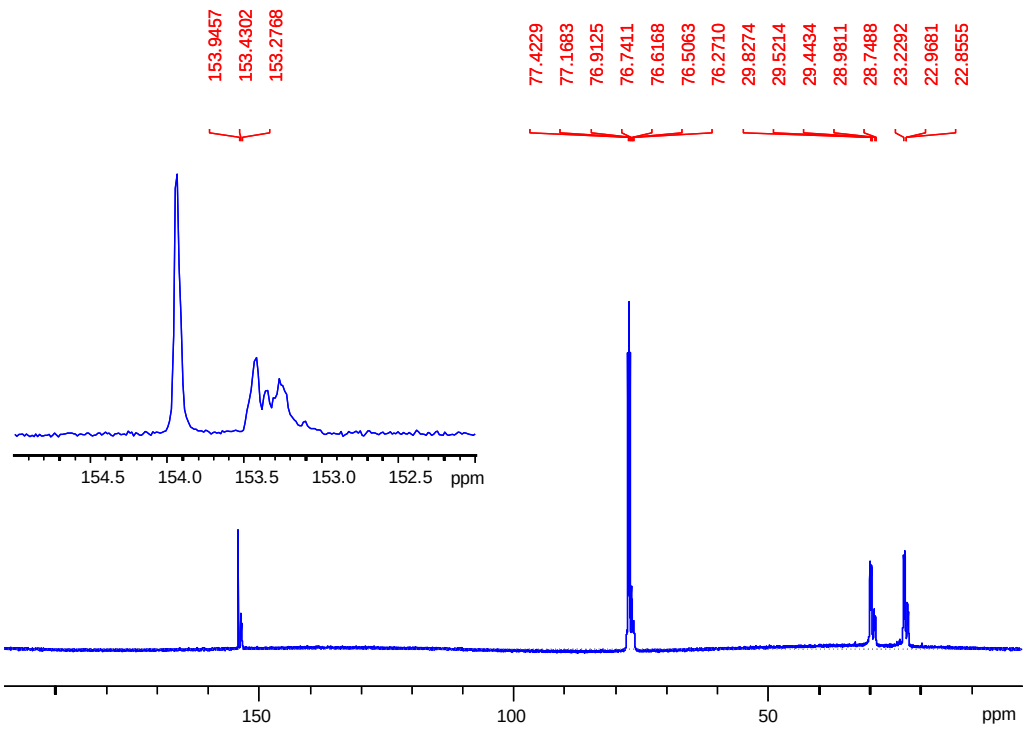

Figure S19. ^{13}C NMR spectrum of PCHC (Table 2, run 3).

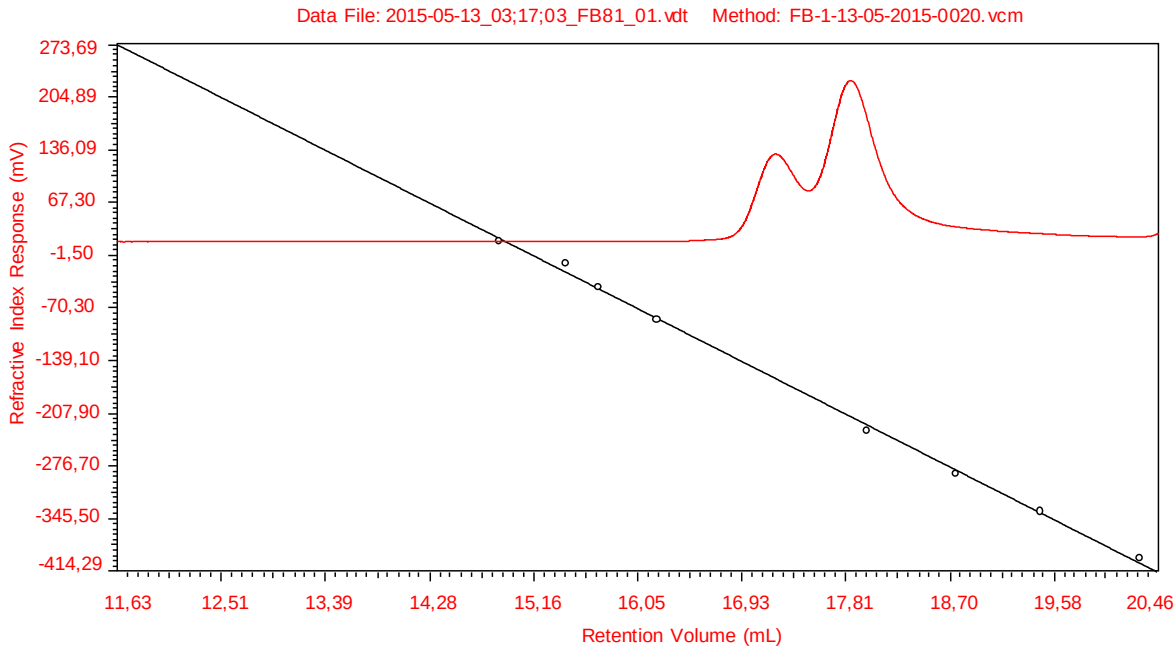

Figure S20. GPC-SEC profile of PCHC (Table 2, run 3).

Table S1. Crystal structure and refinement data for **3**, **4**, **5**, **5''** and **6**.

	3.C_5H_{12}	**4.C_7H_8**	**5**	**5''. C_6H_6**	**6.2C_7H_8**
Formula	$C_{46}H_{78}N_2O_5Zr$	$C_{69}H_{92}N_4O_4Zr$	$C_{70}H_{88}N_4O_4Zr$	$C_{44}H_{58}Cl_2N_2O_3Zr$	$C_{90}H_{120}N_4O_8Zr_2$
Formula weight	830.32	1132.68	1140.66	825.04	1568.33
Temperature/ K	103(2)	103(2)	103(2)	102 (2)	103(2)
Wavelength/ Å	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal size/ mm	0.255×0.210×0.020	0.150×0.050×0.050	0.369×0.314×0.072	0.587×0.376×0.360	0.359 ×0.274 ×0.206
Crystal color	Colorless	Colorless	Colorless, opaque	Colorless	Colorless
Habit	Thin plate	Needle	Flat prism	Irregular prism	Plate
Crystal system	Triclinic	Monoclinic	Triclinic	Monoclinic	Monoclinic
Space group	Pī (No. 2)	*P2₁/c* (No.14)	Pī (No. 2)	*P*2₁/c (No. 14)	*C*2/c (No. 15)
a/ Å	9.627(2)	13.823(4)	15.231(3)	11.3763(8)	60.365(5)
b/ Å	13.587(3)	26.109(5)	15.917(3)	17.4465(12)	17.11443(15)
c/ Å	19.235(4)	17.864(3)	16.457(3)	21.9304(15)	25.466(2)
α/ Å	72.856(3)	90	96.633(2)°	90	90
β/ Å	78.644(3)	102.250(3)	102.016(2)°	97.6800(10)	106.3950(10)
γ/ Å	78.358(3)	90	94.047(2)°	90	90
V/ Å³	2329.2(9)	6300(3)	3857.4(11)	4313.6(5)	25239(4)
Z	2	4	2	4	12
d / g cm^{-3}	1.184	1.194	0.982	1.270	1.238
F(000)	896	2424	1216	1736	9984
Absorption coefficient/ mm^{-1}	0.279	0.224	0.183	0.418	0.304
θ Range for data collection/ °	2.172 to 25.025	1.870 to 25.045	1.692 to 25.027	1.806 to 30.535	1.651 to 25.712
Reflections collected	25963	72225	44806	13183	151274
Independent reflections	8211 [R_{int} = 0.0753]	11146 [R_{int} = 0.1306]	13637 [R_{int} = 0.0515]	13183 [R_{int}= 0.0858]	24027 [R_{int} = 0.0671]
Completeness to θ_{max}	99.7%	99.9%	100%	100%	100%
Absorption correction	Numerical	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F²	Full-matrix least-squares on F²	Full-matrix least-squares on F²	Full-matrix least-squares on F²	Full-matrix least-squares on F²
Data/ restraints/ parameters	8211/0/505	11146 / 824 / 720	11998/60/465	13183/0/487	8673/24/283
Goodness-of-fit on F^2	1.015	1.017	1.084	1.069	1.091
Final *R* indices [$I > 2\sigma(I)$]	R_1 = 0.0532, wR_2 = 0.1291	R_1 = 0.0608, wR_2 = 0.1304	R_1 = 0.0733, wR_2 = 0.1829	R_1 = 0.0410, wR_2 = 0.1093	R_1 = 0.0428, wR_2 = 0.1020
R indices (all data)	R_1 =0.0796, wR_2 = 0.1424	R_1 = 0.1104, wR_2 = 0.1533	R_1 = 0.0767, wR_2 = 0.1844	R_1 = 0.0512, wR_2 = 0.1144	R_1 = 0.0625, wR_1 = 0.1131
Largest diff. peak/ hole/ e Å³	0.878 and -0.672	0.806 and -0.508	0.980 and -0.787	1.521 and -0.657	1.329 and -0.678

Table S2. Bond lengths [Å] and angles [°] for **3**.

Zr(01)-O(4)	1.947(2)	C(15)-H(15C)	0.9800
Zr(01)-O(3)	1.961(3)	C(16)-H(16A)	0.9800
Zr(01)-O(1)	2.007(2)	C(16)-H(16B)	0.9800
Zr(01)-O(2)	2.019(2)	C(16)-H(16C)	0.9800
Zr(01)-C(1)	2.398(3)	C(17)-H(17A)	0.9800
Zr(01)-O(5)	2.406(3)	C(17)-H(17B)	0.9800
O(1)-C(19)	1.337(4)	C(17)-H(17C)	0.9800
N(1)-C(1)	1.338(4)	C(18)-C(23)	1.397(5)
N(1)-C(18)	1.423(4)	C(18)-C(19)	1.415(5)
N(1)-C(2)	1.480(4)	C(19)-C(20)	1.407(5)
C(1)-N(2)	1.353(4)	C(20)-C(21)	1.398(5)
O(2)-C(5)	1.338(4)	C(20)-C(24)	1.545(5)
N(2)-C(4)	1.431(4)	C(21)-C(22)	1.386(5)
N(2)-C(3)	1.487(4)	C(21)-H(21)	0.9500
C(2)-C(3)	1.515(5)	C(22)-C(23)	1.380(5)
C(2)-H(2A)	0.9900	C(22)-C(28)	1.542(5)
C(2)-H(2B)	0.9900	C(23)-H(23)	0.9500
O(3)-C(32)	1.411(5)	C(24)-C(25)	1.531(5)
C(3)-H(3A)	0.9900	C(24)-C(26)	1.533(5)
C(3)-H(3B)	0.9900	C(24)-C(27)	1.546(5)
O(4)-C(35)	1.413(4)	C(25)-H(25A)	0.9800
C(4)-C(9)	1.395(5)	C(25)-H(25B)	0.9800
C(4)-C(5)	1.414(5)	C(25)-H(25C)	0.9800
O(5)-C(38)	1.411(5)	C(26)-H(26A)	0.9800
O(5)-C(41)	1.446(5)	C(26)-H(26B)	0.9800
C(5)-C(6)	1.403(5)	C(26)-H(26C)	0.9800
C(6)-C(7)	1.386(5)	C(27)-H(27A)	0.9800
C(6)-C(10)	1.543(5)	C(27)-H(27B)	0.9800
C(7)-C(8)	1.387(5)	C(27)-H(27C)	0.9800
C(7)-H(7)	0.9500	C(28)-C(31)	1.520(5)
C(8)-C(9)	1.390(5)	C(28)-C(29)	1.521(6)
C(8)-C(14)	1.533(5)	C(28)-C(30)	1.533(6)
C(9)-H(9)	0.9500	C(29)-H(29A)	0.9800
C(10)-C(13)	1.527(5)	C(29)-H(29B)	0.9800
C(10)-C(12)	1.533(5)	C(29)-H(29C)	0.9800
C(10)-C(11)	1.536(5)	C(30)-H(30A)	0.9800
C(11)-H(11A)	0.9800	C(30)-H(30B)	0.9800
C(11)-H(11B)	0.9800	C(30)-H(30C)	0.9800
C(11)-H(11C)	0.9800	C(31)-H(31A)	0.9800
C(12)-H(12A)	0.9800	C(31)-H(31B)	0.9800
C(12)-H(12B)	0.9800	C(31)-H(31C)	0.9800
C(12)-H(12C)	0.9800	C(32)-C(33)	1.486(7)
C(13)-H(13A)	0.9800	C(32)-C(34)	1.495(6)
C(13)-H(13B)	0.9800	C(32)-H(32)	1.0000
C(13)-H(13C)	0.9800	C(33)-H(33A)	0.9800
C(14)-C(16)	1.527(5)	C(33)-H(33B)	0.9800
C(14)-C(15)	1.537(5)	C(33)-H(33C)	0.9800
C(14)-C(17)	1.541(5)	C(34)-H(34A)	0.9800
C(15)-H(15A)	0.9800	C(34)-H(34B)	0.9800
C(15)-H(15B)	0.9800	C(34)-H(34C)	0.9800

C(35)-C(37)	1.510(5)	C(19)-O(1)-Zr(01)	145.5(2)
C(35)-C(36)	1.512(5)	C(1)-N(1)-C(18)	128.4(3)
C(35)-H(35)	1.0000	C(1)-N(1)-C(2)	112.5(3)
C(36)-H(36A)	0.9800	C(18)-N(1)-C(2)	119.1(3)
C(36)-H(36B)	0.9800	N(1)-C(1)-N(2)	108.8(3)
C(36)-H(36C)	0.9800	N(1)-C(1)-Zr(01)	125.2(2)
C(37)-H(37A)	0.9800	N(2)-C(1)-Zr(01)	126.0(2)
C(37)-H(37B)	0.9800	C(5)-O(2)-Zr(01)	146.2(2)
C(37)-H(37C)	0.9800	C(1)-N(2)-C(4)	127.9(3)
C(38)-C(39)	1.487(7)	C(1)-N(2)-C(3)	112.3(3)
C(38)-H(38A)	0.9900	C(4)-N(2)-C(3)	119.2(3)
C(38)-H(38B)	0.9900	N(1)-C(2)-C(3)	103.3(3)
C(39)-C(40)	1.460(7)	N(1)-C(2)-H(2A)	111.1
C(39)-H(39A)	0.9900	C(3)-C(2)-H(2A)	111.1
C(39)-H(39B)	0.9900	N(1)-C(2)-H(2B)	111.1
C(40)-C(41)	1.494(6)	C(3)-C(2)-H(2B)	111.1
C(40)-H(40A)	0.9900	H(2A)-C(2)-H(2B)	109.1
C(40)-H(40B)	0.9900	C(32)-O(3)-Zr(01)	165.1(3)
C(41)-H(41A)	0.9900	N(2)-C(3)-C(2)	102.6(3)
C(41)-H(41B)	0.9900	N(2)-C(3)-H(3A)	111.2
C(42)-C(43)	1.495(7)	C(2)-C(3)-H(3A)	111.2
C(42)-H(42A)	0.9800	N(2)-C(3)-H(3B)	111.2
C(42)-H(42B)	0.9800	C(2)-C(3)-H(3B)	111.2
C(42)-H(42C)	0.9800	H(3A)-C(3)-H(3B)	109.2
C(43)-C(44)	1.488(7)	C(35)-O(4)-Zr(01)	152.7(2)
C(43)-H(43A)	0.9900	C(9)-C(4)-C(5)	119.4(3)
C(43)-H(43B)	0.9900	C(9)-C(4)-N(2)	118.6(3)
C(44)-C(45)	1.497(7)	C(5)-C(4)-N(2)	122.0(3)
C(44)-H(44A)	0.9900	C(38)-O(5)-C(41)	107.8(3)
C(44)-H(44B)	0.9900	C(38)-O(5)-Zr(01)	129.7(2)
C(45)-C(46)	1.514(8)	C(41)-O(5)-Zr(01)	121.3(2)
C(45)-H(45A)	0.9900	O(2)-C(5)-C(6)	120.5(3)
C(45)-H(45B)	0.9900	O(2)-C(5)-C(4)	120.0(3)
C(46)-H(46A)	0.9800	C(6)-C(5)-C(4)	119.5(3)
C(46)-H(46B)	0.9800	C(7)-C(6)-C(5)	118.5(3)
C(46)-H(46C)	0.9800	C(7)-C(6)-C(10)	120.9(3)
		C(5)-C(6)-C(10)	120.6(3)
O(4)-Zr(01)-O(3)	102.52(11)	C(6)-C(7)-C(8)	123.5(3)
O(4)-Zr(01)-O(1)	97.18(10)	C(6)-C(7)-H(7)	118.2
O(3)-Zr(01)-O(1)	101.32(10)	C(8)-C(7)-H(7)	118.2
O(4)-Zr(01)-O(2)	96.38(10)	C(7)-C(8)-C(9)	117.2(3)
O(3)-Zr(01)-O(2)	100.53(10)	C(7)-C(8)-C(14)	123.0(3)
O(1)-Zr(01)-O(2)	151.05(10)	C(9)-C(8)-C(14)	119.8(3)
O(4)-Zr(01)-C(1)	98.74(11)	C(8)-C(9)-C(4)	121.8(3)
O(3)-Zr(01)-C(1)	158.72(12)	C(8)-C(9)-H(9)	119.1
O(1)-Zr(01)-C(1)	76.67(10)	C(4)-C(9)-H(9)	119.1
O(2)-Zr(01)-C(1)	76.06(10)	C(13)-C(10)-C(12)	107.3(3)
O(4)-Zr(01)-O(5)	175.44(10)	C(13)-C(10)-C(11)	106.3(3)
O(3)-Zr(01)-O(5)	81.97(11)	C(12)-C(10)-C(11)	110.4(3)
O(1)-Zr(01)-O(5)	81.04(10)	C(13)-C(10)-C(6)	112.7(3)
O(2)-Zr(01)-O(5)	83.45(9)	C(12)-C(10)-C(6)	109.1(3)
C(1)-Zr(01)-O(5)	76.78(11)	C(11)-C(10)-C(6)	111.0(3)

C(10)-C(11)-H(11A)	109.5	C(22)-C(21)-H(21)	118.5
C(10)-C(11)-H(11B)	109.5	C(20)-C(21)-H(21)	118.5
H(11A)-C(11)-H(11B)	109.5	C(23)-C(22)-C(21)	118.1(3)
C(10)-C(11)-H(11C)	109.5	C(23)-C(22)-C(28)	119.2(3)
H(11A)-C(11)-H(11C)	109.5	C(21)-C(22)-C(28)	122.7(3)
H(11B)-C(11)-H(11C)	109.5	C(22)-C(23)-C(18)	121.8(3)
C(10)-C(12)-H(12A)	109.5	C(22)-C(23)-H(23)	119.1
C(10)-C(12)-H(12B)	109.5	C(18)-C(23)-H(23)	119.1
H(12A)-C(12)-H(12B)	109.5	C(25)-C(24)-C(26)	107.4(3)
C(10)-C(12)-H(12C)	109.5	C(25)-C(24)-C(20)	112.5(3)
H(12A)-C(12)-H(12C)	109.5	C(26)-C(24)-C(20)	111.4(3)
H(12B)-C(12)-H(12C)	109.5	C(25)-C(24)-C(27)	107.2(3)
C(10)-C(13)-H(13A)	109.5	C(26)-C(24)-C(27)	108.8(3)
C(10)-C(13)-H(13B)	109.5	C(20)-C(24)-C(27)	109.3(3)
H(13A)-C(13)-H(13B)	109.5	C(24)-C(25)-H(25A)	109.5
C(10)-C(13)-H(13C)	109.5	C(24)-C(25)-H(25B)	109.5
H(13A)-C(13)-H(13C)	109.5	H(25A)-C(25)-H(25B)	109.5
H(13B)-C(13)-H(13C)	109.5	C(24)-C(25)-H(25C)	109.5
C(16)-C(14)-C(8)	110.5(3)	H(25A)-C(25)-H(25C)	109.5
C(16)-C(14)-C(15)	108.1(3)	H(25B)-C(25)-H(25C)	109.5
C(8)-C(14)-C(15)	112.6(3)	C(24)-C(26)-H(26A)	109.5
C(16)-C(14)-C(17)	109.5(3)	C(24)-C(26)-H(26B)	109.5
C(8)-C(14)-C(17)	108.8(3)	H(26A)-C(26)-H(26B)	109.5
C(15)-C(14)-C(17)	107.4(3)	C(24)-C(26)-H(26C)	109.5
C(14)-C(15)-H(15A)	109.5	H(26A)-C(26)-H(26C)	109.5
C(14)-C(15)-H(15B)	109.5	H(26B)-C(26)-H(26C)	109.5
H(15A)-C(15)-H(15B)	109.5	C(24)-C(27)-H(27A)	109.5
C(14)-C(15)-H(15C)	109.5	C(24)-C(27)-H(27B)	109.5
H(15A)-C(15)-H(15C)	109.5	H(27A)-C(27)-H(27B)	109.5
H(15B)-C(15)-H(15C)	109.5	C(24)-C(27)-H(27C)	109.5
C(14)-C(16)-H(16A)	109.5	H(27A)-C(27)-H(27C)	109.5
C(14)-C(16)-H(16B)	109.5	H(27B)-C(27)-H(27C)	109.5
H(16A)-C(16)-H(16B)	109.5	C(31)-C(28)-C(29)	108.1(3)
C(14)-C(16)-H(16C)	109.5	C(31)-C(28)-C(30)	108.1(3)
H(16A)-C(16)-H(16C)	109.5	C(29)-C(28)-C(30)	109.9(4)
H(16B)-C(16)-H(16C)	109.5	C(31)-C(28)-C(22)	112.0(3)
C(14)-C(17)-H(17A)	109.5	C(29)-C(28)-C(22)	108.8(3)
C(14)-C(17)-H(17B)	109.5	C(30)-C(28)-C(22)	109.9(3)
H(17A)-C(17)-H(17B)	109.5	C(28)-C(29)-H(29A)	109.5
C(14)-C(17)-H(17C)	109.5	C(28)-C(29)-H(29B)	109.5
H(17A)-C(17)-H(17C)	109.5	H(29A)-C(29)-H(29B)	109.5
H(17B)-C(17)-H(17C)	109.5	C(28)-C(29)-H(29C)	109.5
C(23)-C(18)-C(19)	119.2(3)	H(29A)-C(29)-H(29C)	109.5
C(23)-C(18)-N(1)	118.0(3)	H(29B)-C(29)-H(29C)	109.5
C(19)-C(18)-N(1)	122.7(3)	C(28)-C(30)-H(30A)	109.5
O(1)-C(19)-C(20)	120.2(3)	C(28)-C(30)-H(30B)	109.5
O(1)-C(19)-C(18)	120.0(3)	H(30A)-C(30)-H(30B)	109.5
C(20)-C(19)-C(18)	119.8(3)	C(28)-C(30)-H(30C)	109.5
C(21)-C(20)-C(19)	118.1(3)	H(30A)-C(30)-H(30C)	109.5
C(21)-C(20)-C(24)	120.6(3)	H(30B)-C(30)-H(30C)	109.5
C(19)-C(20)-C(24)	121.3(3)	C(28)-C(31)-H(31A)	109.5
C(22)-C(21)-C(20)	123.0(3)	C(28)-C(31)-H(31B)	109.5

H(31A)-C(31)-H(31B)	109.5	C(40)-C(39)-H(39A)	111.1
C(28)-C(31)-H(31C)	109.5	C(38)-C(39)-H(39A)	111.1
H(31A)-C(31)-H(31C)	109.5	C(40)-C(39)-H(39B)	111.1
H(31B)-C(31)-H(31C)	109.5	C(38)-C(39)-H(39B)	111.1
O(3)-C(32)-C(33)	109.9(4)	H(39A)-C(39)-H(39B)	109.1
O(3)-C(32)-C(34)	109.7(4)	C(39)-C(40)-C(41)	103.0(4)
C(33)-C(32)-C(34)	112.3(4)	C(39)-C(40)-H(40A)	111.2
O(3)-C(32)-H(32)	108.3	C(41)-C(40)-H(40A)	111.2
C(33)-C(32)-H(32)	108.3	C(39)-C(40)-H(40B)	111.2
C(34)-C(32)-H(32)	108.3	C(41)-C(40)-H(40B)	111.2
C(32)-C(33)-H(33A)	109.5	H(40A)-C(40)-H(40B)	109.1
C(32)-C(33)-H(33B)	109.5	O(5)-C(41)-C(40)	106.8(4)
H(33A)-C(33)-H(33B)	109.5	O(5)-C(41)-H(41A)	110.4
C(32)-C(33)-H(33C)	109.5	C(40)-C(41)-H(41A)	110.4
H(33A)-C(33)-H(33C)	109.5	O(5)-C(41)-H(41B)	110.4
H(33B)-C(33)-H(33C)	109.5	C(40)-C(41)-H(41B)	110.4
C(32)-C(34)-H(34A)	109.5	H(41A)-C(41)-H(41B)	108.6
C(32)-C(34)-H(34B)	109.5	C(43)-C(42)-H(42A)	109.5
H(34A)-C(34)-H(34B)	109.5	C(43)-C(42)-H(42B)	109.5
C(32)-C(34)-H(34C)	109.5	H(42A)-C(42)-H(42B)	109.5
H(34A)-C(34)-H(34C)	109.5	C(43)-C(42)-H(42C)	109.5
H(34B)-C(34)-H(34C)	109.5	H(42A)-C(42)-H(42C)	109.5
O(4)-C(35)-C(37)	109.8(3)	H(42B)-C(42)-H(42C)	109.5
O(4)-C(35)-C(36)	110.1(3)	C(44)-C(43)-C(42)	115.7(5)
C(37)-C(35)-C(36)	112.4(3)	C(44)-C(43)-H(43A)	108.3
O(4)-C(35)-H(35)	108.1	C(42)-C(43)-H(43A)	108.3
C(37)-C(35)-H(35)	108.1	C(44)-C(43)-H(43B)	108.3
C(36)-C(35)-H(35)	108.1	C(42)-C(43)-H(43B)	108.3
C(35)-C(36)-H(36A)	109.5	H(43A)-C(43)-H(43B)	107.4
C(35)-C(36)-H(36B)	109.5	C(43)-C(44)-C(45)	115.9(5)
H(36A)-C(36)-H(36B)	109.5	C(43)-C(44)-H(44A)	108.3
C(35)-C(36)-H(36C)	109.5	C(45)-C(44)-H(44A)	108.3
H(36A)-C(36)-H(36C)	109.5	C(43)-C(44)-H(44B)	108.3
H(36B)-C(36)-H(36C)	109.5	C(45)-C(44)-H(44B)	108.3
C(35)-C(37)-H(37A)	109.5	H(44A)-C(44)-H(44B)	107.4
C(35)-C(37)-H(37B)	109.5	C(44)-C(45)-C(46)	115.5(5)
H(37A)-C(37)-H(37B)	109.5	C(44)-C(45)-H(45A)	108.4
C(35)-C(37)-H(37C)	109.5	C(46)-C(45)-H(45A)	108.4
H(37A)-C(37)-H(37C)	109.5	C(44)-C(45)-H(45B)	108.4
H(37B)-C(37)-H(37C)	109.5	C(46)-C(45)-H(45B)	108.4
O(5)-C(38)-C(39)	106.2(4)	H(45A)-C(45)-H(45B)	107.5
O(5)-C(38)-H(38A)	110.5	C(45)-C(46)-H(46A)	109.5
C(39)-C(38)-H(38A)	110.5	C(45)-C(46)-H(46B)	109.5
O(5)-C(38)-H(38B)	110.5	H(46A)-C(46)-H(46B)	109.5
C(39)-C(38)-H(38B)	110.5	C(45)-C(46)-H(46C)	109.5
H(38A)-C(38)-H(38B)	108.7	H(46A)-C(46)-H(46C)	109.5
C(40)-C(39)-C(38)	103.3(4)	H(46B)-C(46)-H(46C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S3. Torsion angles [°] for **3**.

C(18)-N(1)-C(1)-N(2)	75.9(3)	C(1)-N(1)-C(18)-C(23)	-177.2(3)
C(2)-N(1)-C(1)-N(2)	4.7(4)	C(2)-N(1)-C(18)-C(23)	2.2(4)
C(18)-N(1)-C(1)-Zr(01)	5.5(5)	C(1)-N(1)-C(18)-C(19)	3.2(5)
C(2)-N(1)-C(1)-Zr(01)	-173.9(2)	C(2)-N(1)-C(18)-C(19)	-177.5(3)
N(1)-C(1)-N(2)-C(4)	170.8(3)	Zr(01)-O(1)-C(19)-C(20)	167.0(3)
Zr(01)-C(1)-N(2)-C(4)	-10.5(5)	Zr(01)-O(1)-C(19)-C(18)	-11.7(6)
N(1)-C(1)-N(2)-C(3)	-0.1(4)	C(23)-C(18)-C(19)-O(1)	177.8(3)
Zr(01)-C(1)-N(2)-C(3)	178.5(2)	N(1)-C(18)-C(19)-O(1)	-2.6(5)
C(1)-N(1)-C(2)-C(3)	-7.2(4)	C(23)-C(18)-C(19)-C(20)	-0.8(5)
C(18)-N(1)-C(2)-C(3)	173.4(3)	N(1)-C(18)-C(19)-C(20)	178.8(3)
C(1)-N(2)-C(3)-C(2)	-4.2(4)	O(1)-C(19)-C(20)-C(21)	-178.8(3)
C(4)-N(2)-C(3)-C(2)	-176.0(3)	C(18)-C(19)-C(20)-C(21)	-0.1(5)
N(1)-C(2)-C(3)-N(2)	6.4(3)	O(1)-C(19)-C(20)-C(24)	-1.4(5)
C(1)-N(2)-C(4)-C(9)	-168.9(3)	C(18)-C(19)-C(20)-C(24)	177.2(3)
C(3)-N(2)-C(4)-C(9)	1.5(4)	C(19)-C(20)-C(21)-C(22)	0.7(5)
C(1)-N(2)-C(4)-C(5)	9.8(5)	C(24)-C(20)-C(21)-C(22)	-176.7(3)
C(3)-N(2)-C(4)-C(5)	-179.8(3)	C(20)-C(21)-C(22)-C(23)	-0.2(5)
Zr(01)-O(2)-C(5)-C(6)	163.2(3)	C(20)-C(21)-C(22)-C(28)	177.7(3)
Zr(01)-O(2)-C(5)-C(4)	-16.9(6)	C(21)-C(22)-C(23)-C(18)	-0.8(5)
C(9)-C(4)-C(5)-O(2)	-179.4(3)	C(28)-C(22)-C(23)-C(18)	-178.8(3)
N(2)-C(4)-C(5)-O(2)	1.9(5)	C(19)-C(18)-C(23)-C(22)	1.3(5)
C(9)-C(4)-C(5)-C(6)	0.5(5)	N(1)-C(18)-C(23)-C(22)	-178.3(3)
N(2)-C(4)-C(5)-C(6)	-178.2(3)	C(21)-C(20)-C(24)-C(25)	-2.7(5)
O(2)-C(5)-C(6)-C(7)	-178.2(3)	C(19)-C(20)-C(24)-C(25)	-180.0(3)
C(4)-C(5)-C(6)-C(7)	1.9(5)	C(21)-C(20)-C(24)-C(26)	-123.4(4)
O(2)-C(5)-C(6)-C(10)	2.7(5)	C(19)-C(20)-C(24)-C(26)	59.3(5)
C(4)-C(5)-C(6)-C(10)	-177.2(3)	C(21)-C(20)-C(24)-C(27)	116.3(4)
C(5)-C(6)-C(7)-C(8)	-1.5(5)	C(19)-C(20)-C(24)-C(27)	-61.0(4)
C(10)-C(6)-C(7)-C(8)	177.6(3)	C(23)-C(22)-C(28)-C(31)	-174.8(3)
C(6)-C(7)-C(8)-C(9)	-1.4(5)	C(21)-C(22)-C(28)-C(31)	7.3(5)
C(6)-C(7)-C(8)-C(14)	176.8(3)	C(23)-C(22)-C(28)-C(29)	65.8(4)
C(7)-C(8)-C(9)-C(4)	4.0(5)	C(21)-C(22)-C(28)-C(29)	-112.1(4)
C(14)-C(8)-C(9)-C(4)	-174.3(3)	C(23)-C(22)-C(28)-C(30)	-54.6(4)
C(5)-C(4)-C(9)-C(8)	-3.6(5)	C(21)-C(22)-C(28)-C(30)	127.5(4)
N(2)-C(4)-C(9)-C(8)	175.2(3)	Zr(01)-O(3)-C(32)-C(33)	136.2(9)
C(7)-C(6)-C(10)-C(13)	1.7(5)	Zr(01)-O(3)-C(32)-C(34)	-99.9(11)
C(5)-C(6)-C(10)-C(13)	-179.3(3)	Zr(01)-O(4)-C(35)-C(37)	-50.8(6)
C(7)-C(6)-C(10)-C(12)	-117.4(4)	Zr(01)-O(4)-C(35)-C(36)	73.5(6)
C(5)-C(6)-C(10)-C(12)	61.7(4)	C(41)-O(5)-C(38)-C(39)	18.5(6)
C(7)-C(6)-C(10)-C(11)	120.8(4)	Zr(01)-O(5)-C(38)-C(39)	-148.7(4)
C(5)-C(6)-C(10)-C(11)	-60.1(4)	O(5)-C(38)-C(39)-C(40)	-33.9(6)
C(7)-C(8)-C(14)-C(16)	118.2(4)	C(38)-C(39)-C(40)-C(41)	35.0(6)
C(9)-C(8)-C(14)-C(16)	-63.6(4)	C(38)-O(5)-C(41)-C(40)	3.7(7)
C(7)-C(8)-C(14)-C(15)	-2.7(5)	Zr(01)-O(5)-C(41)-C(40)	172.3(3)
C(9)-C(8)-C(14)-C(15)	175.5(3)	C(39)-C(40)-C(41)-O(5)	-24.6(7)
C(7)-C(8)-C(14)-C(17)	-121.6(4)	C(42)-C(43)-C(44)-C(45)	175.0(5)
C(9)-C(8)-C(14)-C(17)	56.6(4)	C(43)-C(44)-C(45)-C(46)	180.0(5)

Symmetry transformations used to generate equivalent atoms:

Table S4. Bond lengths [Å] and angles [°] for **4**.

Zr(1)-O(1)	2.006(3)	C(14)-C(16A)	1.510(10)
Zr(1)-O(4)	2.015(3)	C(14)-C(17)	1.514(7)
Zr(1)-O(3)	2.021(3)	C(14)-C(15)	1.517(7)
Zr(1)-O(2)	2.036(3)	C(14)-C(16)	1.569(6)
Zr(1)-C(32)	2.351(4)	C(14)-C(17A)	1.592(10)
Zr(1)-C(1)	2.352(4)	C(15)-H(15A)	0.9800
O(1)-C(5)	1.339(5)	C(15)-H(15B)	0.9800
N(1)-C(1)	1.370(5)	C(15)-H(15C)	0.9800
N(1)-C(2)	1.385(5)	C(16)-H(16A)	0.9800
N(1)-C(18)	1.435(5)	C(16)-H(16B)	0.9800
C(1)-N(2)	1.370(5)	C(16)-H(16C)	0.9800
O(2)-C(19)	1.337(5)	C(17)-H(17A)	0.9800
N(2)-C(3)	1.388(5)	C(17)-H(17B)	0.9800
N(2)-C(4)	1.433(5)	C(17)-H(17C)	0.9800
C(2)-C(3)	1.334(5)	C(15A)-H(15D)	0.9800
C(2)-H(2)	0.9500	C(15A)-H(15E)	0.9800
O(3)-C(36)	1.339(5)	C(15A)-H(15F)	0.9800
N(3)-C(32)	1.361(5)	C(16A)-H(16D)	0.9800
N(3)-C(33)	1.381(5)	C(16A)-H(16E)	0.9800
N(3)-C(49)	1.440(5)	C(16A)-H(16F)	0.9800
C(3)-H(3)	0.9500	C(17A)-H(17D)	0.9800
O(4)-C(50)	1.339(5)	C(17A)-H(17E)	0.9800
N(4)-C(32)	1.361(5)	C(17A)-H(17F)	0.9800
N(4)-C(34)	1.389(5)	C(18)-C(23)	1.375(6)
N(4)-C(35)	1.431(5)	C(18)-C(19)	1.399(5)
C(4)-C(9)	1.391(5)	C(19)-C(20)	1.419(6)
C(4)-C(5)	1.402(5)	C(20)-C(21)	1.371(6)
C(5)-C(6)	1.412(6)	C(20)-C(24)	1.544(6)
C(6)-C(7)	1.380(6)	C(21)-C(22)	1.386(6)
C(6)-C(10)	1.538(6)	C(21)-H(21)	0.9500
C(7)-C(8)	1.395(6)	C(22)-C(23)	1.384(6)
C(7)-H(7)	0.9500	C(22)-C(28)	1.522(7)
C(8)-C(9)	1.384(5)	C(23)-H(23)	0.9500
C(8)-C(14)	1.527(6)	C(24)-C(26)	1.527(7)
C(9)-H(9)	0.9500	C(24)-C(27)	1.535(6)
C(10)-C(13)	1.518(9)	C(24)-C(25)	1.540(6)
C(10)-C(11)	1.543(7)	C(25)-H(25A)	0.9800
C(10)-C(12)	1.545(8)	C(25)-H(25B)	0.9800
C(11)-H(11A)	0.9800	C(25)-H(25C)	0.9800
C(11)-H(11B)	0.9800	C(26)-H(26A)	0.9800
C(11)-H(11C)	0.9800	C(26)-H(26B)	0.9800
C(12)-H(12A)	0.9800	C(26)-H(26C)	0.9800
C(12)-H(12B)	0.9800	C(27)-H(27A)	0.9800
C(12)-H(12C)	0.9800	C(27)-H(27B)	0.9800
C(13)-H(13A)	0.9800	C(27)-H(27C)	0.9800
C(13)-H(13B)	0.9800	C(28)-C(30)	1.533(10)
C(13)-H(13C)	0.9800	C(28)-C(31)	1.534(9)
C(14)-C(15A)	1.483(11)	C(28)-C(29)	1.535(7)

C(29)-H(29A)	0.9800	C(52)-H(52)	0.9500
C(29)-H(29B)	0.9800	C(53)-C(54)	1.382(6)
C(29)-H(29C)	0.9800	C(53)-C(59)	1.530(7)
C(30)-H(30A)	0.9800	C(54)-H(54)	0.9500
C(30)-H(30B)	0.9800	C(55)-C(57)	1.531(8)
C(30)-H(30C)	0.9800	C(55)-C(56)	1.532(6)
C(31)-H(31A)	0.9800	C(55)-C(58)	1.540(6)
C(31)-H(31B)	0.9800	C(56)-H(56A)	0.9800
C(31)-H(31C)	0.9800	C(56)-H(56B)	0.9800
C(33)-C(34)	1.326(5)	C(56)-H(56C)	0.9800
C(33)-H(33)	0.9500	C(57)-H(57A)	0.9800
C(34)-H(34)	0.9500	C(57)-H(57B)	0.9800
C(35)-C(40)	1.393(5)	C(57)-H(57C)	0.9800
C(35)-C(36)	1.393(6)	C(58)-H(58A)	0.9800
C(36)-C(37)	1.410(6)	C(58)-H(58B)	0.9800
C(37)-C(38)	1.390(6)	C(58)-H(58C)	0.9800
C(37)-C(41)	1.545(6)	C(59)-C(61)	1.449(9)
C(38)-C(39)	1.391(6)	C(59)-C(62)	1.524(7)
C(38)-H(38)	0.9500	C(59)-C(60)	1.558(8)
C(39)-C(40)	1.372(6)	C(60)-H(60A)	0.9800
C(39)-C(45)	1.536(6)	C(60)-H(60B)	0.9800
C(40)-H(40)	0.9500	C(60)-H(60C)	0.9800
C(41)-C(44)	1.526(7)	C(61)-H(61A)	0.9800
C(41)-C(42)	1.533(6)	C(61)-H(61B)	0.9800
C(41)-C(43)	1.535(7)	C(61)-H(61C)	0.9800
C(42)-H(42A)	0.9800	C(62)-H(62A)	0.9800
C(42)-H(42B)	0.9800	C(62)-H(62B)	0.9800
C(42)-H(42C)	0.9800	C(62)-H(62C)	0.9800
C(43)-H(43A)	0.9800	C(1SA)-C(2SA)	1.3900
C(43)-H(43B)	0.9800	C(1SA)-C(6SA)	1.3900
C(43)-H(43C)	0.9800	C(1SA)-C(7SA)	1.511(11)
C(44)-H(44A)	0.9800	C(2SA)-C(3SA)	1.3900
C(44)-H(44B)	0.9800	C(2SA)-H(2SA)	0.9500
C(44)-H(44C)	0.9800	C(3SA)-C(4SA)	1.3900
C(45)-C(46)	1.503(6)	C(3SA)-H(3SA)	0.9500
C(45)-C(48)	1.513(7)	C(4SA)-C(5SA)	1.3900
C(45)-C(47)	1.534(7)	C(4SA)-H(4SA)	0.9500
C(46)-H(46A)	0.9800	C(5SA)-C(6SA)	1.3900
C(46)-H(46B)	0.9800	C(5SA)-H(5SA)	0.9500
C(46)-H(46C)	0.9800	C(6SA)-H(6SA)	0.9500
C(47)-H(47A)	0.9800	C(7SA)-H(7S1)	0.9800
C(47)-H(47B)	0.9800	C(7SA)-H(7S2)	0.9800
C(47)-H(47C)	0.9800	C(7SA)-H(7S3)	0.9800
C(48)-H(48A)	0.9800	C(1SB)-C(2SB)	1.3900
C(48)-H(48B)	0.9800	C(1SB)-C(6SB)	1.3900
C(48)-H(48C)	0.9800	C(1SB)-C(7SB)	1.501(12)
C(49)-C(54)	1.381(6)	C(2SB)-C(3SB)	1.3900
C(49)-C(50)	1.403(5)	C(2SB)-H(2SB)	0.9500
C(50)-C(51)	1.410(6)	C(3SB)-C(4SB)	1.3900
C(51)-C(52)	1.389(6)	C(3SB)-H(3SB)	0.9500
C(51)-C(55)	1.554(6)	C(4SB)-C(5SB)	1.3900
C(52)-C(53)	1.380(6)	C(4SB)-H(4SB)	0.9500

C(5SB)-C(6SB)	1.3900	C(4)-C(5)-C(6)	118.6(4)
C(5SB)-H(5SB)	0.9500	C(7)-C(6)-C(5)	118.2(4)
C(6SB)-H(6SB)	0.9500	C(7)-C(6)-C(10)	121.4(4)
C(7SB)-H(7S4)	0.9800	C(5)-C(6)-C(10)	120.4(4)
C(7SB)-H(7S5)	0.9800	C(6)-C(7)-C(8)	124.2(4)
C(7SB)-H(7S6)	0.9800	C(6)-C(7)-H(7)	117.9
		C(8)-C(7)-H(7)	117.9
O(1)-Zr(1)-O(4)	93.46(13)	C(9)-C(8)-C(7)	116.6(4)
O(1)-Zr(1)-O(3)	111.97(11)	C(9)-C(8)-C(14)	123.2(4)
O(4)-Zr(1)-O(3)	139.70(11)	C(7)-C(8)-C(14)	120.2(4)
O(1)-Zr(1)-O(2)	142.81(11)	C(8)-C(9)-C(4)	121.4(4)
O(4)-Zr(1)-O(2)	87.22(12)	C(8)-C(9)-H(9)	119.3
O(3)-Zr(1)-O(2)	89.95(11)	C(4)-C(9)-H(9)	119.3
O(1)-Zr(1)-C(32)	87.25(12)	C(13)-C(10)-C(6)	110.1(5)
O(4)-Zr(1)-C(32)	75.51(12)	C(13)-C(10)-C(11)	108.6(5)
O(3)-Zr(1)-C(32)	75.11(12)	C(6)-C(10)-C(11)	111.0(4)
O(2)-Zr(1)-C(32)	128.48(12)	C(13)-C(10)-C(12)	111.9(5)
O(1)-Zr(1)-C(1)	74.21(12)	C(6)-C(10)-C(12)	108.4(4)
O(4)-Zr(1)-C(1)	127.97(12)	C(11)-C(10)-C(12)	106.7(5)
O(3)-Zr(1)-C(1)	89.96(12)	C(10)-C(11)-H(11A)	109.5
O(2)-Zr(1)-C(1)	76.24(12)	C(10)-C(11)-H(11B)	109.5
C(32)-Zr(1)-C(1)	149.99(13)	H(11A)-C(11)-H(11B)	109.5
C(5)-O(1)-Zr(1)	147.1(3)	C(10)-C(11)-H(11C)	109.5
C(1)-N(1)-C(2)	110.3(3)	H(11A)-C(11)-H(11C)	109.5
C(1)-N(1)-C(18)	125.6(3)	H(11B)-C(11)-H(11C)	109.5
C(2)-N(1)-C(18)	123.9(3)	C(10)-C(12)-H(12A)	109.5
N(1)-C(1)-N(2)	104.6(3)	C(10)-C(12)-H(12B)	109.5
N(1)-C(1)-Zr(1)	126.1(3)	H(12A)-C(12)-H(12B)	109.5
N(2)-C(1)-Zr(1)	128.7(3)	C(10)-C(12)-H(12C)	109.5
C(19)-O(2)-Zr(1)	138.5(2)	H(12A)-C(12)-H(12C)	109.5
C(1)-N(2)-C(3)	110.1(3)	H(12B)-C(12)-H(12C)	109.5
C(1)-N(2)-C(4)	126.2(3)	C(10)-C(13)-H(13A)	109.5
C(3)-N(2)-C(4)	123.7(3)	C(10)-C(13)-H(13B)	109.5
C(3)-C(2)-N(1)	107.5(3)	H(13A)-C(13)-H(13B)	109.5
C(3)-C(2)-H(2)	126.3	C(10)-C(13)-H(13C)	109.5
N(1)-C(2)-H(2)	126.3	H(13A)-C(13)-H(13C)	109.5
C(36)-O(3)-Zr(1)	142.3(3)	H(13B)-C(13)-H(13C)	109.5
C(32)-N(3)-C(33)	110.5(3)	C(15A)-C(14)-C(16A)	113.7(8)
C(32)-N(3)-C(49)	125.2(3)	C(17)-C(14)-C(15)	110.5(4)
C(33)-N(3)-C(49)	124.2(3)	C(15A)-C(14)-C(8)	109.5(7)
C(2)-C(3)-N(2)	107.5(3)	C(16A)-C(14)-C(8)	114.0(7)
C(2)-C(3)-H(3)	126.3	C(17)-C(14)-C(8)	109.2(4)
N(2)-C(3)-H(3)	126.3	C(15)-C(14)-C(8)	113.1(4)
C(50)-O(4)-Zr(1)	140.8(3)	C(17)-C(14)-C(16)	107.8(4)
C(32)-N(4)-C(34)	110.5(3)	C(15)-C(14)-C(16)	106.3(4)
C(32)-N(4)-C(35)	125.5(3)	C(8)-C(14)-C(16)	109.8(4)
C(34)-N(4)-C(35)	124.0(3)	C(15A)-C(14)-C(17A)	107.9(7)
C(9)-C(4)-C(5)	120.9(4)	C(16A)-C(14)-C(17A)	105.5(7)
C(9)-C(4)-N(2)	119.0(3)	C(8)-C(14)-C(17A)	105.8(6)
C(5)-C(4)-N(2)	120.1(3)	C(14)-C(15)-H(15A)	109.5
O(1)-C(5)-C(4)	120.4(4)	C(14)-C(15)-H(15B)	109.5
O(1)-C(5)-C(6)	121.0(4)	H(15A)-C(15)-H(15B)	109.5

C(14)-C(15)-H(15C)	109.5	C(26)-C(24)-C(25)	110.9(4)
H(15A)-C(15)-H(15C)	109.5	C(27)-C(24)-C(25)	107.3(4)
H(15B)-C(15)-H(15C)	109.5	C(26)-C(24)-C(20)	109.8(4)
C(14)-C(16)-H(16A)	109.5	C(27)-C(24)-C(20)	111.4(4)
C(14)-C(16)-H(16B)	109.5	C(25)-C(24)-C(20)	109.8(3)
H(16A)-C(16)-H(16B)	109.5	C(24)-C(25)-H(25A)	109.5
C(14)-C(16)-H(16C)	109.5	C(24)-C(25)-H(25B)	109.5
H(16A)-C(16)-H(16C)	109.5	H(25A)-C(25)-H(25B)	109.5
H(16B)-C(16)-H(16C)	109.5	C(24)-C(25)-H(25C)	109.5
C(14)-C(17)-H(17A)	109.5	H(25A)-C(25)-H(25C)	109.5
C(14)-C(17)-H(17B)	109.5	H(25B)-C(25)-H(25C)	109.5
H(17A)-C(17)-H(17B)	109.5	C(24)-C(26)-H(26A)	109.5
C(14)-C(17)-H(17C)	109.5	C(24)-C(26)-H(26B)	109.5
H(17A)-C(17)-H(17C)	109.5	H(26A)-C(26)-H(26B)	109.5
H(17B)-C(17)-H(17C)	109.5	C(24)-C(26)-H(26C)	109.5
C(14)-C(15A)-H(15D)	109.5	H(26A)-C(26)-H(26C)	109.5
C(14)-C(15A)-H(15E)	109.5	H(26B)-C(26)-H(26C)	109.5
H(15D)-C(15A)-H(15E)	109.5	C(24)-C(27)-H(27A)	109.5
C(14)-C(15A)-H(15F)	109.5	C(24)-C(27)-H(27B)	109.5
H(15D)-C(15A)-H(15F)	109.5	H(27A)-C(27)-H(27B)	109.5
H(15E)-C(15A)-H(15F)	109.5	C(24)-C(27)-H(27C)	109.5
C(14)-C(16A)-H(16D)	109.5	H(27A)-C(27)-H(27C)	109.5
C(14)-C(16A)-H(16E)	109.5	H(27B)-C(27)-H(27C)	109.5
H(16D)-C(16A)-H(16E)	109.5	C(22)-C(28)-C(30)	108.3(6)
C(14)-C(16A)-H(16F)	109.5	C(22)-C(28)-C(31)	109.9(5)
H(16D)-C(16A)-H(16F)	109.5	C(30)-C(28)-C(31)	111.6(6)
H(16E)-C(16A)-H(16F)	109.5	C(22)-C(28)-C(29)	111.8(4)
C(14)-C(17A)-H(17D)	109.5	C(30)-C(28)-C(29)	109.5(5)
C(14)-C(17A)-H(17E)	109.5	C(31)-C(28)-C(29)	105.9(6)
H(17D)-C(17A)-H(17E)	109.5	C(28)-C(29)-H(29A)	109.5
C(14)-C(17A)-H(17F)	109.5	C(28)-C(29)-H(29B)	109.5
H(17D)-C(17A)-H(17F)	109.5	H(29A)-C(29)-H(29B)	109.5
H(17E)-C(17A)-H(17F)	109.5	C(28)-C(29)-H(29C)	109.5
C(23)-C(18)-C(19)	120.9(4)	H(29A)-C(29)-H(29C)	109.5
C(23)-C(18)-N(1)	118.0(3)	H(29B)-C(29)-H(29C)	109.5
C(19)-C(18)-N(1)	121.1(4)	C(28)-C(30)-H(30A)	109.5
O(2)-C(19)-C(18)	120.7(4)	C(28)-C(30)-H(30B)	109.5
O(2)-C(19)-C(20)	120.9(4)	H(30A)-C(30)-H(30B)	109.5
C(18)-C(19)-C(20)	118.4(4)	C(28)-C(30)-H(30C)	109.5
C(21)-C(20)-C(19)	118.0(4)	H(30A)-C(30)-H(30C)	109.5
C(21)-C(20)-C(24)	121.4(4)	H(30B)-C(30)-H(30C)	109.5
C(19)-C(20)-C(24)	120.5(4)	C(28)-C(31)-H(31A)	109.5
C(20)-C(21)-C(22)	124.3(4)	C(28)-C(31)-H(31B)	109.5
C(20)-C(21)-H(21)	117.9	H(31A)-C(31)-H(31B)	109.5
C(22)-C(21)-H(21)	117.9	C(28)-C(31)-H(31C)	109.5
C(23)-C(22)-C(21)	116.6(4)	H(31A)-C(31)-H(31C)	109.5
C(23)-C(22)-C(28)	122.6(4)	H(31B)-C(31)-H(31C)	109.5
C(21)-C(22)-C(28)	120.7(4)	N(3)-C(32)-N(4)	104.4(3)
C(18)-C(23)-C(22)	121.7(4)	N(3)-C(32)-Zr(1)	127.6(3)
C(18)-C(23)-H(23)	119.1	N(4)-C(32)-Zr(1)	127.3(3)
C(22)-C(23)-H(23)	119.1	C(34)-C(33)-N(3)	107.6(3)
C(26)-C(24)-C(27)	107.6(4)	C(34)-C(33)-H(33)	126.2

N(3)-C(33)-H(33)	126.2	C(45)-C(46)-H(46A)	109.5
C(33)-C(34)-N(4)	107.0(3)	C(45)-C(46)-H(46B)	109.5
C(33)-C(34)-H(34)	126.5	H(46A)-C(46)-H(46B)	109.5
N(4)-C(34)-H(34)	126.5	C(45)-C(46)-H(46C)	109.5
C(40)-C(35)-C(36)	121.1(4)	H(46A)-C(46)-H(46C)	109.5
C(40)-C(35)-N(4)	118.3(4)	H(46B)-C(46)-H(46C)	109.5
C(36)-C(35)-N(4)	120.6(3)	C(45)-C(47)-H(47A)	109.5
O(3)-C(36)-C(35)	120.4(4)	C(45)-C(47)-H(47B)	109.5
O(3)-C(36)-C(37)	120.7(4)	H(47A)-C(47)-H(47B)	109.5
C(35)-C(36)-C(37)	118.9(4)	C(45)-C(47)-H(47C)	109.5
C(38)-C(37)-C(36)	117.7(4)	H(47A)-C(47)-H(47C)	109.5
C(38)-C(37)-C(41)	121.7(4)	H(47B)-C(47)-H(47C)	109.5
C(36)-C(37)-C(41)	120.7(4)	C(45)-C(48)-H(48A)	109.5
C(37)-C(38)-C(39)	123.5(4)	C(45)-C(48)-H(48B)	109.5
C(37)-C(38)-H(38)	118.2	H(48A)-C(48)-H(48B)	109.5
C(39)-C(38)-H(38)	118.2	C(45)-C(48)-H(48C)	109.5
C(40)-C(39)-C(38)	117.7(4)	H(48A)-C(48)-H(48C)	109.5
C(40)-C(39)-C(45)	120.1(4)	H(48B)-C(48)-H(48C)	109.5
C(38)-C(39)-C(45)	122.0(4)	C(54)-C(49)-C(50)	121.3(4)
C(39)-C(40)-C(35)	120.7(4)	C(54)-C(49)-N(3)	118.4(4)
C(39)-C(40)-H(40)	119.6	C(50)-C(49)-N(3)	120.3(3)
C(35)-C(40)-H(40)	119.6	O(4)-C(50)-C(49)	120.9(4)
C(44)-C(41)-C(42)	107.1(5)	O(4)-C(50)-C(51)	121.0(4)
C(44)-C(41)-C(43)	110.0(4)	C(49)-C(50)-C(51)	118.1(4)
C(42)-C(41)-C(43)	107.9(4)	C(52)-C(51)-C(50)	118.6(4)
C(44)-C(41)-C(37)	109.8(4)	C(52)-C(51)-C(55)	121.8(4)
C(42)-C(41)-C(37)	111.9(4)	C(50)-C(51)-C(55)	119.7(4)
C(43)-C(41)-C(37)	110.2(4)	C(53)-C(52)-C(51)	123.3(4)
C(41)-C(42)-H(42A)	109.5	C(53)-C(52)-H(52)	118.4
C(41)-C(42)-H(42B)	109.5	C(51)-C(52)-H(52)	118.4
H(42A)-C(42)-H(42B)	109.5	C(52)-C(53)-C(54)	117.7(4)
C(41)-C(42)-H(42C)	109.5	C(52)-C(53)-C(59)	122.1(4)
H(42A)-C(42)-H(42C)	109.5	C(54)-C(53)-C(59)	120.1(4)
H(42B)-C(42)-H(42C)	109.5	C(49)-C(54)-C(53)	121.0(4)
C(41)-C(43)-H(43A)	109.5	C(49)-C(54)-H(54)	119.5
C(41)-C(43)-H(43B)	109.5	C(53)-C(54)-H(54)	119.5
H(43A)-C(43)-H(43B)	109.5	C(57)-C(55)-C(56)	110.8(5)
C(41)-C(43)-H(43C)	109.5	C(57)-C(55)-C(58)	108.6(4)
H(43A)-C(43)-H(43C)	109.5	C(56)-C(55)-C(58)	106.9(4)
H(43B)-C(43)-H(43C)	109.5	C(57)-C(55)-C(51)	109.3(4)
C(41)-C(44)-H(44A)	109.5	C(56)-C(55)-C(51)	110.5(4)
C(41)-C(44)-H(44B)	109.5	C(58)-C(55)-C(51)	110.7(4)
H(44A)-C(44)-H(44B)	109.5	C(55)-C(56)-H(56A)	109.5
C(41)-C(44)-H(44C)	109.5	C(55)-C(56)-H(56B)	109.5
H(44A)-C(44)-H(44C)	109.5	H(56A)-C(56)-H(56B)	109.5
H(44B)-C(44)-H(44C)	109.5	C(55)-C(56)-H(56C)	109.5
C(46)-C(45)-C(48)	109.1(5)	H(56A)-C(56)-H(56C)	109.5
C(46)-C(45)-C(47)	106.3(5)	H(56B)-C(56)-H(56C)	109.5
C(48)-C(45)-C(47)	110.5(5)	C(55)-C(57)-H(57A)	109.5
C(46)-C(45)-C(39)	111.2(4)	C(55)-C(57)-H(57B)	109.5
C(48)-C(45)-C(39)	107.9(4)	H(57A)-C(57)-H(57B)	109.5
C(47)-C(45)-C(39)	111.8(4)	C(55)-C(57)-H(57C)	109.5

H(57A)-C(57)-H(57C)	109.5	C(4SA)-C(3SA)-H(3SA)	120.0
H(57B)-C(57)-H(57C)	109.5	C(5SA)-C(4SA)-C(3SA)	120.0
C(55)-C(58)-H(58A)	109.5	C(5SA)-C(4SA)-H(4SA)	120.0
C(55)-C(58)-H(58B)	109.5	C(3SA)-C(4SA)-H(4SA)	120.0
H(58A)-C(58)-H(58B)	109.5	C(6SA)-C(5SA)-C(4SA)	120.0
C(55)-C(58)-H(58C)	109.5	C(6SA)-C(5SA)-H(5SA)	120.0
H(58A)-C(58)-H(58C)	109.5	C(4SA)-C(5SA)-H(5SA)	120.0
H(58B)-C(58)-H(58C)	109.5	C(5SA)-C(6SA)-C(1SA)	120.0
C(61)-C(59)-C(62)	111.1(5)	C(5SA)-C(6SA)-H(6SA)	120.0
C(61)-C(59)-C(53)	110.5(5)	C(1SA)-C(6SA)-H(6SA)	120.0
C(62)-C(59)-C(53)	109.7(4)	C(1SA)-C(7SA)-H(7S1)	109.5
C(61)-C(59)-C(60)	111.9(6)	C(1SA)-C(7SA)-H(7S2)	109.5
C(62)-C(59)-C(60)	103.1(5)	H(7S1)-C(7SA)-H(7S2)	109.5
C(53)-C(59)-C(60)	110.2(5)	C(1SA)-C(7SA)-H(7S3)	109.5
C(59)-C(60)-H(60A)	109.5	H(7S1)-C(7SA)-H(7S3)	109.5
C(59)-C(60)-H(60B)	109.5	H(7S2)-C(7SA)-H(7S3)	109.5
H(60A)-C(60)-H(60B)	109.5	C(2SB)-C(1SB)-C(6SB)	120.0
C(59)-C(60)-H(60C)	109.5	C(2SB)-C(1SB)-C(7SB)	120.5(9)
H(60A)-C(60)-H(60C)	109.5	C(6SB)-C(1SB)-C(7SB)	119.5(9)
H(60B)-C(60)-H(60C)	109.5	C(3SB)-C(2SB)-C(1SB)	120.0
C(59)-C(61)-H(61A)	109.5	C(3SB)-C(2SB)-H(2SB)	120.0
C(59)-C(61)-H(61B)	109.5	C(1SB)-C(2SB)-H(2SB)	120.0
H(61A)-C(61)-H(61B)	109.5	C(2SB)-C(3SB)-C(4SB)	120.0
C(59)-C(61)-H(61C)	109.5	C(2SB)-C(3SB)-H(3SB)	120.0
H(61A)-C(61)-H(61C)	109.5	C(4SB)-C(3SB)-H(3SB)	120.0
H(61B)-C(61)-H(61C)	109.5	C(3SB)-C(4SB)-C(5SB)	120.0
C(59)-C(62)-H(62A)	109.5	C(3SB)-C(4SB)-H(4SB)	120.0
C(59)-C(62)-H(62B)	109.5	C(5SB)-C(4SB)-H(4SB)	120.0
H(62A)-C(62)-H(62B)	109.5	C(4SB)-C(5SB)-C(6SB)	120.0
C(59)-C(62)-H(62C)	109.5	C(4SB)-C(5SB)-H(5SB)	120.0
H(62A)-C(62)-H(62C)	109.5	C(6SB)-C(5SB)-H(5SB)	120.0
H(62B)-C(62)-H(62C)	109.5	C(5SB)-C(6SB)-C(1SB)	120.0
C(2SA)-C(1SA)-C(6SA)	120.0	C(5SB)-C(6SB)-H(6SB)	120.0
C(2SA)-C(1SA)-C(7SA)	120.1(8)	C(1SB)-C(6SB)-H(6SB)	120.0
C(6SA)-C(1SA)-C(7SA)	119.7(8)	C(1SB)-C(7SB)-H(7S4)	109.5
C(3SA)-C(2SA)-C(1SA)	120.0	C(1SB)-C(7SB)-H(7S5)	109.5
C(3SA)-C(2SA)-H(2SA)	120.0	H(7S4)-C(7SB)-H(7S5)	109.5
C(1SA)-C(2SA)-H(2SA)	120.0	C(1SB)-C(7SB)-H(7S6)	109.5
C(2SA)-C(3SA)-C(4SA)	120.0	H(7S4)-C(7SB)-H(7S6)	109.5
C(2SA)-C(3SA)-H(3SA)	120.0	H(7S5)-C(7SB)-H(7S6)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S5. Torsion angles [°] for **4**.

C(2)-N(1)-C(1)-N(2)	-1.0(4)	Zr(1)-C(1)-N(2)-C(3)	-170.8(3)
C(18)-N(1)-C(1)-N(2)	174.3(3)	N(1)-C(1)-N(2)-C(4)	-179.8(3)
C(2)-N(1)-C(1)-Zr(1)	170.8(3)	Zr(1)-C(1)-N(2)-C(4)	8.7(5)
C(18)-N(1)-C(1)-Zr(1)	-13.9(5)	C(1)-N(1)-C(2)-C(3)	0.9(4)
N(1)-C(1)-N(2)-C(3)	0.7(4)	C(18)-N(1)-C(2)-C(3)	-174.5(3)

N(1)-C(2)-C(3)-N(2)	-0.4(4)
C(1)-N(2)-C(3)-C(2)	-0.2(4)
C(4)-N(2)-C(3)-C(2)	-179.8(3)
C(1)-N(2)-C(4)-C(9)	164.6(4)
C(3)-N(2)-C(4)-C(9)	-16.0(5)
C(1)-N(2)-C(4)-C(5)	-15.0(5)
C(3)-N(2)-C(4)-C(5)	164.5(4)
Zr(1)-O(1)-C(5)-C(4)	19.8(7)
Zr(1)-O(1)-C(5)-C(6)	-159.5(4)
C(9)-C(4)-C(5)-O(1)	-175.3(4)
N(2)-C(4)-C(5)-O(1)	4.3(6)
C(9)-C(4)-C(5)-C(6)	4.1(6)
N(2)-C(4)-C(5)-C(6)	-176.4(4)
O(1)-C(5)-C(6)-C(7)	176.2(4)
C(4)-C(5)-C(6)-C(7)	-3.2(6)
O(1)-C(5)-C(6)-C(10)	-2.8(7)
C(4)-C(5)-C(6)-C(10)	177.9(4)
C(5)-C(6)-C(7)-C(8)	0.0(7)
C(10)-C(6)-C(7)-C(8)	179.0(5)
C(6)-C(7)-C(8)-C(9)	2.2(6)
C(6)-C(7)-C(8)-C(14)	-175.1(4)
C(7)-C(8)-C(9)-C(4)	-1.3(6)
C(14)-C(8)-C(9)-C(4)	175.9(4)
C(5)-C(4)-C(9)-C(8)	-1.8(6)
N(2)-C(4)-C(9)-C(8)	178.7(3)
C(7)-C(6)-C(10)-C(13)	122.7(5)
C(5)-C(6)-C(10)-C(13)	-58.4(6)
C(7)-C(6)-C(10)-C(11)	2.3(8)
C(5)-C(6)-C(10)-C(11)	-178.7(5)
C(7)-C(6)-C(10)-C(12)	-114.6(5)
C(5)-C(6)-C(10)-C(12)	64.3(7)
C(9)-C(8)-C(14)-C(15A)	63.1(8)
C(7)-C(8)-C(14)-C(15A)	-119.8(7)
C(9)-C(8)-C(14)-C(16A)	-168.3(8)
C(7)-C(8)-C(14)-C(16A)	8.8(9)
C(9)-C(8)-C(14)-C(17)	-113.0(5)
C(7)-C(8)-C(14)-C(17)	64.1(5)
C(9)-C(8)-C(14)-C(15)	10.5(6)
C(7)-C(8)-C(14)-C(15)	-172.4(4)
C(9)-C(8)-C(14)-C(16)	129.0(4)
C(7)-C(8)-C(14)-C(16)	-53.8(5)
C(9)-C(8)-C(14)-C(17A)	-52.9(7)
C(7)-C(8)-C(14)-C(17A)	124.2(7)
C(1)-N(1)-C(18)-C(23)	-157.1(4)
C(2)-N(1)-C(18)-C(23)	17.5(6)
C(1)-N(1)-C(18)-C(19)	23.2(6)
C(2)-N(1)-C(18)-C(19)	-162.1(4)
Zr(1)-O(2)-C(19)-C(18)	-39.9(6)
Zr(1)-O(2)-C(19)-C(20)	141.5(3)
C(23)-C(18)-C(19)-O(2)	179.9(4)
N(1)-C(18)-C(19)-O(2)	-0.4(6)
C(23)-C(18)-C(19)-C(20)	-1.4(6)
N(1)-C(18)-C(19)-C(20)	178.2(3)
O(2)-C(19)-C(20)-C(21)	179.1(4)
C(18)-C(19)-C(20)-C(21)	0.4(6)
O(2)-C(19)-C(20)-C(24)	0.0(6)
C(18)-C(19)-C(20)-C(24)	-178.6(4)
C(19)-C(20)-C(21)-C(22)	-0.1(7)
C(24)-C(20)-C(21)-C(22)	178.9(4)
C(20)-C(21)-C(22)-C(23)	0.7(7)
C(20)-C(21)-C(22)-C(28)	178.2(5)
C(19)-C(18)-C(23)-C(22)	2.1(7)
N(1)-C(18)-C(23)-C(22)	-177.5(4)
C(21)-C(22)-C(23)-C(18)	-1.7(7)
C(28)-C(22)-C(23)-C(18)	-179.1(5)
C(21)-C(20)-C(24)-C(26)	-118.3(5)
C(19)-C(20)-C(24)-C(26)	60.7(5)
C(21)-C(20)-C(24)-C(27)	0.8(6)
C(19)-C(20)-C(24)-C(27)	179.8(4)
C(21)-C(20)-C(24)-C(25)	119.5(5)
C(19)-C(20)-C(24)-C(25)	-61.4(5)
C(23)-C(22)-C(28)-C(30)	92.7(6)
C(21)-C(22)-C(28)-C(30)	-84.6(6)
C(23)-C(22)-C(28)-C(31)	-29.3(8)
C(21)-C(22)-C(28)-C(31)	153.4(6)
C(23)-C(22)-C(28)-C(29)	-146.6(5)
C(21)-C(22)-C(28)-C(29)	36.1(8)
C(33)-N(3)-C(32)-N(4)	-0.7(4)
C(49)-N(3)-C(32)-N(4)	174.6(3)
C(33)-N(3)-C(32)-Zr(1)	169.7(3)
C(49)-N(3)-C(32)-Zr(1)	-15.0(5)
C(34)-N(4)-C(32)-N(3)	0.5(4)
C(35)-N(4)-C(32)-N(3)	-179.4(3)
C(34)-N(4)-C(32)-Zr(1)	-169.9(3)
C(35)-N(4)-C(32)-Zr(1)	10.2(5)
C(32)-N(3)-C(33)-C(34)	0.7(4)
C(49)-N(3)-C(33)-C(34)	-174.7(3)
N(3)-C(33)-C(34)-N(4)	-0.3(4)
C(32)-N(4)-C(34)-C(33)	-0.1(4)
C(35)-N(4)-C(34)-C(33)	179.8(3)
C(32)-N(4)-C(35)-C(40)	158.0(4)
C(34)-N(4)-C(35)-C(40)	-21.8(6)
C(32)-N(4)-C(35)-C(36)	-24.4(6)
C(34)-N(4)-C(35)-C(36)	155.7(4)
Zr(1)-O(3)-C(36)-C(35)	28.6(6)
Zr(1)-O(3)-C(36)-C(37)	-152.0(3)
C(40)-C(35)-C(36)-O(3)	-173.3(4)
N(4)-C(35)-C(36)-O(3)	9.2(6)
C(40)-C(35)-C(36)-C(37)	7.3(6)
N(4)-C(35)-C(36)-C(37)	-170.2(4)
O(3)-C(36)-C(37)-C(38)	174.7(4)
C(35)-C(36)-C(37)-C(38)	-5.9(6)
O(3)-C(36)-C(37)-C(41)	-5.5(6)
C(35)-C(36)-C(37)-C(41)	173.9(4)

C(36)-C(37)-C(38)-C(39)	1.1(7)	C(55)-C(51)-C(52)-C(53)	179.2(4)
C(41)-C(37)-C(38)-C(39)	-178.8(4)	C(51)-C(52)-C(53)-C(54)	-0.6(7)
C(37)-C(38)-C(39)-C(40)	2.7(7)	C(51)-C(52)-C(53)-C(59)	-178.7(4)
C(37)-C(38)-C(39)-C(45)	-173.0(4)	C(50)-C(49)-C(54)-C(53)	0.9(6)
C(38)-C(39)-C(40)-C(35)	-1.4(6)	N(3)-C(49)-C(54)-C(53)	-179.7(4)
C(45)-C(39)-C(40)-C(35)	174.4(4)	C(52)-C(53)-C(54)-C(49)	0.0(6)
C(36)-C(35)-C(40)-C(39)	-3.6(6)	C(59)-C(53)-C(54)-C(49)	178.2(4)
N(4)-C(35)-C(40)-C(39)	174.0(4)	C(52)-C(51)-C(55)-C(57)	-116.6(5)
C(38)-C(37)-C(41)-C(44)	123.1(5)	C(50)-C(51)-C(55)-C(57)	62.3(5)
C(36)-C(37)-C(41)-C(44)	-56.8(6)	C(52)-C(51)-C(55)-C(56)	121.2(5)
C(38)-C(37)-C(41)-C(42)	4.4(7)	C(50)-C(51)-C(55)-C(56)	-59.9(6)
C(36)-C(37)-C(41)-C(42)	-175.5(5)	C(52)-C(51)-C(55)-C(58)	2.9(6)
C(38)-C(37)-C(41)-C(43)	-115.6(5)	C(50)-C(51)-C(55)-C(58)	-178.2(4)
C(36)-C(37)-C(41)-C(43)	64.5(5)	C(52)-C(53)-C(59)-C(61)	111.8(6)
C(40)-C(39)-C(45)-C(46)	36.5(6)	C(54)-C(53)-C(59)-C(61)	-66.3(6)
C(38)-C(39)-C(45)-C(46)	-147.9(5)	C(52)-C(53)-C(59)-C(62)	-125.3(5)
C(40)-C(39)-C(45)-C(48)	-83.0(6)	C(54)-C(53)-C(59)-C(62)	56.6(7)
C(38)-C(39)-C(45)-C(48)	92.6(6)	C(52)-C(53)-C(59)-C(60)	-12.4(7)
C(40)-C(39)-C(45)-C(47)	155.2(5)	C(54)-C(53)-C(59)-C(60)	169.5(5)
C(38)-C(39)-C(45)-C(47)	-29.2(7)	C(6SA)-C(1SA)-C(2SA)-C(3SA)	0.0
C(32)-N(3)-C(49)-C(54)	-157.9(4)	C(7SA)-C(1SA)-C(2SA)-C(3SA)	174.9(9)
C(33)-N(3)-C(49)-C(54)	16.8(5)	C(1SA)-C(2SA)-C(3SA)-C(4SA)	0.0
C(32)-N(3)-C(49)-C(50)	21.4(6)	C(2SA)-C(3SA)-C(4SA)-C(5SA)	0.0
C(33)-N(3)-C(49)-C(50)	-163.8(4)	C(3SA)-C(4SA)-C(5SA)-C(6SA)	0.0
Zr(1)-O(4)-C(50)-C(49)	-37.6(6)	C(4SA)-C(5SA)-C(6SA)-C(1SA)	0.0
Zr(1)-O(4)-C(50)-C(51)	143.3(4)	C(2SA)-C(1SA)-C(6SA)-C(5SA)	0.0
C(54)-C(49)-C(50)-O(4)	179.6(4)	C(7SA)-C(1SA)-C(6SA)-C(5SA)	-174.9(9)
N(3)-C(49)-C(50)-O(4)	0.2(6)	C(6SB)-C(1SB)-C(2SB)-C(3SB)	0.0
C(54)-C(49)-C(50)-C(51)	-1.3(6)	C(7SB)-C(1SB)-C(2SB)-C(3SB)	-178.7(9)
N(3)-C(49)-C(50)-C(51)	179.4(3)	C(1SB)-C(2SB)-C(3SB)-C(4SB)	0.0
O(4)-C(50)-C(51)-C(52)	179.8(4)	C(2SB)-C(3SB)-C(4SB)-C(5SB)	0.0
C(49)-C(50)-C(51)-C(52)	0.7(6)	C(3SB)-C(4SB)-C(5SB)-C(6SB)	0.0
O(4)-C(50)-C(51)-C(55)	0.9(6)	C(4SB)-C(5SB)-C(6SB)-C(1SB)	0.0
C(49)-C(50)-C(51)-C(55)	-178.3(4)	C(2SB)-C(1SB)-C(6SB)-C(5SB)	0.0
C(50)-C(51)-C(52)-C(53)	0.2(6)	C(7SB)-C(1SB)-C(6SB)-C(5SB)	178.7(9)

Symmetry transformations used to generate equivalent atoms:

Table S6. Bond lengths [Å] and angles [°] for **5**.

Zr(1)-O(4)	2.010(3)	O(2)-C(23)	1.331(5)
Zr(1)-O(2)	2.020(3)	N(2)-C(21)	1.399(6)
Zr(1)-O(3)	2.021(3)	N(2)-C(22)	1.441(5)
Zr(1)-O(1)	2.028(3)	C(2)-C(7)	1.386(6)
Zr(1)-C(1)	2.393(4)	C(2)-C(3)	1.395(6)
Zr(1)-C(36)	2.401(4)	O(3)-C(38)	1.337(5)
O(1)-C(3)	1.324(5)	N(3)-C(36)	1.352(5)
N(1)-C(1)	1.358(5)	N(3)-C(51)	1.400(6)
N(1)-C(16)	1.396(5)	N(3)-C(37)	1.435(5)
N(1)-C(2)	1.448(5)	C(3)-C(4)	1.430(6)
C(1)-N(2)	1.361(5)	O(4)-C(58)	1.325(5)

N(4)-C(36)	1.354(5)	C(26)-C(32)	1.547(9)
N(4)-C(56)	1.394(6)	C(26)-C(32A)	1.551(8)
N(4)-C(57)	1.444(6)	C(27)-H(27)	0.9500
C(4)-C(5)	1.386(6)	C(28)-C(31)	1.529(6)
C(4)-C(8)	1.544(6)	C(28)-C(29)	1.531(7)
C(5)-C(6)	1.388(7)	C(28)-C(30)	1.537(7)
C(5)-H(5)	0.9500	C(29)-H(29A)	0.9800
C(6)-C(7)	1.379(6)	C(29)-H(29B)	0.9800
C(6)-C(12)	1.531(6)	C(29)-H(29C)	0.9800
C(7)-H(7)	0.9500	C(30)-H(30A)	0.9800
C(8)-C(11)	1.519(7)	C(30)-H(30B)	0.9800
C(8)-C(9)	1.534(7)	C(30)-H(30C)	0.9800
C(8)-C(10)	1.546(7)	C(31)-H(31A)	0.9800
C(9)-H(9A)	0.9800	C(31)-H(31B)	0.9800
C(9)-H(9B)	0.9800	C(31)-H(31C)	0.9800
C(9)-H(9C)	0.9800	C(32)-C(35)	1.507(9)
C(10)-H(10A)	0.9800	C(32)-C(33)	1.509(9)
C(10)-H(10B)	0.9800	C(32)-C(34)	1.514(9)
C(10)-H(10C)	0.9800	C(33)-H(33A)	0.9800
C(11)-H(11A)	0.9800	C(33)-H(33B)	0.9800
C(11)-H(11B)	0.9800	C(33)-H(33C)	0.9800
C(11)-H(11C)	0.9800	C(34)-H(34A)	0.9800
C(12)-C(13)	1.523(8)	C(34)-H(34B)	0.9800
C(12)-C(15)	1.527(7)	C(34)-H(34C)	0.9800
C(12)-C(14)	1.533(8)	C(35)-H(35A)	0.9800
C(13)-H(13A)	0.9800	C(35)-H(35B)	0.9800
C(13)-H(13B)	0.9800	C(35)-H(35C)	0.9800
C(13)-H(13C)	0.9800	C(32A)-C(35A)	1.496(17)
C(14)-H(14A)	0.9800	C(32A)-C(34A)	1.504(16)
C(14)-H(14B)	0.9800	C(32A)-C(33A)	1.546(15)
C(14)-H(14C)	0.9800	C(33A)-H(33D)	0.9800
C(15)-H(15A)	0.9800	C(33A)-H(33E)	0.9800
C(15)-H(15B)	0.9800	C(33A)-H(33F)	0.9800
C(15)-H(15C)	0.9800	C(34A)-H(34D)	0.9800
C(16)-C(17)	1.386(6)	C(34A)-H(34E)	0.9800
C(16)-C(21)	1.402(6)	C(34A)-H(34F)	0.9800
C(17)-C(18)	1.385(6)	C(35A)-H(35D)	0.9800
C(17)-H(17)	0.9500	C(35A)-H(35E)	0.9800
C(18)-C(19)	1.388(7)	C(35A)-H(35F)	0.9800
C(18)-H(18)	0.9500	C(37)-C(42)	1.380(6)
C(19)-C(20)	1.379(7)	C(37)-C(38)	1.407(6)
C(19)-H(19)	0.9500	C(38)-C(39)	1.408(6)
C(20)-C(21)	1.402(6)	C(39)-C(40)	1.396(3)
C(20)-H(20)	0.9500	C(39)-C(43)	1.540(6)
C(22)-C(27)	1.373(6)	C(40)-C(41)	1.396(2)
C(22)-C(23)	1.404(6)	C(40)-H(40)	0.9500
C(23)-C(24)	1.411(6)	C(41)-C(42)	1.396(3)
C(24)-C(25)	1.386(7)	C(41)-C(47)	1.524(6)
C(24)-C(28)	1.542(6)	C(42)-H(42)	0.9500
C(25)-C(26)	1.389(7)	C(43)-C(46)	1.535(7)
C(25)-H(25)	0.9500	C(43)-C(44)	1.535(6)
C(26)-C(27)	1.384(7)	C(43)-C(45)	1.539(6)

C(44)-H(44A)	0.9800	C(61)-C(62)	1.397(3)
C(44)-H(44B)	0.9800	C(61)-C(67)	1.542(8)
C(44)-H(44C)	0.9800	C(62)-H(62)	0.9500
C(45)-H(45A)	0.9800	C(67)-C(70)	1.516(6)
C(45)-H(45B)	0.9800	C(67)-C(68)	1.516(6)
C(45)-H(45C)	0.9800	C(67)-C(69)	1.516(6)
C(46)-H(46A)	0.9800	C(68)-H(68A)	0.9800
C(46)-H(46B)	0.9800	C(68)-H(68B)	0.9800
C(46)-H(46C)	0.9800	C(68)-H(68C)	0.9800
C(47)-C(49)	1.506(7)	C(69)-H(69A)	0.9800
C(47)-C(48)	1.524(7)	C(69)-H(69B)	0.9800
C(47)-C(50)	1.532(8)	C(69)-H(69C)	0.9800
C(48)-H(48A)	0.9800	C(70)-H(70A)	0.9800
C(48)-H(48B)	0.9800	C(70)-H(70B)	0.9800
C(48)-H(48C)	0.9800	C(70)-H(70C)	0.9800
C(49)-H(49A)	0.9800	C(60A)-C(61A)	1.396(3)
C(49)-H(49B)	0.9800	C(60A)-H(60A)	0.9500
C(49)-H(49C)	0.9800	C(61A)-C(62A)	1.396(3)
C(50)-H(50A)	0.9800	C(61A)-C(67A)	1.542(8)
C(50)-H(50B)	0.9800	C(62A)-H(62A)	0.9500
C(50)-H(50C)	0.9800	C(67A)-C(68A)	1.516(6)
C(51)-C(56)	1.384(6)	C(67A)-C(69A)	1.516(6)
C(51)-C(52)	1.398(6)	C(67A)-C(70A)	1.516(6)
C(52)-C(53)	1.375(7)	C(68A)-H(68D)	0.9800
C(52)-H(52)	0.9500	C(68A)-H(68E)	0.9800
C(53)-C(54)	1.388(8)	C(68A)-H(68F)	0.9800
C(53)-H(53)	0.9500	C(69A)-H(69D)	0.9800
C(54)-C(55)	1.395(8)	C(69A)-H(69E)	0.9800
C(54)-H(54)	0.9500	C(69A)-H(69F)	0.9800
C(55)-C(56)	1.393(7)	C(70A)-H(70D)	0.9800
C(55)-H(55)	0.9500	C(70A)-H(70E)	0.9800
C(57)-C(62A)	1.367(12)	C(70A)-H(70F)	0.9800
C(57)-C(62)	1.397(3)		
C(57)-C(58)	1.400(6)	O(4)-Zr(1)-O(2)	100.56(12)
C(58)-C(59)	1.418(6)	O(4)-Zr(1)-O(3)	149.29(12)
C(59)-C(60A)	1.397(3)	O(2)-Zr(1)-O(3)	91.55(12)
C(59)-C(60)	1.397(3)	O(4)-Zr(1)-O(1)	91.54(12)
C(59)-C(63)	1.548(6)	O(2)-Zr(1)-O(1)	149.74(12)
C(63)-C(64)	1.525(7)	O(3)-Zr(1)-O(1)	91.90(12)
C(63)-C(66)	1.529(7)	O(4)-Zr(1)-C(1)	96.02(13)
C(63)-C(65)	1.531(7)	O(2)-Zr(1)-C(1)	75.13(13)
C(64)-H(64A)	0.9800	O(3)-Zr(1)-C(1)	114.42(13)
C(64)-H(64B)	0.9800	O(1)-Zr(1)-C(1)	76.10(13)
C(64)-H(64C)	0.9800	O(4)-Zr(1)-C(36)	75.46(13)
C(65)-H(65A)	0.9800	O(2)-Zr(1)-C(36)	94.33(13)
C(65)-H(65B)	0.9800	O(3)-Zr(1)-C(36)	75.56(13)
C(65)-H(65C)	0.9800	O(1)-Zr(1)-C(36)	115.62(13)
C(66)-H(66A)	0.9800	C(1)-Zr(1)-C(36)	165.23(14)
C(66)-H(66B)	0.9800	C(3)-O(1)-Zr(1)	140.3(3)
C(66)-H(66C)	0.9800	C(1)-N(1)-C(16)	111.5(3)
C(60)-C(61)	1.397(3)	C(1)-N(1)-C(2)	122.6(3)
C(60)-H(60)	0.9500	C(16)-N(1)-C(2)	124.9(3)

N(1)-C(1)-N(2)	105.9(4)	C(8)-C(11)-H(11B)	109.5
N(1)-C(1)-Zr(1)	122.1(3)	H(11A)-C(11)-H(11B)	109.5
N(2)-C(1)-Zr(1)	124.1(3)	C(8)-C(11)-H(11C)	109.5
C(23)-O(2)-Zr(1)	142.1(3)	H(11A)-C(11)-H(11C)	109.5
C(1)-N(2)-C(21)	110.6(3)	H(11B)-C(11)-H(11C)	109.5
C(1)-N(2)-C(22)	123.0(4)	C(13)-C(12)-C(15)	106.7(5)
C(21)-N(2)-C(22)	126.2(4)	C(13)-C(12)-C(6)	112.8(4)
C(7)-C(2)-C(3)	123.0(4)	C(15)-C(12)-C(6)	110.5(4)
C(7)-C(2)-N(1)	117.7(4)	C(13)-C(12)-C(14)	108.8(5)
C(3)-C(2)-N(1)	119.0(4)	C(15)-C(12)-C(14)	110.5(4)
C(38)-O(3)-Zr(1)	138.2(3)	C(6)-C(12)-C(14)	107.6(4)
C(36)-N(3)-C(51)	110.2(4)	C(12)-C(13)-H(13A)	109.5
C(36)-N(3)-C(37)	122.5(3)	C(12)-C(13)-H(13B)	109.5
C(51)-N(3)-C(37)	126.3(4)	H(13A)-C(13)-H(13B)	109.5
O(1)-C(3)-C(2)	121.0(4)	C(12)-C(13)-H(13C)	109.5
O(1)-C(3)-C(4)	122.2(4)	H(13A)-C(13)-H(13C)	109.5
C(2)-C(3)-C(4)	116.8(4)	H(13B)-C(13)-H(13C)	109.5
C(58)-O(4)-Zr(1)	141.2(3)	C(12)-C(14)-H(14A)	109.5
C(36)-N(4)-C(56)	110.1(4)	C(12)-C(14)-H(14B)	109.5
C(36)-N(4)-C(57)	122.7(4)	H(14A)-C(14)-H(14B)	109.5
C(56)-N(4)-C(57)	126.2(4)	C(12)-C(14)-H(14C)	109.5
C(5)-C(4)-C(3)	118.2(4)	H(14A)-C(14)-H(14C)	109.5
C(5)-C(4)-C(8)	121.7(4)	H(14B)-C(14)-H(14C)	109.5
C(3)-C(4)-C(8)	120.0(4)	C(12)-C(15)-H(15A)	109.5
C(4)-C(5)-C(6)	124.3(4)	C(12)-C(15)-H(15B)	109.5
C(4)-C(5)-H(5)	117.9	H(15A)-C(15)-H(15B)	109.5
C(6)-C(5)-H(5)	117.9	C(12)-C(15)-H(15C)	109.5
C(7)-C(6)-C(5)	117.1(4)	H(15A)-C(15)-H(15C)	109.5
C(7)-C(6)-C(12)	121.9(4)	H(15B)-C(15)-H(15C)	109.5
C(5)-C(6)-C(12)	120.9(4)	C(17)-C(16)-N(1)	132.9(4)
C(6)-C(7)-C(2)	120.4(4)	C(17)-C(16)-C(21)	121.5(4)
C(6)-C(7)-H(7)	119.8	N(1)-C(16)-C(21)	105.3(4)
C(2)-C(7)-H(7)	119.8	C(18)-C(17)-C(16)	117.1(4)
C(11)-C(8)-C(9)	107.3(4)	C(18)-C(17)-H(17)	121.4
C(11)-C(8)-C(4)	110.3(4)	C(16)-C(17)-H(17)	121.4
C(9)-C(8)-C(4)	111.3(4)	C(17)-C(18)-C(19)	121.8(4)
C(11)-C(8)-C(10)	111.4(4)	C(17)-C(18)-H(18)	119.1
C(9)-C(8)-C(10)	107.2(4)	C(19)-C(18)-H(18)	119.1
C(4)-C(8)-C(10)	109.3(4)	C(20)-C(19)-C(18)	121.6(4)
C(8)-C(9)-H(9A)	109.5	C(20)-C(19)-H(19)	119.2
C(8)-C(9)-H(9B)	109.5	C(18)-C(19)-H(19)	119.2
H(9A)-C(9)-H(9B)	109.5	C(19)-C(20)-C(21)	117.3(4)
C(8)-C(9)-H(9C)	109.5	C(19)-C(20)-H(20)	121.3
H(9A)-C(9)-H(9C)	109.5	C(21)-C(20)-H(20)	121.3
H(9B)-C(9)-H(9C)	109.5	N(2)-C(21)-C(16)	106.5(4)
C(8)-C(10)-H(10A)	109.5	N(2)-C(21)-C(20)	132.6(4)
C(8)-C(10)-H(10B)	109.5	C(16)-C(21)-C(20)	120.6(4)
H(10A)-C(10)-H(10B)	109.5	C(27)-C(22)-C(23)	121.8(4)
C(8)-C(10)-H(10C)	109.5	C(27)-C(22)-N(2)	119.1(4)
H(10A)-C(10)-H(10C)	109.5	C(23)-C(22)-N(2)	118.8(4)
H(10B)-C(10)-H(10C)	109.5	O(2)-C(23)-C(22)	120.5(4)
C(8)-C(11)-H(11A)	109.5	O(2)-C(23)-C(24)	121.3(4)

C(22)-C(23)-C(24)	118.2(4)	C(32)-C(34)-H(34B)	109.5
C(25)-C(24)-C(23)	117.7(4)	H(34A)-C(34)-H(34B)	109.5
C(25)-C(24)-C(28)	121.8(4)	C(32)-C(34)-H(34C)	109.5
C(23)-C(24)-C(28)	120.5(4)	H(34A)-C(34)-H(34C)	109.5
C(24)-C(25)-C(26)	124.0(4)	H(34B)-C(34)-H(34C)	109.5
C(24)-C(25)-H(25)	118.0	C(32)-C(35)-H(35A)	109.5
C(26)-C(25)-H(25)	118.0	C(32)-C(35)-H(35B)	109.5
C(27)-C(26)-C(25)	117.3(4)	H(35A)-C(35)-H(35B)	109.5
C(27)-C(26)-C(32)	119.6(6)	C(32)-C(35)-H(35C)	109.5
C(25)-C(26)-C(32)	122.7(6)	H(35A)-C(35)-H(35C)	109.5
C(27)-C(26)-C(32A)	120.6(6)	H(35B)-C(35)-H(35C)	109.5
C(25)-C(26)-C(32A)	121.1(6)	C(35A)-C(32A)-C(34A)	109.9(9)
C(22)-C(27)-C(26)	120.6(4)	C(35A)-C(32A)-C(33A)	107.6(9)
C(22)-C(27)-H(27)	119.7	C(34A)-C(32A)-C(33A)	107.2(10)
C(26)-C(27)-H(27)	119.7	C(35A)-C(32A)-C(26)	112.9(9)
C(31)-C(28)-C(29)	107.3(4)	C(34A)-C(32A)-C(26)	110.4(9)
C(31)-C(28)-C(30)	108.1(4)	C(33A)-C(32A)-C(26)	108.7(12)
C(29)-C(28)-C(30)	110.1(4)	C(32A)-C(33A)-H(33D)	109.5
C(31)-C(28)-C(24)	111.5(4)	C(32A)-C(33A)-H(33E)	109.5
C(29)-C(28)-C(24)	110.1(4)	H(33D)-C(33A)-H(33E)	109.5
C(30)-C(28)-C(24)	109.7(4)	C(32A)-C(33A)-H(33F)	109.5
C(28)-C(29)-H(29A)	109.5	H(33D)-C(33A)-H(33F)	109.5
C(28)-C(29)-H(29B)	109.5	H(33E)-C(33A)-H(33F)	109.5
H(29A)-C(29)-H(29B)	109.5	C(32A)-C(34A)-H(34D)	109.5
C(28)-C(29)-H(29C)	109.5	C(32A)-C(34A)-H(34E)	109.5
H(29A)-C(29)-H(29C)	109.5	H(34D)-C(34A)-H(34E)	109.5
H(29B)-C(29)-H(29C)	109.5	C(32A)-C(34A)-H(34F)	109.5
C(28)-C(30)-H(30A)	109.5	H(34D)-C(34A)-H(34F)	109.5
C(28)-C(30)-H(30B)	109.5	H(34E)-C(34A)-H(34F)	109.5
H(30A)-C(30)-H(30B)	109.5	C(32A)-C(35A)-H(35D)	109.5
C(28)-C(30)-H(30C)	109.5	C(32A)-C(35A)-H(35E)	109.5
H(30A)-C(30)-H(30C)	109.5	H(35D)-C(35A)-H(35E)	109.5
H(30B)-C(30)-H(30C)	109.5	C(32A)-C(35A)-H(35F)	109.5
C(28)-C(31)-H(31A)	109.5	H(35D)-C(35A)-H(35F)	109.5
C(28)-C(31)-H(31B)	109.5	H(35E)-C(35A)-H(35F)	109.5
H(31A)-C(31)-H(31B)	109.5	N(3)-C(36)-N(4)	106.8(4)
C(28)-C(31)-H(31C)	109.5	N(3)-C(36)-Zr(1)	123.4(3)
H(31A)-C(31)-H(31C)	109.5	N(4)-C(36)-Zr(1)	123.6(3)
H(31B)-C(31)-H(31C)	109.5	C(42)-C(37)-C(38)	122.2(4)
C(35)-C(32)-C(33)	109.4(7)	C(42)-C(37)-N(3)	118.0(4)
C(35)-C(32)-C(34)	108.8(7)	C(38)-C(37)-N(3)	119.5(4)
C(33)-C(32)-C(34)	108.5(7)	O(3)-C(38)-C(37)	119.7(4)
C(35)-C(32)-C(26)	106.2(9)	O(3)-C(38)-C(39)	122.6(4)
C(33)-C(32)-C(26)	111.9(13)	C(37)-C(38)-C(39)	117.7(4)
C(34)-C(32)-C(26)	111.8(8)	C(40)-C(39)-C(38)	118.7(4)
C(32)-C(33)-H(33A)	109.5	C(40)-C(39)-C(43)	121.1(4)
C(32)-C(33)-H(33B)	109.5	C(38)-C(39)-C(43)	120.2(3)
H(33A)-C(33)-H(33B)	109.5	C(39)-C(40)-C(41)	123.7(4)
C(32)-C(33)-H(33C)	109.5	C(39)-C(40)-H(40)	118.1
H(33A)-C(33)-H(33C)	109.5	C(41)-C(40)-H(40)	118.1
H(33B)-C(33)-H(33C)	109.5	C(42)-C(41)-C(40)	116.6(4)
C(32)-C(34)-H(34A)	109.5	C(42)-C(41)-C(47)	122.3(3)

C(40)-C(41)-C(47)	121.1(3)	C(56)-C(51)-C(52)	121.6(4)
C(37)-C(42)-C(41)	121.0(4)	C(56)-C(51)-N(3)	106.1(4)
C(37)-C(42)-H(42)	119.5	C(52)-C(51)-N(3)	132.2(4)
C(41)-C(42)-H(42)	119.5	C(53)-C(52)-C(51)	116.9(5)
C(46)-C(43)-C(44)	107.4(4)	C(53)-C(52)-H(52)	121.6
C(46)-C(43)-C(45)	110.5(4)	C(51)-C(52)-H(52)	121.6
C(44)-C(43)-C(45)	106.3(4)	C(52)-C(53)-C(54)	122.3(5)
C(46)-C(43)-C(39)	109.4(4)	C(52)-C(53)-H(53)	118.9
C(44)-C(43)-C(39)	112.5(4)	C(54)-C(53)-H(53)	118.9
C(45)-C(43)-C(39)	110.5(4)	C(53)-C(54)-C(55)	120.8(5)
C(43)-C(44)-H(44A)	109.5	C(53)-C(54)-H(54)	119.6
C(43)-C(44)-H(44B)	109.5	C(55)-C(54)-H(54)	119.6
H(44A)-C(44)-H(44B)	109.5	C(56)-C(55)-C(54)	117.3(5)
C(43)-C(44)-H(44C)	109.5	C(56)-C(55)-H(55)	121.3
H(44A)-C(44)-H(44C)	109.5	C(54)-C(55)-H(55)	121.3
H(44B)-C(44)-H(44C)	109.5	C(51)-C(56)-C(55)	121.1(5)
C(43)-C(45)-H(45A)	109.5	C(51)-C(56)-N(4)	106.7(4)
C(43)-C(45)-H(45B)	109.5	C(55)-C(56)-N(4)	132.0(4)
H(45A)-C(45)-H(45B)	109.5	C(62A)-C(57)-C(58)	123.5(5)
C(43)-C(45)-H(45C)	109.5	C(62)-C(57)-C(58)	119.8(5)
H(45A)-C(45)-H(45C)	109.5	C(62A)-C(57)-N(4)	116.7(5)
H(45B)-C(45)-H(45C)	109.5	C(62)-C(57)-N(4)	118.9(5)
C(43)-C(46)-H(46A)	109.5	C(58)-C(57)-N(4)	118.8(4)
C(43)-C(46)-H(46B)	109.5	O(4)-C(58)-C(57)	121.1(4)
H(46A)-C(46)-H(46B)	109.5	O(4)-C(58)-C(59)	121.4(4)
C(43)-C(46)-H(46C)	109.5	C(57)-C(58)-C(59)	117.5(4)
H(46A)-C(46)-H(46C)	109.5	C(60A)-C(59)-C(58)	117.3(5)
H(46B)-C(46)-H(46C)	109.5	C(60)-C(59)-C(58)	118.6(5)
C(49)-C(47)-C(48)	107.9(5)	C(60A)-C(59)-C(63)	121.6(5)
C(49)-C(47)-C(41)	110.8(4)	C(60)-C(59)-C(63)	119.7(5)
C(48)-C(47)-C(41)	112.8(4)	C(58)-C(59)-C(63)	119.7(4)
C(49)-C(47)-C(50)	109.0(5)	C(64)-C(63)-C(66)	106.9(4)
C(48)-C(47)-C(50)	107.0(5)	C(64)-C(63)-C(65)	110.2(4)
C(41)-C(47)-C(50)	109.2(4)	C(66)-C(63)-C(65)	107.7(4)
C(47)-C(48)-H(48A)	109.5	C(64)-C(63)-C(59)	110.4(4)
C(47)-C(48)-H(48B)	109.5	C(66)-C(63)-C(59)	111.3(4)
H(48A)-C(48)-H(48B)	109.5	C(65)-C(63)-C(59)	110.3(4)
C(47)-C(48)-H(48C)	109.5	C(63)-C(64)-H(64A)	109.5
H(48A)-C(48)-H(48C)	109.5	C(63)-C(64)-H(64B)	109.5
H(48B)-C(48)-H(48C)	109.5	H(64A)-C(64)-H(64B)	109.5
C(47)-C(49)-H(49A)	109.5	C(63)-C(64)-H(64C)	109.5
C(47)-C(49)-H(49B)	109.5	H(64A)-C(64)-H(64C)	109.5
H(49A)-C(49)-H(49B)	109.5	H(64B)-C(64)-H(64C)	109.5
C(47)-C(49)-H(49C)	109.5	C(63)-C(65)-H(65A)	109.5
H(49A)-C(49)-H(49C)	109.5	C(63)-C(65)-H(65B)	109.5
H(49B)-C(49)-H(49C)	109.5	H(65A)-C(65)-H(65B)	109.5
C(47)-C(50)-H(50A)	109.5	C(63)-C(65)-H(65C)	109.5
C(47)-C(50)-H(50B)	109.5	H(65A)-C(65)-H(65C)	109.5
H(50A)-C(50)-H(50B)	109.5	H(65B)-C(65)-H(65C)	109.5
C(47)-C(50)-H(50C)	109.5	C(63)-C(66)-H(66A)	109.5
H(50A)-C(50)-H(50C)	109.5	C(63)-C(66)-H(66B)	109.5
H(50B)-C(50)-H(50C)	109.5	H(66A)-C(66)-H(66B)	109.5

C(63)-C(66)-H(66C)	109.5	H(70B)-C(70)-H(70C)	109.5
H(66A)-C(66)-H(66C)	109.5	C(61A)-C(60A)-C(59)	123.0(6)
H(66B)-C(66)-H(66C)	109.5	C(61A)-C(60A)-H(60A)	118.5
C(61)-C(60)-C(59)	123.3(6)	C(59)-C(60A)-H(60A)	118.5
C(61)-C(60)-H(60)	118.4	C(62A)-C(61A)-C(60A)	118.1(8)
C(59)-C(60)-H(60)	118.4	C(62A)-C(61A)-C(67A)	119.7(7)
C(62)-C(61)-C(60)	115.8(6)	C(60A)-C(61A)-C(67A)	122.1(6)
C(62)-C(61)-C(67)	124.2(5)	C(57)-C(62A)-C(61A)	118.5(8)
C(60)-C(61)-C(67)	120.0(5)	C(57)-C(62A)-H(62A)	120.7
C(61)-C(62)-C(57)	122.6(6)	C(61A)-C(62A)-H(62A)	120.7
C(61)-C(62)-H(62)	118.7	C(68A)-C(67A)-C(69A)	111.0(10)
C(57)-C(62)-H(62)	118.7	C(68A)-C(67A)-C(70A)	109.8(14)
C(70)-C(67)-C(68)	107.8(10)	C(69A)-C(67A)-C(70A)	107.1(11)
C(70)-C(67)-C(69)	111.6(9)	C(68A)-C(67A)-C(61A)	108.2(12)
C(68)-C(67)-C(69)	108.3(9)	C(69A)-C(67A)-C(61A)	108.1(7)
C(70)-C(67)-C(61)	108.6(9)	C(70A)-C(67A)-C(61A)	112.7(10)
C(68)-C(67)-C(61)	111.9(9)	C(67A)-C(68A)-H(68D)	109.5
C(69)-C(67)-C(61)	108.5(7)	C(67A)-C(68A)-H(68E)	109.5
C(67)-C(68)-H(68A)	109.5	H(68D)-C(68A)-H(68E)	109.5
C(67)-C(68)-H(68B)	109.5	C(67A)-C(68A)-H(68F)	109.5
H(68A)-C(68)-H(68B)	109.5	H(68D)-C(68A)-H(68F)	109.5
C(67)-C(68)-H(68C)	109.5	H(68E)-C(68A)-H(68F)	109.5
H(68A)-C(68)-H(68C)	109.5	C(67A)-C(69A)-H(69D)	109.5
H(68B)-C(68)-H(68C)	109.5	C(67A)-C(69A)-H(69E)	109.5
C(67)-C(69)-H(69A)	109.5	H(69D)-C(69A)-H(69E)	109.5
C(67)-C(69)-H(69B)	109.5	C(67A)-C(69A)-H(69F)	109.5
H(69A)-C(69)-H(69B)	109.5	H(69D)-C(69A)-H(69F)	109.5
C(67)-C(69)-H(69C)	109.5	H(69E)-C(69A)-H(69F)	109.5
H(69A)-C(69)-H(69C)	109.5	C(67A)-C(70A)-H(70D)	109.5
H(69B)-C(69)-H(69C)	109.5	C(67A)-C(70A)-H(70E)	109.5
C(67)-C(70)-H(70A)	109.5	H(70D)-C(70A)-H(70E)	109.5
C(67)-C(70)-H(70B)	109.5	C(67A)-C(70A)-H(70F)	109.5
H(70A)-C(70)-H(70B)	109.5	H(70D)-C(70A)-H(70F)	109.5
C(67)-C(70)-H(70C)	109.5	H(70E)-C(70A)-H(70F)	109.5
H(70A)-C(70)-H(70C)	109.5		

Symmetry transformations used to generate equivalent atoms:

Table S7. Torsion angles [°] for **5**.

C(16)-N(1)-C(1)-N(2)	-4.5(5)	Zr(1)-O(1)-C(3)-C(2)	-41.0(6)
C(2)-N(1)-C(1)-N(2)	164.6(4)	Zr(1)-O(1)-C(3)-C(4)	138.9(4)
C(16)-N(1)-C(1)-Zr(1)	145.7(3)	C(7)-C(2)-C(3)-O(1)	178.4(4)
C(2)-N(1)-C(1)-Zr(1)	-45.3(5)	N(1)-C(2)-C(3)-O(1)	4.4(6)
N(1)-C(1)-N(2)-C(21)	3.0(5)	C(7)-C(2)-C(3)-C(4)	-1.4(6)
Zr(1)-C(1)-N(2)-C(21)	-146.4(3)	N(1)-C(2)-C(3)-C(4)	-175.5(4)
N(1)-C(1)-N(2)-C(22)	-171.5(4)	O(1)-C(3)-C(4)-C(5)	178.8(4)
Zr(1)-C(1)-N(2)-C(22)	39.2(5)	C(2)-C(3)-C(4)-C(5)	-1.3(6)
C(1)-N(1)-C(2)-C(7)	-137.8(4)	O(1)-C(3)-C(4)-C(8)	-2.3(6)
C(16)-N(1)-C(2)-C(7)	29.7(6)	C(2)-C(3)-C(4)-C(8)	177.6(4)
C(1)-N(1)-C(2)-C(3)	36.6(6)	C(3)-C(4)-C(5)-C(6)	2.1(7)
C(16)-N(1)-C(2)-C(3)	-155.9(4)	C(8)-C(4)-C(5)-C(6)	-176.7(4)

C(4)-C(5)-C(6)-C(7)	-0.2(7)
C(4)-C(5)-C(6)-C(12)	-178.4(4)
C(5)-C(6)-C(7)-C(2)	-2.6(6)
C(12)-C(6)-C(7)-C(2)	175.6(4)
C(3)-C(2)-C(7)-C(6)	3.5(7)
N(1)-C(2)-C(7)-C(6)	177.6(4)
C(5)-C(4)-C(8)-C(11)	-120.2(5)
C(3)-C(4)-C(8)-C(11)	60.9(6)
C(5)-C(4)-C(8)-C(9)	-1.3(6)
C(3)-C(4)-C(8)-C(9)	179.9(4)
C(5)-C(4)-C(8)-C(10)	116.9(5)
C(3)-C(4)-C(8)-C(10)	-61.9(5)
C(7)-C(6)-C(12)-C(13)	10.3(7)
C(5)-C(6)-C(12)-C(13)	-171.5(5)
C(7)-C(6)-C(12)-C(15)	129.6(5)
C(5)-C(6)-C(12)-C(15)	-52.2(6)
C(7)-C(6)-C(12)-C(14)	-109.7(5)
C(5)-C(6)-C(12)-C(14)	68.5(6)
C(1)-N(1)-C(16)-C(17)	-170.4(5)
C(2)-N(1)-C(16)-C(17)	20.8(7)
C(1)-N(1)-C(16)-C(21)	4.2(5)
C(2)-N(1)-C(16)-C(21)	-164.5(4)
N(1)-C(16)-C(17)-C(18)	175.3(5)
C(21)-C(16)-C(17)-C(18)	1.4(7)
C(16)-C(17)-C(18)-C(19)	-0.2(7)
C(17)-C(18)-C(19)-C(20)	-0.6(8)
C(18)-C(19)-C(20)-C(21)	0.2(8)
C(1)-N(2)-C(21)-C(16)	-0.5(5)
C(22)-N(2)-C(21)-C(16)	173.8(4)
C(1)-N(2)-C(21)-C(20)	173.8(5)
C(22)-N(2)-C(21)-C(20)	-12.0(8)
C(17)-C(16)-C(21)-N(2)	173.2(4)
N(1)-C(16)-C(21)-N(2)	-2.2(5)
C(17)-C(16)-C(21)-C(20)	-1.9(7)
N(1)-C(16)-C(21)-C(20)	-177.2(4)
C(19)-C(20)-C(21)-N(2)	-172.6(5)
C(19)-C(20)-C(21)-C(16)	1.0(7)
C(1)-N(2)-C(22)-C(27)	137.0(4)
C(21)-N(2)-C(22)-C(27)	-36.5(6)
C(1)-N(2)-C(22)-C(23)	-37.6(6)
C(21)-N(2)-C(22)-C(23)	148.8(4)
Zr(1)-O(2)-C(23)-C(22)	37.4(7)
Zr(1)-O(2)-C(23)-C(24)	-141.7(4)
C(27)-C(22)-C(23)-O(2)	-171.6(4)
N(2)-C(22)-C(23)-O(2)	2.9(6)
C(27)-C(22)-C(23)-C(24)	7.5(7)
N(2)-C(22)-C(23)-C(24)	-178.0(4)
O(2)-C(23)-C(24)-C(25)	173.3(4)
C(22)-C(23)-C(24)-C(25)	-5.9(6)
O(2)-C(23)-C(24)-C(28)	-4.3(7)
C(22)-C(23)-C(24)-C(28)	176.5(4)
C(23)-C(24)-C(25)-C(26)	1.3(7)
C(28)-C(24)-C(25)-C(26)	178.9(5)
C(24)-C(25)-C(26)-C(27)	1.9(8)
C(24)-C(25)-C(26)-C(32)	174.9(7)
C(24)-C(25)-C(26)-C(32A)	-166.6(7)
C(23)-C(22)-C(27)-C(26)	-4.3(7)
N(2)-C(22)-C(27)-C(26)	-178.8(4)
C(25)-C(26)-C(27)-C(22)	-0.5(7)
C(32)-C(26)-C(27)-C(22)	-173.7(6)
C(32A)-C(26)-C(27)-C(22)	168.1(7)
C(25)-C(24)-C(28)-C(31)	8.1(7)
C(23)-C(24)-C(28)-C(31)	-174.5(5)
C(25)-C(24)-C(28)-C(29)	127.0(5)
C(23)-C(24)-C(28)-C(29)	-55.5(6)
C(25)-C(24)-C(28)-C(30)	-111.6(5)
C(23)-C(24)-C(28)-C(30)	65.8(6)
C(27)-C(26)-C(32)-C(35)	-45.2(9)
C(25)-C(26)-C(32)-C(35)	142.0(9)
C(27)-C(26)-C(32)-C(33)	-164.6(8)
C(25)-C(26)-C(32)-C(33)	22.6(11)
C(27)-C(26)-C(32)-C(34)	73.4(10)
C(25)-C(26)-C(32)-C(34)	-99.4(10)
C(27)-C(26)-C(32A)-C(35A)	-80.2(12)
C(25)-C(26)-C(32A)-C(35A)	87.9(13)
C(27)-C(26)-C(32A)-C(34A)	43.2(13)
C(25)-C(26)-C(32A)-C(34A)	-148.6(11)
C(27)-C(26)-C(32A)-C(33A)	160.5(11)
C(25)-C(26)-C(32A)-C(33A)	-31.4(15)
C(51)-N(3)-C(36)-N(4)	-3.2(5)
C(37)-N(3)-C(36)-N(4)	166.1(4)
C(51)-N(3)-C(36)-Zr(1)	149.8(3)
C(37)-N(3)-C(36)-Zr(1)	-40.9(5)
C(56)-N(4)-C(36)-N(3)	2.6(5)
C(57)-N(4)-C(36)-N(3)	-166.5(4)
C(56)-N(4)-C(36)-Zr(1)	-150.3(3)
C(57)-N(4)-C(36)-Zr(1)	40.6(6)
C(36)-N(3)-C(37)-C(42)	-137.6(4)
C(51)-N(3)-C(37)-C(42)	29.9(6)
C(36)-N(3)-C(37)-C(38)	35.9(6)
C(51)-N(3)-C(37)-C(38)	-156.5(4)
Zr(1)-O(3)-C(38)-C(37)	-49.0(6)
Zr(1)-O(3)-C(38)-C(39)	131.0(4)
C(42)-C(37)-C(38)-O(3)	178.7(4)
N(3)-C(37)-C(38)-O(3)	5.4(6)
C(42)-C(37)-C(38)-C(39)	-1.4(6)
N(3)-C(37)-C(38)-C(39)	-174.6(4)
O(3)-C(38)-C(39)-C(40)	179.3(4)
C(37)-C(38)-C(39)-C(40)	-0.6(6)
O(3)-C(38)-C(39)-C(43)	-1.7(6)
C(37)-C(38)-C(39)-C(43)	178.3(4)
C(38)-C(39)-C(40)-C(41)	1.5(7)
C(43)-C(39)-C(40)-C(41)	-177.4(4)
C(39)-C(40)-C(41)-C(42)	-0.4(7)

C(39)-C(40)-C(41)-C(47)	179.5(4)	C(62A)-C(57)-C(58)-C(59)	-13.2(10)
C(38)-C(37)-C(42)-C(41)	2.6(6)	C(62)-C(57)-C(58)-C(59)	16.6(8)
N(3)-C(37)-C(42)-C(41)	175.9(4)	N(4)-C(57)-C(58)-C(59)	178.7(4)
C(40)-C(41)-C(42)-C(37)	-1.7(6)	O(4)-C(58)-C(59)-C(60A)	-169.4(7)
C(47)-C(41)-C(42)-C(37)	178.5(4)	C(57)-C(58)-C(59)-C(60A)	11.9(9)
C(40)-C(39)-C(43)-C(46)	-120.0(4)	O(4)-C(58)-C(59)-C(60)	161.5(6)
C(38)-C(39)-C(43)-C(46)	61.2(5)	C(57)-C(58)-C(59)-C(60)	-17.2(9)
C(40)-C(39)-C(43)-C(44)	-0.6(6)	O(4)-C(58)-C(59)-C(63)	-2.7(7)
C(38)-C(39)-C(43)-C(44)	-179.5(4)	C(57)-C(58)-C(59)-C(63)	178.6(5)
C(40)-C(39)-C(43)-C(45)	118.1(5)	C(60A)-C(59)-C(63)-C(64)	108.9(8)
C(38)-C(39)-C(43)-C(45)	-60.8(5)	C(60)-C(59)-C(63)-C(64)	138.8(7)
C(42)-C(41)-C(47)-C(49)	-127.0(5)	C(58)-C(59)-C(63)-C(64)	-57.2(6)
C(40)-C(41)-C(47)-C(49)	53.2(6)	C(60A)-C(59)-C(63)-C(66)	-9.6(9)
C(42)-C(41)-C(47)-C(48)	-5.9(7)	C(60)-C(59)-C(63)-C(66)	20.3(8)
C(40)-C(41)-C(47)-C(48)	174.3(5)	C(58)-C(59)-C(63)-C(66)	-175.8(5)
C(42)-C(41)-C(47)-C(50)	112.9(5)	C(60A)-C(59)-C(63)-C(65)	-129.1(8)
C(40)-C(41)-C(47)-C(50)	-67.0(6)	C(60)-C(59)-C(63)-C(65)	-99.2(7)
C(36)-N(3)-C(51)-C(56)	2.6(5)	C(58)-C(59)-C(63)-C(65)	64.8(6)
C(37)-N(3)-C(51)-C(56)	-166.2(4)	C(58)-C(59)-C(60)-C(61)	11.2(13)
C(36)-N(3)-C(51)-C(52)	-173.8(5)	C(63)-C(59)-C(60)-C(61)	175.4(8)
C(37)-N(3)-C(51)-C(52)	17.4(8)	C(59)-C(60)-C(61)-C(62)	-3.8(15)
C(56)-C(51)-C(52)-C(53)	0.0(8)	C(59)-C(60)-C(61)-C(67)	177.4(9)
N(3)-C(51)-C(52)-C(53)	175.9(6)	C(60)-C(61)-C(62)-C(57)	2.8(14)
C(51)-C(52)-C(53)-C(54)	-0.7(11)	C(67)-C(61)-C(62)-C(57)	-178.4(9)
C(52)-C(53)-C(54)-C(55)	1.2(13)	C(58)-C(57)-C(62)-C(61)	-9.7(12)
C(53)-C(54)-C(55)-C(56)	-0.9(13)	N(4)-C(57)-C(62)-C(61)	-171.8(8)
C(52)-C(51)-C(56)-C(55)	0.2(9)	C(62)-C(61)-C(67)-C(70)	123.7(12)
N(3)-C(51)-C(56)-C(55)	-176.6(6)	C(60)-C(61)-C(67)-C(70)	-57.6(13)
C(52)-C(51)-C(56)-N(4)	175.9(5)	C(62)-C(61)-C(67)-C(68)	4.7(14)
N(3)-C(51)-C(56)-N(4)	-0.9(5)	C(60)-C(61)-C(67)-C(68)	-176.5(11)
C(54)-C(55)-C(56)-C(51)	0.2(10)	C(62)-C(61)-C(67)-C(69)	-114.8(10)
C(54)-C(55)-C(56)-N(4)	-174.2(7)	C(60)-C(61)-C(67)-C(69)	64.0(11)
C(36)-N(4)-C(56)-C(51)	-1.0(6)	C(58)-C(59)-C(60A)-C(61A)	-11.2(14)
C(57)-N(4)-C(56)-C(51)	167.6(5)	C(63)-C(59)-C(60A)-C(61A)	-177.7(8)
C(36)-N(4)-C(56)-C(55)	174.0(7)	C(59)-C(60A)-C(61A)-C(62A)	10.5(17)
C(57)-N(4)-C(56)-C(55)	-17.4(10)	C(59)-C(60A)-C(61A)-C(67A)	-172.1(10)
C(36)-N(4)-C(57)-C(62A)	154.3(7)	C(58)-C(57)-C(62A)-C(61A)	12.5(14)
C(56)-N(4)-C(57)-C(62A)	-13.0(9)	N(4)-C(57)-C(62A)-C(61A)	-179.2(8)
C(36)-N(4)-C(57)-C(62)	125.5(7)	C(60A)-C(61A)-C(62A)-C(57)	-10.6(16)
C(56)-N(4)-C(57)-C(62)	-41.8(8)	C(67A)-C(61A)-C(62A)-C(57)	172.0(9)
C(36)-N(4)-C(57)-C(58)	-36.8(7)	C(62A)-C(61A)-C(67A)-C(68A)	-58.0(14)
C(56)-N(4)-C(57)-C(58)	155.9(5)	C(60A)-C(61A)-C(67A)-C(68A)	124.6(13)
Zr(1)-O(4)-C(58)-C(57)	39.7(7)	C(62A)-C(61A)-C(67A)-C(69A)	62.2(12)
Zr(1)-O(4)-C(58)-C(59)	-139.0(4)	C(60A)-C(61A)-C(67A)-C(69A)	-115.1(11)
C(62A)-C(57)-C(58)-O(4)	168.1(7)	C(62A)-C(61A)-C(67A)-C(70A)	-179.6(13)
C(62)-C(57)-C(58)-O(4)	-162.1(6)	C(60A)-C(61A)-C(67A)-C(70A)	3.1(16)
N(4)-C(57)-C(58)-O(4)	0.0(7)		

Symmetry transformations used to generate equivalent atoms:

Table S8. Bond lengths [Å] and angles [°] for **5''**.

Zr(1)-O(3)	1.8901(11)	C(19)-H(19A)	0.9800
Zr(1)-O(1)	1.9732(10)	C(19)-H(19B)	0.9800
Zr(1)-O(2)	1.9777(10)	C(19)-H(19C)	0.9800
Zr(1)-Cl(2)	2.4675(5)	C(20)-H(20A)	0.9800
Zr(1)-Cl(1)	2.5322(4)	C(20)-H(20B)	0.9800
O(1)-C(9)	1.3337(16)	C(20)-H(20C)	0.9800
N(1)-C(1)	1.3370(17)	C(21)-H(21A)	0.9800
N(1)-C(2)	1.3961(17)	C(21)-H(21B)	0.9800
N(1)-C(8)	1.4369(17)	C(21)-H(21C)	0.9800
C(1)-N(2)	1.3355(17)	C(22)-C(27)	1.3846(19)
C(1)-H(1)	0.936(19)	C(22)-C(23)	1.4029(18)
O(2)-C(23)	1.3343(16)	C(23)-C(24)	1.4142(19)
N(2)-C(3)	1.3972(17)	C(24)-C(25)	1.3983(19)
N(2)-C(22)	1.4391(17)	C(24)-C(28)	1.5381(19)
C(2)-C(3)	1.391(2)	C(25)-C(26)	1.3973(19)
C(2)-C(7)	1.3922(19)	C(25)-H(25)	0.9500
O(3)-C(36)	1.4188(18)	C(26)-C(27)	1.3939(19)
C(3)-C(4)	1.3936(19)	C(26)-C(32)	1.5302(19)
C(4)-C(5)	1.380(2)	C(27)-H(27)	0.9500
C(4)-H(4)	0.9500	C(28)-C(31)	1.535(2)
C(5)-C(6)	1.412(2)	C(28)-C(29)	1.535(2)
C(5)-H(5)	0.9500	C(28)-C(30)	1.543(2)
C(6)-C(7)	1.378(2)	C(29)-H(29A)	0.9800
C(6)-H(6)	0.9500	C(29)-H(29B)	0.9800
C(7)-H(7)	0.9500	C(29)-H(29C)	0.9800
C(8)-C(13)	1.3915(18)	C(30)-H(30A)	0.9800
C(8)-C(9)	1.3994(19)	C(30)-H(30B)	0.9800
C(9)-C(10)	1.4176(19)	C(30)-H(30C)	0.9800
C(10)-C(11)	1.3944(19)	C(31)-H(31A)	0.9800
C(10)-C(14)	1.5305(19)	C(31)-H(31B)	0.9800
C(11)-C(12)	1.4029(19)	C(31)-H(31C)	0.9800
C(11)-H(11)	0.9500	C(32)-C(34)	1.528(2)
C(12)-C(13)	1.3869(19)	C(32)-C(35)	1.531(2)
C(12)-C(18)	1.5307(19)	C(32)-C(33)	1.531(2)
C(13)-H(13)	0.9500	C(33)-H(33A)	0.9800
C(14)-C(17)	1.536(2)	C(33)-H(33B)	0.9800
C(14)-C(15)	1.542(2)	C(33)-H(33C)	0.9800
C(14)-C(16)	1.544(2)	C(34)-H(34A)	0.9800
C(15)-H(15A)	0.9800	C(34)-H(34B)	0.9800
C(15)-H(15B)	0.9800	C(34)-H(34C)	0.9800
C(15)-H(15C)	0.9800	C(35)-H(35A)	0.9800
C(16)-H(16A)	0.9800	C(35)-H(35B)	0.9800
C(16)-H(16B)	0.9800	C(35)-H(35C)	0.9800
C(16)-H(16C)	0.9800	C(36)-C(37)	1.510(2)
C(17)-H(17A)	0.9800	C(36)-C(38)	1.514(2)
C(17)-H(17B)	0.9800	C(36)-H(36)	1.0000
C(17)-H(17C)	0.9800	C(37)-H(37A)	0.9800
C(18)-C(20)	1.521(2)	C(37)-H(37B)	0.9800
C(18)-C(19)	1.523(2)	C(37)-H(37C)	0.9800
C(18)-C(21)	1.526(2)	C(38)-H(38A)	0.9800

C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(1S)-C(2S)	1.382(3)
C(1S)-C(6S)	1.386(3)
C(1S)-H(1S)	0.9500
C(2S)-C(3S)	1.387(3)
C(2S)-H(2S)	0.9500
C(3S)-C(4S)	1.384(3)
C(3S)-H(3S)	0.9500
C(4S)-C(5S)	1.380(3)
C(4S)-H(4S)	0.9500
C(5S)-C(6S)	1.381(3)
C(5S)-H(5S)	0.9500
C(6S)-H(6S)	0.9500

O(3)-Zr(1)-O(1)	117.11(5)
O(3)-Zr(1)-O(2)	115.61(5)
O(1)-Zr(1)-O(2)	127.17(4)
O(3)-Zr(1)-Cl(2)	94.87(5)
O(1)-Zr(1)-Cl(2)	88.18(3)
O(2)-Zr(1)-Cl(2)	90.66(3)
O(3)-Zr(1)-Cl(1)	96.23(4)
O(1)-Zr(1)-Cl(1)	85.31(3)
O(2)-Zr(1)-Cl(1)	86.03(3)
Cl(2)-Zr(1)-Cl(1)	168.780(17)
C(9)-O(1)-Zr(1)	163.62(9)
C(1)-N(1)-C(2)	108.20(12)
C(1)-N(1)-C(8)	125.99(12)
C(2)-N(1)-C(8)	125.32(11)
N(2)-C(1)-N(1)	110.26(12)
N(2)-C(1)-H(1)	125.2(10)
N(1)-C(1)-H(1)	124.6(10)
C(23)-O(2)-Zr(1)	161.41(9)
C(1)-N(2)-C(3)	108.17(11)
C(1)-N(2)-C(22)	125.51(12)
C(3)-N(2)-C(22)	125.82(11)
C(3)-C(2)-C(7)	121.84(13)
C(3)-C(2)-N(1)	106.66(11)
C(7)-C(2)-N(1)	131.50(13)
C(36)-O(3)-Zr(1)	160.85(11)
C(2)-C(3)-C(4)	121.83(12)
C(2)-C(3)-N(2)	106.70(12)
C(4)-C(3)-N(2)	131.47(13)
C(5)-C(4)-C(3)	116.44(14)
C(5)-C(4)-H(4)	121.8
C(3)-C(4)-H(4)	121.8
C(4)-C(5)-C(6)	121.63(14)
C(4)-C(5)-H(5)	119.2
C(6)-C(5)-H(5)	119.2
C(7)-C(6)-C(5)	121.73(13)
C(7)-C(6)-H(6)	119.1
C(5)-C(6)-H(6)	119.1
C(6)-C(7)-C(2)	116.51(14)
C(6)-C(7)-H(7)	121.7
C(2)-C(7)-H(7)	121.7
C(13)-C(8)-C(9)	122.87(13)
C(13)-C(8)-N(1)	118.30(12)
C(9)-C(8)-N(1)	118.72(12)
O(1)-C(9)-C(8)	119.38(12)
O(1)-C(9)-C(10)	122.21(12)
C(8)-C(9)-C(10)	118.39(12)
C(11)-C(10)-C(9)	117.17(12)
C(11)-C(10)-C(14)	122.15(12)
C(9)-C(10)-C(14)	120.68(12)
C(10)-C(11)-C(12)	124.54(13)
C(10)-C(11)-H(11)	117.7
C(12)-C(11)-H(11)	117.7
C(13)-C(12)-C(11)	117.26(13)
C(13)-C(12)-C(18)	122.23(13)
C(11)-C(12)-C(18)	120.51(12)
C(12)-C(13)-C(8)	119.74(13)
C(12)-C(13)-H(13)	120.1
C(8)-C(13)-H(13)	120.1
C(10)-C(14)-C(17)	111.77(12)
C(10)-C(14)-C(15)	110.03(11)
C(17)-C(14)-C(15)	106.88(12)
C(10)-C(14)-C(16)	109.92(11)
C(17)-C(14)-C(16)	107.87(12)
C(15)-C(14)-C(16)	110.30(12)
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(14)-C(17)-H(17A)	109.5
C(14)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(14)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(20)-C(18)-C(19)	110.06(17)
C(20)-C(18)-C(21)	108.28(15)
C(19)-C(18)-C(21)	106.97(16)
C(20)-C(18)-C(12)	109.85(12)
C(19)-C(18)-C(12)	109.41(13)
C(21)-C(18)-C(12)	112.22(13)
C(18)-C(19)-H(19A)	109.5

C(18)-C(19)-H(19B)	109.5	H(30B)-C(30)-H(30C)	109.5
H(19A)-C(19)-H(19B)	109.5	C(28)-C(31)-H(31A)	109.5
C(18)-C(19)-H(19C)	109.5	C(28)-C(31)-H(31B)	109.5
H(19A)-C(19)-H(19C)	109.5	H(31A)-C(31)-H(31B)	109.5
H(19B)-C(19)-H(19C)	109.5	C(28)-C(31)-H(31C)	109.5
C(18)-C(20)-H(20A)	109.5	H(31A)-C(31)-H(31C)	109.5
C(18)-C(20)-H(20B)	109.5	H(31B)-C(31)-H(31C)	109.5
H(20A)-C(20)-H(20B)	109.5	C(34)-C(32)-C(26)	108.55(12)
C(18)-C(20)-H(20C)	109.5	C(34)-C(32)-C(35)	108.47(14)
H(20A)-C(20)-H(20C)	109.5	C(26)-C(32)-C(35)	111.77(12)
H(20B)-C(20)-H(20C)	109.5	C(34)-C(32)-C(33)	109.61(14)
C(18)-C(21)-H(21A)	109.5	C(26)-C(32)-C(33)	110.80(12)
C(18)-C(21)-H(21B)	109.5	C(35)-C(32)-C(33)	107.59(14)
H(21A)-C(21)-H(21B)	109.5	C(32)-C(33)-H(33A)	109.5
C(18)-C(21)-H(21C)	109.5	C(32)-C(33)-H(33B)	109.5
H(21A)-C(21)-H(21C)	109.5	H(33A)-C(33)-H(33B)	109.5
H(21B)-C(21)-H(21C)	109.5	C(32)-C(33)-H(33C)	109.5
C(27)-C(22)-C(23)	123.05(12)	H(33A)-C(33)-H(33C)	109.5
C(27)-C(22)-N(2)	118.32(12)	H(33B)-C(33)-H(33C)	109.5
C(23)-C(22)-N(2)	118.58(12)	C(32)-C(34)-H(34A)	109.5
O(2)-C(23)-C(22)	119.43(12)	C(32)-C(34)-H(34B)	109.5
O(2)-C(23)-C(24)	122.39(12)	H(34A)-C(34)-H(34B)	109.5
C(22)-C(23)-C(24)	118.17(12)	C(32)-C(34)-H(34C)	109.5
C(25)-C(24)-C(23)	117.34(12)	H(34A)-C(34)-H(34C)	109.5
C(25)-C(24)-C(28)	121.48(12)	H(34B)-C(34)-H(34C)	109.5
C(23)-C(24)-C(28)	121.18(12)	C(32)-C(35)-H(35A)	109.5
C(26)-C(25)-C(24)	124.56(13)	C(32)-C(35)-H(35B)	109.5
C(26)-C(25)-H(25)	117.7	H(35A)-C(35)-H(35B)	109.5
C(24)-C(25)-H(25)	117.7	C(32)-C(35)-H(35C)	109.5
C(27)-C(26)-C(25)	117.10(12)	H(35A)-C(35)-H(35C)	109.5
C(27)-C(26)-C(32)	120.44(12)	H(35B)-C(35)-H(35C)	109.5
C(25)-C(26)-C(32)	122.41(12)	O(3)-C(36)-C(37)	109.24(12)
C(22)-C(27)-C(26)	119.78(13)	O(3)-C(36)-C(38)	108.59(12)
C(22)-C(27)-H(27)	120.1	C(37)-C(36)-C(38)	112.79(13)
C(26)-C(27)-H(27)	120.1	O(3)-C(36)-H(36)	108.7
C(31)-C(28)-C(29)	106.94(12)	C(37)-C(36)-H(36)	108.7
C(31)-C(28)-C(24)	110.44(11)	C(38)-C(36)-H(36)	108.7
C(29)-C(28)-C(24)	112.02(12)	C(36)-C(37)-H(37A)	109.5
C(31)-C(28)-C(30)	110.23(12)	C(36)-C(37)-H(37B)	109.5
C(29)-C(28)-C(30)	107.49(12)	H(37A)-C(37)-H(37B)	109.5
C(24)-C(28)-C(30)	109.66(12)	C(36)-C(37)-H(37C)	109.5
C(28)-C(29)-H(29A)	109.5	H(37A)-C(37)-H(37C)	109.5
C(28)-C(29)-H(29B)	109.5	H(37B)-C(37)-H(37C)	109.5
H(29A)-C(29)-H(29B)	109.5	C(36)-C(38)-H(38A)	109.5
C(28)-C(29)-H(29C)	109.5	C(36)-C(38)-H(38B)	109.5
H(29A)-C(29)-H(29C)	109.5	H(38A)-C(38)-H(38B)	109.5
H(29B)-C(29)-H(29C)	109.5	C(36)-C(38)-H(38C)	109.5
C(28)-C(30)-H(30A)	109.5	H(38A)-C(38)-H(38C)	109.5
C(28)-C(30)-H(30B)	109.5	H(38B)-C(38)-H(38C)	109.5
H(30A)-C(30)-H(30B)	109.5	C(2S)-C(1S)-C(6S)	120.03(19)
C(28)-C(30)-H(30C)	109.5	C(2S)-C(1S)-H(1S)	120.0
H(30A)-C(30)-H(30C)	109.5	C(6S)-C(1S)-H(1S)	120.0

C(1S)-C(2S)-C(3S)	119.96(19)	C(3S)-C(4S)-H(4S)	120.0
C(1S)-C(2S)-H(2S)	120.0	C(4S)-C(5S)-C(6S)	120.2(2)
C(3S)-C(2S)-H(2S)	120.0	C(4S)-C(5S)-H(5S)	119.9
C(4S)-C(3S)-C(2S)	119.8(2)	C(6S)-C(5S)-H(5S)	119.9
C(4S)-C(3S)-H(3S)	120.1	C(5S)-C(6S)-C(1S)	119.9(2)
C(2S)-C(3S)-H(3S)	120.1	C(5S)-C(6S)-H(6S)	120.1
C(5S)-C(4S)-C(3S)	120.0(2)	C(1S)-C(6S)-H(6S)	120.1
C(5S)-C(4S)-H(4S)	120.0		

Symmetry transformations used to generate equivalent atoms:

Table S9. Torsion angles [°] for **5''**.

C(2)-N(1)-C(1)-N(2)	1.01(16)	C(13)-C(8)-C(9)-C(10)	-1.8(2)
C(8)-N(1)-C(1)-N(2)	-171.35(12)	N(1)-C(8)-C(9)-C(10)	174.34(12)
N(1)-C(1)-N(2)-C(3)	-1.31(16)	O(1)-C(9)-C(10)-C(11)	179.91(12)
N(1)-C(1)-N(2)-C(22)	170.90(12)	C(8)-C(9)-C(10)-C(11)	1.34(19)
C(1)-N(1)-C(2)-C(3)	-0.30(15)	O(1)-C(9)-C(10)-C(14)	0.2(2)
C(8)-N(1)-C(2)-C(3)	172.13(12)	C(8)-C(9)-C(10)-C(14)	-178.32(12)
C(1)-N(1)-C(2)-C(7)	-179.87(15)	C(9)-C(10)-C(11)-C(12)	0.3(2)
C(8)-N(1)-C(2)-C(7)	-7.4(2)	C(14)-C(10)-C(11)-C(12)	179.93(13)
O(1)-Zr(1)-O(3)-C(36)	-76.2(3)	C(10)-C(11)-C(12)-C(13)	-1.5(2)
O(2)-Zr(1)-O(3)-C(36)	107.3(3)	C(10)-C(11)-C(12)-C(18)	178.86(13)
Cl(2)-Zr(1)-O(3)-C(36)	14.3(3)	C(11)-C(12)-C(13)-C(8)	1.1(2)
Cl(1)-Zr(1)-O(3)-C(36)	-164.1(3)	C(18)-C(12)-C(13)-C(8)	-179.30(13)
C(7)-C(2)-C(3)-C(4)	-1.1(2)	C(9)-C(8)-C(13)-C(12)	0.5(2)
N(1)-C(2)-C(3)-C(4)	179.27(13)	N(1)-C(8)-C(13)-C(12)	-175.61(13)
C(7)-C(2)-C(3)-N(2)	179.14(13)	C(11)-C(10)-C(14)-C(17)	-2.87(19)
N(1)-C(2)-C(3)-N(2)	-0.47(14)	C(9)-C(10)-C(14)-C(17)	176.78(13)
C(1)-N(2)-C(3)-C(2)	1.09(15)	C(11)-C(10)-C(14)-C(15)	-121.45(14)
C(22)-N(2)-C(3)-C(2)	-171.10(12)	C(9)-C(10)-C(14)-C(15)	58.20(17)
C(1)-N(2)-C(3)-C(4)	-178.62(15)	C(11)-C(10)-C(14)-C(16)	116.88(14)
C(22)-N(2)-C(3)-C(4)	9.2(2)	C(9)-C(10)-C(14)-C(16)	-63.47(17)
C(2)-C(3)-C(4)-C(5)	-0.2(2)	C(13)-C(12)-C(18)-C(20)	-114.32(17)
N(2)-C(3)-C(4)-C(5)	179.47(14)	C(11)-C(12)-C(18)-C(20)	65.29(19)
C(3)-C(4)-C(5)-C(6)	0.9(2)	C(13)-C(12)-C(18)-C(19)	124.75(17)
C(4)-C(5)-C(6)-C(7)	-0.4(2)	C(11)-C(12)-C(18)-C(19)	-55.63(19)
C(5)-C(6)-C(7)-C(2)	-0.8(2)	C(13)-C(12)-C(18)-C(21)	6.2(2)
C(3)-C(2)-C(7)-C(6)	1.6(2)	C(11)-C(12)-C(18)-C(21)	-174.20(15)
N(1)-C(2)-C(7)-C(6)	-178.89(15)	C(1)-N(2)-C(22)-C(27)	128.48(15)
C(1)-N(1)-C(8)-C(13)	-129.61(15)	C(3)-N(2)-C(22)-C(27)	-60.65(19)
C(2)-N(1)-C(8)-C(13)	59.29(19)	C(1)-N(2)-C(22)-C(23)	-54.03(19)
C(1)-N(1)-C(8)-C(9)	54.1(2)	C(3)-N(2)-C(22)-C(23)	116.84(15)
C(2)-N(1)-C(8)-C(9)	-117.02(15)	Zr(1)-O(2)-C(23)-C(22)	37.2(4)
Zr(1)-O(1)-C(9)-C(8)	-19.5(4)	Zr(1)-O(2)-C(23)-C(24)	-144.2(2)
Zr(1)-O(1)-C(9)-C(10)	161.9(3)	C(27)-C(22)-C(23)-O(2)	178.33(13)
C(13)-C(8)-C(9)-O(1)	179.60(13)	N(2)-C(22)-C(23)-O(2)	0.97(19)
N(1)-C(8)-C(9)-O(1)	-4.27(19)	C(27)-C(22)-C(23)-C(24)	-0.3(2)

N(2)-C(22)-C(23)-C(24)	-177.62(12)	C(25)-C(24)-C(28)-C(30)	-117.97(15)
O(2)-C(23)-C(24)-C(25)	-178.61(13)	C(23)-C(24)-C(28)-C(30)	63.06(17)
C(22)-C(23)-C(24)-C(25)	-0.07(19)	C(27)-C(26)-C(32)-C(34)	80.86(17)
O(2)-C(23)-C(24)-C(28)	0.4(2)	C(25)-C(26)-C(32)-C(34)	-96.43(17)
C(22)-C(23)-C(24)-C(28)	178.94(12)	C(27)-C(26)-C(32)-C(35)	-159.55(14)
C(23)-C(24)-C(25)-C(26)	0.0(2)	C(25)-C(26)-C(32)-C(35)	23.2(2)
C(28)-C(24)-C(25)-C(26)	-178.97(13)	C(27)-C(26)-C(32)-C(33)	-39.55(19)
C(24)-C(25)-C(26)-C(27)	0.3(2)	C(25)-C(26)-C(32)-C(33)	143.17(15)
C(24)-C(25)-C(26)-C(32)	177.68(13)	Zr(1)-O(3)-C(36)-C(37)	-139.5(3)
C(23)-C(22)-C(27)-C(26)	0.6(2)	Zr(1)-O(3)-C(36)-C(38)	97.1(3)
N(2)-C(22)-C(27)-C(26)	177.99(12)	C(6S)-C(1S)-C(2S)-C(3S)	0.4(3)
C(25)-C(26)-C(27)-C(22)	-0.6(2)	C(1S)-C(2S)-C(3S)-C(4S)	-0.1(3)
C(32)-C(26)-C(27)-C(22)	-178.04(13)	C(2S)-C(3S)-C(4S)-C(5S)	-0.4(3)
C(25)-C(24)-C(28)-C(31)	120.36(14)	C(3S)-C(4S)-C(5S)-C(6S)	0.5(3)
C(23)-C(24)-C(28)-C(31)	-58.61(17)	C(4S)-C(5S)-C(6S)-C(1S)	-0.2(3)
C(25)-C(24)-C(28)-C(29)	1.28(19)	C(2S)-C(1S)-C(6S)-C(5S)	-0.3(3)
C(23)-C(24)-C(28)-C(29)	-177.69(13)		

Symmetry transformations used to generate equivalent atoms:

Table S10. Bond lengths [Å] and angles [°] for **6**.

Zr(1)-O(4)	1.9263(17)	C(2T)-H(2T)	0.9500
Zr(1)-O(2)	2.0429(17)	Zr(3)-O(12)	1.9231(17)
Zr(1)-O(1)	2.0498(18)	Zr(3)-O(9)	2.0517(17)
Zr(1)-O(3)#1	2.1289(19)	Zr(3)-O(10)	2.0524(17)
Zr(1)-O(3)	2.146(2)	Zr(3)-O(11)	2.1335(19)
Zr(1)-C(1)	2.400(3)	Zr(3)-O(7)	2.1399(18)
Zr(1)-Zr(1)#1	3.5346(5)	Zr(3)-C(71)	2.402(3)
O(1)-C(7)	1.346(3)	O(3)-H(3O)	0.65(4)
N(1)-C(1)	1.359(3)	N(3)-C(36)	1.355(3)
N(1)-C(16)	1.398(3)	N(3)-C(51)	1.403(3)
N(1)-C(2)	1.431(3)	N(3)-C(37)	1.437(3)
C(1)-N(2)	1.360(3)	C(3)-C(4)	1.380(4)
C(1T)-C(6T)	1.368(5)	C(3)-H(3)	0.9500
C(1T)-C(2T)	1.398(5)	C(3T)-C(4T)	1.363(6)
C(1T)-C(7T)	1.487(5)	C(3T)-H(3T)	0.9500
Zr(2)-O(8)	1.9257(17)	O(4)-C(106)	1.410(3)
Zr(2)-O(6)	2.0413(17)	N(4)-C(36)	1.361(3)
Zr(2)-O(5)	2.0531(17)	N(4)-C(56)	1.406(3)
Zr(2)-O(7)	2.1284(18)	N(4)-C(57)	1.435(3)
Zr(2)-O(11)	2.1340(19)	C(4)-C(5)	1.398(4)
Zr(2)-C(36)	2.415(3)	C(4)-C(8)	1.540(4)
Zr(2)-Zr(3)	3.5343(4)	C(4T)-C(5T)	1.384(6)
O(2)-C(23)	1.345(3)	C(4T)-H(4T)	0.9500
N(2)-C(21)	1.396(3)	O(5)-C(42)	1.337(3)
N(2)-C(22)	1.433(3)	N(5)-C(71)	1.350(3)
C(2)-C(7)	1.394(4)	N(5)-C(86)	1.402(3)
C(2)-C(3)	1.395(4)	N(5)-C(72)	1.430(3)
C(2T)-C(3T)	1.372(5)	C(5)-C(6)	1.391(4)

C(5)-H(5)	0.9500	C(14T)-H(14D)	0.9800
C(5T)-C(6T)	1.389(5)	C(14T)-H(14E)	0.9800
C(5T)-H(5T)	0.9500	C(14T)-H(14F)	0.9800
O(6)-C(58)	1.346(3)	C(15)-H(15A)	0.9800
N(6)-C(71)	1.359(3)	C(15)-H(15B)	0.9800
N(6)-C(91)	1.395(3)	C(15)-H(15C)	0.9800
N(6)-C(92)	1.432(3)	C(15T)-C(16T)	1.383(4)
C(6)-C(7)	1.425(4)	C(15T)-C(20T)	1.394(4)
C(6)-C(12)	1.534(4)	C(15T)-C(21T)	1.505(5)
C(6T)-H(6T)	0.9500	C(16)-C(21)	1.391(4)
O(7)-H(7O)	0.76(4)	C(16)-C(17)	1.393(4)
C(7T)-H(7TA)	0.9800	C(16T)-C(17T)	1.383(5)
C(7T)-H(7TB)	0.9800	C(16T)-H(16T)	0.9500
C(7T)-H(7TC)	0.9800	C(17)-C(18)	1.378(4)
O(8)-C(109)	1.413(3)	C(17)-H(17)	0.9500
C(8)-C(10)	1.527(4)	C(17T)-C(18T)	1.375(5)
C(8)-C(11)	1.531(4)	C(17T)-H(17T)	0.9500
C(8)-C(9)	1.531(4)	C(18)-C(19)	1.408(4)
C(8T)-C(13T)	1.348(7)	C(18)-H(18)	0.9500
C(8T)-C(9T)	1.449(7)	C(18T)-C(19T)	1.380(4)
C(8T)-C(14T)	1.502(7)	C(18T)-H(18T)	0.9500
O(9)-C(73)	1.345(3)	C(19)-C(20)	1.378(4)
C(9)-H(9A)	0.9800	C(19)-H(19)	0.9500
C(9)-H(9B)	0.9800	C(19T)-C(20T)	1.376(4)
C(9)-H(9C)	0.9800	C(19T)-H(19T)	0.9500
C(9T)-C(10T)	1.402(6)	C(20)-C(21)	1.395(4)
C(9T)-H(9T)	0.9500	C(20)-H(20)	0.9500
O(10)-C(93)	1.346(3)	C(20T)-H(20T)	0.9500
C(10)-H(10A)	0.9800	C(21T)-H(21A)	0.9800
C(10)-H(10B)	0.9800	C(21T)-H(21B)	0.9800
C(10)-H(10C)	0.9800	C(21T)-H(21C)	0.9800
C(10T)-C(11T)	1.410(7)	C(22)-C(27)	1.384(4)
C(10T)-H(10T)	0.9500	C(22)-C(23)	1.407(4)
O(11)-H(11O)	0.70(4)	C(23)-C(24)	1.415(4)
C(11)-H(11A)	0.9800	C(24)-C(25)	1.400(4)
C(11)-H(11B)	0.9800	C(24)-C(28)	1.532(4)
C(11)-H(11C)	0.9800	C(25)-C(26)	1.390(4)
C(11T)-C(12T)	1.353(6)	C(25)-H(25)	0.9500
C(11T)-H(11T)	0.9500	C(26)-C(27)	1.393(4)
O(12)-C(112)	1.412(3)	C(26)-C(32)	1.535(4)
C(12)-C(15)	1.530(4)	C(27)-H(27)	0.9500
C(12)-C(13)	1.536(4)	C(28)-C(31)	1.535(4)
C(12)-C(14)	1.542(4)	C(28)-C(29)	1.537(4)
C(12T)-C(13T)	1.425(7)	C(28)-C(30)	1.542(4)
C(12T)-H(12T)	0.9500	C(29)-H(29A)	0.9800
C(13)-H(13A)	0.9800	C(29)-H(29B)	0.9800
C(13)-H(13B)	0.9800	C(29)-H(29C)	0.9800
C(13)-H(13C)	0.9800	C(30)-H(30A)	0.9800
C(13T)-H(13T)	0.9500	C(30)-H(30B)	0.9800
C(14)-H(14A)	0.9800	C(30)-H(30C)	0.9800
C(14)-H(14B)	0.9800	C(31)-H(31A)	0.9800
C(14)-H(14C)	0.9800	C(31)-H(31B)	0.9800

C(31)-H(31C)	0.9800	C(53)-H(53)	0.9500
C(32)-C(34)	1.531(4)	C(54)-C(55)	1.384(4)
C(32)-C(33)	1.532(4)	C(54)-H(54)	0.9500
C(32)-C(35)	1.532(4)	C(55)-C(56)	1.392(4)
C(33)-H(33A)	0.9800	C(55)-H(55)	0.9500
C(33)-H(33B)	0.9800	C(57)-C(62)	1.385(4)
C(33)-H(33C)	0.9800	C(57)-C(58)	1.409(4)
C(34)-H(34A)	0.9800	C(58)-C(59)	1.413(4)
C(34)-H(34B)	0.9800	C(59)-C(60)	1.395(4)
C(34)-H(34C)	0.9800	C(59)-C(63)	1.540(4)
C(35)-H(35A)	0.9800	C(60)-C(61)	1.389(4)
C(35)-H(35B)	0.9800	C(60)-H(60)	0.9500
C(35)-H(35C)	0.9800	C(61)-C(62)	1.392(4)
C(37)-C(38)	1.384(4)	C(61)-C(67)	1.540(4)
C(37)-C(42)	1.409(4)	C(62)-H(62)	0.9500
C(38)-C(39)	1.393(4)	C(63)-C(66)	1.530(4)
C(38)-H(38)	0.9500	C(63)-C(65)	1.535(4)
C(39)-C(40)	1.393(4)	C(63)-C(64)	1.541(4)
C(39)-C(43)	1.539(4)	C(64)-H(64A)	0.9800
C(40)-C(41)	1.393(4)	C(64)-H(64B)	0.9800
C(40)-H(40)	0.9500	C(64)-H(64C)	0.9800
C(41)-C(42)	1.422(4)	C(65)-H(65A)	0.9800
C(41)-C(47)	1.539(4)	C(65)-H(65B)	0.9800
C(43)-C(46)	1.531(4)	C(65)-H(65C)	0.9800
C(43)-C(45)	1.533(4)	C(66)-H(66A)	0.9800
C(43)-C(44)	1.538(4)	C(66)-H(66B)	0.9800
C(44)-H(44A)	0.9800	C(66)-H(66C)	0.9800
C(44)-H(44B)	0.9800	C(67)-C(69)	1.531(4)
C(44)-H(44C)	0.9800	C(67)-C(70)	1.536(4)
C(45)-H(45A)	0.9800	C(67)-C(68)	1.537(4)
C(45)-H(45B)	0.9800	C(68)-H(68A)	0.9800
C(45)-H(45C)	0.9800	C(68)-H(68B)	0.9800
C(46)-H(46A)	0.9800	C(68)-H(68C)	0.9800
C(46)-H(46B)	0.9800	C(69)-H(69A)	0.9800
C(46)-H(46C)	0.9800	C(69)-H(69B)	0.9800
C(47)-C(50)	1.530(4)	C(69)-H(69C)	0.9800
C(47)-C(49)	1.533(4)	C(70)-H(70A)	0.9800
C(47)-C(48)	1.536(4)	C(70)-H(70B)	0.9800
C(48)-H(48A)	0.9800	C(70)-H(70C)	0.9800
C(48)-H(48B)	0.9800	C(72)-C(77)	1.385(4)
C(48)-H(48C)	0.9800	C(72)-C(73)	1.402(4)
C(49)-H(49A)	0.9800	C(73)-C(74)	1.419(4)
C(49)-H(49B)	0.9800	C(74)-C(75)	1.394(4)
C(49)-H(49C)	0.9800	C(74)-C(78)	1.538(4)
C(50)-H(50A)	0.9800	C(75)-C(76)	1.397(4)
C(50)-H(50B)	0.9800	C(75)-H(75)	0.9500
C(50)-H(50C)	0.9800	C(76)-C(77)	1.384(4)
C(51)-C(52)	1.389(4)	C(76)-C(82)	1.535(4)
C(51)-C(56)	1.393(4)	C(77)-H(77)	0.9500
C(52)-C(53)	1.380(4)	C(78)-C(79)	1.526(4)
C(52)-H(52)	0.9500	C(78)-C(81)	1.536(4)
C(53)-C(54)	1.395(4)	C(78)-C(80)	1.537(4)

C(79)-H(79A)	0.9800	C(101)-H(10I)	0.9800
C(79)-H(79B)	0.9800	C(102)-C(14A)	1.472(10)
C(79)-H(79C)	0.9800	C(102)-C(103)	1.509(5)
C(80)-H(80A)	0.9800	C(102)-C(105)	1.517(5)
C(80)-H(80B)	0.9800	C(102)-C(13A)	1.520(10)
C(80)-H(80C)	0.9800	C(102)-C(104)	1.554(5)
C(81)-H(81A)	0.9800	C(102)-C(15A)	1.588(10)
C(81)-H(81B)	0.9800	C(103)-H(10J)	0.9800
C(81)-H(81C)	0.9800	C(103)-H(10K)	0.9800
C(82)-C(85)	1.525(4)	C(103)-H(10L)	0.9800
C(82)-C(84)	1.530(4)	C(104)-H(10M)	0.9800
C(82)-C(83)	1.531(4)	C(104)-H(10N)	0.9800
C(83)-H(83A)	0.9800	C(104)-H(10O)	0.9800
C(83)-H(83B)	0.9800	C(105)-H(10P)	0.9800
C(83)-H(83C)	0.9800	C(105)-H(10Q)	0.9800
C(84)-H(84A)	0.9800	C(105)-H(10R)	0.9800
C(84)-H(84B)	0.9800	C(13A)-H(13D)	0.9800
C(84)-H(84C)	0.9800	C(13A)-H(13E)	0.9800
C(85)-H(85A)	0.9800	C(13A)-H(13F)	0.9800
C(85)-H(85B)	0.9800	C(14A)-H(14G)	0.9800
C(85)-H(85C)	0.9800	C(14A)-H(14H)	0.9800
C(86)-C(91)	1.391(4)	C(14A)-H(14I)	0.9800
C(86)-C(87)	1.393(4)	C(15A)-H(15D)	0.9800
C(87)-C(88)	1.376(4)	C(15A)-H(15E)	0.9800
C(87)-H(87)	0.9500	C(15A)-H(15F)	0.9800
C(88)-C(89)	1.396(4)	C(106)-C(108)	1.513(4)
C(88)-H(88)	0.9500	C(106)-C(107)	1.513(4)
C(89)-C(90)	1.379(4)	C(106)-H(106)	1.0000
C(89)-H(89)	0.9500	C(107)-H(10S)	0.9800
C(90)-C(91)	1.396(4)	C(107)-H(10U)	0.9800
C(90)-H(90)	0.9500	C(107)-H(10V)	0.9800
C(92)-C(97)	1.379(4)	C(108)-H(10W)	0.9800
C(92)-C(93)	1.410(4)	C(108)-H(10X)	0.9800
C(93)-C(94)	1.413(4)	C(108)-H(10Y)	0.9800
C(94)-C(95)	1.396(4)	C(109)-C(111)	1.512(4)
C(94)-C(98)	1.535(4)	C(109)-C(110)	1.515(4)
C(95)-C(96)	1.396(4)	C(109)-H(109)	1.0000
C(95)-H(95)	0.9500	C(110)-H(11D)	0.9800
C(96)-C(97)	1.389(4)	C(110)-H(11E)	0.9800
C(96)-C(102)	1.539(4)	C(110)-H(11F)	0.9800
C(97)-H(97)	0.9500	C(111)-H(11G)	0.9800
C(98)-C(100)	1.529(4)	C(111)-H(11H)	0.9800
C(98)-C(99)	1.540(4)	C(111)-H(11I)	0.9800
C(98)-C(101)	1.543(4)	C(112)-C(114)	1.508(4)
C(99)-H(99A)	0.9800	C(112)-C(113)	1.515(4)
C(99)-H(99B)	0.9800	C(112)-H(112)	1.0000
C(99)-H(99C)	0.9800	C(113)-H(11J)	0.9800
C(100)-H(10D)	0.9800	C(113)-H(11K)	0.9800
C(100)-H(10E)	0.9800	C(113)-H(11L)	0.9800
C(100)-H(10F)	0.9800	C(114)-H(11N)	0.9800
C(101)-H(10G)	0.9800	C(114)-H(11M)	0.9800
C(101)-H(10H)	0.9800	C(114)-H(11P)	0.9800

O(4)-Zr(1)-O(2)	97.25(7)
O(4)-Zr(1)-O(1)	95.10(7)
O(2)-Zr(1)-O(1)	113.84(7)
O(4)-Zr(1)-O(3)#1	102.12(8)
O(2)-Zr(1)-O(3)#1	150.07(7)
O(1)-Zr(1)-O(3)#1	87.07(7)
O(4)-Zr(1)-O(3)	102.74(8)
O(2)-Zr(1)-O(3)	85.22(7)
O(1)-Zr(1)-O(3)	152.11(7)
O(3)#1-Zr(1)-O(3)	68.46(9)
O(4)-Zr(1)-C(1)	161.56(8)
O(2)-Zr(1)-C(1)	74.16(8)
O(1)-Zr(1)-C(1)	74.39(8)
O(3)#1-Zr(1)-C(1)	92.58(8)
O(3)-Zr(1)-C(1)	92.92(8)
O(4)-Zr(1)-Zr(1)#1	105.09(6)
O(2)-Zr(1)-Zr(1)#1	118.12(5)
O(1)-Zr(1)-Zr(1)#1	120.39(5)
O(3)#1-Zr(1)-Zr(1)#1	34.39(5)
O(3)-Zr(1)-Zr(1)#1	34.07(5)
C(1)-Zr(1)-Zr(1)#1	93.33(6)
C(7)-O(1)-Zr(1)	130.50(15)
C(1)-N(1)-C(16)	111.3(2)
C(1)-N(1)-C(2)	122.8(2)
C(16)-N(1)-C(2)	125.8(2)
N(1)-C(1)-N(2)	105.3(2)
N(1)-C(1)-Zr(1)	124.35(18)
N(2)-C(1)-Zr(1)	125.13(18)
C(6T)-C(1T)-C(2T)	117.7(3)
C(6T)-C(1T)-C(7T)	121.9(3)
C(2T)-C(1T)-C(7T)	120.4(3)
O(8)-Zr(2)-O(6)	98.30(7)
O(8)-Zr(2)-O(5)	95.99(7)
O(6)-Zr(2)-O(5)	113.35(7)
O(8)-Zr(2)-O(7)	103.07(7)
O(6)-Zr(2)-O(7)	86.22(7)
O(5)-Zr(2)-O(7)	150.44(7)
O(8)-Zr(2)-O(11)	99.70(7)
O(6)-Zr(2)-O(11)	151.47(7)
O(5)-Zr(2)-O(11)	86.56(7)
O(7)-Zr(2)-O(11)	68.26(7)
O(8)-Zr(2)-C(36)	163.03(8)
O(6)-Zr(2)-C(36)	74.33(8)
O(5)-Zr(2)-C(36)	73.81(8)
O(7)-Zr(2)-C(36)	91.82(8)
O(11)-Zr(2)-C(36)	93.30(8)
O(8)-Zr(2)-Zr(3)	104.88(5)
O(6)-Zr(2)-Zr(3)	119.17(5)
O(5)-Zr(2)-Zr(3)	118.88(5)
O(7)-Zr(2)-Zr(3)	34.21(5)
O(11)-Zr(2)-Zr(3)	34.08(5)
C(36)-Zr(2)-Zr(3)	92.00(6)
C(23)-O(2)-Zr(1)	130.78(15)
C(1)-N(2)-C(21)	111.5(2)
C(1)-N(2)-C(22)	122.6(2)
C(21)-N(2)-C(22)	125.6(2)
C(7)-C(2)-C(3)	122.7(2)
C(7)-C(2)-N(1)	119.0(2)
C(3)-C(2)-N(1)	118.3(2)
C(3T)-C(2T)-C(1T)	120.5(4)
C(3T)-C(2T)-H(2T)	119.8
C(1T)-C(2T)-H(2T)	119.8
O(12)-Zr(3)-O(9)	96.39(7)
O(12)-Zr(3)-O(10)	93.60(7)
O(9)-Zr(3)-O(10)	116.55(7)
O(12)-Zr(3)-O(11)	101.03(7)
O(9)-Zr(3)-O(11)	150.10(7)
O(10)-Zr(3)-O(11)	86.54(7)
O(12)-Zr(3)-O(7)	104.74(7)
O(9)-Zr(3)-O(7)	84.15(7)
O(10)-Zr(3)-O(7)	150.86(7)
O(11)-Zr(3)-O(7)	68.06(7)
O(12)-Zr(3)-C(71)	158.56(8)
O(9)-Zr(3)-C(71)	74.89(8)
O(10)-Zr(3)-C(71)	73.82(8)
O(11)-Zr(3)-C(71)	95.56(8)
O(7)-Zr(3)-C(71)	93.97(8)
O(12)-Zr(3)-Zr(2)	104.52(5)
O(9)-Zr(3)-Zr(2)	117.67(5)
O(10)-Zr(3)-Zr(2)	119.73(5)
O(11)-Zr(3)-Zr(2)	34.09(5)
O(7)-Zr(3)-Zr(2)	34.00(5)
C(71)-Zr(3)-Zr(2)	96.84(6)
Zr(1)#1-O(3)-Zr(1)	111.55(8)
Zr(1)#1-O(3)-H(3O)	121(3)
Zr(1)-O(3)-H(3O)	128(3)
C(36)-N(3)-C(51)	111.7(2)
C(36)-N(3)-C(37)	122.9(2)
C(51)-N(3)-C(37)	125.1(2)
C(4)-C(3)-C(2)	120.3(3)
C(4)-C(3)-H(3)	119.8
C(2)-C(3)-H(3)	119.8
C(4T)-C(3T)-C(2T)	121.3(4)
C(4T)-C(3T)-H(3T)	119.3
C(2T)-C(3T)-H(3T)	119.3
C(106)-O(4)-Zr(1)	169.88(18)
C(36)-N(4)-C(56)	111.1(2)
C(36)-N(4)-C(57)	123.7(2)
C(56)-N(4)-C(57)	125.0(2)
C(3)-C(4)-C(5)	117.0(2)
C(3)-C(4)-C(8)	122.1(2)
C(5)-C(4)-C(8)	120.8(2)
C(3T)-C(4T)-C(5T)	119.2(4)

C(3T)-C(4T)-H(4T)	120.4	C(10T)-C(9T)-H(9T)	122.7
C(5T)-C(4T)-H(4T)	120.4	C(8T)-C(9T)-H(9T)	122.7
C(42)-O(5)-Zr(2)	130.23(15)	C(93)-O(10)-Zr(3)	129.65(15)
C(71)-N(5)-C(86)	111.3(2)	C(8)-C(10)-H(10A)	109.5
C(71)-N(5)-C(72)	123.0(2)	C(8)-C(10)-H(10B)	109.5
C(86)-N(5)-C(72)	125.6(2)	H(10A)-C(10)-H(10B)	109.5
C(6)-C(5)-C(4)	124.5(3)	C(8)-C(10)-H(10C)	109.5
C(6)-C(5)-H(5)	117.8	H(10A)-C(10)-H(10C)	109.5
C(4)-C(5)-H(5)	117.8	H(10B)-C(10)-H(10C)	109.5
C(4T)-C(5T)-C(6T)	119.3(4)	C(9T)-C(10T)-C(11T)	125.9(4)
C(4T)-C(5T)-H(5T)	120.3	C(9T)-C(10T)-H(10T)	117.1
C(6T)-C(5T)-H(5T)	120.3	C(11T)-C(10T)-H(10T)	117.1
C(58)-O(6)-Zr(2)	131.97(15)	Zr(3)-O(11)-Zr(2)	111.83(9)
C(71)-N(6)-C(91)	111.1(2)	Zr(3)-O(11)-H(11O)	120(3)
C(71)-N(6)-C(92)	122.2(2)	Zr(2)-O(11)-H(11O)	128(3)
C(91)-N(6)-C(92)	126.6(2)	C(8)-C(11)-H(11A)	109.5
C(5)-C(6)-C(7)	117.5(2)	C(8)-C(11)-H(11B)	109.5
C(5)-C(6)-C(12)	121.7(2)	H(11A)-C(11)-H(11B)	109.5
C(7)-C(6)-C(12)	120.8(2)	C(8)-C(11)-H(11C)	109.5
C(1T)-C(6T)-C(5T)	121.9(4)	H(11A)-C(11)-H(11C)	109.5
C(1T)-C(6T)-H(6T)	119.0	H(11B)-C(11)-H(11C)	109.5
C(5T)-C(6T)-H(6T)	119.0	C(12T)-C(11T)-C(10T)	118.0(5)
Zr(2)-O(7)-Zr(3)	111.80(8)	C(12T)-C(11T)-H(11T)	121.0
Zr(2)-O(7)-H(7O)	122(3)	C(10T)-C(11T)-H(11T)	121.0
Zr(3)-O(7)-H(7O)	126(3)	C(112)-O(12)-Zr(3)	164.79(17)
O(1)-C(7)-C(2)	120.4(2)	C(15)-C(12)-C(6)	110.2(2)
O(1)-C(7)-C(6)	121.7(2)	C(15)-C(12)-C(13)	107.8(2)
C(2)-C(7)-C(6)	117.9(2)	C(6)-C(12)-C(13)	112.2(2)
C(1T)-C(7T)-H(7TA)	109.5	C(15)-C(12)-C(14)	109.2(2)
C(1T)-C(7T)-H(7TB)	109.5	C(6)-C(12)-C(14)	110.3(2)
H(7TA)-C(7T)-H(7TB)	109.5	C(13)-C(12)-C(14)	107.0(2)
C(1T)-C(7T)-H(7TC)	109.5	C(11T)-C(12T)-C(13T)	117.6(6)
H(7TA)-C(7T)-H(7TC)	109.5	C(11T)-C(12T)-H(12T)	121.2
H(7TB)-C(7T)-H(7TC)	109.5	C(13T)-C(12T)-H(12T)	121.2
C(109)-O(8)-Zr(2)	166.93(17)	C(12)-C(13)-H(13A)	109.5
C(10)-C(8)-C(11)	109.9(3)	C(12)-C(13)-H(13B)	109.5
C(10)-C(8)-C(9)	108.0(2)	H(13A)-C(13)-H(13B)	109.5
C(11)-C(8)-C(9)	107.5(2)	C(12)-C(13)-H(13C)	109.5
C(10)-C(8)-C(4)	108.9(2)	H(13A)-C(13)-H(13C)	109.5
C(11)-C(8)-C(4)	110.7(2)	H(13B)-C(13)-H(13C)	109.5
C(9)-C(8)-C(4)	111.7(2)	C(8T)-C(13T)-C(12T)	125.5(4)
C(13T)-C(8T)-C(9T)	118.4(5)	C(8T)-C(13T)-H(13T)	117.2
C(13T)-C(8T)-C(14T)	124.8(4)	C(12T)-C(13T)-H(13T)	117.2
C(9T)-C(8T)-C(14T)	116.7(5)	C(12)-C(14)-H(14A)	109.5
C(73)-O(9)-Zr(3)	129.20(15)	C(12)-C(14)-H(14B)	109.5
C(8)-C(9)-H(9A)	109.5	H(14A)-C(14)-H(14B)	109.5
C(8)-C(9)-H(9B)	109.5	C(12)-C(14)-H(14C)	109.5
H(9A)-C(9)-H(9B)	109.5	H(14A)-C(14)-H(14C)	109.5
C(8)-C(9)-H(9C)	109.5	H(14B)-C(14)-H(14C)	109.5
H(9A)-C(9)-H(9C)	109.5	C(8T)-C(14T)-H(14D)	109.5
H(9B)-C(9)-H(9C)	109.5	C(8T)-C(14T)-H(14E)	109.5
C(10T)-C(9T)-C(8T)	114.6(6)	H(14D)-C(14T)-H(14E)	109.5

C(8T)-C(14T)-H(14F)	109.5	C(27)-C(22)-N(2)	118.9(2)
H(14D)-C(14T)-H(14F)	109.5	C(23)-C(22)-N(2)	118.9(2)
H(14E)-C(14T)-H(14F)	109.5	O(2)-C(23)-C(22)	120.7(2)
C(12)-C(15)-H(15A)	109.5	O(2)-C(23)-C(24)	121.1(2)
C(12)-C(15)-H(15B)	109.5	C(22)-C(23)-C(24)	118.2(2)
H(15A)-C(15)-H(15B)	109.5	C(25)-C(24)-C(23)	117.6(2)
C(12)-C(15)-H(15C)	109.5	C(25)-C(24)-C(28)	121.6(2)
H(15A)-C(15)-H(15C)	109.5	C(23)-C(24)-C(28)	120.8(2)
H(15B)-C(15)-H(15C)	109.5	C(26)-C(25)-C(24)	124.3(3)
C(16T)-C(15T)-C(20T)	117.8(3)	C(26)-C(25)-H(25)	117.9
C(16T)-C(15T)-C(21T)	121.6(3)	C(24)-C(25)-H(25)	117.9
C(20T)-C(15T)-C(21T)	120.6(3)	C(25)-C(26)-C(27)	117.2(2)
C(21)-C(16)-C(17)	121.4(3)	C(25)-C(26)-C(32)	123.6(3)
C(21)-C(16)-N(1)	106.1(2)	C(27)-C(26)-C(32)	119.3(2)
C(17)-C(16)-N(1)	132.3(3)	C(22)-C(27)-C(26)	120.4(2)
C(15T)-C(16T)-C(17T)	121.2(3)	C(22)-C(27)-H(27)	119.8
C(15T)-C(16T)-H(16T)	119.4	C(26)-C(27)-H(27)	119.8
C(17T)-C(16T)-H(16T)	119.4	C(24)-C(28)-C(31)	112.0(2)
C(18)-C(17)-C(16)	117.3(3)	C(24)-C(28)-C(29)	110.4(2)
C(18)-C(17)-H(17)	121.3	C(31)-C(28)-C(29)	107.2(2)
C(16)-C(17)-H(17)	121.3	C(24)-C(28)-C(30)	109.9(2)
C(18T)-C(17T)-C(16T)	120.3(3)	C(31)-C(28)-C(30)	107.2(2)
C(18T)-C(17T)-H(17T)	119.9	C(29)-C(28)-C(30)	110.0(2)
C(16T)-C(17T)-H(17T)	119.9	C(28)-C(29)-H(29A)	109.5
C(17)-C(18)-C(19)	121.3(3)	C(28)-C(29)-H(29B)	109.5
C(17)-C(18)-H(18)	119.3	H(29A)-C(29)-H(29B)	109.5
C(19)-C(18)-H(18)	119.3	C(28)-C(29)-H(29C)	109.5
C(17T)-C(18T)-C(19T)	119.3(3)	H(29A)-C(29)-H(29C)	109.5
C(17T)-C(18T)-H(18T)	120.3	H(29B)-C(29)-H(29C)	109.5
C(19T)-C(18T)-H(18T)	120.3	C(28)-C(30)-H(30A)	109.5
C(20)-C(19)-C(18)	121.3(3)	C(28)-C(30)-H(30B)	109.5
C(20)-C(19)-H(19)	119.4	H(30A)-C(30)-H(30B)	109.5
C(18)-C(19)-H(19)	119.4	C(28)-C(30)-H(30C)	109.5
C(20T)-C(19T)-C(18T)	120.3(3)	H(30A)-C(30)-H(30C)	109.5
C(20T)-C(19T)-H(19T)	119.8	H(30B)-C(30)-H(30C)	109.5
C(18T)-C(19T)-H(19T)	119.8	C(28)-C(31)-H(31A)	109.5
C(19)-C(20)-C(21)	117.4(3)	C(28)-C(31)-H(31B)	109.5
C(19)-C(20)-H(20)	121.3	H(31A)-C(31)-H(31B)	109.5
C(21)-C(20)-H(20)	121.3	C(28)-C(31)-H(31C)	109.5
C(19T)-C(20T)-C(15T)	121.1(3)	H(31A)-C(31)-H(31C)	109.5
C(19T)-C(20T)-H(20T)	119.5	H(31B)-C(31)-H(31C)	109.5
C(15T)-C(20T)-H(20T)	119.5	C(34)-C(32)-C(33)	108.4(2)
C(16)-C(21)-C(20)	121.1(3)	C(34)-C(32)-C(35)	109.0(3)
C(16)-C(21)-N(2)	105.9(2)	C(33)-C(32)-C(35)	108.7(3)
C(20)-C(21)-N(2)	132.8(3)	C(34)-C(32)-C(26)	109.2(2)
C(15T)-C(21T)-H(21A)	109.5	C(33)-C(32)-C(26)	111.6(2)
C(15T)-C(21T)-H(21B)	109.5	C(35)-C(32)-C(26)	109.9(2)
H(21A)-C(21T)-H(21B)	109.5	C(32)-C(33)-H(33A)	109.5
C(15T)-C(21T)-H(21C)	109.5	C(32)-C(33)-H(33B)	109.5
H(21A)-C(21T)-H(21C)	109.5	H(33A)-C(33)-H(33B)	109.5
H(21B)-C(21T)-H(21C)	109.5	C(32)-C(33)-H(33C)	109.5
C(27)-C(22)-C(23)	122.2(2)	H(33A)-C(33)-H(33C)	109.5

H(33B)-C(33)-H(33C)	109.5	C(43)-C(46)-H(46A)	109.5
C(32)-C(34)-H(34A)	109.5	C(43)-C(46)-H(46B)	109.5
C(32)-C(34)-H(34B)	109.5	H(46A)-C(46)-H(46B)	109.5
H(34A)-C(34)-H(34B)	109.5	C(43)-C(46)-H(46C)	109.5
C(32)-C(34)-H(34C)	109.5	H(46A)-C(46)-H(46C)	109.5
H(34A)-C(34)-H(34C)	109.5	H(46B)-C(46)-H(46C)	109.5
H(34B)-C(34)-H(34C)	109.5	C(50)-C(47)-C(49)	108.3(2)
C(32)-C(35)-H(35A)	109.5	C(50)-C(47)-C(48)	106.9(2)
C(32)-C(35)-H(35B)	109.5	C(49)-C(47)-C(48)	108.9(2)
H(35A)-C(35)-H(35B)	109.5	C(50)-C(47)-C(41)	111.5(2)
C(32)-C(35)-H(35C)	109.5	C(49)-C(47)-C(41)	110.3(2)
H(35A)-C(35)-H(35C)	109.5	C(48)-C(47)-C(41)	110.9(2)
H(35B)-C(35)-H(35C)	109.5	C(47)-C(48)-H(48A)	109.5
N(3)-C(36)-N(4)	105.5(2)	C(47)-C(48)-H(48B)	109.5
N(3)-C(36)-Zr(2)	124.56(17)	H(48A)-C(48)-H(48B)	109.5
N(4)-C(36)-Zr(2)	124.25(17)	C(47)-C(48)-H(48C)	109.5
C(38)-C(37)-C(42)	122.4(2)	H(48A)-C(48)-H(48C)	109.5
C(38)-C(37)-N(3)	119.0(2)	H(48B)-C(48)-H(48C)	109.5
C(42)-C(37)-N(3)	118.6(2)	C(47)-C(49)-H(49A)	109.5
C(37)-C(38)-C(39)	120.7(2)	C(47)-C(49)-H(49B)	109.5
C(37)-C(38)-H(38)	119.6	H(49A)-C(49)-H(49B)	109.5
C(39)-C(38)-H(38)	119.6	C(47)-C(49)-H(49C)	109.5
C(40)-C(39)-C(38)	116.9(2)	H(49A)-C(49)-H(49C)	109.5
C(40)-C(39)-C(43)	123.3(2)	H(49B)-C(49)-H(49C)	109.5
C(38)-C(39)-C(43)	119.8(2)	C(47)-C(50)-H(50A)	109.5
C(39)-C(40)-C(41)	124.3(2)	C(47)-C(50)-H(50B)	109.5
C(39)-C(40)-H(40)	117.8	H(50A)-C(50)-H(50B)	109.5
C(41)-C(40)-H(40)	117.8	C(47)-C(50)-H(50C)	109.5
C(40)-C(41)-C(42)	118.1(2)	H(50A)-C(50)-H(50C)	109.5
C(40)-C(41)-C(47)	121.4(2)	H(50B)-C(50)-H(50C)	109.5
C(42)-C(41)-C(47)	120.4(2)	C(52)-C(51)-C(56)	121.1(2)
O(5)-C(42)-C(37)	120.3(2)	C(52)-C(51)-N(3)	133.0(2)
O(5)-C(42)-C(41)	122.2(2)	C(56)-C(51)-N(3)	105.7(2)
C(37)-C(42)-C(41)	117.5(2)	C(53)-C(52)-C(51)	117.6(2)
C(46)-C(43)-C(45)	108.5(2)	C(53)-C(52)-H(52)	121.2
C(46)-C(43)-C(44)	108.8(2)	C(51)-C(52)-H(52)	121.2
C(45)-C(43)-C(44)	108.1(2)	C(52)-C(53)-C(54)	121.2(2)
C(46)-C(43)-C(39)	109.9(2)	C(52)-C(53)-H(53)	119.4
C(45)-C(43)-C(39)	112.1(2)	C(54)-C(53)-H(53)	119.4
C(44)-C(43)-C(39)	109.3(2)	C(55)-C(54)-C(53)	121.8(3)
C(43)-C(44)-H(44A)	109.5	C(55)-C(54)-H(54)	119.1
C(43)-C(44)-H(44B)	109.5	C(53)-C(54)-H(54)	119.1
H(44A)-C(44)-H(44B)	109.5	C(54)-C(55)-C(56)	116.8(2)
C(43)-C(44)-H(44C)	109.5	C(54)-C(55)-H(55)	121.6
H(44A)-C(44)-H(44C)	109.5	C(56)-C(55)-H(55)	121.6
H(44B)-C(44)-H(44C)	109.5	C(55)-C(56)-C(51)	121.6(2)
C(43)-C(45)-H(45A)	109.5	C(55)-C(56)-N(4)	132.2(2)
C(43)-C(45)-H(45B)	109.5	C(51)-C(56)-N(4)	106.1(2)
H(45A)-C(45)-H(45B)	109.5	C(62)-C(57)-C(58)	122.2(2)
C(43)-C(45)-H(45C)	109.5	C(62)-C(57)-N(4)	119.0(2)
H(45A)-C(45)-H(45C)	109.5	C(58)-C(57)-N(4)	118.8(2)
H(45B)-C(45)-H(45C)	109.5	O(6)-C(58)-C(57)	120.4(2)

O(6)-C(58)-C(59)	121.8(2)	H(69A)-C(69)-H(69B)	109.5
C(57)-C(58)-C(59)	117.8(2)	C(67)-C(69)-H(69C)	109.5
C(60)-C(59)-C(58)	118.2(2)	H(69A)-C(69)-H(69C)	109.5
C(60)-C(59)-C(63)	121.0(2)	H(69B)-C(69)-H(69C)	109.5
C(58)-C(59)-C(63)	120.9(2)	C(67)-C(70)-H(70A)	109.5
C(61)-C(60)-C(59)	124.2(2)	C(67)-C(70)-H(70B)	109.5
C(61)-C(60)-H(60)	117.9	H(70A)-C(70)-H(70B)	109.5
C(59)-C(60)-H(60)	117.9	C(67)-C(70)-H(70C)	109.5
C(60)-C(61)-C(62)	117.0(2)	H(70A)-C(70)-H(70C)	109.5
C(60)-C(61)-C(67)	123.3(2)	H(70B)-C(70)-H(70C)	109.5
C(62)-C(61)-C(67)	119.7(2)	N(5)-C(71)-N(6)	105.6(2)
C(57)-C(62)-C(61)	120.6(2)	N(5)-C(71)-Zr(3)	123.78(17)
C(57)-C(62)-H(62)	119.7	N(6)-C(71)-Zr(3)	124.64(18)
C(61)-C(62)-H(62)	119.7	C(77)-C(72)-C(73)	122.7(2)
C(66)-C(63)-C(65)	107.7(2)	C(77)-C(72)-N(5)	118.7(2)
C(66)-C(63)-C(59)	111.8(2)	C(73)-C(72)-N(5)	118.6(2)
C(65)-C(63)-C(59)	110.0(2)	O(9)-C(73)-C(72)	120.6(2)
C(66)-C(63)-C(64)	107.3(2)	O(9)-C(73)-C(74)	121.7(2)
C(65)-C(63)-C(64)	109.6(2)	C(72)-C(73)-C(74)	117.6(2)
C(59)-C(63)-C(64)	110.3(2)	C(75)-C(74)-C(73)	118.0(2)
C(63)-C(64)-H(64A)	109.5	C(75)-C(74)-C(78)	121.3(2)
C(63)-C(64)-H(64B)	109.5	C(73)-C(74)-C(78)	120.7(2)
H(64A)-C(64)-H(64B)	109.5	C(74)-C(75)-C(76)	124.0(2)
C(63)-C(64)-H(64C)	109.5	C(74)-C(75)-H(75)	118.0
H(64A)-C(64)-H(64C)	109.5	C(76)-C(75)-H(75)	118.0
H(64B)-C(64)-H(64C)	109.5	C(77)-C(76)-C(75)	117.2(2)
C(63)-C(65)-H(65A)	109.5	C(77)-C(76)-C(82)	121.7(2)
C(63)-C(65)-H(65B)	109.5	C(75)-C(76)-C(82)	120.9(2)
H(65A)-C(65)-H(65B)	109.5	C(76)-C(77)-C(72)	120.4(2)
C(63)-C(65)-H(65C)	109.5	C(76)-C(77)-H(77)	119.8
H(65A)-C(65)-H(65C)	109.5	C(72)-C(77)-H(77)	119.8
H(65B)-C(65)-H(65C)	109.5	C(79)-C(78)-C(81)	107.7(2)
C(63)-C(66)-H(66A)	109.5	C(79)-C(78)-C(80)	107.3(2)
C(63)-C(66)-H(66B)	109.5	C(81)-C(78)-C(80)	109.6(2)
H(66A)-C(66)-H(66B)	109.5	C(79)-C(78)-C(74)	111.7(2)
C(63)-C(66)-H(66C)	109.5	C(81)-C(78)-C(74)	109.4(2)
H(66A)-C(66)-H(66C)	109.5	C(80)-C(78)-C(74)	111.1(2)
H(66B)-C(66)-H(66C)	109.5	C(78)-C(79)-H(79A)	109.5
C(69)-C(67)-C(70)	109.1(2)	C(78)-C(79)-H(79B)	109.5
C(69)-C(67)-C(68)	108.1(2)	H(79A)-C(79)-H(79B)	109.5
C(70)-C(67)-C(68)	108.1(2)	C(78)-C(79)-H(79C)	109.5
C(69)-C(67)-C(61)	109.5(2)	H(79A)-C(79)-H(79C)	109.5
C(70)-C(67)-C(61)	109.9(2)	H(79B)-C(79)-H(79C)	109.5
C(68)-C(67)-C(61)	112.1(2)	C(78)-C(80)-H(80A)	109.5
C(67)-C(68)-H(68A)	109.5	C(78)-C(80)-H(80B)	109.5
C(67)-C(68)-H(68B)	109.5	H(80A)-C(80)-H(80B)	109.5
H(68A)-C(68)-H(68B)	109.5	C(78)-C(80)-H(80C)	109.5
C(67)-C(68)-H(68C)	109.5	H(80A)-C(80)-H(80C)	109.5
H(68A)-C(68)-H(68C)	109.5	H(80B)-C(80)-H(80C)	109.5
H(68B)-C(68)-H(68C)	109.5	C(78)-C(81)-H(81A)	109.5
C(67)-C(69)-H(69A)	109.5	C(78)-C(81)-H(81B)	109.5
C(67)-C(69)-H(69B)	109.5	H(81A)-C(81)-H(81B)	109.5

C(78)-C(81)-H(81C)	109.5	C(95)-C(94)-C(98)	121.1(2)
H(81A)-C(81)-H(81C)	109.5	C(93)-C(94)-C(98)	120.9(2)
H(81B)-C(81)-H(81C)	109.5	C(96)-C(95)-C(94)	124.2(3)
C(85)-C(82)-C(84)	109.6(3)	C(96)-C(95)-H(95)	117.9
C(85)-C(82)-C(83)	107.6(3)	C(94)-C(95)-H(95)	117.9
C(84)-C(82)-C(83)	108.6(3)	C(97)-C(96)-C(95)	116.9(2)
C(85)-C(82)-C(76)	111.7(2)	C(97)-C(96)-C(102)	120.5(2)
C(84)-C(82)-C(76)	107.4(2)	C(95)-C(96)-C(102)	122.5(2)
C(83)-C(82)-C(76)	112.0(2)	C(92)-C(97)-C(96)	120.6(2)
C(82)-C(83)-H(83A)	109.5	C(92)-C(97)-H(97)	119.7
C(82)-C(83)-H(83B)	109.5	C(96)-C(97)-H(97)	119.7
H(83A)-C(83)-H(83B)	109.5	C(100)-C(98)-C(94)	112.6(2)
C(82)-C(83)-H(83C)	109.5	C(100)-C(98)-C(99)	107.2(2)
H(83A)-C(83)-H(83C)	109.5	C(94)-C(98)-C(99)	110.6(2)
H(83B)-C(83)-H(83C)	109.5	C(100)-C(98)-C(101)	107.7(2)
C(82)-C(84)-H(84A)	109.5	C(94)-C(98)-C(101)	109.4(2)
C(82)-C(84)-H(84B)	109.5	C(99)-C(98)-C(101)	109.2(2)
H(84A)-C(84)-H(84B)	109.5	C(98)-C(99)-H(99A)	109.5
C(82)-C(84)-H(84C)	109.5	C(98)-C(99)-H(99B)	109.5
H(84A)-C(84)-H(84C)	109.5	H(99A)-C(99)-H(99B)	109.5
H(84B)-C(84)-H(84C)	109.5	C(98)-C(99)-H(99C)	109.5
C(82)-C(85)-H(85A)	109.5	H(99A)-C(99)-H(99C)	109.5
C(82)-C(85)-H(85B)	109.5	H(99B)-C(99)-H(99C)	109.5
H(85A)-C(85)-H(85B)	109.5	C(98)-C(100)-H(10D)	109.5
C(82)-C(85)-H(85C)	109.5	C(98)-C(100)-H(10E)	109.5
H(85A)-C(85)-H(85C)	109.5	H(10D)-C(100)-H(10E)	109.5
H(85B)-C(85)-H(85C)	109.5	C(98)-C(100)-H(10F)	109.5
C(91)-C(86)-C(87)	121.9(2)	H(10D)-C(100)-H(10F)	109.5
C(91)-C(86)-N(5)	105.7(2)	H(10E)-C(100)-H(10F)	109.5
C(87)-C(86)-N(5)	132.3(3)	C(98)-C(101)-H(10G)	109.5
C(88)-C(87)-C(86)	116.8(3)	C(98)-C(101)-H(10H)	109.5
C(88)-C(87)-H(87)	121.6	H(10G)-C(101)-H(10H)	109.5
C(86)-C(87)-H(87)	121.6	C(98)-C(101)-H(10I)	109.5
C(87)-C(88)-C(89)	121.5(3)	H(10G)-C(101)-H(10I)	109.5
C(87)-C(88)-H(88)	119.2	H(10H)-C(101)-H(10I)	109.5
C(89)-C(88)-H(88)	119.2	C(103)-C(102)-C(105)	110.6(3)
C(90)-C(89)-C(88)	121.8(3)	C(14A)-C(102)-C(13A)	113.0(7)
C(90)-C(89)-H(89)	119.1	C(14A)-C(102)-C(96)	112.2(6)
C(88)-C(89)-H(89)	119.1	C(103)-C(102)-C(96)	110.0(2)
C(89)-C(90)-C(91)	117.1(3)	C(105)-C(102)-C(96)	109.5(2)
C(89)-C(90)-H(90)	121.5	C(13A)-C(102)-C(96)	109.0(6)
C(91)-C(90)-H(90)	121.5	C(103)-C(102)-C(104)	107.7(3)
C(86)-C(91)-N(6)	106.1(2)	C(105)-C(102)-C(104)	106.9(3)
C(86)-C(91)-C(90)	120.8(2)	C(96)-C(102)-C(104)	112.1(3)
N(6)-C(91)-C(90)	132.9(3)	C(14A)-C(102)-C(15A)	107.0(7)
C(97)-C(92)-C(93)	122.5(2)	C(13A)-C(102)-C(15A)	104.5(7)
C(97)-C(92)-N(6)	119.6(2)	C(96)-C(102)-C(15A)	110.8(5)
C(93)-C(92)-N(6)	117.9(2)	C(102)-C(103)-H(10J)	109.5
O(10)-C(93)-C(92)	120.0(2)	C(102)-C(103)-H(10K)	109.5
O(10)-C(93)-C(94)	122.2(2)	H(10J)-C(103)-H(10K)	109.5
C(92)-C(93)-C(94)	117.7(2)	C(102)-C(103)-H(10L)	109.5
C(95)-C(94)-C(93)	117.9(2)	H(10J)-C(103)-H(10L)	109.5

H(10K)-C(103)-H(10L)	109.5	C(106)-C(108)-H(10W)	109.5
C(102)-C(104)-H(10M)	109.5	C(106)-C(108)-H(10X)	109.5
C(102)-C(104)-H(10N)	109.5	H(10W)-C(108)-H(10X)	109.5
H(10M)-C(104)-H(10N)	109.5	C(106)-C(108)-H(10Y)	109.5
C(102)-C(104)-H(10O)	109.5	H(10W)-C(108)-H(10Y)	109.5
H(10M)-C(104)-H(10O)	109.5	H(10X)-C(108)-H(10Y)	109.5
H(10N)-C(104)-H(10O)	109.5	O(8)-C(109)-C(111)	109.7(2)
C(102)-C(105)-H(10P)	109.5	O(8)-C(109)-C(110)	109.8(2)
C(102)-C(105)-H(10Q)	109.5	C(111)-C(109)-C(110)	111.1(2)
H(10P)-C(105)-H(10Q)	109.5	O(8)-C(109)-H(109)	108.7
C(102)-C(105)-H(10R)	109.5	C(111)-C(109)-H(109)	108.7
H(10P)-C(105)-H(10R)	109.5	C(110)-C(109)-H(109)	108.7
H(10Q)-C(105)-H(10R)	109.5	C(109)-C(110)-H(11D)	109.5
C(102)-C(13A)-H(13D)	109.5	C(109)-C(110)-H(11E)	109.5
C(102)-C(13A)-H(13E)	109.5	H(11D)-C(110)-H(11E)	109.5
H(13D)-C(13A)-H(13E)	109.5	C(109)-C(110)-H(11F)	109.5
C(102)-C(13A)-H(13F)	109.5	H(11D)-C(110)-H(11F)	109.5
H(13D)-C(13A)-H(13F)	109.5	H(11E)-C(110)-H(11F)	109.5
H(13E)-C(13A)-H(13F)	109.5	C(109)-C(111)-H(11G)	109.5
C(102)-C(14A)-H(14G)	109.5	C(109)-C(111)-H(11H)	109.5
C(102)-C(14A)-H(14H)	109.5	H(11G)-C(111)-H(11H)	109.5
H(14G)-C(14A)-H(14H)	109.5	C(109)-C(111)-H(11I)	109.5
C(102)-C(14A)-H(14I)	109.5	H(11G)-C(111)-H(11I)	109.5
H(14G)-C(14A)-H(14I)	109.5	H(11H)-C(111)-H(11I)	109.5
H(14H)-C(14A)-H(14I)	109.5	O(12)-C(112)-C(114)	109.6(2)
C(102)-C(15A)-H(15D)	109.5	O(12)-C(112)-C(113)	109.6(2)
C(102)-C(15A)-H(15E)	109.5	C(114)-C(112)-C(113)	112.4(2)
H(15D)-C(15A)-H(15E)	109.5	O(12)-C(112)-H(112)	108.4
C(102)-C(15A)-H(15F)	109.5	C(114)-C(112)-H(112)	108.4
H(15D)-C(15A)-H(15F)	109.5	C(113)-C(112)-H(112)	108.4
H(15E)-C(15A)-H(15F)	109.5	C(112)-C(113)-H(11J)	109.5
O(4)-C(106)-C(108)	109.9(2)	C(112)-C(113)-H(11K)	109.5
O(4)-C(106)-C(107)	109.4(2)	H(11J)-C(113)-H(11K)	109.5
C(108)-C(106)-C(107)	111.4(3)	C(112)-C(113)-H(11L)	109.5
O(4)-C(106)-H(106)	108.7	H(11J)-C(113)-H(11L)	109.5
C(108)-C(106)-H(106)	108.7	H(11K)-C(113)-H(11L)	109.5
C(107)-C(106)-H(106)	108.7	C(112)-C(114)-H(11N)	109.5
C(106)-C(107)-H(10S)	109.5	C(112)-C(114)-H(11M)	109.5
C(106)-C(107)-H(10U)	109.5	H(11N)-C(114)-H(11M)	109.5
H(10S)-C(107)-H(10U)	109.5	C(112)-C(114)-H(11P)	109.5
C(106)-C(107)-H(10V)	109.5	H(11N)-C(114)-H(11P)	109.5
H(10S)-C(107)-H(10V)	109.5	H(11M)-C(114)-H(11P)	109.5
H(10U)-C(107)-H(10V)	109.5		

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

Table S11. Torsion angles [°] for **6**.

C(16)-N(1)-C(1)-N(2)	-1.4(3)	C(2)-N(1)-C(1)-Zr(1)	-22.6(3)
C(2)-N(1)-C(1)-N(2)	-178.0(2)	N(1)-C(1)-N(2)-C(21)	1.1(3)
C(16)-N(1)-C(1)-Zr(1)	153.98(19)	Zr(1)-C(1)-N(2)-C(21)	-154.06(18)

N(1)-C(1)-N(2)-C(22)	174.9(2)
Zr(1)-C(1)-N(2)-C(22)	19.8(3)
C(1)-N(1)-C(2)-C(7)	39.6(4)
C(16)-N(1)-C(2)-C(7)	-136.5(3)
C(1)-N(1)-C(2)-C(3)	-140.8(3)
C(16)-N(1)-C(2)-C(3)	43.2(4)
C(6T)-C(1T)-C(2T)-C(3T)	-0.2(5)
C(7T)-C(1T)-C(2T)-C(3T)	179.3(3)
C(7)-C(2)-C(3)-C(4)	2.5(4)
N(1)-C(2)-C(3)-C(4)	-177.2(2)
C(1T)-C(2T)-C(3T)-C(4T)	0.9(5)
C(2)-C(3)-C(4)-C(5)	0.0(4)
C(2)-C(3)-C(4)-C(8)	178.9(2)
C(2T)-C(3T)-C(4T)-C(5T)	-0.6(6)
C(3)-C(4)-C(5)-C(6)	-1.9(4)
C(8)-C(4)-C(5)-C(6)	179.3(2)
C(3T)-C(4T)-C(5T)-C(6T)	-0.4(6)
C(4)-C(5)-C(6)-C(7)	1.2(4)
C(4)-C(5)-C(6)-C(12)	-178.6(2)
C(2T)-C(1T)-C(6T)-C(5T)	-0.8(5)
C(7T)-C(1T)-C(6T)-C(5T)	179.7(3)
C(4T)-C(5T)-C(6T)-C(1T)	1.1(6)
Zr(1)-O(1)-C(7)-C(2)	-54.4(3)
Zr(1)-O(1)-C(7)-C(6)	124.2(2)
C(3)-C(2)-C(7)-O(1)	175.5(2)
N(1)-C(2)-C(7)-O(1)	-4.9(4)
C(3)-C(2)-C(7)-C(6)	-3.1(4)
N(1)-C(2)-C(7)-C(6)	176.5(2)
C(5)-C(6)-C(7)-O(1)	-177.3(2)
C(12)-C(6)-C(7)-O(1)	2.5(4)
C(5)-C(6)-C(7)-C(2)	1.3(4)
C(12)-C(6)-C(7)-C(2)	-178.9(2)
C(3)-C(4)-C(8)-C(10)	-107.2(3)
C(5)-C(4)-C(8)-C(10)	71.6(3)
C(3)-C(4)-C(8)-C(11)	131.8(3)
C(5)-C(4)-C(8)-C(11)	-49.4(3)
C(3)-C(4)-C(8)-C(9)	12.1(4)
C(5)-C(4)-C(8)-C(9)	-169.1(2)
C(13T)-C(8T)-C(9T)-C(10T)	0.1(6)
C(14T)-C(8T)-C(9T)-C(10T)	177.6(4)
C(8T)-C(9T)-C(10T)-C(11T)	0.8(6)
C(9T)-C(10T)-C(11T)-C(12T)	-1.3(7)
C(5)-C(6)-C(12)-C(15)	-121.7(3)
C(7)-C(6)-C(12)-C(15)	58.5(3)
C(5)-C(6)-C(12)-C(13)	-1.6(4)
C(7)-C(6)-C(12)-C(13)	178.6(3)
C(5)-C(6)-C(12)-C(14)	117.7(3)
C(7)-C(6)-C(12)-C(14)	-62.1(3)
C(10T)-C(11T)-C(12T)-C(13T)	0.9(6)
C(9T)-C(8T)-C(13T)-C(12T)	-0.5(7)
C(14T)-C(8T)-C(13T)-C(12T)	-177.8(4)
C(11T)-C(12T)-C(13T)-C(8T)	0.0(7)
C(1)-N(1)-C(16)-C(21)	1.2(3)
C(2)-N(1)-C(16)-C(21)	177.6(2)
C(1)-N(1)-C(16)-C(17)	-173.2(3)
C(2)-N(1)-C(16)-C(17)	3.2(5)
C(20T)-C(15T)-C(16T)-C(17T)	-0.6(4)
C(21T)-C(15T)-C(16T)-C(17T)	178.4(3)
C(21)-C(16)-C(17)-C(18)	1.9(5)
N(1)-C(16)-C(17)-C(18)	175.6(3)
C(15T)-C(16T)-C(17T)-C(18T)	-0.3(5)
C(16)-C(17)-C(18)-C(19)	-0.1(5)
C(16T)-C(17T)-C(18T)-C(19T)	0.7(5)
C(17)-C(18)-C(19)-C(20)	-1.9(5)
C(17T)-C(18T)-C(19T)-C(20T)	-0.2(5)
C(18)-C(19)-C(20)-C(21)	2.1(4)
C(18T)-C(19T)-C(20T)-C(15T)	-0.6(5)
C(16T)-C(15T)-C(20T)-C(19T)	1.0(4)
C(21T)-C(15T)-C(20T)-C(19T)	-178.0(3)
C(17)-C(16)-C(21)-C(20)	-1.7(4)
N(1)-C(16)-C(21)-C(20)	-176.9(2)
C(17)-C(16)-C(21)-N(2)	174.6(3)
N(1)-C(16)-C(21)-N(2)	-0.5(3)
C(19)-C(20)-C(21)-C(16)	-0.3(4)
C(19)-C(20)-C(21)-N(2)	-175.6(3)
C(1)-N(2)-C(21)-C(16)	-0.3(3)
C(22)-N(2)-C(21)-C(16)	-174.0(2)
C(1)-N(2)-C(21)-C(20)	175.4(3)
C(22)-N(2)-C(21)-C(20)	1.8(5)
C(1)-N(2)-C(22)-C(27)	143.6(3)
C(21)-N(2)-C(22)-C(27)	-43.5(4)
C(1)-N(2)-C(22)-C(23)	-37.7(4)
C(21)-N(2)-C(22)-C(23)	135.3(3)
Zr(1)-O(2)-C(23)-C(22)	53.9(3)
Zr(1)-O(2)-C(23)-C(24)	-125.5(2)
C(27)-C(22)-C(23)-O(2)	-176.1(2)
N(2)-C(22)-C(23)-O(2)	5.2(4)
C(27)-C(22)-C(23)-C(24)	3.3(4)
N(2)-C(22)-C(23)-C(24)	-175.4(2)
O(2)-C(23)-C(24)-C(25)	178.1(2)
C(22)-C(23)-C(24)-C(25)	-1.3(4)
O(2)-C(23)-C(24)-C(28)	-2.4(4)
C(22)-C(23)-C(24)-C(28)	178.1(2)
C(23)-C(24)-C(25)-C(26)	-0.4(4)
C(28)-C(24)-C(25)-C(26)	-179.9(2)
C(24)-C(25)-C(26)-C(27)	0.3(4)
C(24)-C(25)-C(26)-C(32)	179.2(2)
C(23)-C(22)-C(27)-C(26)	-3.5(4)
N(2)-C(22)-C(27)-C(26)	175.2(2)
C(25)-C(26)-C(27)-C(22)	1.7(4)
C(32)-C(26)-C(27)-C(22)	-177.3(2)
C(25)-C(24)-C(28)-C(31)	3.5(4)
C(23)-C(24)-C(28)-C(31)	-175.9(2)
C(25)-C(24)-C(28)-C(29)	122.9(3)

C(23)-C(24)-C(28)-C(29)	-56.5(3)
C(25)-C(24)-C(28)-C(30)	-115.6(3)
C(23)-C(24)-C(28)-C(30)	65.0(3)
C(25)-C(26)-C(32)-C(34)	-125.6(3)
C(27)-C(26)-C(32)-C(34)	53.3(3)
C(25)-C(26)-C(32)-C(33)	-5.9(4)
C(27)-C(26)-C(32)-C(33)	173.0(2)
C(25)-C(26)-C(32)-C(35)	114.8(3)
C(27)-C(26)-C(32)-C(35)	-66.3(3)
C(51)-N(3)-C(36)-N(4)	0.8(3)
C(37)-N(3)-C(36)-N(4)	175.6(2)
C(51)-N(3)-C(36)-Zr(2)	-153.34(17)
C(37)-N(3)-C(36)-Zr(2)	21.5(3)
C(56)-N(4)-C(36)-N(3)	-1.3(3)
C(57)-N(4)-C(36)-N(3)	-175.3(2)
C(56)-N(4)-C(36)-Zr(2)	152.88(17)
C(57)-N(4)-C(36)-Zr(2)	-21.1(3)
C(36)-N(3)-C(37)-C(38)	143.2(2)
C(51)-N(3)-C(37)-C(38)	-42.7(3)
C(36)-N(3)-C(37)-C(42)	-38.1(3)
C(51)-N(3)-C(37)-C(42)	135.9(2)
C(42)-C(37)-C(38)-C(39)	-2.3(4)
N(3)-C(37)-C(38)-C(39)	176.2(2)
C(37)-C(38)-C(39)-C(40)	1.7(4)
C(37)-C(38)-C(39)-C(43)	-177.8(2)
C(38)-C(39)-C(40)-C(41)	-0.2(4)
C(43)-C(39)-C(40)-C(41)	179.3(2)
C(39)-C(40)-C(41)-C(42)	-0.8(4)
C(39)-C(40)-C(41)-C(47)	-179.9(2)
Zr(2)-O(5)-C(42)-C(37)	57.0(3)
Zr(2)-O(5)-C(42)-C(41)	-122.5(2)
C(38)-C(37)-C(42)-O(5)	-178.3(2)
N(3)-C(37)-C(42)-O(5)	3.1(3)
C(38)-C(37)-C(42)-C(41)	1.2(4)
N(3)-C(37)-C(42)-C(41)	-177.3(2)
C(40)-C(41)-C(42)-O(5)	179.8(2)
C(47)-C(41)-C(42)-O(5)	-1.1(4)
C(40)-C(41)-C(42)-C(37)	0.3(4)
C(47)-C(41)-C(42)-C(37)	179.4(2)
C(40)-C(39)-C(43)-C(46)	116.0(3)
C(38)-C(39)-C(43)-C(46)	-64.5(3)
C(40)-C(39)-C(43)-C(45)	-4.8(4)
C(38)-C(39)-C(43)-C(45)	174.7(2)
C(40)-C(39)-C(43)-C(44)	-124.7(3)
C(38)-C(39)-C(43)-C(44)	54.8(3)
C(40)-C(41)-C(47)-C(50)	-1.7(4)
C(42)-C(41)-C(47)-C(50)	179.2(2)
C(40)-C(41)-C(47)-C(49)	118.6(3)
C(42)-C(41)-C(47)-C(49)	-60.5(3)
C(40)-C(41)-C(47)-C(48)	-120.7(3)
C(42)-C(41)-C(47)-C(48)	60.2(3)
C(36)-N(3)-C(51)-C(52)	174.6(3)
C(37)-N(3)-C(51)-C(52)	0.0(4)
C(36)-N(3)-C(51)-C(56)	0.1(3)
C(37)-N(3)-C(51)-C(56)	-174.6(2)
C(56)-C(51)-C(52)-C(53)	-0.6(4)
N(3)-C(51)-C(52)-C(53)	-174.5(3)
C(51)-C(52)-C(53)-C(54)	1.4(4)
C(52)-C(53)-C(54)-C(55)	-0.8(4)
C(53)-C(54)-C(55)-C(56)	-0.6(4)
C(54)-C(55)-C(56)-C(51)	1.5(4)
C(54)-C(55)-C(56)-N(4)	175.4(3)
C(52)-C(51)-C(56)-C(55)	-0.9(4)
N(3)-C(51)-C(56)-C(55)	174.5(2)
C(52)-C(51)-C(56)-N(4)	-176.2(2)
N(3)-C(51)-C(56)-N(4)	-0.9(3)
C(36)-N(4)-C(56)-C(55)	-173.2(3)
C(57)-N(4)-C(56)-C(55)	0.7(4)
C(36)-N(4)-C(56)-C(51)	1.4(3)
C(57)-N(4)-C(56)-C(51)	175.3(2)
C(36)-N(4)-C(57)-C(62)	-144.4(2)
C(56)-N(4)-C(57)-C(62)	42.4(4)
C(36)-N(4)-C(57)-C(58)	37.4(3)
C(56)-N(4)-C(57)-C(58)	-135.7(2)
Zr(2)-O(6)-C(58)-C(57)	-53.7(3)
Zr(2)-O(6)-C(58)-C(59)	125.4(2)
C(62)-C(57)-C(58)-O(6)	177.6(2)
N(4)-C(57)-C(58)-O(6)	-4.4(3)
C(62)-C(57)-C(58)-C(59)	-1.6(4)
N(4)-C(57)-C(58)-C(59)	176.5(2)
O(6)-C(58)-C(59)-C(60)	-179.8(2)
C(57)-C(58)-C(59)-C(60)	-0.7(3)
O(6)-C(58)-C(59)-C(63)	0.8(4)
C(57)-C(58)-C(59)-C(63)	180.0(2)
C(58)-C(59)-C(60)-C(61)	1.7(4)
C(63)-C(59)-C(60)-C(61)	-178.9(2)
C(59)-C(60)-C(61)-C(62)	-0.5(4)
C(59)-C(60)-C(61)-C(67)	-180.0(2)
C(58)-C(57)-C(62)-C(61)	2.8(4)
N(4)-C(57)-C(62)-C(61)	-175.2(2)
C(60)-C(61)-C(62)-C(57)	-1.7(4)
C(67)-C(61)-C(62)-C(57)	177.7(2)
C(60)-C(59)-C(63)-C(66)	-0.9(3)
C(58)-C(59)-C(63)-C(66)	178.4(2)
C(60)-C(59)-C(63)-C(65)	-120.6(3)
C(58)-C(59)-C(63)-C(65)	58.8(3)
C(60)-C(59)-C(63)-C(64)	118.4(3)
C(58)-C(59)-C(63)-C(64)	-62.2(3)
C(60)-C(61)-C(67)-C(69)	123.7(3)
C(62)-C(61)-C(67)-C(69)	-55.7(3)
C(60)-C(61)-C(67)-C(70)	-116.4(3)
C(62)-C(61)-C(67)-C(70)	64.2(3)
C(60)-C(61)-C(67)-C(68)	3.8(4)
C(62)-C(61)-C(67)-C(68)	-175.6(2)

C(86)-N(5)-C(71)-N(6)	-1.7(3)
C(72)-N(5)-C(71)-N(6)	-178.5(2)
C(86)-N(5)-C(71)-Zr(3)	152.11(17)
C(72)-N(5)-C(71)-Zr(3)	-24.7(3)
C(91)-N(6)-C(71)-N(5)	1.6(3)
C(92)-N(6)-C(71)-N(5)	-179.5(2)
C(91)-N(6)-C(71)-Zr(3)	-151.92(18)
C(92)-N(6)-C(71)-Zr(3)	26.9(3)
C(71)-N(5)-C(72)-C(77)	-138.8(3)
C(86)-N(5)-C(72)-C(77)	44.8(4)
C(71)-N(5)-C(72)-C(73)	40.9(3)
C(86)-N(5)-C(72)-C(73)	-135.4(3)
Zr(3)-O(9)-C(73)-C(72)	-55.5(3)
Zr(3)-O(9)-C(73)-C(74)	124.1(2)
C(77)-C(72)-C(73)-O(9)	175.9(2)
N(5)-C(72)-C(73)-O(9)	-3.9(3)
C(77)-C(72)-C(73)-C(74)	-3.7(4)
N(5)-C(72)-C(73)-C(74)	176.5(2)
O(9)-C(73)-C(74)-C(75)	-178.0(2)
C(72)-C(73)-C(74)-C(75)	1.6(3)
O(9)-C(73)-C(74)-C(78)	3.0(4)
C(72)-C(73)-C(74)-C(78)	-177.4(2)
C(73)-C(74)-C(75)-C(76)	1.5(4)
C(78)-C(74)-C(75)-C(76)	-179.6(2)
C(74)-C(75)-C(76)-C(77)	-2.4(4)
C(74)-C(75)-C(76)-C(82)	-179.3(2)
C(75)-C(76)-C(77)-C(72)	0.3(4)
C(82)-C(76)-C(77)-C(72)	177.1(2)
C(73)-C(72)-C(77)-C(76)	2.8(4)
N(5)-C(72)-C(77)-C(76)	-177.5(2)
C(75)-C(74)-C(78)-C(79)	0.0(3)
C(73)-C(74)-C(78)-C(79)	178.9(2)
C(75)-C(74)-C(78)-C(81)	-119.1(3)
C(73)-C(74)-C(78)-C(81)	59.8(3)
C(75)-C(74)-C(78)-C(80)	119.8(3)
C(73)-C(74)-C(78)-C(80)	-61.3(3)
C(77)-C(76)-C(82)-C(85)	139.0(3)
C(75)-C(76)-C(82)-C(85)	-44.3(3)
C(77)-C(76)-C(82)-C(84)	-100.8(3)
C(75)-C(76)-C(82)-C(84)	75.9(3)
C(77)-C(76)-C(82)-C(83)	18.3(4)
C(75)-C(76)-C(82)-C(83)	-165.0(3)
C(71)-N(5)-C(86)-C(91)	1.2(3)
C(72)-N(5)-C(86)-C(91)	177.9(2)
C(71)-N(5)-C(86)-C(87)	-175.0(3)
C(72)-N(5)-C(86)-C(87)	1.7(4)
C(91)-C(86)-C(87)-C(88)	0.7(4)
N(5)-C(86)-C(87)-C(88)	176.4(3)
C(86)-C(87)-C(88)-C(89)	-1.5(4)
C(87)-C(88)-C(89)-C(90)	1.1(4)
C(88)-C(89)-C(90)-C(91)	0.2(4)
C(87)-C(86)-C(91)-N(6)	176.5(2)
N(5)-C(86)-C(91)-N(6)	-0.2(3)
C(87)-C(86)-C(91)-C(90)	0.5(4)
N(5)-C(86)-C(91)-C(90)	-176.2(2)
C(71)-N(6)-C(91)-C(86)	-0.9(3)
C(92)-N(6)-C(91)-C(86)	-179.7(2)
C(71)-N(6)-C(91)-C(90)	174.4(3)
C(92)-N(6)-C(91)-C(90)	-4.4(5)
C(89)-C(90)-C(91)-C(86)	-0.9(4)
C(89)-C(90)-C(91)-N(6)	-175.7(3)
C(71)-N(6)-C(92)-C(97)	136.9(3)
C(91)-N(6)-C(92)-C(97)	-44.4(4)
C(71)-N(6)-C(92)-C(93)	-41.5(3)
C(91)-N(6)-C(92)-C(93)	137.2(3)
Zr(3)-O(10)-C(93)-C(92)	58.4(3)
Zr(3)-O(10)-C(93)-C(94)	-120.7(2)
C(97)-C(92)-C(93)-O(10)	-175.6(2)
N(6)-C(92)-C(93)-O(10)	2.8(3)
C(97)-C(92)-C(93)-C(94)	3.6(4)
N(6)-C(92)-C(93)-C(94)	-178.0(2)
O(10)-C(93)-C(94)-C(95)	176.4(2)
C(92)-C(93)-C(94)-C(95)	-2.8(4)
O(10)-C(93)-C(94)-C(98)	-4.9(4)
C(92)-C(93)-C(94)-C(98)	176.0(2)
C(93)-C(94)-C(95)-C(96)	0.1(4)
C(98)-C(94)-C(95)-C(96)	-178.7(2)
C(94)-C(95)-C(96)-C(97)	1.9(4)
C(94)-C(95)-C(96)-C(102)	-177.6(2)
C(93)-C(92)-C(97)-C(96)	-1.6(4)
N(6)-C(92)-C(97)-C(96)	-180.0(2)
C(95)-C(96)-C(97)-C(92)	-1.1(4)
C(102)-C(96)-C(97)-C(92)	178.4(2)
C(95)-C(94)-C(98)-C(100)	0.4(3)
C(93)-C(94)-C(98)-C(100)	-178.3(2)
C(95)-C(94)-C(98)-C(99)	-119.5(3)
C(93)-C(94)-C(98)-C(99)	61.8(3)
C(95)-C(94)-C(98)-C(101)	120.2(3)
C(93)-C(94)-C(98)-C(101)	-58.6(3)
C(97)-C(96)-C(102)-C(14A)	119.7(6)
C(95)-C(96)-C(102)-C(14A)	-60.8(7)
C(97)-C(96)-C(102)-C(103)	-62.5(3)
C(95)-C(96)-C(102)-C(103)	117.0(3)
C(97)-C(96)-C(102)-C(105)	59.2(4)
C(95)-C(96)-C(102)-C(105)	-121.3(3)
C(97)-C(96)-C(102)-C(13A)	-114.4(6)
C(95)-C(96)-C(102)-C(13A)	65.1(6)
C(97)-C(96)-C(102)-C(104)	177.7(3)
C(95)-C(96)-C(102)-C(104)	-2.8(4)
C(97)-C(96)-C(102)-C(15A)	0.1(6)
C(95)-C(96)-C(102)-C(15A)	179.7(6)
Zr(1)-O(4)-C(106)-C(107)	55.8(11)
Zr(2)-O(8)-C(109)-C(111)	-155.2(7)
Zr(2)-O(8)-C(109)-C(110)	-32.8(9)

Zr(3)-O(12)-C(112)-C(114)	146.8(5)	Zr(3)-O(12)-C(112)-C(113)	-89.4(6)

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