Supporting data for the manuscript

Polymerization of Propylene Promoted by Zirconium Benzamidinates

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Crystal data of the complexes

1. Crystal data of complex 9

Table 1. Crystal data and structure refinement for complex 9.

Identification code	zrpmethox
Empirical formula	C28 H50 Cl2 N4 O2 Si4 Zr
Formula weight	749.20
Temperature	230.0(1) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 11.1770(3) A alpha = 64.6330(15) deg. b = 13.2410(4) A beta = 88.4740(15) deg. c = 15.1640(5) A gamma = 72.6430(15) deg.
Volume	1922.11(10) A^3
Z, Calculated density	2, 1.294 Mg/m^3
Absorption coefficient	0.579 mm^-1
F(000)	784
Crystal size	0.36 x 0.30 x 0.09 mm
Theta range for data collection	1.50 to 27.47 deg.
Limiting indices	-14<=h<=14, -17<=k<=17, -19<=l<=19
Reflections collected / unique	14549 / 8760 [R(int) = 0.0357]
Completeness to theta = 27.47	99.3 %
Absorption correction	None
Max. and min. transmission	0.9498 and 0.8187
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8760 / 0 / 380
Goodness-of-fit on F^2	0.969
Final R indices [I>2sigma(I)]	R1 = 0.0415, wR2 = 0.1094
R indices (all data)	R1 = 0.0669, wR2 = 0.1164
Largest diff. peak and hole	0.538 and -0.709 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for complex 9.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Zr(1)	6552(1)	6685(1)	-2537(1)	31(1)
Cl(1)	4564(1)	8266(1)	-2996(1)	55(1)
Cl(2)	7020(1)	6673(1)	-980(1)	55(1)
Si(1)	3952(1)	5402(1)	-2299(1)	37(1)
Si(2)	9246(1)	3996(1)	-1436(1)	37(1)
Si(3)	6740(1)	6229(1)	-4849(1)	37(1)
Si(4)	8249(1)	8904(1)	-3365(1)	39(1)
O(1)	6522(2)	-144(2)	566(2)	65(1)
O(2)	10253(2)	9047(2)	-7446(2)	50(1)
N(1)	5532(2)	5380(2)	-2212(2)	35(1)
N(2)	7655(2)	4795(2)	-1902(2)	32(1)
N(3)	6990(2)	6783(2)	-4024(2)	35(1)
N(4)	7710(2)	7780(2)	-3378(2)	36(1)
C(1)	3117(3)	5925(3)	-1430(3)	49(1)
C(2)	3778(3)	3955(3)	-2065(3)	52(1)
C(3)	3229(3)	6445(3)	-3583(2)	52(1)
C(4)	6603(2)	4491(2)	-1768(2)	32(1)
C(5)	6610(2)	3255(2)	-1144(2)	33(1)
C(6)	7149(3)	2345(3)	-1412(2)	45(1)
C(7)	7101(3)	1222(3)	-837(3)	50(1)
C(8)	6541(3)	977(3)	24(2)	45(1)
C(9)	6028(3)	1865(3)	307(2)	46(1)
C(10)	6046(3)	2993(3)	-283(2)	41(1)
C(11)	5747(6)	-419(5)	1335(4)	67(2)
C(11A)	6791(15)	-942(12)	233(13)	89(6)
C(12)	9456(4)	2842(4)	-164(3)	80(1)
C(13)	10018(3)	5063(3)	-1482(3)	70(1)
C(14)	9976(3)	3375(4)	-2276(4)	80(1)
C(15)	6471(3)	4795(3)	-4123(2)	48(1)
C(16)	8130(3)	5892(3)	-5502(3)	53(1)
C(17)	5356(3)	7303(3)	-5751(3)	56(1)
C(18)	7657(2)	7506(2)	-4129(2)	33(1)
C(19)	8325(2)	7950(2)	-5013(2)	33(1)
C(20)	9626(3)	7489(3)	-4952(2)	37(1)
C(21)	10239(3)	7862(3)	-5775(2)	40(1)
C(22)	9562(3)	8730(3)	-6673(2)	39(1)
C(23)	8262(3)	9211(3)	-6732(2)	43(1)
C(24)	7656(3)	8810(2)	-5904(2)	38(1)
C(25)	9560(4)	9854(4)	-8392(3)	69(1)
C(26)	7371(4)	9421(4)	-2510(3)	77(1)
C(27)	9961(3)	8302(3)	-2940(3)	69(1)
C(28)	7948(4)	10195(3)	-4580(3)	70(1)

Table 3. Bond lengths [A] and angles [deg] for complex 9.

Zr(1)-N(4)	2.202(2)
Zr(1)-N(2)	2.206(2)
Zr(1)-N(1)	2.224(2)
Zr(1)-N(3)	2.251(2)
Zr(1)-Cl(1)	2.4219(8)
Zr(1)-Cl(2)	2.4234(8)
Si(1)-N(1)	1.765(2)
Si(1)-C(1)	1.849(3)
Si(1)-C(3)	1.861(3)
Si(1)-C(2)	1.863(3)
Si(2)-N(2)	1.756(2)
Si(2)-C(13)	1.841(3)
Si(2)-C(12)	1.843(4)
Si(2)-C(14)	1.845(3)
Si(3)-N(3)	1.763(2)
Si(3)-C(17)	1.850(3)
Si(3)-C(15)	1.855(3)
Si(3)-C(16)	1.865(3)
Si(4)-N(4)	1.772(2)
Si(4)-C(26)	1.846(4)
Si(4)-C(28)	1.849(4)
Si(4)-C(27)	1.852(3)
O(1)-C(11A)	1.312(16)
O(1)-C(8)	1.361(4)
O(1)-C(11)	1.419(6)
O(2)-C(22)	1.367(3)
O(2)-C(25)	1.432(4)
N(1)-C(4)	1.340(3)
N(2)-C(4)	1.336(3)
N(3)-C(18)	1.336(3)
N(4)-C(18)	1.342(3)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(1)-H(1C)	0.9700
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(2)-H(2C)	0.9700
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(3)-H(3C)	0.9700
C(4)-C(5)	1.496(4)
C(5)-C(10)	1.387(4)
C(5)-C(6)	1.397(4)
C(6)-C(7)	1.383(4)
C(6)-H(6)	0.9400
C(7)-C(8)	1.383(5)
C(7)-H(7)	0.9400
C(8)-C(9)	1.383(4)
C(9)-C(10)	1.380(4)
C(9)-H(9)	0.9400
C(10)-H(10)	0.9400
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(11)-H(11C)	0.9700
C(11A)-H(11D)	0.9700
C(11A)-H(11E)	0.9700
C(11A)-H(11F)	0.9700
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(12)-H(12C)	0.9700
C(13)-H(13A)	0.9700
C(13)-H(13B)	0.9700
C(13)-H(13C)	0.9700
C(14)-H(14A)	0.9700

C(14)-H(14B)	0.9700
C(14)-H(14C)	0.9700
C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700
C(15)-H(15C)	0.9700
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(16)-H(16C)	0.9700
C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700
C(17)-H(17C)	0.9700
C(18)-C(19)	1.495(4)
C(19)-C(24)	1.382(4)
C(19)-C(20)	1.387(4)
C(20)-C(21)	1.378(4)
C(20)-H(20)	0.9400
C(21)-C(22)	1.394(4)
C(21)-H(21)	0.9400
C(22)-C(23)	1.390(4)
C(23)-C(24)	1.384(4)
C(23)-H(23)	0.9400
C(24)-H(24)	0.9400
C(25)-H(25A)	0.9700
C(25)-H(25B)	0.9700
C(25)-H(25C)	0.9700
C(26)-H(26A)	0.9700
C(26)-H(26B)	0.9700
C(26)-H(26C)	0.9700
C(27)-H(27A)	0.9700
C(27)-H(27B)	0.9700
C(27)-H(27C)	0.9700
C(28)-H(28A)	0.9700
C(28)-H(28B)	0.9700
C(28)-H(28C)	0.9700

N(4)-Zr(1)-N(2)	110.97(8)
N(4)-Zr(1)-N(1)	155.73(8)
N(2)-Zr(1)-N(1)	61.30(8)
N(4)-Zr(1)-N(3)	61.14(8)
N(2)-Zr(1)-N(3)	87.70(8)
N(1)-Zr(1)-N(3)	94.82(8)
N(4)-Zr(1)-Cl(1)	96.78(6)
N(2)-Zr(1)-Cl(1)	151.36(6)
N(1)-Zr(1)-Cl(1)	90.46(6)
N(3)-Zr(1)-Cl(1)	100.16(6)
N(4)-Zr(1)-Cl(2)	96.44(6)
N(2)-Zr(1)-Cl(2)	88.80(6)
N(1)-Zr(1)-Cl(2)	105.98(7)
N(3)-Zr(1)-Cl(2)	154.01(6)
Cl(1)-Zr(1)-Cl(2)	95.17(3)
N(1)-Si(1)-C(1)	108.56(13)
N(1)-Si(1)-C(3)	107.41(13)
C(1)-Si(1)-C(3)	110.12(16)
N(1)-Si(1)-C(2)	114.15(13)
C(1)-Si(1)-C(2)	109.94(16)
C(3)-Si(1)-C(2)	106.59(16)
N(2)-Si(2)-C(13)	106.92(14)
N(2)-Si(2)-C(12)	113.15(15)
C(13)-Si(2)-C(12)	109.4(2)
N(2)-Si(2)-C(14)	108.17(16)
C(13)-Si(2)-C(14)	107.4(2)
C(12)-Si(2)-C(14)	111.6(2)
N(3)-Si(3)-C(17)	108.82(14)
N(3)-Si(3)-C(15)	107.77(13)
C(17)-Si(3)-C(15)	111.21(16)
N(3)-Si(3)-C(16)	114.01(13)
C(17)-Si(3)-C(16)	109.91(17)
C(15)-Si(3)-C(16)	105.09(15)

N(4)-Si(4)-C(26)	107.67(15)
N(4)-Si(4)-C(28)	112.85(15)
C(26)-Si(4)-C(28)	107.2(2)
N(4)-Si(4)-C(27)	109.64(14)
C(26)-Si(4)-C(27)	110.0(2)
C(28)-Si(4)-C(27)	109.4(2)
C(11A)-O(1)-C(8)	123.2(8)
C(11A)-O(1)-C(11)	110.6(7)
C(8)-O(1)-C(11)	121.6(3)
C(22)-O(2)-C(25)	116.8(2)
C(4)-N(1)-Si(1)	131.5(2)
Si(1)-N(1)-Zr(1)	137.26(12)
C(4)-N(2)-Si(2)	132.6(2)
Si(2)-N(2)-Zr(1)	133.70(12)
C(18)-N(3)-Si(3)	127.7(2)
Si(3)-N(3)-Zr(1)	141.60(13)
C(18)-N(4)-Si(4)	127.2(2)
Si(4)-N(4)-Zr(1)	138.61(12)
Si(1)-C(1)-H(1A)	109.5
Si(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
Si(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
Si(1)-C(2)-H(2A)	109.5
Si(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
Si(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
Si(1)-C(3)-H(3A)	109.5
Si(1)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
Si(1)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
N(2)-C(4)-N(1)	115.1(2)
N(2)-C(4)-C(5)	122.7(2)
N(1)-C(4)-C(5)	122.1(2)
C(10)-C(5)-C(6)	118.2(3)
C(10)-C(5)-C(4)	119.9(2)
C(6)-C(5)-C(4)	122.0(3)
C(7)-C(6)-C(5)	120.5(3)
C(7)-C(6)-H(6)	119.8
C(5)-C(6)-H(6)	119.8
C(6)-C(7)-C(8)	120.4(3)
C(6)-C(7)-H(7)	119.8
C(8)-C(7)-H(7)	119.8
O(1)-C(8)-C(7)	118.1(3)
O(1)-C(8)-C(9)	122.3(3)
C(7)-C(8)-C(9)	119.6(3)
C(10)-C(9)-C(8)	119.9(3)
C(10)-C(9)-H(9)	120.1
C(8)-C(9)-H(9)	120.1
C(9)-C(10)-C(5)	121.4(3)
C(9)-C(10)-H(10)	119.3
C(5)-C(10)-H(10)	119.3
O(1)-C(11)-H(11A)	109.5
O(1)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
O(1)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
O(1)-C(11A)-H(11D)	109.5
O(1)-C(11A)-H(11E)	109.5
H(11D)-C(11A)-H(11E)	109.5
O(1)-C(11A)-H(11F)	109.5
H(11D)-C(11A)-H(11F)	109.5

H(11E)-C(11A)-H(11F)	109.5
Si(2)-C(12)-H(12A)	109.5
Si(2)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
Si(2)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
Si(2)-C(13)-H(13A)	109.5
Si(2)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
Si(2)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
Si(2)-C(14)-H(14A)	109.5
Si(2)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
Si(2)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
Si(3)-C(15)-H(15A)	109.5
Si(3)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
Si(3)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
Si(3)-C(16)-H(16A)	109.5
Si(3)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
Si(3)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
Si(3)-C(17)-H(17A)	109.5
Si(3)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
Si(3)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
N(3)-C(18)-N(4)	115.5(2)
N(3)-C(18)-C(19)	121.9(2)
N(4)-C(18)-C(19)	122.5(2)
N(3)-C(18)-Zr(1)	58.79(14)
N(4)-C(18)-Zr(1)	56.72(14)
C(19)-C(18)-Zr(1)	178.15(19)
C(24)-C(19)-C(20)	119.1(3)
C(24)-C(19)-C(18)	120.6(2)
C(20)-C(19)-C(18)	120.3(2)
C(21)-C(20)-C(19)	120.4(3)
C(21)-C(20)-H(20)	119.8
C(19)-C(20)-H(20)	119.8
C(20)-C(21)-C(22)	120.3(3)
C(20)-C(21)-H(21)	119.9
C(22)-C(21)-H(21)	119.9
O(2)-C(22)-C(23)	124.6(3)
O(2)-C(22)-C(21)	116.1(3)
C(23)-C(22)-C(21)	119.4(3)
C(24)-C(23)-C(22)	119.6(3)
C(24)-C(23)-H(23)	120.2
C(22)-C(23)-H(23)	120.2
C(19)-C(24)-C(23)	121.1(3)
C(19)-C(24)-H(24)	119.5
C(23)-C(24)-H(24)	119.5
O(2)-C(25)-H(25A)	109.5
O(2)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
O(2)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
Si(4)-C(26)-H(26A)	109.5

Si(4)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
Si(4)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
Si(4)-C(27)-H(27A)	109.5
Si(4)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
Si(4)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
Si(4)-C(28)-H(28A)	109.5
Si(4)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
Si(4)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for complex 9.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Zr(1)	31(1)	30(1)	31(1)	-12(1)	5(1)	-11(1)
Cl(1)	39(1)	43(1)	72(1)	-21(1)	2(1)	-2(1)
Cl(2)	74(1)	56(1)	39(1)	-24(1)	4(1)	-20(1)
Si(1)	30(1)	44(1)	39(1)	-18(1)	3(1)	-15(1)
Si(2)	30(1)	34(1)	40(1)	-12(1)	4(1)	-10(1)
Si(3)	40(1)	44(1)	36(1)	-22(1)	7(1)	-18(1)
Si(4)	45(1)	37(1)	41(1)	-18(1)	6(1)	-20(1)
O(1)	79(2)	40(1)	67(2)	-9(1)	12(1)	-29(1)
O(2)	50(1)	55(1)	42(1)	-15(1)	18(1)	-23(1)
N(1)	33(1)	34(1)	37(1)	-14(1)	4(1)	-14(1)
N(2)	31(1)	32(1)	32(1)	-12(1)	5(1)	-13(1)
N(3)	43(1)	36(1)	32(1)	-17(1)	10(1)	-19(1)
N(4)	41(1)	37(1)	33(1)	-16(1)	7(1)	-17(1)
C(1)	39(2)	63(2)	50(2)	-28(2)	11(1)	-19(2)
C(2)	47(2)	57(2)	59(2)	-24(2)	2(2)	-27(2)
C(3)	41(2)	66(2)	46(2)	-22(2)	-2(1)	-15(2)
C(4)	34(1)	35(1)	29(1)	-15(1)	5(1)	-12(1)
C(5)	31(1)	33(1)	36(2)	-14(1)	2(1)	-12(1)
C(6)	49(2)	42(2)	50(2)	-23(2)	19(2)	-19(1)
C(7)	53(2)	39(2)	63(2)	-26(2)	18(2)	-17(2)
C(8)	43(2)	33(2)	52(2)	-10(2)	0(1)	-16(1)
C(9)	54(2)	47(2)	35(2)	-12(2)	8(1)	-22(2)
C(10)	47(2)	42(2)	38(2)	-19(1)	8(1)	-18(1)
C(11)	88(4)	62(3)	55(4)	-10(3)	14(3)	-53(3)
C(11A)	80(10)	45(8)	122(15)	-16(8)	15(9)	-24(7)
C(12)	50(2)	87(3)	55(2)	8(2)	-6(2)	-17(2)
C(13)	40(2)	57(2)	109(4)	-30(2)	-4(2)	-18(2)
C(14)	46(2)	113(4)	106(4)	-78(3)	23(2)	-17(2)
C(15)	60(2)	52(2)	46(2)	-29(2)	13(2)	-28(2)
C(16)	54(2)	68(2)	60(2)	-42(2)	20(2)	-29(2)
C(17)	54(2)	61(2)	51(2)	-21(2)	-3(2)	-21(2)
C(18)	29(1)	30(1)	33(2)	-10(1)	2(1)	-8(1)
C(19)	35(1)	33(1)	32(2)	-14(1)	5(1)	-15(1)
C(20)	36(1)	38(2)	35(2)	-12(1)	3(1)	-14(1)
C(21)	34(1)	40(2)	44(2)	-17(2)	8(1)	-13(1)
C(22)	44(2)	38(2)	38(2)	-16(1)	14(1)	-20(1)
C(23)	44(2)	39(2)	37(2)	-8(1)	4(1)	-12(1)

C(24)	32(1)	35(2)	40(2)	-12(1)	5(1)	-7(1)
C(25)	74(3)	71(3)	44(2)	-11(2)	23(2)	-24(2)
C(26)	99(3)	76(3)	97(3)	-61(3)	46(3)	-53(3)
C(27)	56(2)	59(2)	101(3)	-42(2)	-11(2)	-20(2)
C(28)	110(3)	42(2)	57(2)	-12(2)	-6(2)	-34(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for complex 9.

	x	y	z	U(eq)
H(1A)	3211	6679	-1557	74
H(1B)	3473	5356	-762	74
H(1C)	2228	6015	-1515	74
H(2A)	4216	3687	-2524	79
H(2B)	2890	4042	-2149	79
H(2C)	4137	3383	-1398	79
H(3A)	3676	6165	-4033	78
H(3B)	3285	7218	-3734	78
H(3C)	2350	6496	-3650	78
H(6)	7548	2498	-1988	54
H(7)	7451	620	-1031	60
H(9)	5669	1700	900	55
H(10)	5668	3597	-97	49
H(11A)	5576	168	1584	101
H(11B)	6178	-1190	1861	101
H(11C)	4959	-421	1086	101
H(11D)	6720	-1676	737	134
H(11E)	7646	-1069	57	134
H(11F)	6206	-672	-343	134
H(12A)	9052	2278	-140	119
H(12B)	9078	3199	259	119
H(12C)	10350	2443	57	119
H(13A)	9910	5670	-2152	106
H(13B)	10911	4661	-1259	106
H(13C)	9640	5422	-1059	106
H(14A)	9594	2802	-2265	119
H(14B)	10874	2994	-2067	119
H(14C)	9843	4003	-2939	119
H(15A)	7212	4249	-3659	71
H(15B)	6316	4477	-4562	71
H(15C)	5746	4909	-3769	71
H(16A)	8324	6611	-5901	80
H(16B)	7938	5562	-5921	80
H(16C)	8852	5328	-5025	80
H(17A)	5522	8043	-6121	84
H(17B)	4623	7433	-5408	84
H(17C)	5196	6997	-6198	84
H(20)	10092	6918	-4346	45
H(21)	11119	7531	-5730	48
H(23)	7797	9807	-7331	52
H(24)	6774	9127	-5949	46
H(25A)	10144	10010	-8880	103
H(25B)	9070	10585	-8376	103
H(25C)	8998	9512	-8560	103
H(26A)	7510	8764	-1862	115
H(26B)	6477	9747	-2743	115
H(26C)	7664	10024	-2474	115
H(27A)	10121	7623	-2304	103
H(27B)	10241	8901	-2883	103
H(27C)	10419	8068	-3409	103
H(28A)	8401	9955	-5048	105
H(28B)	8234	10792	-4527	105

H(28C)	7050	10515	-4801	105

Table 6. Torsion angles [deg] for complex 9.

C(1)-Si(1)-N(1)-C(4)	102.8(3)
C(3)-Si(1)-N(1)-C(4)	-138.2(3)
C(2)-Si(1)-N(1)-C(4)	-20.2(3)
C(1)-Si(1)-N(1)-Zr(1)	-65.9(2)
C(3)-Si(1)-N(1)-Zr(1)	53.1(2)
C(2)-Si(1)-N(1)-Zr(1)	171.08(18)
N(4)-Zr(1)-N(1)-Si(1)	-104.2(2)
N(2)-Zr(1)-N(1)-Si(1)	178.6(2)
N(3)-Zr(1)-N(1)-Si(1)	-96.64(19)
Cl(1)-Zr(1)-N(1)-Si(1)	3.59(18)
Cl(2)-Zr(1)-N(1)-Si(1)	99.11(18)
C(13)-Si(2)-N(2)-C(4)	-155.2(3)
C(12)-Si(2)-N(2)-C(4)	-34.7(3)
C(14)-Si(2)-N(2)-C(4)	89.4(3)
C(13)-Si(2)-N(2)-Zr(1)	3.2(2)
C(12)-Si(2)-N(2)-Zr(1)	123.7(2)
C(14)-Si(2)-N(2)-Zr(1)	-112.2(2)
N(4)-Zr(1)-N(2)-Si(2)	34.04(19)
N(1)-Zr(1)-N(2)-Si(2)	-171.4(2)
N(3)-Zr(1)-N(2)-Si(2)	91.85(17)
Cl(1)-Zr(1)-N(2)-Si(2)	-161.01(9)
Cl(2)-Zr(1)-N(2)-Si(2)	-62.40(16)
C(17)-Si(3)-N(3)-C(18)	-86.7(3)
C(15)-Si(3)-N(3)-C(18)	152.6(2)
C(16)-Si(3)-N(3)-C(18)	36.4(3)
C(17)-Si(3)-N(3)-Zr(1)	95.5(2)
C(15)-Si(3)-N(3)-Zr(1)	-25.2(3)
C(16)-Si(3)-N(3)-Zr(1)	-141.4(2)
N(4)-Zr(1)-N(3)-Si(3)	178.6(2)
N(2)-Zr(1)-N(3)-Si(3)	63.0(2)
N(1)-Zr(1)-N(3)-Si(3)	2.1(2)
Cl(1)-Zr(1)-N(3)-Si(3)	-89.2(2)
Cl(2)-Zr(1)-N(3)-Si(3)	145.54(14)
C(26)-Si(4)-N(4)-C(18)	149.8(3)
C(28)-Si(4)-N(4)-C(18)	31.7(3)
C(27)-Si(4)-N(4)-C(18)	-90.5(3)
C(26)-Si(4)-N(4)-Zr(1)	-11.7(3)
C(28)-Si(4)-N(4)-Zr(1)	-129.8(2)
C(27)-Si(4)-N(4)-Zr(1)	108.0(2)
N(2)-Zr(1)-N(4)-Si(4)	-120.03(19)
N(1)-Zr(1)-N(4)-Si(4)	173.63(16)
N(3)-Zr(1)-N(4)-Si(4)	165.1(2)
Cl(1)-Zr(1)-N(4)-Si(4)	67.2(2)
Cl(2)-Zr(1)-N(4)-Si(4)	-28.8(2)
Si(2)-N(2)-C(4)-N(1)	176.0(2)
Si(2)-N(2)-C(4)-C(5)	-2.2(4)
Si(1)-N(1)-C(4)-N(2)	176.27(19)
Si(1)-N(1)-C(4)-C(5)	-5.5(4)
N(2)-C(4)-C(5)-C(10)	113.8(3)
N(1)-C(4)-C(5)-C(10)	-64.3(4)
N(2)-C(4)-C(5)-C(6)	-67.6(4)
N(1)-C(4)-C(5)-C(6)	114.3(3)
C(10)-C(5)-C(6)-C(7)	0.9(5)
C(4)-C(5)-C(6)-C(7)	-177.7(3)
C(5)-C(6)-C(7)-C(8)	-1.4(5)
C(11A)-O(1)-C(8)-C(7)	-13.0(9)
C(11)-O(1)-C(8)-C(7)	-166.5(4)
C(11A)-O(1)-C(8)-C(9)	167.3(9)
C(11)-O(1)-C(8)-C(9)	13.8(5)
C(6)-C(7)-C(8)-O(1)	-179.8(3)
C(6)-C(7)-C(8)-C(9)	0.0(5)

O(1)-C(8)-C(9)-C(10)	-178.4(3)
C(7)-C(8)-C(9)-C(10)	1.9(5)
C(8)-C(9)-C(10)-C(5)	-2.3(5)
C(6)-C(5)-C(10)-C(9)	1.0(4)
C(4)-C(5)-C(10)-C(9)	179.6(3)
Si(3)-N(3)-C(18)-N(4)	-179.10(19)
Si(3)-N(3)-C(18)-C(19)	-0.7(4)
Si(3)-N(3)-C(18)-Zr(1)	-178.7(3)
Si(4)-N(4)-C(18)-N(3)	-167.4(2)
Si(4)-N(4)-C(18)-C(19)	14.1(4)
N(3)-C(18)-C(19)-C(24)	74.3(4)
N(4)-C(18)-C(19)-C(24)	-107.4(3)
N(3)-C(18)-C(19)-C(20)	-104.7(3)
N(4)-C(18)-C(19)-C(20)	73.6(4)
C(24)-C(19)-C(20)-C(21)	-1.5(4)
C(18)-C(19)-C(20)-C(21)	177.4(3)
C(19)-C(20)-C(21)-C(22)	1.5(4)
C(25)-O(2)-C(22)-C(23)	-5.9(4)
C(25)-O(2)-C(22)-C(21)	174.3(3)
C(20)-C(21)-C(22)-O(2)	179.7(3)
C(20)-C(21)-C(22)-C(23)	-0.2(4)
O(2)-C(22)-C(23)-C(24)	179.0(3)
C(21)-C(22)-C(23)-C(24)	-1.2(4)
C(20)-C(19)-C(24)-C(23)	0.2(4)
C(18)-C(19)-C(24)-C(23)	-178.8(3)
C(22)-C(23)-C(24)-C(19)	1.2(5)

Symmetry transformations used to generate equivalent atoms:

2. **Crystal data for complex 10**

Table 1. Crystal data and structure refinement for complex 10.

Identification code	zrpetdim
Empirical formula	C30 H54 Cl2 N4 Si4 Zr
Formula weight	745.25
Temperature	230.0(1) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C 2/c
Unit cell dimensions	a = 28.3540(11) A alpha = 90 deg. b = 8.8490(5) A beta = 128.046(3) deg. c = 20.4080(10) A gamma = 90 deg.
Volume	4032.4(3) A^3
Z, Calculated density	4, 1.228 Mg/m^3
Absorption coefficient	0.548 mm^-1
F(000)	1568
Crystal size	0.24 x 0.16 x 0.12 mm
Theta range for data collection	1.82 to 25.05 deg.
Limiting indices	-33<=h<=33, -10<=k<=10, -24<=l<=24

Reflections collected / unique	6258 / 3544 [R(int) = 0.0467]
Completeness to theta = 25.05	98.9 %
Absorption correction	None
Max. and min. transmission	0.9372 and 0.8797
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3544 / 0 / 187
Goodness-of-fit on F^2	0.941
Final R indices [I>2sigma(I)]	R1 = 0.0402, wR2 = 0.0957
R indices (all data)	R1 = 0.0648, wR2 = 0.1010
Extinction coefficient	0.00147(19)
Largest diff. peak and hole	0.330 and -0.471 e.A^-3

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

	x	y	z	U(eq)
Zr(1)	0	4599(1)	2500	40(1)
Si(1)	-380(1)	1612(1)	3367(1)	53(1)
Si(2)	1587(1)	5185(1)	4300(1)	52(1)
Cl(1)	-405(1)	6396(1)	2921(1)	74(1)
N(1)	96(1)	2840(3)	3338(1)	43(1)
N(2)	902(1)	4201(3)	3711(1)	41(1)
C(1)	4(2)	-48(4)	4041(2)	66(1)
C(2)	-934(2)	953(5)	2276(2)	92(2)
C(3)	-742(2)	2658(5)	3727(3)	94(1)
C(4)	658(1)	3246(3)	3935(2)	40(1)
C(5)	993(1)	2722(3)	4814(2)	42(1)
C(6)	1353(2)	1452(4)	5102(2)	52(1)
C(7)	1657(1)	981(4)	5919(2)	56(1)
C(8)	1608(1)	1772(4)	6459(2)	51(1)
C(9)	1241(2)	3024(4)	6161(2)	57(1)
C(10)	934(1)	3497(3)	5348(2)	50(1)
C(11)	1979(2)	1312(4)	7373(2)	67(1)
C(12)	2613(2)	1844(5)	7866(2)	109(2)
C(13)	1886(2)	5168(5)	3705(2)	84(1)
C(14)	1434(2)	7142(4)	4442(2)	87(1)
C(15)	2183(1)	4356(4)	5338(2)	72(1)

Table 3. Bond lengths [A] and angles [deg] for complex 10.

Zr(1)-N(1)#1	2.202(2)
Zr(1)-N(1)	2.202(2)
Zr(1)-N(2)	2.233(2)
Zr(1)-N(2)#1	2.233(2)
Zr(1)-Cl(1)	2.4089(9)
Zr(1)-Cl(1)#1	2.4089(9)
Si(1)-N(1)	1.762(2)
Si(1)-C(1)	1.840(3)
Si(1)-C(3)	1.839(4)
Si(1)-C(2)	1.859(3)
Si(2)-N(2)	1.759(2)
Si(2)-C(14)	1.851(4)
Si(2)-C(13)	1.863(4)
Si(2)-C(15)	1.863(3)
N(1)-C(4)	1.326(4)
N(2)-C(4)	1.339(3)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(1)-H(1C)	0.9700
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(2)-H(2C)	0.9700
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(3)-H(3C)	0.9700
C(4)-C(5)	1.495(4)
C(5)-C(10)	1.381(4)
C(5)-C(6)	1.383(4)
C(6)-C(7)	1.388(4)
C(6)-H(6)	0.9400
C(7)-C(8)	1.382(4)
C(7)-H(7)	0.9400
C(8)-C(9)	1.380(4)
C(8)-C(11)	1.527(4)
C(9)-C(10)	1.381(4)
C(9)-H(9)	0.9400
C(10)-H(10)	0.9400
C(11)-C(12)	1.495(5)
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(12)-H(12C)	0.9700
C(13)-H(13A)	0.9700
C(13)-H(13B)	0.9700
C(13)-H(13C)	0.9700
C(14)-H(14A)	0.9700
C(14)-H(14B)	0.9700
C(14)-H(14C)	0.9700
C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700
C(15)-H(15C)	0.9700

N(1)#1-Zr(1)-N(1)	89.99(12)
N(1)#1-Zr(1)-N(2)	104.92(8)
N(1)-Zr(1)-N(2)	61.27(8)
N(1)#1-Zr(1)-N(2)#1	61.27(8)
N(1)-Zr(1)-N(2)#1	104.92(8)
N(2)-Zr(1)-N(2)#1	161.84(12)
N(1)#1-Zr(1)-Cl(1)	152.35(7)
N(1)-Zr(1)-Cl(1)	92.74(6)
N(2)-Zr(1)-Cl(1)	100.47(6)
N(2)#1-Zr(1)-Cl(1)	91.52(6)
N(1)#1-Zr(1)-Cl(1)#1	92.74(7)

N(1)-Zr(1)-Cl(1)#1	152.35(7)
N(2)-Zr(1)-Cl(1)#1	91.52(6)
N(2)#1-Zr(1)-Cl(1)#1	100.48(6)
Cl(1)-Zr(1)-Cl(1)#1	97.38(5)
N(1)-Si(1)-C(1)	113.86(14)
N(1)-Si(1)-C(3)	109.31(15)
C(1)-Si(1)-C(3)	108.77(18)
N(1)-Si(1)-C(2)	104.66(14)
C(1)-Si(1)-C(2)	108.61(18)
C(3)-Si(1)-C(2)	111.6(2)
N(2)-Si(2)-C(14)	107.70(15)
N(2)-Si(2)-C(13)	107.77(15)
C(14)-Si(2)-C(13)	110.7(2)
N(2)-Si(2)-C(15)	115.35(15)
C(14)-Si(2)-C(15)	109.06(17)
C(13)-Si(2)-C(15)	106.21(17)
C(4)-N(1)-Si(1)	130.3(2)
C(4)-N(1)-Zr(1)	91.49(17)
Si(1)-N(1)-Zr(1)	136.99(13)
C(4)-N(2)-Si(2)	131.6(2)
C(4)-N(2)-Zr(1)	89.83(17)
Si(2)-N(2)-Zr(1)	134.99(13)
Si(1)-C(1)-H(1A)	109.5
Si(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
Si(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
Si(1)-C(2)-H(2A)	109.5
Si(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
Si(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
Si(1)-C(3)-H(3A)	109.5
Si(1)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
Si(1)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
N(1)-C(4)-N(2)	116.0(2)
N(1)-C(4)-C(5)	122.2(2)
N(2)-C(4)-C(5)	121.7(3)
N(1)-C(4)-Zr(1)	57.85(15)
N(2)-C(4)-Zr(1)	59.18(14)
C(5)-C(4)-Zr(1)	168.17(19)
C(10)-C(5)-C(6)	119.0(3)
C(10)-C(5)-C(4)	119.8(3)
C(6)-C(5)-C(4)	121.2(3)
C(5)-C(6)-C(7)	120.3(3)
C(5)-C(6)-H(6)	119.9
C(7)-C(6)-H(6)	119.9
C(8)-C(7)-C(6)	120.9(3)
C(8)-C(7)-H(7)	119.6
C(6)-C(7)-H(7)	119.6
C(9)-C(8)-C(7)	118.3(3)
C(9)-C(8)-C(11)	121.1(3)
C(7)-C(8)-C(11)	120.5(3)
C(10)-C(9)-C(8)	121.3(3)
C(10)-C(9)-H(9)	119.4
C(8)-C(9)-H(9)	119.4
C(9)-C(10)-C(5)	120.3(3)
C(9)-C(10)-H(10)	119.9
C(5)-C(10)-H(10)	119.9
C(12)-C(11)-C(8)	112.0(3)
C(12)-C(11)-H(11A)	109.2
C(8)-C(11)-H(11A)	109.2
C(12)-C(11)-H(11B)	109.2

C(8)-C(11)-H(11B)	109.2
H(11A)-C(11)-H(11B)	107.9
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
Si(2)-C(13)-H(13A)	109.5
Si(2)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
Si(2)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
Si(2)-C(14)-H(14A)	109.5
Si(2)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
Si(2)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
Si(2)-C(15)-H(15A)	109.5
Si(2)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
Si(2)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,-z+1/2

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

	U11	U22	U33	U23	U13	U12
Zr(1)	35(1)	40(1)	42(1)	0	21(1)	0
Si(1)	49(1)	55(1)	56(1)	1(1)	33(1)	-10(1)
Si(2)	35(1)	57(1)	53(1)	0(1)	22(1)	-6(1)
Cl(1)	66(1)	68(1)	81(1)	-20(1)	41(1)	9(1)
N(1)	36(2)	46(1)	45(1)	-1(1)	23(1)	-5(1)
N(2)	38(1)	44(1)	40(1)	-3(1)	23(1)	-4(1)
C(1)	73(3)	57(2)	71(2)	0(2)	45(2)	-14(2)
C(2)	78(3)	110(3)	65(2)	0(2)	33(2)	-51(3)
C(3)	88(3)	84(3)	152(4)	8(3)	95(3)	0(2)
C(4)	44(2)	35(2)	45(2)	-2(1)	30(2)	5(1)
C(5)	38(2)	48(2)	40(2)	-1(1)	24(2)	-2(1)
C(6)	60(2)	55(2)	45(2)	1(2)	34(2)	8(2)
C(7)	55(2)	57(2)	51(2)	9(2)	31(2)	11(2)
C(8)	49(2)	61(2)	44(2)	3(2)	29(2)	-7(2)
C(9)	64(2)	65(2)	53(2)	-8(2)	42(2)	-3(2)
C(10)	53(2)	50(2)	52(2)	-1(2)	36(2)	7(2)
C(11)	73(3)	75(3)	48(2)	8(2)	34(2)	-8(2)
C(12)	85(3)	142(4)	49(2)	14(3)	15(2)	-41(3)
C(13)	47(2)	127(4)	74(3)	4(2)	36(2)	-18(2)
C(14)	72(3)	53(2)	97(3)	-14(2)	31(3)	-14(2)
C(15)	41(2)	91(3)	63(2)	2(2)	22(2)	-8(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for complex 10.

	x	y	z	U(eq)
H(1A)	197	-608	3857	100
H(1B)	-286	-692	4010	100
H(1C)	303	282	4611	100
H(2A)	-730	388	2110	138
H(2B)	-1134	1819	1912	138
H(2C)	-1228	309	2236	138
H(3A)	-948	3532	3374	142
H(3B)	-440	2988	4296	142
H(3C)	-1028	2007	3702	142
H(6)	1392	906	4743	63
H(7)	1899	114	6108	67
H(9)	1198	3565	6519	68
H(10)	683	4349	5157	60
H(11A)	1796	1738	7613	81
H(11B)	1974	209	7411	81
H(12A)	2832	1533	8442	164
H(12B)	2620	2937	7838	164
H(12C)	2798	1406	7639	164
H(13A)	1961	4134	3635	126
H(13B)	2257	5738	4006	126
H(13C)	1596	5624	3163	126
H(14A)	1280	7127	4755	131
H(14B)	1140	7600	3902	131
H(14C)	1802	7725	4743	131
H(15A)	2266	3330	5268	108
H(15B)	2050	4347	5676	108
H(15C)	2544	4959	5611	108

Table 6. Torsion angles [deg] for complex 10.

C(1)-Si(1)-N(1)-C(4)	-37.3(3)
C(3)-Si(1)-N(1)-C(4)	84.6(3)
C(2)-Si(1)-N(1)-C(4)	-155.7(3)
C(1)-Si(1)-N(1)-Zr(1)	158.88(18)
C(3)-Si(1)-N(1)-Zr(1)	-79.3(2)
C(2)-Si(1)-N(1)-Zr(1)	40.4(2)
N(1)#1-Zr(1)-N(1)-Si(1)	-78.08(18)
N(2)-Zr(1)-N(1)-Si(1)	174.8(2)
N(2)#1-Zr(1)-N(1)-Si(1)	-17.9(2)
Cl(1)-Zr(1)-N(1)-Si(1)	74.39(18)
Cl(1)#1-Zr(1)-N(1)-Si(1)	-173.99(9)
C(4)#1-Zr(1)-N(1)-Si(1)	-49.7(2)
C(4)-Zr(1)-N(1)-Si(1)	167.7(3)
C(14)-Si(2)-N(2)-C(4)	-99.3(3)
C(13)-Si(2)-N(2)-C(4)	141.2(3)
C(15)-Si(2)-N(2)-C(4)	22.7(3)
C(14)-Si(2)-N(2)-Zr(1)	52.7(2)
C(13)-Si(2)-N(2)-Zr(1)	-66.8(2)
C(15)-Si(2)-N(2)-Zr(1)	174.75(17)
N(1)#1-Zr(1)-N(2)-C(4)	-88.62(15)
N(1)-Zr(1)-N(2)-C(4)	-7.03(15)
Cl(1)-Zr(1)-N(2)-C(4)	80.34(15)
Cl(1)#1-Zr(1)-N(2)-C(4)	178.13(15)
C(4)#1-Zr(1)-N(2)-C(4)	-84.5(2)
N(1)#1-Zr(1)-N(2)-Si(2)	111.90(17)
N(1)-Zr(1)-N(2)-Si(2)	-166.5(2)

N(2)#1-Zr(1)-N(2)-Si(2)	150.31(17)
Cl(1)-Zr(1)-N(2)-Si(2)	-79.14(17)
Cl(1)#1-Zr(1)-N(2)-Si(2)	18.65(17)
C(4)#1-Zr(1)-N(2)-Si(2)	116.00(18)
C(4)-Zr(1)-N(2)-Si(2)	-159.5(3)
Si(1)-N(1)-C(4)-N(2)	179.35(19)
Zr(1)-N(1)-C(4)-N(2)	-11.6(2)
Si(1)-N(1)-C(4)-C(5)	-3.0(4)
Zr(1)-N(1)-C(4)-C(5)	166.0(2)
Si(1)-N(1)-C(4)-Zr(1)	-169.0(3)
Si(2)-N(2)-C(4)-N(1)	172.1(2)
Zr(1)-N(2)-C(4)-N(1)	11.4(2)
Si(2)-N(2)-C(4)-C(5)	-5.6(4)
Zr(1)-N(2)-C(4)-C(5)	-166.2(2)
Si(2)-N(2)-C(4)-Zr(1)	160.6(3)
N(1)#1-Zr(1)-C(4)-N(1)	-68.9(2)
N(2)-Zr(1)-C(4)-N(1)	-167.8(3)
N(2)#1-Zr(1)-C(4)-N(1)	-7.8(2)
Cl(1)-Zr(1)-C(4)-N(1)	88.52(16)
Cl(1)#1-Zr(1)-C(4)-N(1)	-170.06(14)
C(4)#1-Zr(1)-C(4)-N(1)	-46.61(15)
N(1)#1-Zr(1)-C(4)-N(2)	98.97(15)
N(1)-Zr(1)-C(4)-N(2)	167.8(3)
N(2)#1-Zr(1)-C(4)-N(2)	160.07(14)
Cl(1)-Zr(1)-C(4)-N(2)	-103.63(15)
Cl(1)#1-Zr(1)-C(4)-N(2)	-2.21(17)
C(4)#1-Zr(1)-C(4)-N(2)	121.24(16)
N(1)#1-Zr(1)-C(4)-C(5)	-163.1(10)
N(1)-Zr(1)-C(4)-C(5)	-94.2(10)
N(2)-Zr(1)-C(4)-C(5)	98.0(10)
N(2)#1-Zr(1)-C(4)-C(5)	-102.0(10)
Cl(1)-Zr(1)-C(4)-C(5)	-5.7(10)
Cl(1)#1-Zr(1)-C(4)-C(5)	95.7(10)
C(4)#1-Zr(1)-C(4)-C(5)	-140.8(10)
N(1)-C(4)-C(5)-C(10)	-84.8(4)
N(2)-C(4)-C(5)-C(10)	92.6(3)
Zr(1)-C(4)-C(5)-C(10)	1.9(12)
N(1)-C(4)-C(5)-C(6)	93.8(4)
N(2)-C(4)-C(5)-C(6)	-88.7(4)
C(10)-C(5)-C(6)-C(7)	-1.0(5)
C(4)-C(5)-C(6)-C(7)	-179.6(3)
C(5)-C(6)-C(7)-C(8)	-0.3(5)
C(6)-C(7)-C(8)-C(9)	1.3(5)
C(6)-C(7)-C(8)-C(11)	-175.6(3)
C(7)-C(8)-C(9)-C(10)	-0.9(5)
C(11)-C(8)-C(9)-C(10)	175.9(3)
C(8)-C(9)-C(10)-C(5)	-0.4(5)
C(6)-C(5)-C(10)-C(9)	1.3(5)
C(4)-C(5)-C(10)-C(9)	-180.0(3)
C(9)-C(8)-C(11)-C(12)	-98.6(4)
C(7)-C(8)-C(11)-C(12)	78.2(5)

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,-z+1/2

Table 1 3. Tables for Complex 11

Experimental details

Crystal data	
Chemical formula	$3(C_{34}H_{62}Cl_2N_4Si_4Zr)$
M_r	2404.08
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	230
a, b, c (Å)	18.8580 (2), 22.1300 (3), 32.6300 (4)
β (°)	98.5150 (11)
V (Å^3)	13467.3 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.50
Crystal size (mm)	0.27 × 0.20 × 0.12
Data collection	
Diffractometer	KappaCCD diffractometer
Absorption correction	–
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18690, 18690, 9964
R_{int}	0.0000
θ_{max} (°)	23.0
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.550
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.055, 0.146, 1.01
No. of reflections	18690
No. of parameters	1226
No. of restraints	0
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.44, −0.34

Computer programs: Nonius (1997), KappaCCD Collect Program, *HKL SCALEPACK* (Otwinowski & Minor 1997), *HKL DENZO* and *SCALEPACK* (Otwinowski & Minor 1997), S.Mackay, C.J.Gilmore, C.Edwards, M. Tremayne, N. Stuart, K.Shankland "*maXus*": a computer program for the solution and refinement of crystal structures from diffraction data University of Glasgow, Scotland, UK, Nonius BV, Delft, The Netherlands and MacScience Co. Ltd., Yokohama, Japan (1998), *SHELXL97* (Sheldrick, 1997), Molecular Structure Corporation (1999). *ORTEP*. *TEXRAY* Structure Analysis Package. MSC, 3200 Research Forest Drive, The Woodlands,TX 77381, USA..

3. Tables for Complex 11

Computing details

Data collection: Nonius (1997), KappaCCD Collect Program; cell refinement: *HKL SCALEPACK* (Otwinowski & Minor 1997); data reduction: *HKL DENZO* and *SCALEPACK* (Otwinowski & Minor 1997); program(s) used to solve structure: S.Mackay, C.J.Gilmore, C.Edwards, M. Tremayne, N. Stuart, K.Shankland "*maXus*": a computer program for the solution and refinement of crystal structures from diffraction data University of Glasgow, Scotland, UK, Nonius BV, Delft, The Netherlands and MacScience Co. Ltd., Yokohama, Japan (1998); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: Molecular Structure Corporation (1999). *ORTEP*. *TEXRAY* Structure Analysis Package. MSC, 3200 Research Forest Drive, The Woodlands,TX 77381, USA.; software used to prepare material for publication: *SHELXL97* (Sheldrick, 1997).

(zrnbudim)

Crystal data

$3(C_{34}H_{62}Cl_2N_4Si_4Zr)$
$M_r = 2404.08$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 18.8580$ (2) Å
$b = 22.1300$ (3) Å
$c = 32.6300$ (4) Å
$\beta = 98.5150$ (11)°
$V = 13467.3$ (3) Å^3
$Z = 4$
$F(000) = 5088$
$D_x = 1.186$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 60215 reflections
$\theta = 1.0$–27.5°
$\mu = 0.50$ mm^{-1}
$T = 230$ K
Prism, colorless
0.27 × 0.20 × 0.12 mm

Data collection

KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
CCD scans
18690 measured reflections
18690 independent reflections
9964 reflections with $I > 2\sigma(I)$
$R_{int} = 0.0000$
$\theta_{max} = 23.0°$, $\theta_{min} = 1.1°$
$h = 0 \rightarrow 20$
$k = 0 \rightarrow 24$
$l = -35 \rightarrow 35$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.146$
$S = 1.01$
18690 reflections
1226 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0685P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.010$
$\Delta\rho_{max} = 0.44$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

Special details

Refinement

Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Zr1A	−0.06400 (3)	0.31974 (3)	0.482221 (15)	0.05832 (18)	
Cl1A	−0.07727 (9)	0.38630 (7)	0.53952 (5)	0.0822 (5)	
Cl2A	−0.16000 (9)	0.36292 (8)	0.43389 (5)	0.0891 (5)	
Si1A	0.09896 (10)	0.29943 (9)	0.55625 (5)	0.0739 (5)	
Si2A	0.01254 (10)	0.39925 (9)	0.39816 (5)	0.0758 (5)	
Si3A	−0.20267 (10)	0.24903 (9)	0.53530 (5)	0.0740 (5)	
Si4A	−0.01667 (10)	0.18291 (9)	0.42387 (5)	0.0764 (5)	
N1A	0.0512 (2)	0.3154 (2)	0.50711 (12)	0.0619 (13)	
N2A	0.0137 (2)	0.3592 (2)	0.44519 (12)	0.0596 (12)	
N3A	−0.1321 (2)	0.2496 (2)	0.50567 (12)	0.0628 (13)	
N4A	−0.0600 (2)	0.2259 (2)	0.45820 (13)	0.0611 (12)	
C1A	0.0365 (4)	0.2528 (3)	0.58228 (18)	0.108 (2)	
H1A1	−0.0060	0.2763	0.5851	0.161*	
H1A2	0.0601	0.2409	0.6095	0.161*	
H1A3	0.0228	0.2171	0.5658	0.161*	
C2A	0.1226 (3)	0.3694 (3)	0.58655 (16)	0.093 (2)	
H2A1	0.0795	0.3925	0.5883	0.140*	
H2A2	0.1554	0.3934	0.5730	0.140*	
H2A3	0.1454	0.3588	0.6143	0.140*	
C3A	0.1803 (4)	0.2539 (3)	0.5520 (2)	0.112 (3)	
H3A1	0.1667	0.2176	0.5362	0.169*	
H3A2	0.2036	0.2430	0.5795	0.169*	
H3A3	0.2131	0.2775	0.5382	0.169*	
C4A	0.0662 (3)	0.3529 (3)	0.47730 (16)	0.0599 (16)	
C5A	0.1347 (3)	0.3879 (3)	0.48146 (15)	0.0600 (15)	
C6A	0.1983 (4)	0.3611 (3)	0.47536 (17)	0.0810 (19)	
H6A	0.1995	0.3194	0.4700	0.097*	
C7A	0.2611 (4)	0.3953 (4)	0.4771 (2)	0.094 (2)	
H7A	0.3043	0.3760	0.4737	0.113*	
C8A	0.2610 (3)	0.4565 (4)	0.4837 (2)	0.094 (2)	
C9A	0.1982 (4)	0.4826 (3)	0.49161 (18)	0.088 (2)	
H9A	0.1980	0.5239	0.4984	0.106*	
C10A	0.1343 (3)	0.4491 (3)	0.48971 (16)	0.0725 (17)	
H10A	0.0915	0.4683	0.4940	0.087*	
C11A	0.3275 (4)	0.4961 (5)	0.4822 (2)	0.141 (3)	
H11A	0.3594	0.4745	0.4660	0.169*	
H11B	0.3120	0.5332	0.4670	0.169*	
C12A	0.3661 (4)	0.5120 (4)	0.5190 (2)	0.128 (3)	
H12A	0.3855	0.4750	0.5330	0.153*	
H12B	0.3333	0.5300	0.5362	0.153*	
C13A	0.4296 (4)	0.5569 (4)	0.5176 (2)	0.117 (3)	
H13A	0.4579	0.5435	0.4964	0.140*	
H13B	0.4103	0.5970	0.5097	0.140*	
C14A	0.4756 (5)	0.5610 (4)	0.5568 (2)	0.151 (4)	

H14A	0.5137	0.5898	0.5547	0.227*
H14B	0.4962	0.5217	0.5643	0.227*
H14C	0.4479	0.5744	0.5779	0.227*
C15A	−0.0264 (4)	0.4742 (3)	0.40328 (19)	0.105 (2)
H15A	0.0035	0.4967	0.4248	0.158*
H15B	−0.0741	0.4700	0.4105	0.158*
H15C	−0.0290	0.4957	0.3772	0.158*
C16A	−0.0424 (4)	0.3550 (3)	0.35668 (16)	0.099 (2)
H16A	−0.0210	0.3155	0.3546	0.149*
H16B	−0.0444	0.3761	0.3305	0.149*
H16C	−0.0906	0.3503	0.3633	0.149*
C17A	0.1045 (3)	0.4045 (4)	0.38219 (18)	0.118 (3)
H17A	0.1237	0.3642	0.3799	0.177*
H17B	0.1360	0.4272	0.4028	0.177*
H17C	0.1011	0.4249	0.3556	0.177*
C18A	−0.2642 (3)	0.1831 (3)	0.52619 (18)	0.093 (2)
H18A	−0.2842	0.1812	0.4971	0.140*
H18B	−0.3026	0.1874	0.5427	0.140*
H18C	−0.2377	0.1463	0.5341	0.140*
C19A	−0.2587 (3)	0.3179 (3)	0.5204 (2)	0.106 (2)
H19A	−0.2784	0.3158	0.4912	0.159*
H19B	−0.2291	0.3538	0.5254	0.159*
H19C	−0.2975	0.3198	0.5368	0.159*
C20A	−0.1660 (4)	0.2523 (3)	0.59097 (16)	0.108 (3)
H20A	−0.1342	0.2868	0.5961	0.162*
H20B	−0.1395	0.2156	0.5989	0.162*
H20C	−0.2050	0.2563	0.6071	0.162*
C21A	−0.1078 (3)	0.2078 (3)	0.48184 (17)	0.0601 (15)
C22A	−0.1314 (3)	0.1434 (3)	0.48282 (18)	0.0692 (17)
C23A	−0.1061 (4)	0.1075 (3)	0.5157 (2)	0.105 (3)
H23A	−0.0746	0.1235	0.5380	0.126*
C24A	−0.1269 (4)	0.0472 (4)	0.5161 (2)	0.123 (3)
H24A	−0.1089	0.0224	0.5386	0.147*
C25A	−0.1748 (4)	0.0233 (3)	0.4829 (3)	0.100 (2)
C26A	−0.2019 (4)	0.0607 (4)	0.4512 (2)	0.095 (2)
H26A	−0.2363	0.0459	0.4298	0.115*
C27A	−0.1793 (3)	0.1198 (3)	0.45014 (18)	0.0749 (18)
H27A	−0.1962	0.1443	0.4273	0.090*
C28A	−0.1950 (5)	−0.0439 (4)	0.4845 (3)	0.150 (4)
H28A	−0.2212	−0.0562	0.4576	0.180*
H28B	−0.1513	−0.0683	0.4900	0.180*
C29A	−0.2410 (6)	−0.0552 (4)	0.5177 (3)	0.154 (4)
H29A	−0.2862	−0.0330	0.5114	0.185*
H29B	−0.2162	−0.0409	0.5445	0.185*
C30A	−0.2572 (6)	−0.1280 (7)	0.5202 (4)	0.228 (7)
H30A	−0.2934	−0.1409	0.4972	0.274*
H30B	−0.2134	−0.1518	0.5199	0.274*
C31A	−0.2804 (7)	−0.1330 (6)	0.5548 (3)	0.255 (8)
H31A	−0.2907	−0.1751	0.5596	0.382*
H31B	−0.3238	−0.1093	0.5541	0.382*
H31C	−0.2443	−0.1185	0.5768	0.382*
C32A	−0.0760 (3)	0.1793 (3)	0.37274 (16)	0.096 (2)
H32A	−0.1202	0.1586	0.3760	0.144*
H32B	−0.0518	0.1575	0.3531	0.144*

H32C	−0.0870	0.2200	0.3626	0.144*
C33A	0.0686 (3)	0.2221 (3)	0.41854 (18)	0.095 (2)
H33A	0.0987	0.2238	0.4453	0.142*
H33B	0.0582	0.2628	0.4084	0.142*
H33C	0.0933	0.2002	0.3991	0.142*
C34A	0.0081 (3)	0.1056 (3)	0.4435 (2)	0.105 (2)
H34A	−0.0351	0.0832	0.4466	0.157*
H34B	0.0386	0.1084	0.4701	0.157*
H34C	0.0336	0.0848	0.4239	0.157*
Zr1B	−0.05135 (3)	0.33734 (3)	0.147149 (15)	0.05657 (18)
Cl1B	−0.06142 (8)	0.39735 (8)	0.20789 (5)	0.0825 (5)
Cl2B	−0.15279 (8)	0.37911 (9)	0.10215 (5)	0.0894 (5)
Si1B	0.11885 (9)	0.31018 (8)	0.21369 (5)	0.0714 (5)
Si2B	0.01269 (9)	0.43420 (8)	0.06685 (5)	0.0677 (5)
Si3B	−0.18122 (9)	0.25788 (9)	0.20191 (5)	0.0744 (5)
Si4B	−0.00613 (9)	0.20790 (8)	0.08181 (5)	0.0676 (5)
N1B	0.0650 (2)	0.3336 (2)	0.16819 (12)	0.0553 (12)
N2B	0.0204 (2)	0.38622 (19)	0.11055 (12)	0.0563 (12)
N3B	−0.1131 (2)	0.2634 (2)	0.17020 (12)	0.0614 (13)
N4B	−0.0472 (2)	0.2458 (2)	0.11912 (12)	0.0563 (12)
C1B	0.2026 (3)	0.2750 (3)	0.2017 (2)	0.113 (3)
H1B1	0.2319	0.3054	0.1910	0.169*
H1B2	0.1909	0.2434	0.1812	0.169*
H1B3	0.2289	0.2576	0.2268	0.169*
C2B	0.1377 (4)	0.3722 (3)	0.25117 (17)	0.107 (2)
H2B1	0.1666	0.4026	0.2401	0.160*
H2B2	0.1635	0.3566	0.2769	0.160*
H2B3	0.0929	0.3901	0.2563	0.160*
C3B	0.0645 (4)	0.2521 (3)	0.2347 (2)	0.129 (3)
H3B1	0.0545	0.2195	0.2148	0.193*
H3B2	0.0198	0.2697	0.2401	0.193*
H3B3	0.0906	0.2363	0.2604	0.193*
C4B	0.0759 (3)	0.3766 (3)	0.14125 (16)	0.0567 (15)
C5B	0.1423 (3)	0.4139 (3)	0.14454 (15)	0.0582 (15)
C6B	0.2038 (3)	0.3911 (3)	0.13245 (16)	0.0707 (17)
H6B	0.2049	0.3509	0.1233	0.085*
C7B	0.2645 (3)	0.4274 (4)	0.1337 (2)	0.093 (2)
H7B	0.3060	0.4112	0.1251	0.112*
C8B	0.2652 (4)	0.4866 (4)	0.1473 (2)	0.095 (2)
C9B	0.2038 (4)	0.5081 (3)	0.1606 (2)	0.092 (2)
H9B	0.2035	0.5478	0.1708	0.111*
C10B	0.1414 (3)	0.4725 (3)	0.15932 (17)	0.0752 (18)
H10B	0.1000	0.4882	0.1683	0.090*
C11B	0.3312 (4)	0.5275 (5)	0.1459 (3)	0.162 (4)
H11C	0.3593	0.5096	0.1260	0.194*
H11D	0.3137	0.5667	0.1345	0.194*
C12B	0.3743 (5)	0.5377 (5)	0.1795 (2)	0.154 (4)
H12C	0.3940	0.4987	0.1898	0.185*
H12D	0.3454	0.5529	0.2000	0.185*
C13B	0.4378 (4)	0.5814 (4)	0.1796 (2)	0.134 (3)
H13C	0.4671	0.5673	0.1591	0.161*
H13D	0.4190	0.6213	0.1707	0.161*
C14B	0.4819 (4)	0.5874 (4)	0.2177 (2)	0.131 (3)
H14D	0.5197	0.6163	0.2151	0.197*

H14E	0.5029	0.5486	0.2262	0.197*	
H14F	0.4537	0.6017	0.2383	0.197*	
C15B	−0.0374 (3)	0.3906 (3)	0.02367 (16)	0.089 (2)	
H15D	−0.0838	0.3791	0.0307	0.134*	
H15E	−0.0106	0.3546	0.0188	0.134*	
H15F	−0.0443	0.4153	−0.0012	0.134*	
C16B	−0.0363 (3)	0.5031 (3)	0.07835 (18)	0.094 (2)	
H16D	−0.0083	0.5249	0.1010	0.141*	
H16E	−0.0822	0.4918	0.0862	0.141*	
H16F	−0.0440	0.5287	0.0539	0.141*	
C17B	0.0996 (3)	0.4545 (3)	0.05100 (17)	0.097 (2)	
H17D	0.1278	0.4776	0.0729	0.145*	
H17E	0.0914	0.4786	0.0259	0.145*	
H17F	0.1254	0.4180	0.0459	0.145*	
C18B	−0.1377 (3)	0.2517 (3)	0.25659 (15)	0.091 (2)	
H18D	−0.1049	0.2853	0.2632	0.137*	
H18E	−0.1113	0.2140	0.2605	0.137*	
H18F	−0.1740	0.2526	0.2747	0.137*	
C19B	−0.2354 (3)	0.3283 (3)	0.1929 (2)	0.103 (2)	
H19D	−0.2046	0.3631	0.1996	0.155*	
H19E	−0.2727	0.3281	0.2104	0.155*	
H19F	−0.2571	0.3303	0.1641	0.155*	
C20B	−0.2440 (3)	0.1941 (3)	0.18878 (19)	0.110 (3)	
H20D	−0.2666	0.1978	0.1602	0.166*	
H20E	−0.2805	0.1948	0.2069	0.166*	
H20F	−0.2179	0.1563	0.1924	0.166*	
C21B	−0.0908 (3)	0.2245 (3)	0.14379 (15)	0.0573 (15)	
C22B	−0.1131 (3)	0.1587 (3)	0.14272 (16)	0.0585 (15)	
C23B	−0.0841 (3)	0.1209 (3)	0.17518 (18)	0.0738 (18)	
H23B	−0.0520	0.1364	0.1975	0.089*	
C24B	−0.1028 (4)	0.0615 (3)	0.1743 (2)	0.090 (2)	
H24B	−0.0825	0.0362	0.1961	0.107*	
C25B	−0.1508 (4)	0.0368 (3)	0.1422 (2)	0.0806 (19)	
C26B	−0.1803 (3)	0.0757 (3)	0.11036 (18)	0.0752 (18)	
H26B	−0.2140	0.0607	0.0886	0.090*	
C27B	−0.1604 (3)	0.1363 (3)	0.11047 (16)	0.0635 (16)	
H27B	−0.1794	0.1617	0.0885	0.076*	
C28B	−0.1747 (5)	−0.0298 (3)	0.1418 (2)	0.124 (3)	
H28C	−0.1330	−0.0555	0.1509	0.149*	
H28D	−0.1945	−0.0415	0.1135	0.149*	
C29B	−0.2329 (8)	−0.0401 (8)	0.1711 (6)	0.319 (12)	
H29C	−0.2303	−0.0842	0.1737	0.383*	
H29D	−0.2063	−0.0253	0.1972	0.383*	
C30B	−0.2765 (12)	−0.0343 (12)	0.1760 (7)	0.160 (11)*	0.59 (3)
C30E	−0.2541 (18)	−0.1035 (18)	0.1857 (9)	0.21 (2)*	0.41 (3)
C31B	−0.3042 (7)	−0.0706 (7)	0.2120 (3)	0.210 (5)	
C32B	0.0213 (3)	0.1290 (3)	0.09669 (19)	0.095 (2)	
H32D	−0.0208	0.1053	0.0998	0.142*	
H32E	0.0538	0.1294	0.1227	0.142*	
H32F	0.0454	0.1112	0.0753	0.142*	
C33B	0.0766 (3)	0.2491 (3)	0.07643 (18)	0.094 (2)	
H33D	0.1084	0.2486	0.1027	0.141*	
H33E	0.0649	0.2906	0.0685	0.141*	
H33F	0.1001	0.2300	0.0553	0.141*	

C34B	−0.0667 (3)	0.2076 (3)	0.03173 (16)	0.099 (2)	
H34D	−0.1099	0.1851	0.0346	0.148*	
H34E	−0.0427	0.1887	0.0107	0.148*	
H34F	−0.0794	0.2488	0.0236	0.148*	
Zr1C	0.44729 (3)	0.20144 (3)	0.302662 (16)	0.06121 (18)	
Cl1C	0.42697 (10)	0.13691 (9)	0.35949 (6)	0.1038 (6)	
Cl2C	0.34387 (9)	0.16842 (9)	0.25593 (6)	0.1078 (7)	
Si1C	0.33445 (10)	0.28887 (9)	0.36428 (5)	0.0796 (6)	
Si2C	0.49912 (9)	0.32776 (8)	0.23712 (5)	0.0626 (5)	
Si3C	0.61809 (10)	0.22242 (9)	0.37105 (5)	0.0846 (6)	
Si4C	0.50833 (10)	0.10040 (9)	0.22426 (5)	0.0729 (5)	
N1C	0.3967 (2)	0.2799 (2)	0.32946 (12)	0.0590 (12)	
N2C	0.4587 (2)	0.29319 (19)	0.27605 (11)	0.0541 (11)	
N3C	0.5632 (2)	0.2000 (2)	0.32539 (13)	0.0628 (13)	
N4C	0.5179 (2)	0.1489 (2)	0.26708 (12)	0.0606 (12)	
C1C	0.3818 (4)	0.2725 (3)	0.41722 (16)	0.109 (3)	
H1C1	0.4193	0.3022	0.4247	0.164*	
H1C2	0.4029	0.2324	0.4177	0.164*	
H1C3	0.3480	0.2742	0.4369	0.164*	
C2C	0.2612 (3)	0.2354 (3)	0.34813 (19)	0.105 (2)	
H2C1	0.2372	0.2462	0.3207	0.157*	
H2C2	0.2271	0.2368	0.3677	0.157*	
H2C3	0.2805	0.1948	0.3475	0.157*	
C3C	0.2938 (4)	0.3658 (3)	0.36555 (19)	0.117 (3)	
H3C1	0.3312	0.3952	0.3741	0.175*	
H3C2	0.2596	0.3660	0.3850	0.175*	
H3C3	0.2694	0.3761	0.3381	0.175*	
C4C	0.4178 (3)	0.3182 (3)	0.30192 (15)	0.0533 (15)	
C5C	0.3983 (3)	0.3836 (3)	0.30031 (16)	0.0531 (14)	
C6C	0.4330 (3)	0.4234 (3)	0.32857 (17)	0.0703 (17)	
H6C	0.4703	0.4096	0.3488	0.084*	
C7C	0.4134 (3)	0.4837 (3)	0.32754 (19)	0.0749 (18)	
H7C	0.4395	0.5106	0.3463	0.090*	
C8C	0.3570 (4)	0.5054 (3)	0.29982 (19)	0.0683 (17)	
C9C	0.3225 (3)	0.4640 (3)	0.27121 (17)	0.0697 (17)	
H9C	0.2843	0.4773	0.2515	0.084*	
C10C	0.3434 (3)	0.4035 (3)	0.27121 (15)	0.0625 (16)	
H10C	0.3200	0.3765	0.2514	0.075*	
C11C	0.3310 (4)	0.5695 (3)	0.3021 (2)	0.095 (2)	
H11E	0.3015	0.5795	0.2756	0.114*	
H11F	0.3728	0.5964	0.3053	0.114*	
C12C	0.2880 (6)	0.5827 (4)	0.3366 (4)	0.133 (3)	
C13C	0.2282 (8)	0.5492 (6)	0.3391 (8)	0.095 (6)	0.72 (4)
C13F	0.271 (4)	0.5538 (18)	0.3649 (14)	0.10 (2)	0.28 (4)
C14C	0.1997 (4)	0.5649 (4)	0.3814 (2)	0.120 (3)	
C15C	0.4335 (3)	0.3305 (3)	0.18863 (15)	0.090 (2)	
H15G	0.3926	0.3549	0.1931	0.134*	
H15H	0.4175	0.2898	0.1809	0.134*	
H15I	0.4560	0.3481	0.1666	0.134*	
C16C	0.5780 (3)	0.2812 (3)	0.22992 (18)	0.090 (2)	
H16G	0.6113	0.2801	0.2556	0.135*	
H16H	0.6015	0.2987	0.2082	0.135*	
H16I	0.5625	0.2405	0.2222	0.135*	
C17C	0.5323 (3)	0.4059 (3)	0.25197 (18)	0.096 (2)	

H17G	0.4922	0.4313	0.2564	0.144*
H17H	0.5554	0.4229	0.2299	0.144*
H17I	0.5665	0.4040	0.2773	0.144*
C18C	0.5758 (4)	0.2918 (4)	0.3872 (2)	0.178 (5)
H18G	0.5765	0.3227	0.3662	0.266*
H18H	0.6021	0.3059	0.4133	0.266*
H18I	0.5266	0.2832	0.3907	0.266*
C19C	0.6187 (5)	0.1632 (4)	0.4108 (2)	0.174 (4)
H19G	0.6405	0.1268	0.4017	0.262*
H19H	0.5698	0.1545	0.4150	0.262*
H19I	0.6460	0.1770	0.4366	0.262*
C20C	0.7107 (4)	0.2407 (4)	0.3638 (2)	0.154 (4)
H20G	0.7101	0.2724	0.3433	0.231*
H20H	0.7334	0.2050	0.3545	0.231*
H20I	0.7373	0.2543	0.3899	0.231*
C21C	0.5728 (3)	0.1566 (3)	0.29801 (17)	0.0618 (16)
C22C	0.6369 (3)	0.1168 (3)	0.30338 (16)	0.0578 (15)
C23C	0.7007 (3)	0.1356 (3)	0.29137 (17)	0.0735 (18)
H23C	0.7039	0.1744	0.2801	0.088*
C24C	0.7596 (3)	0.0981 (3)	0.29582 (18)	0.0748 (18)
H24C	0.8026	0.1121	0.2878	0.090*
C25C	0.7573 (3)	0.0407 (3)	0.31161 (17)	0.0693 (17)
C26C	0.6933 (3)	0.0220 (3)	0.32444 (18)	0.0806 (19)
H26C	0.6904	−0.0163	0.3365	0.097*
C27C	0.6338 (3)	0.0600 (3)	0.31934 (17)	0.0721 (17)
H27C	0.5905	0.0462	0.3271	0.087*
C28C	0.8201 (3)	−0.0020 (3)	0.31575 (19)	0.091 (2)
H28E	0.8041	−0.0401	0.3021	0.109*
H28F	0.8567	0.0152	0.3008	0.109*
C29C	0.8534 (4)	−0.0155 (3)	0.3582 (2)	0.110 (3)
H29E	0.8167	−0.0326	0.3732	0.132*
H29F	0.8696	0.0225	0.3719	0.132*
C30C	0.9159 (4)	−0.0584 (4)	0.3621 (2)	0.129 (3)
H30C	0.8994	−0.0965	0.3486	0.154*
H30D	0.9520	−0.0415	0.3466	0.154*
C31C	0.9494 (6)	−0.0714 (5)	0.4023 (3)	0.226 (6)
H31D	0.9890	−0.0989	0.4011	0.339*
H31E	0.9150	−0.0900	0.4178	0.339*
H31F	0.9672	−0.0343	0.4160	0.339*
C32C	0.4567 (3)	0.0339 (3)	0.23582 (18)	0.096 (2)
H32G	0.4831	0.0120	0.2590	0.144*
H32H	0.4488	0.0077	0.2117	0.144*
H32I	0.4108	0.0467	0.2429	0.144*
C33C	0.4597 (4)	0.1430 (3)	0.17967 (16)	0.112 (3)
H33G	0.4881	0.1776	0.1737	0.167*
H33H	0.4140	0.1567	0.1864	0.167*
H33I	0.4516	0.1169	0.1556	0.167*
C34C	0.5956 (3)	0.0758 (4)	0.20956 (18)	0.126 (3)
H34G	0.6230	0.1111	0.2036	0.188*
H34H	0.5870	0.0503	0.1852	0.188*
H34I	0.6224	0.0533	0.2323	0.188*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zr1A	0.0579 (4)	0.0559 (4)	0.0588 (3)	0.0034 (3)	0.0009 (3)	0.0002 (3)
Cl1A	0.0853 (12)	0.0713 (12)	0.0906 (10)	0.0019 (10)	0.0156 (9)	−0.0203 (9)
Cl2A	0.0664 (11)	0.1008 (14)	0.0944 (11)	0.0061 (10)	−0.0068 (9)	0.0275 (10)
Si1A	0.0753 (13)	0.0746 (14)	0.0652 (10)	0.0120 (11)	−0.0114 (9)	0.0059 (9)
Si2A	0.0759 (13)	0.0897 (15)	0.0593 (10)	−0.0035 (11)	0.0014 (9)	0.0112 (9)
Si3A	0.0843 (13)	0.0727 (14)	0.0663 (10)	−0.0086 (11)	0.0152 (9)	−0.0004 (9)
Si4A	0.0684 (12)	0.0734 (14)	0.0839 (11)	0.0166 (10)	−0.0002 (9)	−0.0176 (10)
N1A	0.060 (3)	0.069 (4)	0.054 (3)	0.007 (3)	−0.001 (2)	0.005 (3)
N2A	0.056 (3)	0.064 (3)	0.056 (3)	0.007 (2)	−0.002 (2)	−0.001 (2)
N3A	0.076 (3)	0.058 (3)	0.055 (3)	0.002 (3)	0.012 (2)	−0.004 (2)
N4A	0.061 (3)	0.056 (3)	0.064 (3)	0.005 (3)	0.002 (2)	−0.002 (2)
C1A	0.117 (6)	0.109 (6)	0.090 (5)	−0.002 (5)	−0.007 (4)	0.039 (4)
C2A	0.099 (5)	0.099 (6)	0.072 (4)	0.006 (4)	−0.019 (4)	−0.009 (4)
C3A	0.113 (6)	0.110 (7)	0.105 (5)	0.049 (5)	−0.016 (4)	0.003 (5)
C4A	0.068 (4)	0.058 (4)	0.052 (3)	0.020 (3)	0.003 (3)	−0.009 (3)
C5A	0.050 (4)	0.066 (5)	0.063 (3)	0.002 (4)	0.004 (3)	−0.003 (3)
C6A	0.072 (5)	0.088 (6)	0.082 (4)	0.004 (5)	0.008 (4)	−0.020 (4)
C7A	0.064 (5)	0.104 (7)	0.112 (5)	0.010 (5)	0.007 (4)	−0.019 (5)
C8A	0.045 (5)	0.136 (8)	0.103 (5)	−0.002 (5)	0.014 (4)	−0.013 (5)
C9A	0.079 (5)	0.082 (6)	0.101 (5)	−0.025 (5)	0.008 (4)	−0.006 (4)
C10A	0.066 (5)	0.072 (5)	0.080 (4)	0.004 (4)	0.009 (3)	0.004 (4)
C11A	0.075 (6)	0.203 (11)	0.143 (7)	−0.038 (6)	0.012 (5)	−0.016 (7)
C12A	0.117 (7)	0.166 (9)	0.099 (6)	−0.050 (7)	0.012 (5)	−0.015 (6)
C13A	0.089 (6)	0.121 (7)	0.134 (6)	−0.032 (5)	−0.002 (5)	0.001 (5)
C14A	0.143 (8)	0.168 (10)	0.144 (7)	−0.034 (7)	0.027 (6)	−0.045 (7)
C15A	0.129 (6)	0.078 (6)	0.098 (5)	−0.007 (5)	−0.017 (4)	0.017 (4)
C16A	0.116 (6)	0.111 (6)	0.063 (4)	0.002 (5)	−0.009 (4)	0.004 (4)
C17A	0.094 (6)	0.187 (9)	0.077 (4)	−0.007 (6)	0.025 (4)	0.020 (5)
C18A	0.100 (5)	0.090 (6)	0.094 (4)	−0.023 (4)	0.030 (4)	−0.007 (4)
C19A	0.085 (5)	0.106 (6)	0.133 (6)	0.007 (5)	0.039 (4)	0.024 (5)
C20A	0.136 (7)	0.123 (7)	0.067 (4)	−0.026 (5)	0.022 (4)	−0.011 (4)
C21A	0.060 (4)	0.052 (4)	0.061 (4)	0.004 (4)	−0.017 (3)	0.006 (3)
C22A	0.067 (4)	0.061 (5)	0.072 (4)	0.004 (4)	−0.012 (3)	0.003 (4)
C23A	0.119 (6)	0.063 (5)	0.116 (5)	−0.028 (5)	−0.042 (5)	0.023 (5)
C24A	0.124 (7)	0.093 (7)	0.132 (6)	−0.011 (6)	−0.044 (5)	0.025 (5)
C25A	0.093 (6)	0.050 (5)	0.149 (7)	−0.021 (4)	−0.008 (5)	−0.014 (5)
C26A	0.088 (6)	0.071 (6)	0.118 (6)	0.009 (5)	−0.017 (4)	−0.013 (5)
C27A	0.083 (5)	0.059 (5)	0.078 (4)	0.011 (4)	−0.003 (4)	−0.009 (4)
C28A	0.121 (8)	0.084 (7)	0.231 (11)	−0.018 (6)	−0.022 (7)	−0.005 (7)
C29A	0.193 (11)	0.067 (7)	0.202 (10)	−0.032 (7)	0.029 (8)	0.013 (7)
C30A	0.161 (12)	0.33 (2)	0.189 (12)	0.007 (12)	−0.006 (9)	0.086 (14)
C31A	0.309 (18)	0.273 (17)	0.176 (11)	−0.134 (14)	0.015 (12)	0.056 (12)
C32A	0.088 (5)	0.118 (6)	0.080 (4)	0.016 (5)	0.008 (4)	−0.021 (4)
C33A	0.079 (5)	0.099 (6)	0.108 (5)	0.016 (4)	0.022 (4)	−0.028 (4)
C34A	0.094 (5)	0.075 (5)	0.140 (6)	0.026 (4)	0.000 (5)	−0.007 (5)
Zr1B	0.0483 (4)	0.0598 (4)	0.0593 (3)	−0.0023 (3)	0.0003 (3)	0.0036 (3)
Cl1B	0.0748 (11)	0.0829 (13)	0.0896 (10)	−0.0038 (9)	0.0111 (9)	−0.0197 (9)
Cl2B	0.0581 (10)	0.1139 (16)	0.0906 (10)	0.0099 (10)	−0.0069 (8)	0.0268 (10)
Si1B	0.0599 (11)	0.0726 (14)	0.0743 (10)	−0.0015 (10)	−0.0140 (9)	0.0164 (9)
Si2B	0.0696 (12)	0.0657 (13)	0.0650 (10)	−0.0008 (10)	0.0006 (9)	0.0130 (9)
Si3B	0.0707 (12)	0.0887 (15)	0.0663 (10)	−0.0197 (11)	0.0181 (9)	−0.0093 (9)

Si4B	0.0658 (12)	0.0698 (13)	0.0676 (10)	−0.0002 (10)	0.0111 (8)	−0.0032 (9)
N1B	0.053 (3)	0.049 (3)	0.061 (3)	−0.006 (2)	−0.002 (2)	0.014 (2)
N2B	0.045 (3)	0.057 (3)	0.064 (3)	0.002 (2)	−0.003 (2)	0.006 (2)
N3B	0.062 (3)	0.069 (4)	0.054 (3)	−0.009 (3)	0.012 (2)	−0.007 (2)
N4B	0.052 (3)	0.064 (3)	0.053 (3)	−0.009 (2)	0.010 (2)	0.005 (2)
C1B	0.098 (6)	0.110 (7)	0.121 (5)	0.040 (5)	−0.017 (4)	0.018 (5)
C2B	0.106 (6)	0.123 (7)	0.079 (4)	0.011 (5)	−0.026 (4)	−0.008 (4)
C3B	0.101 (6)	0.139 (8)	0.132 (6)	−0.034 (5)	−0.030 (5)	0.084 (6)
C4B	0.041 (4)	0.054 (4)	0.073 (4)	0.007 (3)	0.003 (3)	−0.005 (3)
C5B	0.047 (4)	0.064 (5)	0.061 (3)	0.003 (4)	0.000 (3)	0.006 (3)
C6B	0.057 (4)	0.072 (5)	0.079 (4)	0.001 (4)	0.000 (3)	0.008 (3)
C7B	0.048 (5)	0.123 (7)	0.108 (5)	−0.009 (5)	0.010 (4)	0.002 (5)
C8B	0.073 (6)	0.113 (7)	0.094 (5)	−0.035 (6)	−0.006 (4)	0.003 (5)
C9B	0.095 (6)	0.068 (5)	0.107 (5)	−0.011 (5)	−0.006 (5)	−0.004 (4)
C10B	0.058 (4)	0.077 (5)	0.089 (4)	−0.011 (4)	0.004 (3)	−0.008 (4)
C11B	0.122 (8)	0.203 (11)	0.147 (8)	−0.091 (8)	−0.024 (6)	0.022 (7)
C12B	0.148 (8)	0.219 (11)	0.091 (5)	−0.105 (8)	0.005 (5)	0.010 (6)
C13B	0.110 (7)	0.184 (9)	0.104 (6)	−0.097 (7)	0.002 (5)	0.021 (6)
C14B	0.143 (8)	0.134 (8)	0.113 (6)	−0.061 (6)	0.005 (6)	0.011 (5)
C15B	0.102 (5)	0.090 (5)	0.069 (4)	−0.003 (4)	−0.010 (4)	0.012 (4)
C16B	0.106 (6)	0.082 (5)	0.089 (4)	0.009 (4)	−0.004 (4)	0.010 (4)
C17B	0.090 (5)	0.114 (6)	0.086 (4)	−0.011 (5)	0.012 (4)	0.041 (4)
C18B	0.108 (5)	0.105 (6)	0.064 (4)	−0.011 (5)	0.026 (4)	−0.001 (4)
C19B	0.070 (5)	0.114 (7)	0.131 (6)	0.004 (5)	0.032 (4)	0.005 (5)
C20B	0.092 (5)	0.138 (7)	0.110 (5)	−0.057 (5)	0.044 (4)	−0.031 (5)
C21B	0.053 (4)	0.064 (5)	0.049 (3)	0.005 (3)	−0.013 (3)	0.000 (3)
C22B	0.056 (4)	0.056 (4)	0.061 (3)	−0.005 (3)	0.003 (3)	0.002 (3)
C23B	0.069 (4)	0.059 (5)	0.087 (4)	−0.010 (4)	−0.010 (3)	0.010 (4)
C24B	0.089 (5)	0.084 (6)	0.090 (5)	−0.010 (5)	−0.007 (4)	0.017 (4)
C25B	0.095 (5)	0.063 (5)	0.089 (5)	−0.011 (4)	0.033 (4)	0.003 (4)
C26B	0.058 (4)	0.083 (6)	0.082 (4)	−0.009 (4)	0.003 (3)	−0.009 (4)
C27B	0.064 (4)	0.055 (5)	0.068 (4)	−0.006 (3)	0.000 (3)	−0.007 (3)
C28B	0.149 (8)	0.066 (6)	0.155 (7)	−0.017 (6)	0.015 (6)	0.003 (5)
C29B	0.193 (16)	0.207 (16)	0.56 (3)	−0.116 (14)	0.061 (17)	0.156 (17)
C31B	0.246 (14)	0.226 (14)	0.160 (9)	−0.050 (12)	0.033 (9)	0.011 (10)
C32B	0.102 (6)	0.075 (5)	0.113 (5)	0.014 (4)	0.036 (4)	0.002 (4)
C33B	0.090 (5)	0.095 (6)	0.107 (5)	−0.008 (4)	0.050 (4)	−0.016 (4)
C34B	0.112 (6)	0.118 (6)	0.066 (4)	0.009 (5)	0.008 (4)	−0.008 (4)
Zr1C	0.0530 (4)	0.0541 (4)	0.0719 (4)	0.0019 (3)	−0.0060 (3)	0.0023 (3)
Cl1C	0.0995 (14)	0.0847 (14)	0.1286 (14)	0.0027 (11)	0.0216 (11)	0.0378 (11)
Cl2C	0.0657 (12)	0.1072 (16)	0.1371 (14)	0.0109 (11)	−0.0297 (10)	−0.0406 (12)
Si1C	0.0849 (14)	0.0952 (16)	0.0623 (10)	0.0026 (12)	0.0229 (9)	0.0070 (10)
Si2C	0.0589 (11)	0.0605 (12)	0.0687 (10)	−0.0036 (9)	0.0102 (8)	0.0013 (8)
Si3C	0.0698 (13)	0.0814 (15)	0.0910 (12)	0.0066 (11)	−0.0267 (10)	−0.0193 (11)
Si4C	0.0767 (13)	0.0741 (14)	0.0641 (10)	−0.0011 (10)	−0.0030 (9)	−0.0095 (9)
N1C	0.059 (3)	0.062 (3)	0.056 (3)	0.002 (3)	0.006 (2)	0.001 (2)
N2C	0.053 (3)	0.054 (3)	0.055 (3)	0.000 (2)	0.009 (2)	−0.001 (2)
N3C	0.055 (3)	0.056 (3)	0.071 (3)	0.001 (3)	−0.013 (2)	−0.001 (3)
N4C	0.062 (3)	0.059 (3)	0.056 (3)	0.006 (3)	−0.009 (2)	0.005 (2)
C1C	0.128 (6)	0.141 (7)	0.060 (4)	−0.013 (5)	0.015 (4)	0.008 (4)
C2C	0.079 (5)	0.142 (7)	0.099 (5)	−0.016 (5)	0.029 (4)	0.007 (5)
C3C	0.140 (7)	0.115 (7)	0.113 (5)	0.045 (6)	0.075 (5)	0.022 (5)
C4C	0.047 (4)	0.068 (5)	0.041 (3)	−0.006 (3)	−0.006 (3)	0.000 (3)
C5C	0.052 (4)	0.045 (4)	0.062 (3)	0.001 (3)	0.008 (3)	−0.001 (3)

C6C	0.065 (4)	0.066 (5)	0.074 (4)	0.004 (4)	−0.009 (3)	−0.009 (4)
C7C	0.071 (5)	0.055 (5)	0.097 (5)	−0.003 (4)	0.008 (4)	−0.022 (4)
C8C	0.075 (5)	0.057 (5)	0.076 (4)	0.001 (4)	0.024 (4)	0.003 (4)
C9C	0.066 (4)	0.072 (5)	0.071 (4)	0.014 (4)	0.010 (3)	0.017 (4)
C10C	0.057 (4)	0.070 (5)	0.058 (3)	0.004 (4)	−0.003 (3)	−0.002 (3)
C11C	0.105 (6)	0.045 (5)	0.135 (6)	0.003 (4)	0.021 (5)	0.011 (4)
C12C	0.152 (10)	0.081 (7)	0.188 (10)	0.034 (7)	0.101 (8)	−0.010 (7)
C13C	0.061 (9)	0.083 (9)	0.134 (14)	0.014 (7)	−0.004 (9)	−0.007 (8)
C13F	0.14 (5)	0.13 (3)	0.06 (3)	0.07 (3)	0.08 (3)	0.051 (19)
C14C	0.123 (7)	0.140 (8)	0.107 (5)	0.032 (6)	0.046 (5)	0.003 (5)
C15C	0.088 (5)	0.115 (6)	0.065 (4)	−0.007 (4)	0.010 (3)	0.006 (4)
C16C	0.071 (5)	0.091 (6)	0.117 (5)	−0.001 (4)	0.042 (4)	0.009 (4)
C17C	0.110 (6)	0.074 (5)	0.111 (5)	−0.026 (4)	0.040 (4)	−0.006 (4)
C18C	0.122 (7)	0.190 (10)	0.192 (8)	0.075 (7)	−0.071 (6)	−0.126 (8)
C19C	0.220 (11)	0.181 (10)	0.093 (5)	−0.060 (8)	−0.073 (6)	0.040 (6)
C20C	0.080 (6)	0.187 (10)	0.179 (8)	−0.021 (6)	−0.033 (5)	−0.074 (7)
C21C	0.064 (4)	0.057 (4)	0.063 (4)	−0.006 (4)	0.005 (3)	0.008 (3)
C22C	0.052 (4)	0.055 (4)	0.065 (3)	0.002 (3)	0.003 (3)	0.006 (3)
C23C	0.063 (5)	0.064 (5)	0.091 (4)	−0.002 (4)	0.004 (4)	0.014 (3)
C24C	0.056 (4)	0.070 (5)	0.099 (5)	−0.006 (4)	0.012 (3)	0.009 (4)
C25C	0.047 (4)	0.077 (5)	0.081 (4)	0.013 (4)	0.000 (3)	−0.005 (4)
C26C	0.065 (5)	0.061 (5)	0.111 (5)	0.012 (4)	−0.002 (4)	0.015 (4)
C27C	0.054 (4)	0.068 (5)	0.095 (4)	0.006 (4)	0.015 (3)	0.017 (4)
C28C	0.061 (5)	0.098 (6)	0.110 (5)	0.021 (4)	0.003 (4)	0.006 (4)
C29C	0.109 (6)	0.098 (6)	0.110 (5)	0.050 (5)	−0.027 (5)	−0.022 (5)
C30C	0.114 (7)	0.122 (8)	0.135 (7)	0.057 (6)	−0.031 (5)	−0.018 (6)
C31C	0.278 (14)	0.170 (11)	0.191 (10)	0.138 (10)	−0.096 (10)	−0.042 (8)
C32C	0.112 (6)	0.075 (5)	0.092 (4)	−0.004 (4)	−0.016 (4)	0.004 (4)
C33C	0.150 (7)	0.109 (6)	0.065 (4)	−0.035 (5)	−0.018 (4)	0.005 (4)
C34C	0.107 (6)	0.187 (9)	0.082 (4)	0.007 (6)	0.011 (4)	−0.062 (5)

Geometric parameters (Å, º)

Zr1A—N1A	2.206 (4)	C12B—H12C	0.9800
Zr1A—N2A	2.213 (4)	C12B—H12D	0.9800
Zr1A—N3A	2.221 (4)	C13B—C14B	1.396 (8)
Zr1A—N4A	2.225 (4)	C13B—H13C	0.9800
Zr1A—Cl2A	2.4151 (16)	C13B—H13D	0.9800
Zr1A—Cl1A	2.4221 (15)	C14B—H14D	0.9700
Zr1A—C4A	2.590 (6)	C14B—H14E	0.9700
Zr1A—C21A	2.612 (6)	C14B—H14F	0.9700
Si1A—N1A	1.755 (4)	C15B—H15D	0.9700
Si1A—C2A	1.855 (6)	C15B—H15E	0.9700
Si1A—C3A	1.857 (6)	C15B—H15F	0.9700
Si1A—C1A	1.862 (6)	C16B—H16D	0.9700
Si2A—N2A	1.770 (4)	C16B—H16E	0.9700
Si2A—C15A	1.832 (7)	C16B—H16F	0.9700
Si2A—C16A	1.858 (6)	C17B—H17D	0.9700
Si2A—C17A	1.888 (6)	C17B—H17E	0.9700
Si3A—N3A	1.757 (5)	C17B—H17F	0.9700
Si3A—C20A	1.847 (5)	C18B—H18D	0.9700
Si3A—C18A	1.860 (6)	C18B—H18E	0.9700
Si3A—C19A	1.878 (7)	C18B—H18F	0.9700
Si4A—N4A	1.760 (5)	C19B—H19D	0.9700

Si4A—C33A	1.857 (6)	C19B—H19E	0.9700
Si4A—C34A	1.862 (7)	C19B—H19F	0.9700
Si4A—C32A	1.868 (6)	C20B—H20D	0.9700
N1A—C4A	1.340 (6)	C20B—H20E	0.9700
N2A—C4A	1.337 (6)	C20B—H20F	0.9700
N3A—C21A	1.333 (6)	C21B—C22B	1.514 (8)
N4A—C21A	1.333 (6)	C22B—C27B	1.368 (7)
C1A—H1A1	0.9700	C22B—C23B	1.396 (7)
C1A—H1A2	0.9700	C23B—C24B	1.361 (8)
C1A—H1A3	0.9700	C23B—H23B	0.9400
C2A—H2A1	0.9700	C24B—C25B	1.389 (8)
C2A—H2A2	0.9700	C24B—H24B	0.9400
C2A—H2A3	0.9700	C25B—C26B	1.401 (8)
C3A—H3A1	0.9700	C25B—C28B	1.540 (9)
C3A—H3A2	0.9700	C26B—C27B	1.392 (8)
C3A—H3A3	0.9700	C26B—H26B	0.9400
C4A—C5A	1.496 (8)	C27B—H27B	0.9400
C5A—C6A	1.379 (8)	C28B—C29B	1.574 (15)
C5A—C10A	1.380 (8)	C28B—H28C	0.9800
C6A—C7A	1.400 (9)	C28B—H28D	0.9800
C6A—H6A	0.9400	C29B—C30B	0.87 (2)
C7A—C8A	1.372 (9)	C29B—H29C	0.9800
C7A—H7A	0.9400	C29B—H29D	0.9800
C8A—C9A	1.375 (9)	C30B—C31B	1.57 (2)
C8A—C11A	1.536 (10)	C30B—C30E	1.61 (4)
C9A—C10A	1.410 (8)	C30E—C31B	1.55 (3)
C9A—H9A	0.9400	C32B—H32D	0.9700
C10A—H10A	0.9400	C32B—H32E	0.9700
C11A—C12A	1.356 (8)	C32B—H32F	0.9700
C11A—H11A	0.9800	C33B—H33D	0.9700
C11A—H11B	0.9800	C33B—H33E	0.9700
C12A—C13A	1.561 (9)	C33B—H33F	0.9700
C12A—H12A	0.9800	C34B—H34D	0.9700
C12A—H12B	0.9800	C34B—H34E	0.9700
C13A—C14A	1.438 (9)	C34B—H34F	0.9700
C13A—H13A	0.9800	Zr1C—N3C	2.203 (4)
C13A—H13B	0.9800	Zr1C—N4C	2.221 (4)
C14A—H14A	0.9700	Zr1C—N1C	2.222 (4)
C14A—H14B	0.9700	Zr1C—N2C	2.231 (4)
C14A—H14C	0.9700	Zr1C—Cl2C	2.4045 (17)
C15A—H15A	0.9700	Zr1C—Cl1C	2.4155 (17)
C15A—H15B	0.9700	Zr1C—C21C	2.591 (6)
C15A—H15C	0.9700	Zr1C—C4C	2.643 (6)
C16A—H16A	0.9700	Si1C—N1C	1.761 (4)
C16A—H16B	0.9700	Si1C—C2C	1.836 (6)
C16A—H16C	0.9700	Si1C—C1C	1.859 (6)
C17A—H17A	0.9700	Si1C—C3C	1.871 (7)
C17A—H17B	0.9700	Si2C—N2C	1.752 (4)
C17A—H17C	0.9700	Si2C—C16C	1.852 (6)
C18A—H18A	0.9700	Si2C—C15C	1.860 (5)
C18A—H18B	0.9700	Si2C—C17C	1.879 (6)
C18A—H18C	0.9700	Si3C—N3C	1.755 (4)
C19A—H19A	0.9700	Si3C—C20C	1.841 (7)
C19A—H19B	0.9700	Si3C—C18C	1.842 (7)

C19A—H19C	0.9700	Si3C—C19C	1.842 (7)
C20A—H20A	0.9700	Si4C—N4C	1.750 (4)
C20A—H20B	0.9700	Si4C—C32C	1.835 (6)
C20A—H20C	0.9700	Si4C—C33C	1.857 (6)
C21A—C22A	1.495 (8)	Si4C—C34C	1.863 (6)
C22A—C23A	1.361 (8)	N1C—C4C	1.338 (6)
C22A—C27A	1.393 (7)	N2C—C4C	1.344 (6)
C23A—C24A	1.392 (9)	N3C—C21C	1.341 (6)
C23A—H23A	0.9400	N4C—C21C	1.345 (6)
C24A—C25A	1.405 (9)	C1C—H1C1	0.9700
C24A—H24A	0.9400	C1C—H1C2	0.9700
C25A—C26A	1.363 (9)	C1C—H1C3	0.9700
C25A—C28A	1.538 (10)	C2C—H2C1	0.9700
C26A—C27A	1.378 (8)	C2C—H2C2	0.9700
C26A—H26A	0.9400	C2C—H2C3	0.9700
C27A—H27A	0.9400	C3C—H3C1	0.9700
C28A—C29A	1.506 (11)	C3C—H3C2	0.9700
C28A—H28A	0.9800	C3C—H3C3	0.9700
C28A—H28B	0.9800	C4C—C5C	1.493 (7)
C29A—C30A	1.644 (15)	C5C—C10C	1.369 (7)
C29A—H29A	0.9800	C5C—C6C	1.369 (7)
C29A—H29B	0.9800	C6C—C7C	1.383 (8)
C30A—C31A	1.272 (13)	C6C—H6C	0.9400
C30A—H30A	0.9800	C7C—C8C	1.377 (8)
C30A—H30B	0.9800	C7C—H7C	0.9400
C31A—H31A	0.9700	C8C—C9C	1.397 (8)
C31A—H31B	0.9700	C8C—C11C	1.508 (8)
C31A—H31C	0.9700	C9C—C10C	1.398 (7)
C32A—H32A	0.9700	C9C—H9C	0.9400
C32A—H32B	0.9700	C10C—H10C	0.9400
C32A—H32C	0.9700	C11C—C12C	1.511 (10)
C33A—H33A	0.9700	C11C—H11E	0.9800
C33A—H33B	0.9700	C11C—H11F	0.9800
C33A—H33C	0.9700	C12C—C13F	1.20 (2)
C34A—H34A	0.9700	C12C—C13C	1.361 (13)
C34A—H34B	0.9700	C13C—C13F	1.08 (6)
C34A—H34C	0.9700	C13C—C14C	1.59 (2)
Zr1B—N1B	2.202 (4)	C13F—C14C	1.54 (4)
Zr1B—N3B	2.204 (4)	C15C—H15G	0.9700
Zr1B—N2B	2.215 (4)	C15C—H15H	0.9700
Zr1B—N4B	2.228 (4)	C15C—H15I	0.9700
Zr1B—Cl2B	2.4162 (15)	C16C—H16G	0.9700
Zr1B—Cl1B	2.4165 (16)	C16C—H16H	0.9700
Zr1B—C4B	2.585 (5)	C16C—H16I	0.9700
Zr1B—C21B	2.604 (6)	C17C—H17G	0.9700
Si1B—N1B	1.748 (4)	C17C—H17H	0.9700
Si1B—C2B	1.837 (6)	C17C—H17I	0.9700
Si1B—C3B	1.840 (6)	C18C—H18G	0.9700
Si1B—C1B	1.854 (6)	C18C—H18H	0.9700
Si2B—N2B	1.766 (4)	C18C—H18I	0.9700
Si2B—C17B	1.846 (6)	C19C—H19G	0.9700
Si2B—C15B	1.848 (6)	C19C—H19H	0.9700
Si2B—C16B	1.850 (6)	C19C—H19I	0.9700
Si3B—N3B	1.768 (4)	C20C—H20G	0.9700

Si3B—C20B	1.852 (6)	C20C—H20H	0.9700
Si3B—C18B	1.856 (5)	C20C—H20I	0.9700
Si3B—C19B	1.862 (7)	C21C—C22C	1.485 (7)
Si4B—N4B	1.751 (4)	C22C—C27C	1.365 (7)
Si4B—C33B	1.838 (6)	C22C—C23C	1.385 (7)
Si4B—C34B	1.850 (6)	C23C—C24C	1.378 (8)
Si4B—C32B	1.866 (6)	C23C—H23C	0.9400
N1B—C4B	1.331 (6)	C24C—C25C	1.372 (8)
N2B—C4B	1.353 (6)	C24C—H24C	0.9400
N3B—C21B	1.331 (6)	C25C—C26C	1.399 (8)
N4B—C21B	1.320 (6)	C25C—C28C	1.505 (8)
C1B—H1B1	0.9700	C26C—C27C	1.392 (7)
C1B—H1B2	0.9700	C26C—H26C	0.9400
C1B—H1B3	0.9700	C27C—H27C	0.9400
C2B—H2B1	0.9700	C28C—C29C	1.465 (8)
C2B—H2B2	0.9700	C28C—H28E	0.9800
C2B—H2B3	0.9700	C28C—H28F	0.9800
C3B—H3B1	0.9700	C29C—C30C	1.505 (8)
C3B—H3B2	0.9700	C29C—H29E	0.9800
C3B—H3B3	0.9700	C29C—H29F	0.9800
C4B—C5B	1.492 (7)	C30C—C31C	1.400 (9)
C5B—C6B	1.375 (7)	C30C—H30C	0.9800
C5B—C10B	1.384 (8)	C30C—H30D	0.9800
C6B—C7B	1.394 (8)	C31C—H31D	0.9700
C6B—H6B	0.9400	C31C—H31E	0.9700
C7B—C8B	1.384 (10)	C31C—H31F	0.9700
C7B—H7B	0.9400	C32C—H32G	0.9700
C8B—C9B	1.380 (9)	C32C—H32H	0.9700
C8B—C11B	1.545 (9)	C32C—H32I	0.9700
C9B—C10B	1.412 (8)	C33C—H33G	0.9700
C9B—H9B	0.9400	C33C—H33H	0.9700
C10B—H10B	0.9400	C33C—H33I	0.9700
C11B—C12B	1.286 (9)	C34C—H34G	0.9700
C11B—H11C	0.9800	C34C—H34H	0.9700
C11B—H11D	0.9800	C34C—H34I	0.9700
C12B—C13B	1.539 (9)		

N1A—Zr1A—N2A	61.45 (15)	C12B—C11B—H11D	107.5
N1A—Zr1A—N3A	115.53 (17)	C8B—C11B—H11D	107.5
N2A—Zr1A—N3A	158.01 (16)	H11C—C11B—H11D	107.0
N1A—Zr1A—N4A	90.33 (16)	C11B—C12B—C13B	120.3 (7)
N2A—Zr1A—N4A	96.64 (17)	C11B—C12B—H12C	107.2
N3A—Zr1A—N4A	61.38 (16)	C13B—C12B—H12C	107.2
N1A—Zr1A—Cl2A	149.30 (13)	C11B—C12B—H12D	107.2
N2A—Zr1A—Cl2A	88.89 (12)	C13B—C12B—H12D	107.3
N3A—Zr1A—Cl2A	94.91 (12)	H12C—C12B—H12D	106.9
N4A—Zr1A—Cl2A	101.57 (12)	C14B—C13B—C12B	115.0 (6)
N1A—Zr1A—Cl1A	87.20 (12)	C14B—C13B—H13C	108.5
N2A—Zr1A—Cl1A	109.54 (12)	C12B—C13B—H13C	108.5
N3A—Zr1A—Cl1A	91.59 (12)	C14B—C13B—H13D	108.5
N4A—Zr1A—Cl1A	148.48 (12)	C12B—C13B—H13D	108.5
Cl2A—Zr1A—Cl1A	96.33 (6)	H13C—C13B—H13D	107.5
N1A—Zr1A—C4A	31.15 (15)	C13B—C14B—H14D	109.5
N2A—Zr1A—C4A	31.09 (14)	C13B—C14B—H14E	109.5

N3A—Zr1A—C4A	145.18 (17)	H14D—C14B—H14E	109.5
N4A—Zr1A—C4A	99.22 (17)	C13B—C14B—H14F	109.5
Cl2A—Zr1A—C4A	118.26 (13)	H14D—C14B—H14F	109.5
Cl1A—Zr1A—C4A	94.76 (12)	H14E—C14B—H14F	109.5
N1A—Zr1A—C21A	104.72 (17)	Si2B—C15B—H15D	109.5
N2A—Zr1A—C21A	127.32 (18)	Si2B—C15B—H15E	109.5
N3A—Zr1A—C21A	30.69 (15)	H15D—C15B—H15E	109.5
N4A—Zr1A—C21A	30.69 (15)	Si2B—C15B—H15F	109.5
Cl2A—Zr1A—C21A	99.56 (12)	H15D—C15B—H15F	109.5
Cl1A—Zr1A—C21A	120.79 (14)	H15E—C15B—H15F	109.5
C4A—Zr1A—C21A	124.79 (18)	Si2B—C16B—H16D	109.5
N1A—Si1A—C2A	111.7 (3)	Si2B—C16B—H16E	109.5
N1A—Si1A—C3A	111.0 (3)	H16D—C16B—H16E	109.5
C2A—Si1A—C3A	110.8 (3)	Si2B—C16B—H16F	109.5
N1A—Si1A—C1A	104.7 (3)	H16D—C16B—H16F	109.5
C2A—Si1A—C1A	109.7 (3)	H16E—C16B—H16F	109.5
C3A—Si1A—C1A	108.6 (3)	Si2B—C17B—H17D	109.5
N2A—Si2A—C15A	109.2 (3)	Si2B—C17B—H17E	109.5
N2A—Si2A—C16A	107.6 (3)	H17D—C17B—H17E	109.5
C15A—Si2A—C16A	110.9 (3)	Si2B—C17B—H17F	109.5
N2A—Si2A—C17A	112.1 (3)	H17D—C17B—H17F	109.5
C15A—Si2A—C17A	111.5 (3)	H17E—C17B—H17F	109.5
C16A—Si2A—C17A	105.5 (3)	Si3B—C18B—H18D	109.5
N3A—Si3A—C20A	109.7 (3)	Si3B—C18B—H18E	109.5
N3A—Si3A—C18A	115.0 (3)	H18D—C18B—H18E	109.5
C20A—Si3A—C18A	108.8 (3)	Si3B—C18B—H18F	109.5
N3A—Si3A—C19A	107.1 (3)	H18D—C18B—H18F	109.5
C20A—Si3A—C19A	109.7 (3)	H18E—C18B—H18F	109.5
C18A—Si3A—C19A	106.4 (3)	Si3B—C19B—H19D	109.5
N4A—Si4A—C33A	107.2 (3)	Si3B—C19B—H19E	109.5
N4A—Si4A—C34A	113.2 (3)	H19D—C19B—H19E	109.5
C33A—Si4A—C34A	106.6 (3)	Si3B—C19B—H19F	109.5
N4A—Si4A—C32A	108.6 (2)	H19D—C19B—H19F	109.5
C33A—Si4A—C32A	110.4 (3)	H19E—C19B—H19F	109.5
C34A—Si4A—C32A	110.7 (3)	Si3B—C20B—H20D	109.5
C4A—N1A—Si1A	130.8 (4)	Si3B—C20B—H20E	109.5
C4A—N1A—Zr1A	90.4 (3)	H20D—C20B—H20E	109.5
Si1A—N1A—Zr1A	133.6 (2)	Si3B—C20B—H20F	109.5
C4A—N2A—Si2A	130.1 (4)	H20D—C20B—H20F	109.5
C4A—N2A—Zr1A	90.2 (3)	H20E—C20B—H20F	109.5
Si2A—N2A—Zr1A	138.3 (2)	N4B—C21B—N3B	116.7 (5)
C21A—N3A—Si3A	132.0 (4)	N4B—C21B—C22B	121.7 (5)
C21A—N3A—Zr1A	91.1 (3)	N3B—C21B—C22B	121.6 (5)
Si3A—N3A—Zr1A	135.9 (3)	N4B—C21B—Zr1B	58.8 (3)
C21A—N4A—Si4A	128.5 (4)	N3B—C21B—Zr1B	57.8 (3)
C21A—N4A—Zr1A	90.9 (3)	C22B—C21B—Zr1B	178.9 (4)
Si4A—N4A—Zr1A	140.5 (3)	C27B—C22B—C23B	120.3 (6)
Si1A—C1A—H1A1	109.5	C27B—C22B—C21B	120.9 (5)
Si1A—C1A—H1A2	109.5	C23B—C22B—C21B	118.8 (5)
H1A1—C1A—H1A2	109.5	C24B—C23B—C22B	119.4 (6)
Si1A—C1A—H1A3	109.5	C24B—C23B—H23B	120.3
H1A1—C1A—H1A3	109.5	C22B—C23B—H23B	120.3
H1A2—C1A—H1A3	109.5	C23B—C24B—C25B	122.3 (6)
Si1A—C2A—H2A1	109.5	C23B—C24B—H24B	118.8

Si1A—C2A—H2A2	109.5	C25B—C24B—H24B	118.8
H2A1—C2A—H2A2	109.5	C24B—C25B—C26B	117.4 (6)
Si1A—C2A—H2A3	109.5	C24B—C25B—C28B	122.7 (7)
H2A1—C2A—H2A3	109.5	C26B—C25B—C28B	119.9 (7)
H2A2—C2A—H2A3	109.5	C27B—C26B—C25B	120.9 (6)
Si1A—C3A—H3A1	109.5	C27B—C26B—H26B	119.6
Si1A—C3A—H3A2	109.5	C25B—C26B—H26B	119.6
H3A1—C3A—H3A2	109.5	C22B—C27B—C26B	119.7 (6)
Si1A—C3A—H3A3	109.5	C22B—C27B—H27B	120.1
H3A1—C3A—H3A3	109.5	C26B—C27B—H27B	120.1
H3A2—C3A—H3A3	109.5	C25B—C28B—C29B	111.2 (9)
N2A—C4A—N1A	115.0 (5)	C25B—C28B—H28C	109.4
N2A—C4A—C5A	123.1 (5)	C29B—C28B—H28C	109.4
N1A—C4A—C5A	121.8 (5)	C25B—C28B—H28D	109.4
N2A—C4A—Zr1A	58.7 (3)	C29B—C28B—H28D	109.4
N1A—C4A—Zr1A	58.4 (3)	H28C—C28B—H28D	108.0
C5A—C4A—Zr1A	162.8 (4)	C30B—C29B—C28B	149 (3)
C6A—C5A—C10A	118.8 (6)	C30B—C29B—H29C	99.6
C6A—C5A—C4A	121.4 (6)	C28B—C29B—H29C	99.6
C10A—C5A—C4A	119.7 (5)	C30B—C29B—H29D	99.6
C5A—C6A—C7A	120.7 (7)	C28B—C29B—H29D	99.6
C5A—C6A—H6A	119.7	H29C—C29B—H29D	104.1
C7A—C6A—H6A	119.7	C29B—C30B—C31B	119 (3)
C8A—C7A—C6A	121.3 (7)	C29B—C30B—C30E	71 (2)
C8A—C7A—H7A	119.4	C31B—C30B—C30E	58.2 (16)
C6A—C7A—H7A	119.4	C31B—C30E—C30B	59.8 (16)
C7A—C8A—C9A	117.8 (7)	C30E—C31B—C30B	62.0 (15)
C7A—C8A—C11A	122.4 (7)	Si4B—C32B—H32D	109.5
C9A—C8A—C11A	119.8 (8)	Si4B—C32B—H32E	109.5
C8A—C9A—C10A	121.7 (7)	H32D—C32B—H32E	109.5
C8A—C9A—H9A	119.1	Si4B—C32B—H32F	109.5
C10A—C9A—H9A	119.1	H32D—C32B—H32F	109.5
C5A—C10A—C9A	119.6 (6)	H32E—C32B—H32F	109.5
C5A—C10A—H10A	120.2	Si4B—C33B—H33D	109.5
C9A—C10A—H10A	120.2	Si4B—C33B—H33E	109.5
C12A—C11A—C8A	116.9 (7)	H33D—C33B—H33E	109.5
C12A—C11A—H11A	108.1	Si4B—C33B—H33F	109.5
C8A—C11A—H11A	108.1	H33D—C33B—H33F	109.5
C12A—C11A—H11B	108.1	H33E—C33B—H33F	109.5
C8A—C11A—H11B	108.1	Si4B—C34B—H34D	109.5
H11A—C11A—H11B	107.3	Si4B—C34B—H34E	109.5
C11A—C12A—C13A	116.9 (7)	H34D—C34B—H34E	109.5
C11A—C12A—H12A	108.1	Si4B—C34B—H34F	109.5
C13A—C12A—H12A	108.1	H34D—C34B—H34F	109.5
C11A—C12A—H12B	108.1	H34E—C34B—H34F	109.5
C13A—C12A—H12B	108.1	N3C—Zr1C—N4C	61.69 (16)
H12A—C12A—H12B	107.3	N3C—Zr1C—N1C	109.99 (16)
C14A—C13A—C12A	112.3 (7)	N4C—Zr1C—N1C	160.15 (16)
C14A—C13A—H13A	109.2	N3C—Zr1C—N2C	89.81 (16)
C12A—C13A—H13A	109.2	N4C—Zr1C—N2C	99.98 (15)
C14A—C13A—H13B	109.1	N1C—Zr1C—N2C	60.90 (15)
C12A—C13A—H13B	109.1	N3C—Zr1C—Cl2C	151.69 (13)
H13A—C13A—H13B	107.9	N4C—Zr1C—Cl2C	90.14 (12)
C13A—C14A—H14A	109.5	N1C—Zr1C—Cl2C	97.58 (12)

C13A—C14A—H14B	109.5	N2C—Zr1C—Cl2C	98.37 (11)
H14A—C14A—H14B	109.5	N3C—Zr1C—Cl1C	89.72 (12)
C13A—C14A—H14C	109.5	N4C—Zr1C—Cl1C	105.51 (12)
H14A—C14A—H14C	109.5	N1C—Zr1C—Cl1C	91.94 (12)
H14B—C14A—H14C	109.5	N2C—Zr1C—Cl1C	150.71 (12)
Si2A—C15A—H15A	109.5	Cl2C—Zr1C—Cl1C	95.80 (7)
Si2A—C15A—H15B	109.5	N3C—Zr1C—C21C	31.17 (15)
H15A—C15A—H15B	109.5	N4C—Zr1C—C21C	31.26 (15)
Si2A—C15A—H15C	109.5	N1C—Zr1C—C21C	140.48 (18)
H15A—C15A—H15C	109.5	N2C—Zr1C—C21C	100.63 (16)
H15B—C15A—H15C	109.5	Cl2C—Zr1C—C21C	120.56 (14)
Si2A—C16A—H16A	109.5	Cl1C—Zr1C—C21C	93.93 (12)
Si2A—C16A—H16B	109.5	N3C—Zr1C—C4C	102.39 (16)
H16A—C16A—H16B	109.5	N4C—Zr1C—C4C	130.44 (16)
Si2A—C16A—H16C	109.5	N1C—Zr1C—C4C	30.40 (14)
H16A—C16A—H16C	109.5	N2C—Zr1C—C4C	30.54 (13)
H16B—C16A—H16C	109.5	Cl2C—Zr1C—C4C	98.16 (11)
Si2A—C17A—H17A	109.5	Cl1C—Zr1C—C4C	121.88 (12)
Si2A—C17A—H17B	109.5	C21C—Zr1C—C4C	124.51 (17)
H17A—C17A—H17B	109.5	N1C—Si1C—C2C	106.7 (3)
Si2A—C17A—H17C	109.5	N1C—Si1C—C1C	107.6 (3)
H17A—C17A—H17C	109.5	C2C—Si1C—C1C	112.2 (3)
H17B—C17A—H17C	109.5	N1C—Si1C—C3C	115.6 (3)
Si3A—C18A—H18A	109.5	C2C—Si1C—C3C	107.4 (3)
Si3A—C18A—H18B	109.5	C1C—Si1C—C3C	107.4 (3)
H18A—C18A—H18B	109.5	N2C—Si2C—C16C	107.1 (2)
Si3A—C18A—H18C	109.5	N2C—Si2C—C15C	108.9 (2)
H18A—C18A—H18C	109.5	C16C—Si2C—C15C	110.8 (3)
H18B—C18A—H18C	109.5	N2C—Si2C—C17C	112.3 (2)
Si3A—C19A—H19A	109.5	C16C—Si2C—C17C	107.5 (3)
Si3A—C19A—H19B	109.5	C15C—Si2C—C17C	110.1 (3)
H19A—C19A—H19B	109.5	N3C—Si3C—C20C	113.9 (3)
Si3A—C19A—H19C	109.5	N3C—Si3C—C18C	104.7 (3)
H19A—C19A—H19C	109.5	C20C—Si3C—C18C	108.2 (4)
H19B—C19A—H19C	109.5	N3C—Si3C—C19C	109.7 (3)
Si3A—C20A—H20A	109.5	C20C—Si3C—C19C	109.8 (4)
Si3A—C20A—H20B	109.5	C18C—Si3C—C19C	110.4 (4)
H20A—C20A—H20B	109.5	N4C—Si4C—C32C	108.9 (3)
Si3A—C20A—H20C	109.5	N4C—Si4C—C33C	107.2 (3)
H20A—C20A—H20C	109.5	C32C—Si4C—C33C	110.6 (3)
H20B—C20A—H20C	109.5	N4C—Si4C—C34C	113.2 (3)
N4A—C21A—N3A	116.6 (5)	C32C—Si4C—C34C	109.6 (4)
N4A—C21A—C22A	121.9 (6)	C33C—Si4C—C34C	107.4 (3)
N3A—C21A—C22A	121.4 (6)	C4C—N1C—Si1C	130.9 (4)
N4A—C21A—Zr1A	58.4 (3)	C4C—N1C—Zr1C	92.5 (3)
N3A—C21A—Zr1A	58.2 (3)	Si1C—N1C—Zr1C	135.1 (3)
C22A—C21A—Zr1A	178.2 (4)	C4C—N2C—Si2C	128.8 (4)
C23A—C22A—C27A	119.7 (6)	C4C—N2C—Zr1C	91.9 (3)
C23A—C22A—C21A	120.1 (6)	Si2C—N2C—Zr1C	139.2 (2)
C27A—C22A—C21A	120.1 (5)	C21C—N3C—Si3C	130.4 (4)
C22A—C23A—C24A	120.0 (7)	C21C—N3C—Zr1C	90.6 (3)
C22A—C23A—H23A	120.0	Si3C—N3C—Zr1C	135.4 (3)
C24A—C23A—H23A	120.0	C21C—N4C—Si4C	130.9 (4)
C23A—C24A—C25A	120.2 (7)	C21C—N4C—Zr1C	89.7 (3)

C23A—C24A—H24A	119.9	Si4C—N4C—Zr1C	137.7 (2)
C25A—C24A—H24A	119.9	Si1C—C1C—H1C1	109.5
C26A—C25A—C24A	118.8 (7)	Si1C—C1C—H1C2	109.5
C26A—C25A—C28A	123.0 (8)	H1C1—C1C—H1C2	109.5
C24A—C25A—C28A	118.2 (8)	Si1C—C1C—H1C3	109.5
C25A—C26A—C27A	120.8 (7)	H1C1—C1C—H1C3	109.5
C25A—C26A—H26A	119.6	H1C2—C1C—H1C3	109.5
C27A—C26A—H26A	119.6	Si1C—C2C—H2C1	109.5
C26A—C27A—C22A	120.3 (6)	Si1C—C2C—H2C2	109.5
C26A—C27A—H27A	119.8	H2C1—C2C—H2C2	109.5
C22A—C27A—H27A	119.9	Si1C—C2C—H2C3	109.5
C29A—C28A—C25A	110.9 (8)	H2C1—C2C—H2C3	109.5
C29A—C28A—H28A	109.5	H2C2—C2C—H2C3	109.5
C25A—C28A—H28A	109.4	Si1C—C3C—H3C1	109.5
C29A—C28A—H28B	109.5	Si1C—C3C—H3C2	109.5
C25A—C28A—H28B	109.5	H3C1—C3C—H3C2	109.5
H28A—C28A—H28B	108.0	Si1C—C3C—H3C3	109.5
C28A—C29A—C30A	109.3 (9)	H3C1—C3C—H3C3	109.5
C28A—C29A—H29A	109.8	H3C2—C3C—H3C3	109.5
C30A—C29A—H29A	109.8	N1C—C4C—N2C	114.6 (5)
C28A—C29A—H29B	109.8	N1C—C4C—C5C	122.8 (5)
C30A—C29A—H29B	109.8	N2C—C4C—C5C	122.6 (5)
H29A—C29A—H29B	108.3	N1C—C4C—Zr1C	57.1 (3)
C31A—C30A—C29A	102.7 (14)	N2C—C4C—Zr1C	57.5 (3)
C31A—C30A—H30A	111.2	C5C—C4C—Zr1C	177.5 (4)
C29A—C30A—H30A	111.2	C10C—C5C—C6C	119.9 (6)
C31A—C30A—H30B	111.2	C10C—C5C—C4C	119.5 (5)
C29A—C30A—H30B	111.2	C6C—C5C—C4C	120.5 (5)
H30A—C30A—H30B	109.1	C5C—C6C—C7C	120.3 (6)
C30A—C31A—H31A	109.5	C5C—C6C—H6C	119.9
C30A—C31A—H31B	109.5	C7C—C6C—H6C	119.9
H31A—C31A—H31B	109.5	C8C—C7C—C6C	122.0 (6)
C30A—C31A—H31C	109.5	C8C—C7C—H7C	119.0
H31A—C31A—H31C	109.5	C6C—C7C—H7C	119.0
H31B—C31A—H31C	109.5	C7C—C8C—C9C	116.7 (6)
Si4A—C32A—H32A	109.5	C7C—C8C—C11C	121.5 (6)
Si4A—C32A—H32B	109.5	C9C—C8C—C11C	121.8 (6)
H32A—C32A—H32B	109.5	C8C—C9C—C10C	121.6 (6)
Si4A—C32A—H32C	109.5	C8C—C9C—H9C	119.2
H32A—C32A—H32C	109.5	C10C—C9C—H9C	119.2
H32B—C32A—H32C	109.5	C5C—C10C—C9C	119.5 (5)
Si4A—C33A—H33A	109.5	C5C—C10C—H10C	120.3
Si4A—C33A—H33B	109.5	C9C—C10C—H10C	120.3
H33A—C33A—H33B	109.5	C8C—C11C—C12C	115.6 (6)
Si4A—C33A—H33C	109.5	C8C—C11C—H11E	108.4
H33A—C33A—H33C	109.5	C12C—C11C—H11E	108.4
H33B—C33A—H33C	109.5	C8C—C11C—H11F	108.4
Si4A—C34A—H34A	109.5	C12C—C11C—H11F	108.4
Si4A—C34A—H34B	109.5	H11E—C11C—H11F	107.4
H34A—C34A—H34B	109.5	C13F—C12C—C13C	49 (3)
Si4A—C34A—H34C	109.5	C13F—C12C—C11C	134.6 (14)
H34A—C34A—H34C	109.5	C13C—C12C—C11C	118.7 (12)
H34B—C34A—H34C	109.5	C13F—C13C—C12C	57.6 (19)
N1B—Zr1B—N3B	114.75 (16)	C13F—C13C—C14C	67 (2)

N1B—Zr1B—N2B	61.71 (14)	C12C—C13C—C14C	108.8 (13)
N3B—Zr1B—N2B	160.45 (16)	C13C—C13F—C12C	73 (2)
N1B—Zr1B—N4B	90.01 (15)	C13C—C13F—C14C	72 (4)
N3B—Zr1B—N4B	61.17 (15)	C12C—C13F—C14C	122 (3)
N2B—Zr1B—N4B	99.29 (15)	C13F—C14C—C13C	40.4 (19)
N1B—Zr1B—Cl2B	150.08 (12)	Si2C—C15C—H15G	109.5
N3B—Zr1B—Cl2B	94.60 (12)	Si2C—C15C—H15H	109.5
N2B—Zr1B—Cl2B	88.72 (11)	H15G—C15C—H15H	109.5
N4B—Zr1B—Cl2B	99.83 (11)	Si2C—C15C—H15I	109.5
N1B—Zr1B—Cl1B	87.75 (11)	H15G—C15C—H15I	109.5
N3B—Zr1B—Cl1B	91.05 (12)	H15H—C15C—H15I	109.5
N2B—Zr1B—Cl1B	107.60 (12)	Si2C—C16C—H16G	109.5
N4B—Zr1B—Cl1B	147.98 (11)	Si2C—C16C—H16H	109.5
Cl2B—Zr1B—Cl1B	97.87 (6)	H16G—C16C—H16H	109.5
N1B—Zr1B—C4B	31.00 (14)	Si2C—C16C—H16I	109.5
N3B—Zr1B—C4B	144.89 (17)	H16G—C16C—H16I	109.5
N2B—Zr1B—C4B	31.57 (14)	H16H—C16C—H16I	109.5
N4B—Zr1B—C4B	100.71 (16)	Si2C—C17C—H17G	109.5
Cl2B—Zr1B—C4B	119.09 (13)	Si2C—C17C—H17H	109.5
Cl1B—Zr1B—C4B	93.60 (12)	H17G—C17C—H17H	109.5
N1B—Zr1B—C21B	104.03 (16)	Si2C—C17C—H17I	109.5
N3B—Zr1B—C21B	30.72 (15)	H17G—C17C—H17I	109.5
N2B—Zr1B—C21B	129.74 (17)	H17H—C17C—H17I	109.5
N4B—Zr1B—C21B	30.45 (14)	Si3C—C18C—H18G	109.5
Cl2B—Zr1B—C21B	98.38 (12)	Si3C—C18C—H18H	109.5
Cl1B—Zr1B—C21B	120.33 (13)	H18G—C18C—H18H	109.5
C4B—Zr1B—C21B	125.57 (17)	Si3C—C18C—H18I	109.5
N1B—Si1B—C2B	112.0 (3)	H18G—C18C—H18I	109.5
N1B—Si1B—C3B	103.8 (3)	H18H—C18C—H18I	109.5
C2B—Si1B—C3B	109.7 (3)	Si3C—C19C—H19G	109.5
N1B—Si1B—C1B	110.6 (3)	Si3C—C19C—H19H	109.5
C2B—Si1B—C1B	111.5 (3)	H19G—C19C—H19H	109.5
C3B—Si1B—C1B	108.9 (4)	Si3C—C19C—H19I	109.5
N2B—Si2B—C17B	113.7 (2)	H19G—C19C—H19I	109.5
N2B—Si2B—C15B	105.9 (2)	H19H—C19C—H19I	109.5
C17B—Si2B—C15B	106.8 (3)	Si3C—C20C—H20G	109.5
N2B—Si2B—C16B	108.4 (2)	Si3C—C20C—H20H	109.5
C17B—Si2B—C16B	110.3 (3)	H20G—C20C—H20H	109.5
C15B—Si2B—C16B	111.7 (3)	Si3C—C20C—H20I	109.5
N3B—Si3B—C20B	114.4 (3)	H20G—C20C—H20I	109.5
N3B—Si3B—C18B	108.1 (2)	H20H—C20C—H20I	109.5
C20B—Si3B—C18B	110.1 (3)	N3C—C21C—N4C	115.2 (5)
N3B—Si3B—C19B	106.2 (3)	N3C—C21C—C22C	122.2 (5)
C20B—Si3B—C19B	106.5 (3)	N4C—C21C—C22C	122.4 (5)
C18B—Si3B—C19B	111.5 (3)	N3C—C21C—Zr1C	58.2 (3)
N4B—Si4B—C33B	107.3 (2)	N4C—C21C—Zr1C	59.0 (3)
N4B—Si4B—C34B	109.7 (2)	C22C—C21C—Zr1C	162.7 (4)
C33B—Si4B—C34B	109.8 (3)	C27C—C22C—C23C	118.2 (5)
N4B—Si4B—C32B	113.7 (2)	C27C—C22C—C21C	120.8 (5)
C33B—Si4B—C32B	106.4 (3)	C23C—C22C—C21C	121.0 (6)
C34B—Si4B—C32B	109.7 (3)	C24C—C23C—C22C	120.6 (6)
C4B—N1B—Si1B	130.3 (4)	C24C—C23C—H23C	119.7
C4B—N1B—Zr1B	90.6 (3)	C22C—C23C—H23C	119.7
Si1B—N1B—Zr1B	134.6 (2)	C25C—C24C—C23C	121.8 (6)

C4B—N2B—Si2B	130.9 (4)	C25C—C24C—H24C	119.1
C4B—N2B—Zr1B	89.5 (3)	C23C—C24C—H24C	119.1
Si2B—N2B—Zr1B	138.1 (2)	C24C—C25C—C26C	117.6 (6)
C21B—N3B—Si3B	131.4 (4)	C24C—C25C—C28C	123.1 (6)
C21B—N3B—Zr1B	91.5 (3)	C26C—C25C—C28C	119.3 (6)
Si3B—N3B—Zr1B	135.8 (3)	C27C—C26C—C25C	120.1 (6)
C21B—N4B—Si4B	129.2 (4)	C27C—C26C—H26C	120.0
C21B—N4B—Zr1B	90.7 (3)	C25C—C26C—H26C	120.0
Si4B—N4B—Zr1B	140.1 (2)	C22C—C27C—C26C	121.5 (6)
Si1B—C1B—H1B1	109.5	C22C—C27C—H27C	119.2
Si1B—C1B—H1B2	109.5	C26C—C27C—H27C	119.2
H1B1—C1B—H1B2	109.5	C29C—C28C—C25C	115.8 (5)
Si1B—C1B—H1B3	109.5	C29C—C28C—H28E	108.4
H1B1—C1B—H1B3	109.5	C25C—C28C—H28E	108.3
H1B2—C1B—H1B3	109.5	C29C—C28C—H28F	108.3
Si1B—C2B—H2B1	109.5	C25C—C28C—H28F	108.3
Si1B—C2B—H2B2	109.5	H28E—C28C—H28F	107.4
H2B1—C2B—H2B2	109.5	C28C—C29C—C30C	115.4 (6)
Si1B—C2B—H2B3	109.5	C28C—C29C—H29E	108.4
H2B1—C2B—H2B3	109.5	C30C—C29C—H29E	108.4
H2B2—C2B—H2B3	109.5	C28C—C29C—H29F	108.4
Si1B—C3B—H3B1	109.5	C30C—C29C—H29F	108.4
Si1B—C3B—H3B2	109.5	H29E—C29C—H29F	107.5
H3B1—C3B—H3B2	109.5	C31C—C30C—C29C	116.5 (7)
Si1B—C3B—H3B3	109.5	C31C—C30C—H30C	108.1
H3B1—C3B—H3B3	109.5	C29C—C30C—H30C	108.2
H3B2—C3B—H3B3	109.5	C31C—C30C—H30D	108.2
N1B—C4B—N2B	115.1 (5)	C29C—C30C—H30D	108.2
N1B—C4B—C5B	123.9 (5)	H30C—C30C—H30D	107.3
N2B—C4B—C5B	121.0 (5)	C30C—C31C—H31D	109.5
N1B—C4B—Zr1B	58.4 (3)	C30C—C31C—H31E	109.5
N2B—C4B—Zr1B	59.0 (3)	H31D—C31C—H31E	109.5
C5B—C4B—Zr1B	163.7 (4)	C30C—C31C—H31F	109.5
C6B—C5B—C10B	119.9 (6)	H31D—C31C—H31F	109.5
C6B—C5B—C4B	120.8 (6)	H31E—C31C—H31F	109.5
C10B—C5B—C4B	119.3 (5)	Si4C—C32C—H32G	109.5
C5B—C6B—C7B	120.3 (6)	Si4C—C32C—H32H	109.5
C5B—C6B—H6B	119.9	H32G—C32C—H32H	109.5
C7B—C6B—H6B	119.9	Si4C—C32C—H32I	109.5
C8B—C7B—C6B	121.5 (7)	H32G—C32C—H32I	109.5
C8B—C7B—H7B	119.3	H32H—C32C—H32I	109.5
C6B—C7B—H7B	119.2	Si4C—C33C—H33G	109.5
C9B—C8B—C7B	117.4 (7)	Si4C—C33C—H33H	109.5
C9B—C8B—C11B	121.7 (9)	H33G—C33C—H33H	109.5
C7B—C8B—C11B	120.9 (8)	Si4C—C33C—H33I	109.5
C8B—C9B—C10B	122.2 (7)	H33G—C33C—H33I	109.5
C8B—C9B—H9B	118.9	H33H—C33C—H33I	109.5
C10B—C9B—H9B	118.9	Si4C—C34C—H34G	109.5
C5B—C10B—C9B	118.7 (6)	Si4C—C34C—H34H	109.5
C5B—C10B—H10B	120.7	H34G—C34C—H34H	109.5
C9B—C10B—H10B	120.6	Si4C—C34C—H34I	109.5
C12B—C11B—C8B	119.1 (8)	H34G—C34C—H34I	109.5
C12B—C11B—H11C	107.5	H34H—C34C—H34I	109.5
C8B—C11B—H11C	107.5		

C2A—Si1A—N1A—C4A	52.2 (6)	N4B—Zr1B—C4B—N2B	90.3 (3)
C3A—Si1A—N1A—C4A	−72.1 (6)	Cl2B—Zr1B—C4B—N2B	−17.4 (3)
C1A—Si1A—N1A—C4A	170.9 (5)	Cl1B—Zr1B—C4B—N2B	−118.4 (3)
C2A—Si1A—N1A—Zr1A	−94.4 (4)	C21B—Zr1B—C4B—N2B	109.7 (3)
C3A—Si1A—N1A—Zr1A	141.4 (4)	N1B—Zr1B—C4B—C5B	−103.2 (15)
C1A—Si1A—N1A—Zr1A	24.3 (4)	N3B—Zr1B—C4B—C5B	−120.6 (14)
N2A—Zr1A—N1A—C4A	10.1 (3)	N2B—Zr1B—C4B—C5B	94.8 (15)
N3A—Zr1A—N1A—C4A	165.6 (3)	N4B—Zr1B—C4B—C5B	−174.8 (14)
N4A—Zr1A—N1A—C4A	107.5 (3)	Cl2B—Zr1B—C4B—C5B	77.4 (14)
Cl2A—Zr1A—N1A—C4A	−6.3 (4)	Cl1B—Zr1B—C4B—C5B	−23.6 (14)
Cl1A—Zr1A—N1A—C4A	−104.0 (3)	C21B—Zr1B—C4B—C5B	−155.5 (14)
C21A—Zr1A—N1A—C4A	134.9 (3)	N1B—C4B—C5B—C6B	78.7 (7)
N2A—Zr1A—N1A—Si1A	165.4 (4)	N2B—C4B—C5B—C6B	−103.6 (6)
N3A—Zr1A—N1A—Si1A	−39.1 (4)	Zr1B—C4B—C5B—C6B	171.4 (12)
N4A—Zr1A—N1A—Si1A	−97.2 (4)	N1B—C4B—C5B—C10B	−102.4 (7)
Cl2A—Zr1A—N1A—Si1A	149.1 (2)	N2B—C4B—C5B—C10B	75.3 (7)
Cl1A—Zr1A—N1A—Si1A	51.4 (3)	Zr1B—C4B—C5B—C10B	−9.7 (17)
C4A—Zr1A—N1A—Si1A	155.3 (6)	C10B—C5B—C6B—C7B	−2.2 (8)
C21A—Zr1A—N1A—Si1A	−69.8 (4)	C4B—C5B—C6B—C7B	176.7 (5)
C15A—Si2A—N2A—C4A	−95.6 (5)	C5B—C6B—C7B—C8B	0.6 (10)
C16A—Si2A—N2A—C4A	144.0 (5)	C6B—C7B—C8B—C9B	1.5 (11)
C17A—Si2A—N2A—C4A	28.4 (6)	C6B—C7B—C8B—C11B	−176.1 (6)
C15A—Si2A—N2A—Zr1A	67.0 (4)	C7B—C8B—C9B—C10B	−2.0 (10)
C16A—Si2A—N2A—Zr1A	−53.4 (4)	C11B—C8B—C9B—C10B	175.5 (6)
C17A—Si2A—N2A—Zr1A	−168.9 (4)	C6B—C5B—C10B—C9B	1.6 (8)
N1A—Zr1A—N2A—C4A	−10.1 (3)	C4B—C5B—C10B—C9B	−177.3 (5)
N3A—Zr1A—N2A—C4A	−98.0 (5)	C8B—C9B—C10B—C5B	0.5 (10)
N4A—Zr1A—N2A—C4A	−96.9 (3)	C9B—C8B—C11B—C12B	79.8 (13)
Cl2A—Zr1A—N2A—C4A	161.6 (3)	C7B—C8B—C11B—C12B	−102.8 (12)
Cl1A—Zr1A—N2A—C4A	65.3 (3)	C8B—C11B—C12B—C13B	−176.2 (9)
C21A—Zr1A—N2A—C4A	−97.2 (3)	C11B—C12B—C13B—C14B	−178.2 (11)
N1A—Zr1A—N2A—Si2A	−176.9 (4)	Si4B—N4B—C21B—N3B	178.4 (4)
N3A—Zr1A—N2A—Si2A	95.2 (5)	Zr1B—N4B—C21B—N3B	0.0 (4)
N4A—Zr1A—N2A—Si2A	96.3 (4)	Si4B—N4B—C21B—C22B	−0.4 (7)
Cl2A—Zr1A—N2A—Si2A	−5.2 (3)	Zr1B—N4B—C21B—C22B	−178.8 (4)
Cl1A—Zr1A—N2A—Si2A	−101.5 (3)	Si4B—N4B—C21B—Zr1B	178.5 (5)
C4A—Zr1A—N2A—Si2A	−166.8 (6)	Si3B—N3B—C21B—N4B	168.2 (4)
C21A—Zr1A—N2A—Si2A	96.0 (4)	Zr1B—N3B—C21B—N4B	0.0 (4)
C20A—Si3A—N3A—C21A	112.2 (5)	Si3B—N3B—C21B—C22B	−13.0 (7)
C18A—Si3A—N3A—C21A	−10.8 (6)	Zr1B—N3B—C21B—C22B	178.9 (4)
C19A—Si3A—N3A—C21A	−128.8 (5)	Si3B—N3B—C21B—Zr1B	168.2 (5)
C20A—Si3A—N3A—Zr1A	−82.8 (4)	N1B—Zr1B—C21B—N4B	−64.9 (3)
C18A—Si3A—N3A—Zr1A	154.2 (3)	N3B—Zr1B—C21B—N4B	−180.0 (5)
C19A—Si3A—N3A—Zr1A	36.2 (4)	N2B—Zr1B—C21B—N4B	−0.2 (4)
N1A—Zr1A—N3A—C21A	−75.4 (3)	Cl2B—Zr1B—C21B—N4B	95.2 (3)
N2A—Zr1A—N3A—C21A	1.2 (6)	Cl1B—Zr1B—C21B—N4B	−160.6 (2)
N4A—Zr1A—N3A—C21A	0.0 (3)	C4B—Zr1B—C21B—N4B	−40.0 (3)
Cl2A—Zr1A—N3A—C21A	100.5 (3)	N1B—Zr1B—C21B—N3B	115.1 (3)
Cl1A—Zr1A—N3A—C21A	−163.0 (3)	N2B—Zr1B—C21B—N3B	179.8 (3)
C4A—Zr1A—N3A—C21A	−62.3 (4)	N4B—Zr1B—C21B—N3B	180.0 (5)
N1A—Zr1A—N3A—Si3A	115.7 (3)	Cl2B—Zr1B—C21B—N3B	−84.9 (3)
N2A—Zr1A—N3A—Si3A	−167.7 (3)	Cl1B—Zr1B—C21B—N3B	19.4 (3)
N4A—Zr1A—N3A—Si3A	−168.9 (4)	C4B—Zr1B—C21B—N3B	139.9 (3)

Cl2A—Zr1A—N3A—Si3A	−68.4 (3)	N1B—Zr1B—C21B—C22B	56 (23)
Cl1A—Zr1A—N3A—Si3A	28.1 (3)	N3B—Zr1B—C21B—C22B	−60 (23)
C4A—Zr1A—N3A—Si3A	128.7 (3)	N2B—Zr1B—C21B—C22B	120 (23)
C21A—Zr1A—N3A—Si3A	−168.9 (5)	N4B—Zr1B—C21B—C22B	120 (23)
C33A—Si4A—N4A—C21A	−155.5 (5)	Cl2B—Zr1B—C21B—C22B	−144 (23)
C34A—Si4A—N4A—C21A	−38.2 (5)	Cl1B—Zr1B—C21B—C22B	−40 (23)
C32A—Si4A—N4A—C21A	85.2 (5)	C4B—Zr1B—C21B—C22B	80 (23)
C33A—Si4A—N4A—Zr1A	23.4 (4)	N4B—C21B—C22B—C27B	−72.8 (7)
C34A—Si4A—N4A—Zr1A	140.7 (4)	N3B—C21B—C22B—C27B	108.4 (6)
C32A—Si4A—N4A—Zr1A	−95.9 (4)	Zr1B—C21B—C22B—C27B	167 (100)
N1A—Zr1A—N4A—C21A	119.2 (3)	N4B—C21B—C22B—C23B	106.7 (6)
N2A—Zr1A—N4A—C21A	−179.5 (3)	N3B—C21B—C22B—C23B	−72.0 (7)
N3A—Zr1A—N4A—C21A	0.0 (3)	Zr1B—C21B—C22B—C23B	−13 (23)
Cl2A—Zr1A—N4A—C21A	−89.3 (3)	C27B—C22B—C23B—C24B	0.7 (9)
Cl1A—Zr1A—N4A—C21A	34.0 (4)	C21B—C22B—C23B—C24B	−178.9 (6)
C4A—Zr1A—N4A—C21A	149.2 (3)	C22B—C23B—C24B—C25B	−0.9 (10)
N1A—Zr1A—N4A—Si4A	−59.9 (4)	C23B—C24B—C25B—C26B	−0.3 (10)
N2A—Zr1A—N4A—Si4A	1.3 (4)	C23B—C24B—C25B—C28B	−177.4 (7)
N3A—Zr1A—N4A—Si4A	−179.1 (4)	C24B—C25B—C26B—C27B	1.8 (9)
Cl2A—Zr1A—N4A—Si4A	91.6 (4)	C28B—C25B—C26B—C27B	178.9 (6)
Cl1A—Zr1A—N4A—Si4A	−145.1 (3)	C23B—C22B—C27B—C26B	0.8 (8)
C4A—Zr1A—N4A—Si4A	−29.9 (4)	C21B—C22B—C27B—C26B	−179.7 (5)
C21A—Zr1A—N4A—Si4A	−179.2 (6)	C25B—C26B—C27B—C22B	−2.0 (9)
Si2A—N2A—C4A—N1A	−175.2 (4)	C24B—C25B—C28B—C29B	78.2 (11)
Zr1A—N2A—C4A—N1A	16.3 (5)	C26B—C25B—C28B—C29B	−98.7 (10)
Si2A—N2A—C4A—C5A	8.8 (8)	C25B—C28B—C29B—C30B	70 (5)
Zr1A—N2A—C4A—C5A	−159.7 (5)	C28B—C29B—C30B—C31B	169 (3)
Si2A—N2A—C4A—Zr1A	168.5 (5)	C28B—C29B—C30B—C30E	136 (5)
Si1A—N1A—C4A—N2A	−172.8 (4)	C29B—C30B—C30E—C31B	146 (3)
Zr1A—N1A—C4A—N2A	−16.3 (5)	C29B—C30B—C31B—C30E	−37 (3)
Si1A—N1A—C4A—C5A	3.2 (8)	C2C—Si1C—N1C—C4C	115.7 (5)
Zr1A—N1A—C4A—C5A	159.7 (5)	C1C—Si1C—N1C—C4C	−123.7 (5)
Si1A—N1A—C4A—Zr1A	−156.5 (5)	C3C—Si1C—N1C—C4C	−3.7 (6)
N1A—Zr1A—C4A—N2A	162.7 (5)	C2C—Si1C—N1C—Zr1C	−45.8 (4)
N3A—Zr1A—C4A—N2A	139.5 (3)	C1C—Si1C—N1C—Zr1C	74.8 (4)
N4A—Zr1A—C4A—N2A	87.6 (3)	C3C—Si1C—N1C—Zr1C	−165.2 (3)
Cl2A—Zr1A—C4A—N2A	−21.0 (3)	N3C—Zr1C—N1C—C4C	80.3 (3)
Cl1A—Zr1A—C4A—N2A	−120.8 (3)	N4C—Zr1C—N1C—C4C	18.9 (6)
C21A—Zr1A—C4A—N2A	106.1 (3)	N2C—Zr1C—N1C—C4C	2.2 (3)
N2A—Zr1A—C4A—N1A	−162.7 (5)	Cl2C—Zr1C—N1C—C4C	−93.2 (3)
N3A—Zr1A—C4A—N1A	−23.1 (4)	Cl1C—Zr1C—N1C—C4C	170.7 (3)
N4A—Zr1A—C4A—N1A	−75.1 (3)	C21C—Zr1C—N1C—C4C	72.1 (4)
Cl2A—Zr1A—C4A—N1A	176.4 (3)	N3C—Zr1C—N1C—Si1C	−113.6 (3)
Cl1A—Zr1A—C4A—N1A	76.6 (3)	N4C—Zr1C—N1C—Si1C	−175.0 (3)
C21A—Zr1A—C4A—N1A	−56.5 (4)	N2C—Zr1C—N1C—Si1C	168.3 (4)
N1A—Zr1A—C4A—C5A	−96.1 (14)	Cl2C—Zr1C—N1C—Si1C	72.9 (3)
N2A—Zr1A—C4A—C5A	101.2 (14)	Cl1C—Zr1C—N1C—Si1C	−23.2 (3)
N3A—Zr1A—C4A—C5A	−119.3 (13)	C21C—Zr1C—N1C—Si1C	−121.7 (3)
N4A—Zr1A—C4A—C5A	−171.2 (13)	C4C—Zr1C—N1C—Si1C	166.1 (5)
Cl2A—Zr1A—C4A—C5A	80.2 (13)	C16C—Si2C—N2C—C4C	154.2 (4)
Cl1A—Zr1A—C4A—C5A	−19.6 (14)	C15C—Si2C—N2C—C4C	−85.8 (5)
C21A—Zr1A—C4A—C5A	−152.7 (13)	C17C—Si2C—N2C—C4C	36.4 (5)
N2A—C4A—C5A—C6A	−106.7 (7)	C16C—Si2C—N2C—Zr1C	−27.7 (4)
N1A—C4A—C5A—C6A	77.6 (7)	C15C—Si2C—N2C—Zr1C	92.3 (4)

Zr1A—C4A—C5A—C6A	163.0 (11)	C17C—Si2C—N2C—Zr1C	−145.5 (4)
N2A—C4A—C5A—C10A	70.3 (7)	N3C—Zr1C—N2C—C4C	−115.3 (3)
N1A—C4A—C5A—C10A	−105.4 (6)	N4C—Zr1C—N2C—C4C	−176.5 (3)
Zr1A—C4A—C5A—C10A	−20.0 (16)	N1C—Zr1C—N2C—C4C	−2.2 (3)
C10A—C5A—C6A—C7A	−0.6 (9)	Cl2C—Zr1C—N2C—C4C	91.9 (3)
C4A—C5A—C6A—C7A	176.4 (5)	Cl1C—Zr1C—N2C—C4C	−26.2 (4)
C5A—C6A—C7A—C8A	−1.8 (10)	C21C—Zr1C—N2C—C4C	−144.7 (3)
C6A—C7A—C8A—C9A	4.6 (11)	N3C—Zr1C—N2C—Si2C	66.2 (3)
C6A—C7A—C8A—C11A	−174.7 (6)	N4C—Zr1C—N2C—Si2C	5.0 (4)
C7A—C8A—C9A—C10A	−5.1 (10)	N1C—Zr1C—N2C—Si2C	179.3 (4)
C11A—C8A—C9A—C10A	174.3 (6)	Cl2C—Zr1C—N2C—Si2C	−86.6 (3)
C6A—C5A—C10A—C9A	0.2 (8)	Cl1C—Zr1C—N2C—Si2C	155.3 (2)
C4A—C5A—C10A—C9A	−176.9 (5)	C21C—Zr1C—N2C—Si2C	36.8 (4)
C8A—C9A—C10A—C5A	2.8 (9)	C4C—Zr1C—N2C—Si2C	−178.5 (5)
C7A—C8A—C11A—C12A	−100.7 (10)	C20C—Si3C—N3C—C21C	53.6 (6)
C9A—C8A—C11A—C12A	80.0 (11)	C18C—Si3C—N3C—C21C	171.6 (6)
C8A—C11A—C12A—C13A	−174.6 (8)	C19C—Si3C—N3C—C21C	−69.9 (6)
C11A—C12A—C13A—C14A	−168.0 (9)	C20C—Si3C—N3C—Zr1C	−154.3 (4)
Si4A—N4A—C21A—N3A	179.3 (4)	C18C—Si3C—N3C—Zr1C	−36.4 (5)
Zr1A—N4A—C21A—N3A	0.0 (5)	C19C—Si3C—N3C—Zr1C	82.1 (5)
Si4A—N4A—C21A—C22A	1.3 (7)	N4C—Zr1C—N3C—C21C	−9.8 (3)
Zr1A—N4A—C21A—C22A	−178.0 (4)	N1C—Zr1C—N3C—C21C	−170.0 (3)
Si4A—N4A—C21A—Zr1A	179.3 (5)	N2C—Zr1C—N3C—C21C	−111.2 (3)
Si3A—N3A—C21A—N4A	169.7 (4)	Cl2C—Zr1C—N3C—C21C	−3.7 (5)
Zr1A—N3A—C21A—N4A	0.0 (5)	Cl1C—Zr1C—N3C—C21C	98.1 (3)
Si3A—N3A—C21A—C22A	−12.4 (8)	C4C—Zr1C—N3C—C21C	−139.3 (3)
Zr1A—N3A—C21A—C22A	178.0 (4)	N4C—Zr1C—N3C—Si3C	−168.8 (4)
Si3A—N3A—C21A—Zr1A	169.6 (5)	N1C—Zr1C—N3C—Si3C	31.0 (4)
N1A—Zr1A—C21A—N4A	−64.5 (3)	N2C—Zr1C—N3C—Si3C	89.7 (4)
N2A—Zr1A—C21A—N4A	0.6 (4)	Cl2C—Zr1C—N3C—Si3C	−162.8 (2)
N3A—Zr1A—C21A—N4A	−180.0 (5)	Cl1C—Zr1C—N3C—Si3C	−61.0 (3)
Cl2A—Zr1A—C21A—N4A	96.6 (3)	C21C—Zr1C—N3C—Si3C	−159.1 (6)
Cl1A—Zr1A—C21A—N4A	−160.1 (2)	C4C—Zr1C—N3C—Si3C	61.7 (4)
C4A—Zr1A—C21A—N4A	−38.0 (3)	C32C—Si4C—N4C—C21C	98.7 (5)
N1A—Zr1A—C21A—N3A	115.5 (3)	C33C—Si4C—N4C—C21C	−141.6 (5)
N2A—Zr1A—C21A—N3A	−179.4 (3)	C34C—Si4C—N4C—C21C	−23.4 (6)
N4A—Zr1A—C21A—N3A	180.0 (5)	C32C—Si4C—N4C—Zr1C	−61.5 (4)
Cl2A—Zr1A—C21A—N3A	−83.5 (3)	C33C—Si4C—N4C—Zr1C	58.2 (4)
Cl1A—Zr1A—C21A—N3A	19.9 (3)	C34C—Si4C—N4C—Zr1C	176.4 (4)
C4A—Zr1A—C21A—N3A	142.0 (3)	N3C—Zr1C—N4C—C21C	9.7 (3)
N1A—Zr1A—C21A—C22A	36 (17)	N1C—Zr1C—N4C—C21C	79.3 (5)
N2A—Zr1A—C21A—C22A	101 (17)	N2C—Zr1C—N4C—C21C	94.1 (3)
N3A—Zr1A—C21A—C22A	−80 (17)	Cl2C—Zr1C—N4C—C21C	−167.4 (3)
N4A—Zr1A—C21A—C22A	100 (17)	Cl1C—Zr1C—N4C—C21C	−71.3 (3)
Cl2A—Zr1A—C21A—C22A	−163 (17)	C4C—Zr1C—N4C—C21C	91.7 (3)
Cl1A—Zr1A—C21A—C22A	−60 (17)	N3C—Zr1C—N4C—Si4C	174.9 (4)
C4A—Zr1A—C21A—C22A	62 (17)	N1C—Zr1C—N4C—Si4C	−115.5 (5)
N4A—C21A—C22A—C23A	104.0 (7)	N2C—Zr1C—N4C—Si4C	−100.8 (3)
N3A—C21A—C22A—C23A	−73.8 (8)	Cl2C—Zr1C—N4C—Si4C	−2.2 (3)
Zr1A—C21A—C22A—C23A	5 (17)	Cl1C—Zr1C—N4C—Si4C	93.8 (3)
N4A—C21A—C22A—C27A	−76.0 (7)	C21C—Zr1C—N4C—Si4C	165.2 (6)
N3A—C21A—C22A—C27A	106.2 (6)	C4C—Zr1C—N4C—Si4C	−103.1 (4)
Zr1A—C21A—C22A—C27A	−175 (100)	Si1C—N1C—C4C—N2C	−170.6 (4)
C27A—C22A—C23A—C24A	1.4 (11)	Zr1C—N1C—C4C—N2C	−3.5 (4)

C21A—C22A—C23A—C24A	−178.6 (7)	Si1C—N1C—C4C—C5C	10.0 (7)
C22A—C23A—C24A—C25A	−0.9 (13)	Zr1C—N1C—C4C—C5C	177.1 (4)
C23A—C24A—C25A—C26A	−1.9 (13)	Si1C—N1C—C4C—Zr1C	−167.1 (5)
C23A—C24A—C25A—C28A	178.9 (8)	Si2C—N2C—C4C—N1C	−177.8 (3)
C24A—C25A—C26A—C27A	4.2 (12)	Zr1C—N2C—C4C—N1C	3.5 (4)
C28A—C25A—C26A—C27A	−176.6 (7)	Si2C—N2C—C4C—C5C	1.6 (7)
C25A—C26A—C27A—C22A	−3.8 (11)	Zr1C—N2C—C4C—C5C	−177.1 (4)
C23A—C22A—C27A—C26A	0.9 (10)	Si2C—N2C—C4C—Zr1C	178.7 (4)
C21A—C22A—C27A—C26A	−179.1 (6)	N3C—Zr1C—C4C—N1C	−108.5 (3)
C26A—C25A—C28A—C29A	−109.6 (10)	N4C—Zr1C—C4C—N1C	−171.7 (3)
C24A—C25A—C28A—C29A	69.5 (10)	N2C—Zr1C—C4C—N1C	−176.2 (5)
C25A—C28A—C29A—C30A	−176.6 (8)	Cl2C—Zr1C—C4C—N1C	91.1 (3)
C28A—C29A—C30A—C31A	165.0 (11)	Cl1C—Zr1C—C4C—N1C	−11.0 (3)
C2B—Si1B—N1B—C4B	58.5 (6)	C21C—Zr1C—C4C—N1C	−132.7 (3)
C3B—Si1B—N1B—C4B	176.8 (5)	N3C—Zr1C—C4C—N2C	67.7 (3)
C1B—Si1B—N1B—C4B	−66.6 (6)	N4C—Zr1C—C4C—N2C	4.5 (4)
C2B—Si1B—N1B—Zr1B	−90.2 (4)	N1C—Zr1C—C4C—N2C	176.2 (5)
C3B—Si1B—N1B—Zr1B	28.1 (4)	Cl2C—Zr1C—C4C—N2C	−92.7 (3)
C1B—Si1B—N1B—Zr1B	144.8 (4)	Cl1C—Zr1C—C4C—N2C	165.2 (2)
N3B—Zr1B—N1B—C4B	169.1 (3)	C21C—Zr1C—C4C—N2C	43.5 (3)
N2B—Zr1B—N1B—C4B	10.6 (3)	N3C—Zr1C—C4C—C5C	163 (9)
N4B—Zr1B—N1B—C4B	111.1 (3)	N4C—Zr1C—C4C—C5C	99 (9)
Cl2B—Zr1B—N1B—C4B	1.1 (5)	N1C—Zr1C—C4C—C5C	−89 (9)
Cl1B—Zr1B—N1B—C4B	−100.8 (3)	N2C—Zr1C—C4C—C5C	95 (9)
C21B—Zr1B—N1B—C4B	138.4 (3)	Cl2C—Zr1C—C4C—C5C	2 (9)
N3B—Zr1B—N1B—Si1B	−34.3 (4)	Cl1C—Zr1C—C4C—C5C	−100 (9)
N2B—Zr1B—N1B—Si1B	167.2 (4)	C21C—Zr1C—C4C—C5C	138 (9)
N4B—Zr1B—N1B—Si1B	−92.2 (3)	N1C—C4C—C5C—C10C	−100.4 (6)
Cl2B—Zr1B—N1B—Si1B	157.7 (2)	N2C—C4C—C5C—C10C	80.2 (7)
Cl1B—Zr1B—N1B—Si1B	55.8 (3)	Zr1C—C4C—C5C—C10C	−13 (10)
C4B—Zr1B—N1B—Si1B	156.6 (5)	N1C—C4C—C5C—C6C	77.2 (7)
C21B—Zr1B—N1B—Si1B	−64.9 (4)	N2C—C4C—C5C—C6C	−102.2 (6)
C17B—Si2B—N2B—C4B	22.8 (6)	Zr1C—C4C—C5C—C6C	164 (9)
C15B—Si2B—N2B—C4B	139.8 (5)	C10C—C5C—C6C—C7C	−0.8 (9)
C16B—Si2B—N2B—C4B	−100.2 (5)	C4C—C5C—C6C—C7C	−178.4 (5)
C17B—Si2B—N2B—Zr1B	−175.8 (3)	C5C—C6C—C7C—C8C	3.1 (9)
C15B—Si2B—N2B—Zr1B	−58.9 (4)	C6C—C7C—C8C—C9C	−3.2 (9)
C16B—Si2B—N2B—Zr1B	61.2 (4)	C6C—C7C—C8C—C11C	173.1 (6)
N1B—Zr1B—N2B—C4B	−10.4 (3)	C7C—C8C—C9C—C10C	1.1 (8)
N3B—Zr1B—N2B—C4B	−94.9 (5)	C11C—C8C—C9C—C10C	−175.2 (5)
N4B—Zr1B—N2B—C4B	−95.4 (3)	C6C—C5C—C10C—C9C	−1.3 (8)
Cl2B—Zr1B—N2B—C4B	164.9 (3)	C4C—C5C—C10C—C9C	176.4 (5)
Cl1B—Zr1B—N2B—C4B	67.0 (3)	C8C—C9C—C10C—C5C	1.1 (8)
C21B—Zr1B—N2B—C4B	−95.3 (3)	C7C—C8C—C11C—C12C	−74.9 (9)
N1B—Zr1B—N2B—Si2B	−176.4 (4)	C9C—C8C—C11C—C12C	101.1 (9)
N3B—Zr1B—N2B—Si2B	99.0 (5)	C8C—C11C—C12C—C13F	4 (6)
N4B—Zr1B—N2B—Si2B	98.6 (3)	C8C—C11C—C12C—C13C	−56.3 (16)
Cl2B—Zr1B—N2B—Si2B	−1.2 (3)	C11C—C12C—C13C—C13F	126 (2)
Cl1B—Zr1B—N2B—Si2B	−99.0 (3)	C13F—C12C—C13C—C14C	45.8 (19)
C4B—Zr1B—N2B—Si2B	−166.0 (6)	C11C—C12C—C13C—C14C	171.6 (9)
C21B—Zr1B—N2B—Si2B	98.7 (4)	C14C—C13C—C13F—C12C	−132.7 (15)
C20B—Si3B—N3B—C21B	−14.0 (6)	C12C—C13C—C13F—C14C	132.7 (15)
C18B—Si3B—N3B—C21B	109.0 (5)	C11C—C12C—C13F—C13C	−93 (4)
C19B—Si3B—N3B—C21B	−131.2 (5)	C13C—C12C—C13F—C14C	−56 (5)

C20B—Si3B—N3B—Zr1B	148.9 (4)	C11C—C12C—C13F—C14C	−148 (2)
C18B—Si3B—N3B—Zr1B	−88.1 (4)	C12C—C13F—C14C—C13C	56 (4)
C19B—Si3B—N3B—Zr1B	31.7 (4)	C12C—C13C—C14C—C13F	−41.0 (19)
N1B—Zr1B—N3B—C21B	−75.3 (3)	Si3C—N3C—C21C—N4C	176.6 (4)
N2B—Zr1B—N3B—C21B	−0.5 (6)	Zr1C—N3C—C21C—N4C	15.8 (5)
N4B—Zr1B—N3B—C21B	0.0 (3)	Si3C—N3C—C21C—C22C	1.2 (8)
Cl2B—Zr1B—N3B—C21B	98.7 (3)	Zr1C—N3C—C21C—C22C	−159.6 (5)
Cl1B—Zr1B—N3B—C21B	−163.3 (3)	Si3C—N3C—C21C—Zr1C	160.8 (5)
C4B—Zr1B—N3B—C21B	−65.6 (4)	Si4C—N4C—C21C—N3C	177.5 (4)
N1B—Zr1B—N3B—Si3B	117.4 (3)	Zr1C—N4C—C21C—N3C	−15.7 (5)
N2B—Zr1B—N3B—Si3B	−167.8 (3)	Si4C—N4C—C21C—C22C	−7.1 (8)
N4B—Zr1B—N3B—Si3B	−167.3 (4)	Zr1C—N4C—C21C—C22C	159.7 (5)
Cl2B—Zr1B—N3B—Si3B	−68.6 (3)	Si4C—N4C—C21C—Zr1C	−166.8 (5)
Cl1B—Zr1B—N3B—Si3B	29.4 (3)	N4C—Zr1C—C21C—N3C	163.3 (5)
C4B—Zr1B—N3B—Si3B	127.2 (3)	N1C—Zr1C—C21C—N3C	14.9 (4)
C21B—Zr1B—N3B—Si3B	−167.3 (5)	N2C—Zr1C—C21C—N3C	71.5 (3)
C33B—Si4B—N4B—C21B	−153.4 (5)	Cl2C—Zr1C—C21C—N3C	178.0 (3)
C34B—Si4B—N4B—C21B	87.3 (5)	Cl1C—Zr1C—C21C—N3C	−82.9 (3)
C32B—Si4B—N4B—C21B	−36.0 (5)	C4C—Zr1C—C21C—N3C	50.7 (4)
C33B—Si4B—N4B—Zr1B	24.2 (4)	N3C—Zr1C—C21C—N4C	−163.3 (5)
C34B—Si4B—N4B—Zr1B	−95.1 (4)	N1C—Zr1C—C21C—N4C	−148.4 (3)
C32B—Si4B—N4B—Zr1B	141.6 (4)	N2C—Zr1C—C21C—N4C	−91.7 (3)
N1B—Zr1B—N4B—C21B	118.6 (3)	Cl2C—Zr1C—C21C—N4C	14.7 (4)
N3B—Zr1B—N4B—C21B	0.0 (3)	Cl1C—Zr1C—C21C—N4C	113.8 (3)
N2B—Zr1B—N4B—C21B	179.9 (3)	C4C—Zr1C—C21C—N4C	−112.6 (3)
Cl2B—Zr1B—N4B—C21B	−89.8 (3)	N3C—Zr1C—C21C—C22C	96.9 (14)
Cl1B—Zr1B—N4B—C21B	32.8 (4)	N4C—Zr1C—C21C—C22C	−99.8 (15)
C4B—Zr1B—N4B—C21B	147.8 (3)	N1C—Zr1C—C21C—C22C	111.8 (14)
N1B—Zr1B—N4B—Si4B	−59.6 (4)	N2C—Zr1C—C21C—C22C	168.4 (14)
N3B—Zr1B—N4B—Si4B	−178.1 (4)	Cl2C—Zr1C—C21C—C22C	−85.1 (14)
N2B—Zr1B—N4B—Si4B	1.7 (4)	Cl1C—Zr1C—C21C—C22C	14.0 (14)
Cl2B—Zr1B—N4B—Si4B	92.0 (3)	C4C—Zr1C—C21C—C22C	147.6 (14)
Cl1B—Zr1B—N4B—Si4B	−145.4 (2)	N3C—C21C—C22C—C27C	99.0 (7)
C4B—Zr1B—N4B—Si4B	−30.3 (4)	N4C—C21C—C22C—C27C	−76.0 (7)
C21B—Zr1B—N4B—Si4B	−178.2 (5)	Zr1C—C21C—C22C—C27C	13.0 (17)
Si1B—N1B—C4B—N2B	−175.3 (4)	N3C—C21C—C22C—C23C	−82.6 (7)
Zr1B—N1B—C4B—N2B	−17.0 (4)	N4C—C21C—C22C—C23C	102.3 (7)
Si1B—N1B—C4B—C5B	2.5 (8)	Zr1C—C21C—C22C—C23C	−168.6 (11)
Zr1B—N1B—C4B—C5B	160.8 (5)	C27C—C22C—C23C—C24C	−0.5 (9)
Si1B—N1B—C4B—Zr1B	−158.3 (5)	C21C—C22C—C23C—C24C	−179.0 (5)
Si2B—N2B—C4B—N1B	−175.4 (4)	C22C—C23C—C24C—C25C	0.9 (9)
Zr1B—N2B—C4B—N1B	16.9 (4)	C23C—C24C—C25C—C26C	−2.0 (9)
Si2B—N2B—C4B—C5B	6.7 (8)	C23C—C24C—C25C—C28C	178.2 (6)
Zr1B—N2B—C4B—C5B	−161.0 (5)	C24C—C25C—C26C—C27C	2.8 (9)
Si2B—N2B—C4B—Zr1B	167.7 (5)	C28C—C25C—C26C—C27C	−177.5 (6)
N3B—Zr1B—C4B—N1B	−17.4 (5)	C23C—C22C—C27C—C26C	1.4 (9)
N2B—Zr1B—C4B—N1B	−162.0 (5)	C21C—C22C—C27C—C26C	179.8 (5)
N4B—Zr1B—C4B—N1B	−71.7 (3)	C25C—C26C—C27C—C22C	−2.5 (9)
Cl2B—Zr1B—C4B—N1B	−179.4 (3)	C24C—C25C—C28C—C29C	111.2 (7)
Cl1B—Zr1B—C4B—N1B	79.5 (3)	C26C—C25C—C28C—C29C	−68.5 (8)
C21B—Zr1B—C4B—N1B	−52.3 (4)	C25C—C28C—C29C—C30C	179.8 (7)
N1B—Zr1B—C4B—N2B	162.0 (5)	C28C—C29C—C30C—C31C	179.1 (9)
N3B—Zr1B—C4B—N2B	144.6 (3)		

4. Crystal data for complex 12

Table 1. Crystal data and structure refinement for complex 12.

Identification code	zrdimomet
Empirical formula	C28 H50 Cl2 N4 O2 Si4 Zr
Formula weight	749.20
Temperature	230.0(1) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 19.409(2) A alpha = 90 deg. b = 11.8110(14) A beta = 93.611(8) deg. c = 17.5870(17) A gamma = 90 deg.
Volume	4023.6(7) A^3
Z, Calculated density	4, 1.237 Mg/m^3
Absorption coefficient	0.553 mm^-1
F(000)	1568
Crystal size	0.39 x 0.39 x 0.30 mm
Theta range for data collection	1.05 to 23.00 deg.
Limiting indices	-21<=h<=21, -12<=k<=12, -19<=l<=19
Reflections collected / unique	9421 / 5465 [R(int) = 0.0672]
Completeness to theta = 23.00	97.7 %
Absorption correction	None
Max. and min. transmission	0.8517 and 0.8132
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5465 / 0 / 355
Goodness-of-fit on F^2	0.902
Final R indices [I>2sigma(I)]	R1 = 0.0600, wR2 = 0.1523
R indices (all data)	R1 = 0.1171, wR2 = 0.1757
Largest diff. peak and hole	0.745 and -0.522 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for complex 12.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)

Zr(1)	7291(1)	851(1)	2781(1)	58(1)
Cl(1)	7637(1)	2002(2)	1733(1)	118(1)
Cl(2)	6303(1)	-10(2)	2092(1)	84(1)
Si(1)	6962(1)	3891(2)	3145(1)	72(1)
Si(2)	6317(1)	-393(2)	4273(1)	62(1)
Si(3)	8706(1)	1074(3)	4311(1)	94(1)
Si(4)	7982(2)	-1570(3)	1743(2)	121(1)
O(1)	5348(2)	2131(5)	3100(3)	72(1)
O(2)	8680(3)	-2250(7)	3711(4)	108(2)
N(1)	6988(2)	2449(5)	3350(3)	56(2)
N(2)	6727(2)	712(5)	3813(3)	52(1)
N(3)	8264(3)	587(6)	3475(3)	75(2)
N(4)	7972(3)	-557(6)	2480(3)	78(2)
C(1)	7869(4)	4270(9)	2979(6)	127(4)
C(2)	6664(5)	4787(8)	3935(5)	121(4)
C(3)	6384(5)	4147(8)	2287(5)	114(3)
C(4)	6607(3)	1821(7)	3803(3)	51(2)
C(5)	6035(3)	2343(6)	4231(4)	54(2)
C(6)	6128(4)	2693(7)	4979(4)	67(2)
C(7)	5596(5)	3218(8)	5332(5)	89(3)
C(8)	4991(5)	3392(7)	4950(5)	84(3)
C(9)	4866(4)	3031(7)	4206(5)	80(2)
C(10)	5392(3)	2522(7)	3847(4)	64(2)
C(11)	4692(4)	2140(8)	2671(5)	102(3)
C(12)	6744(4)	-1693(7)	3935(5)	88(3)
C(13)	5376(3)	-439(7)	3993(4)	83(3)
C(14)	6487(4)	-265(8)	5332(4)	92(3)
C(15)	8131(4)	1975(10)	4819(4)	113(4)
C(16)	9473(4)	1939(11)	4090(5)	133(4)
C(17)	8908(5)	-179(11)	4968(5)	143(5)
C(18)	8428(2)	-256(4)	3029(2)	87(3)
C(19)	9154(2)	-747(4)	3078(2)	107(3)
C(20)	9728(2)	-242(4)	2787(2)	78(4)
C(20A)	9631(2)	-168(4)	2931(2)	57(13)
C(21)	10367(2)	-776(4)	2864(2)	159(8)
C(21A)	10320(2)	-372(4)	2791(2)	57(12)
C(22)	10432(2)	-1815(4)	3233(2)	161(6)
C(23)	9857(2)	-2320(4)	3525(2)	182(10)
C(23A)	10043(2)	-2120(4)	3454(2)	5(5)
C(24)	9219(2)	-1786(4)	3447(2)	102(3)
C(25)	8850(7)	-3254(11)	4130(6)	171(6)
C(26)	8780(5)	-2281(12)	1647(6)	199(8)
C(27)	7354(7)	-2766(11)	1997(8)	187(6)
C(28)	7605(6)	-1013(12)	885(5)	162(6)

Table 3. Bond lengths [A] and angles [deg] for complex 12.

Zr(1)-N(2)	2.182(5)
Zr(1)-N(3)	2.206(5)
Zr(1)-N(4)	2.209(6)
Zr(1)-N(1)	2.232(6)
Zr(1)-Cl(1)	2.420(2)
Zr(1)-Cl(2)	2.427(2)
Si(1)-N(1)	1.740(6)
Si(1)-C(3)	1.848(9)
Si(1)-C(1)	1.857(8)
Si(1)-C(2)	1.867(9)
Si(2)-N(2)	1.754(6)
Si(2)-C(12)	1.860(8)
Si(2)-C(13)	1.862(7)
Si(2)-C(14)	1.877(7)
Si(3)-N(3)	1.752(6)
Si(3)-C(15)	1.817(8)

Si(3)-C(16)	1.868(9)
Si(3)-C(17)	1.902(11)
Si(4)-C(28)	1.762(10)
Si(4)-N(4)	1.765(7)
Si(4)-C(26)	1.779(9)
Si(4)-C(27)	1.935(13)
O(1)-C(10)	1.389(8)
O(1)-C(11)	1.438(8)
O(2)-C(24)	1.292(7)
O(2)-C(25)	1.425(12)
N(1)-C(4)	1.344(8)
N(2)-C(4)	1.330(8)
N(3)-C(18)	1.319(7)
N(4)-C(18)	1.317(6)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(1)-H(1C)	0.9700
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(2)-H(2C)	0.9700
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(3)-H(3C)	0.9700
C(4)-C(5)	1.511(9)
C(5)-C(6)	1.379(9)
C(5)-C(10)	1.398(9)
C(6)-C(7)	1.384(10)
C(6)-H(6)	0.9400
C(7)-C(8)	1.330(11)
C(7)-H(7)	0.9400
C(8)-C(9)	1.383(11)
C(8)-H(8)	0.9400
C(9)-C(10)	1.373(9)
C(9)-H(9)	0.9400
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(11)-H(11C)	0.9700
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(12)-H(12C)	0.9700
C(13)-H(13A)	0.9700
C(13)-H(13B)	0.9700
C(13)-H(13C)	0.9700
C(14)-H(14A)	0.9700
C(14)-H(14B)	0.9700
C(14)-H(14C)	0.9700
C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700
C(15)-H(15C)	0.9700
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(16)-H(16C)	0.9700
C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700
C(17)-H(17C)	0.9700
C(18)-C(19)	1.5211
C(19)-C(20)	1.3900
C(19)-C(24)	1.3901
C(20)-C(21)	1.3900
C(20)-H(20)	0.9400
C(21)-C(22)	1.3900
C(21)-H(21)	0.9400
C(22)-C(23)	1.3900
C(22)-H(22)	0.9400
C(23)-C(24)	1.3900
C(23)-H(23)	0.9400
C(25)-H(25A)	0.9700
C(25)-H(25B)	0.9700

C(25)-H(25C)	0.9700
C(26)-H(26A)	0.9700
C(26)-H(26B)	0.9700
C(26)-H(26C)	0.9700
C(27)-H(27A)	0.9700
C(27)-H(27B)	0.9700
C(27)-H(27C)	0.9700
C(28)-H(28A)	0.9700
C(28)-H(28B)	0.9700
C(28)-H(28C)	0.9700

N(2)-Zr(1)-N(3)	89.23(18)
N(2)-Zr(1)-N(4)	118.8(2)
N(3)-Zr(1)-N(4)	61.4(2)
N(2)-Zr(1)-N(1)	62.0(2)
N(3)-Zr(1)-N(1)	96.4(2)
N(4)-Zr(1)-N(1)	157.2(2)
N(2)-Zr(1)-Cl(1)	148.56(18)
N(3)-Zr(1)-Cl(1)	103.36(17)
N(4)-Zr(1)-Cl(1)	92.35(18)
N(1)-Zr(1)-Cl(1)	87.70(15)
N(2)-Zr(1)-Cl(2)	87.85(14)
N(3)-Zr(1)-Cl(2)	147.1(2)
N(4)-Zr(1)-Cl(2)	91.75(16)
N(1)-Zr(1)-Cl(2)	110.90(13)
Cl(1)-Zr(1)-Cl(2)	95.93(9)
N(2)-Zr(1)-C(4)	31.2(2)
N(3)-Zr(1)-C(4)	97.98(19)
N(4)-Zr(1)-C(4)	147.8(2)
N(1)-Zr(1)-C(4)	31.5(2)
Cl(1)-Zr(1)-C(4)	117.55(19)
Cl(2)-Zr(1)-C(4)	96.30(14)
N(2)-Zr(1)-C(18)	106.87(16)
N(3)-Zr(1)-C(18)	30.75(17)
N(4)-Zr(1)-C(18)	30.70(16)
N(1)-Zr(1)-C(18)	126.84(14)
Cl(1)-Zr(1)-C(18)	97.90(12)
Cl(2)-Zr(1)-C(18)	120.85(10)
C(4)-Zr(1)-C(18)	125.63(16)
N(1)-Si(1)-C(3)	109.7(4)
N(1)-Si(1)-C(1)	104.7(4)
C(3)-Si(1)-C(1)	111.4(4)
N(1)-Si(1)-C(2)	114.0(4)
C(3)-Si(1)-C(2)	108.4(5)
C(1)-Si(1)-C(2)	108.8(5)
N(2)-Si(2)-C(12)	104.0(3)
N(2)-Si(2)-C(13)	111.5(3)
C(12)-Si(2)-C(13)	110.0(4)
N(2)-Si(2)-C(14)	109.9(3)
C(12)-Si(2)-C(14)	109.2(4)
C(13)-Si(2)-C(14)	111.9(4)
N(3)-Si(3)-C(15)	108.8(3)
N(3)-Si(3)-C(16)	111.1(4)
C(15)-Si(3)-C(16)	107.7(5)
N(3)-Si(3)-C(17)	109.0(4)
C(15)-Si(3)-C(17)	105.5(5)
C(16)-Si(3)-C(17)	114.5(5)
C(28)-Si(4)-N(4)	110.6(5)
C(28)-Si(4)-C(26)	114.3(5)
N(4)-Si(4)-C(26)	116.1(4)
C(28)-Si(4)-C(27)	103.7(6)
N(4)-Si(4)-C(27)	106.8(5)
C(26)-Si(4)-C(27)	104.0(7)
C(10)-O(1)-C(11)	119.6(5)
C(24)-O(2)-C(25)	111.8(8)
C(4)-N(1)-Si(1)	130.7(5)
C(4)-N(1)-Zr(1)	88.2(4)
Si(1)-N(1)-Zr(1)	137.7(3)

C(4)-N(2)-Si(2)	130.9(4)
C(4)-N(2)-Zr(1)	90.7(4)
Si(2)-N(2)-Zr(1)	134.9(3)
C(18)-N(3)-Si(3)	128.6(4)
C(18)-N(3)-Zr(1)	90.5(3)
Si(3)-N(3)-Zr(1)	140.8(3)
C(18)-N(4)-Si(4)	133.1(4)
C(18)-N(4)-Zr(1)	90.3(4)
Si(4)-N(4)-Zr(1)	136.1(3)
Si(1)-C(1)-H(1A)	109.5
Si(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
Si(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
Si(1)-C(2)-H(2A)	109.5
Si(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
Si(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
Si(1)-C(3)-H(3A)	109.5
Si(1)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
Si(1)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
N(2)-C(4)-N(1)	116.6(6)
N(2)-C(4)-C(5)	122.0(6)
N(1)-C(4)-C(5)	121.3(7)
N(2)-C(4)-Zr(1)	58.1(3)
N(1)-C(4)-Zr(1)	60.2(3)
C(5)-C(4)-Zr(1)	163.4(4)
C(6)-C(5)-C(10)	118.3(6)
C(6)-C(5)-C(4)	122.8(6)
C(10)-C(5)-C(4)	118.8(6)
C(5)-C(6)-C(7)	120.4(7)
C(5)-C(6)-H(6)	119.8
C(7)-C(6)-H(6)	119.8
C(8)-C(7)-C(6)	120.1(8)
C(8)-C(7)-H(7)	119.9
C(6)-C(7)-H(7)	119.9
C(7)-C(8)-C(9)	121.8(8)
C(7)-C(8)-H(8)	119.1
C(9)-C(8)-H(8)	119.1
C(10)-C(9)-C(8)	118.6(8)
C(10)-C(9)-H(9)	120.7
C(8)-C(9)-H(9)	120.7
C(9)-C(10)-O(1)	125.3(7)
C(9)-C(10)-C(5)	120.7(7)
O(1)-C(10)-C(5)	114.0(6)
O(1)-C(11)-H(11A)	109.5
O(1)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
O(1)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
Si(2)-C(12)-H(12A)	109.5
Si(2)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
Si(2)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
Si(2)-C(13)-H(13A)	109.5
Si(2)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
Si(2)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5

H(13B)-C(13)-H(13C)	109.5
Si(2)-C(14)-H(14A)	109.5
Si(2)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
Si(2)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
Si(3)-C(15)-H(15A)	109.5
Si(3)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
Si(3)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
Si(3)-C(16)-H(16A)	109.5
Si(3)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
Si(3)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
Si(3)-C(17)-H(17A)	109.5
Si(3)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
Si(3)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
N(4)-C(18)-N(3)	117.6(4)
N(4)-C(18)-C(19)	121.1(3)
N(3)-C(18)-C(19)	120.7(3)
N(4)-C(18)-Zr(1)	59.0(3)
N(3)-C(18)-Zr(1)	58.8(3)
C(19)-C(18)-Zr(1)	169.39(11)
C(20)-C(19)-C(24)	120.0
C(20)-C(19)-C(18)	125.2
C(24)-C(19)-C(18)	114.8
C(19)-C(20)-C(21)	120.0
C(19)-C(20)-H(20)	120.0
C(21)-C(20)-H(20)	120.0
C(22)-C(21)-C(20)	120.0
C(22)-C(21)-H(21)	120.0
C(20)-C(21)-H(21)	120.0
C(21)-C(22)-C(23)	120.0
C(21)-C(22)-H(22)	120.0
C(23)-C(22)-H(22)	120.0
C(22)-C(23)-C(24)	120.0
C(22)-C(23)-H(23)	120.0
C(24)-C(23)-H(23)	120.0
O(2)-C(24)-C(23)	120.6(4)
O(2)-C(24)-C(19)	119.4(4)
C(23)-C(24)-C(19)	120.0
O(2)-C(25)-H(25A)	109.5
O(2)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
O(2)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
Si(4)-C(26)-H(26A)	109.5
Si(4)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
Si(4)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
Si(4)-C(27)-H(27A)	109.5
Si(4)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
Si(4)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
Si(4)-C(28)-H(28A)	109.5

Si(4)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
Si(4)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for complex 12. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Zr(1)	50(1)	81(1)	44(1)	-1(1)	8(1)	-2(1)
Cl(1)	162(2)	121(2)	79(2)	10(1)	53(2)	-25(2)
Cl(2)	70(1)	107(2)	73(1)	-18(1)	-9(1)	-1(1)
Si(1)	71(1)	70(2)	77(1)	6(1)	12(1)	-13(1)
Si(2)	61(1)	69(2)	59(1)	12(1)	16(1)	3(1)
Si(3)	50(1)	173(3)	60(1)	-29(2)	-3(1)	-2(2)
Si(4)	105(2)	169(3)	84(2)	-58(2)	-24(2)	63(2)
O(1)	56(3)	88(4)	70(3)	5(3)	-2(2)	9(3)
O(2)	81(4)	137(7)	108(5)	3(4)	17(3)	-3(4)
N(1)	46(3)	70(4)	51(3)	2(3)	5(2)	-4(3)
N(2)	43(3)	57(5)	56(3)	2(3)	6(2)	0(3)
N(3)	45(3)	132(6)	48(3)	-22(4)	4(2)	12(4)
N(4)	49(3)	123(6)	59(4)	-21(4)	-5(3)	16(4)
C(1)	100(7)	106(9)	177(10)	10(7)	27(7)	-52(6)
C(2)	170(9)	64(7)	136(8)	-15(6)	55(7)	-12(7)
C(3)	117(8)	97(8)	125(8)	37(6)	-4(6)	4(6)
C(4)	46(4)	68(6)	39(4)	-3(4)	2(3)	-3(4)
C(5)	52(4)	53(5)	59(4)	5(4)	13(3)	1(3)
C(6)	79(5)	68(6)	53(4)	-7(4)	10(4)	-7(4)
C(7)	118(7)	88(7)	66(5)	-10(5)	41(6)	5(6)
C(8)	84(6)	72(7)	100(7)	-1(5)	40(5)	16(5)
C(9)	71(5)	74(6)	97(6)	14(5)	29(5)	14(4)
C(10)	57(5)	68(6)	69(5)	6(4)	11(4)	-1(4)
C(11)	69(5)	131(9)	103(6)	-4(6)	-22(5)	19(6)
C(12)	91(6)	66(6)	108(6)	16(5)	31(5)	22(5)
C(13)	69(5)	84(7)	98(6)	19(5)	22(4)	-14(4)
C(14)	97(6)	117(8)	61(5)	24(5)	11(4)	0(5)
C(15)	77(6)	187(12)	74(5)	-46(6)	3(4)	8(6)
C(16)	69(6)	209(14)	122(8)	-21(8)	6(5)	-25(7)
C(17)	147(9)	208(14)	67(6)	-11(7)	-31(6)	36(9)
C(18)	34(4)	163(10)	65(5)	-14(5)	-4(4)	24(5)
C(19)	109(7)	137(10)	72(6)	-39(6)	-9(5)	8(7)
C(20)	36(5)	146(12)	56(6)	-9(6)	35(5)	-2(5)
C(21)	34(7)	300(20)	147(13)	-95(14)	10(6)	37(9)
C(22)	141(11)	190(15)	141(10)	-58(9)	-70(8)	105(10)
C(23)	46(7)	350(30)	152(13)	-146(15)	40(8)	-71(11)
C(24)	145(10)	93(8)	66(6)	-17(5)	1(6)	12(7)
C(25)	273(17)	118(12)	119(9)	37(8)	-19(10)	-34(11)
C(26)	147(10)	286(19)	160(10)	-149(12)	-24(8)	106(11)
C(27)	197(13)	121(12)	241(16)	-47(11)	-12(12)	-2(11)
C(28)	181(11)	226(16)	77(7)	-56(8)	-20(7)	60(10)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for complex 12.

	x	y	z	U(eq)
H(1A)	8159	4122	3437	190
H(1B)	7894	5067	2850	190
H(1C)	8026	3819	2562	190
H(2A)	6961	4660	4392	182
H(2B)	6193	4586	4033	182
H(2C)	6684	5578	3791	182
H(3A)	5917	3929	2388	170
H(3B)	6538	3701	1866	170
H(3C)	6394	4944	2155	170
H(6)	6554	2574	5251	80
H(7)	5662	3452	5842	107
H(8)	4640	3770	5193	101
H(9)	4430	3133	3952	95
H(11A)	4748	1849	2163	153
H(11B)	4518	2910	2637	153
H(11C)	4368	1668	2925	153
H(12A)	7235	-1660	4079	131
H(12B)	6677	-1742	3384	131
H(12C)	6545	-2354	4164	131
H(13A)	5156	241	4172	125
H(13B)	5172	-1099	4219	125
H(13C)	5308	-483	3443	125
H(14A)	6981	-250	5455	137
H(14B)	6286	-907	5581	137
H(14C)	6282	430	5507	137
H(15A)	7725	1547	4938	169
H(15B)	7992	2618	4502	169
H(15C)	8368	2242	5286	169
H(16A)	9790	1477	3818	200
H(16B)	9704	2208	4561	200
H(16C)	9325	2580	3777	200
H(17A)	9221	-690	4730	214
H(17B)	8484	-576	5061	214
H(17C)	9122	91	5447	214
H(20)	9685	461	2537	94
H(21)	10755	-434	2668	191
H(22)	10864	-2176	3286	193
H(23)	9901	-3022	3774	218
H(25A)	8433	-3585	4310	257
H(25B)	9165	-3071	4562	257
H(25C)	9068	-3791	3803	257
H(26A)	8946	-2585	2137	299
H(26B)	9115	-1752	1468	299
H(26C)	8712	-2895	1284	299
H(27A)	6900	-2448	2060	281
H(27B)	7523	-3126	2468	281
H(27C)	7324	-3322	1590	281
H(28A)	7172	-646	983	244
H(28B)	7519	-1622	521	244
H(28C)	7916	-466	680	244

Table 6. Torsion angles [deg] for complex 12.

C(3)-Si(1)-N(1)-C(4)	-92.0(6)
C(1)-Si(1)-N(1)-C(4)	148.4(6)
C(2)-Si(1)-N(1)-C(4)	29.7(7)
C(3)-Si(1)-N(1)-Zr(1)	60.3(5)
C(1)-Si(1)-N(1)-Zr(1)	-59.3(5)
C(2)-Si(1)-N(1)-Zr(1)	-178.0(5)
N(2)-Zr(1)-N(1)-C(4)	-9.1(3)
N(3)-Zr(1)-N(1)-C(4)	-94.8(4)
N(4)-Zr(1)-N(1)-C(4)	-107.4(6)

Cl(1)-Zr(1)-N(1)-C(4)	162.0(3)
Cl(2)-Zr(1)-N(1)-C(4)	66.6(4)
C(18)-Zr(1)-N(1)-C(4)	-99.8(4)
N(2)-Zr(1)-N(1)-Si(1)	-168.4(5)
N(3)-Zr(1)-N(1)-Si(1)	105.9(4)
N(4)-Zr(1)-N(1)-Si(1)	93.3(6)
Cl(1)-Zr(1)-N(1)-Si(1)	2.7(4)
Cl(2)-Zr(1)-N(1)-Si(1)	-92.8(4)
C(4)-Zr(1)-N(1)-Si(1)	-159.4(6)
C(18)-Zr(1)-N(1)-Si(1)	100.8(4)
C(12)-Si(2)-N(2)-C(4)	175.5(6)
C(13)-Si(2)-N(2)-C(4)	57.0(7)
C(14)-Si(2)-N(2)-C(4)	-67.7(7)
C(12)-Si(2)-N(2)-Zr(1)	23.4(5)
C(13)-Si(2)-N(2)-Zr(1)	-95.1(5)
C(14)-Si(2)-N(2)-Zr(1)	140.2(4)
N(3)-Zr(1)-N(2)-C(4)	106.9(4)
N(4)-Zr(1)-N(2)-C(4)	163.3(4)
N(1)-Zr(1)-N(2)-C(4)	9.2(3)
Cl(1)-Zr(1)-N(2)-C(4)	-8.0(5)
Cl(2)-Zr(1)-N(2)-C(4)	-105.9(4)
C(18)-Zr(1)-N(2)-C(4)	132.4(3)
N(3)-Zr(1)-N(2)-Si(2)	-93.9(4)
N(4)-Zr(1)-N(2)-Si(2)	-37.5(5)
N(1)-Zr(1)-N(2)-Si(2)	168.5(5)
Cl(1)-Zr(1)-N(2)-Si(2)	151.2(3)
Cl(2)-Zr(1)-N(2)-Si(2)	53.4(4)
C(4)-Zr(1)-N(2)-Si(2)	159.3(6)
C(18)-Zr(1)-N(2)-Si(2)	-68.3(4)
C(15)-Si(3)-N(3)-C(18)	-164.3(6)
C(16)-Si(3)-N(3)-C(18)	77.3(8)
C(17)-Si(3)-N(3)-C(18)	-49.8(7)
C(15)-Si(3)-N(3)-Zr(1)	8.9(8)
C(16)-Si(3)-N(3)-Zr(1)	-109.5(6)
C(17)-Si(3)-N(3)-Zr(1)	123.5(6)
N(2)-Zr(1)-N(3)-C(18)	126.2(4)
N(4)-Zr(1)-N(3)-C(18)	2.4(3)
N(1)-Zr(1)-N(3)-C(18)	-172.1(4)
Cl(1)-Zr(1)-N(3)-C(18)	-82.9(4)
Cl(2)-Zr(1)-N(3)-C(18)	41.3(5)
C(4)-Zr(1)-N(3)-C(18)	156.2(4)
N(2)-Zr(1)-N(3)-Si(3)	-48.5(6)
N(4)-Zr(1)-N(3)-Si(3)	-172.3(7)
N(1)-Zr(1)-N(3)-Si(3)	13.2(6)
Cl(1)-Zr(1)-N(3)-Si(3)	102.4(6)
Cl(2)-Zr(1)-N(3)-Si(3)	-133.4(5)
C(4)-Zr(1)-N(3)-Si(3)	-18.5(6)
C(18)-Zr(1)-N(3)-Si(3)	-174.7(9)
C(28)-Si(4)-N(4)-C(18)	-138.2(8)
C(26)-Si(4)-N(4)-C(18)	-5.9(10)
C(27)-Si(4)-N(4)-C(18)	109.6(8)
C(28)-Si(4)-N(4)-Zr(1)	31.7(8)
C(26)-Si(4)-N(4)-Zr(1)	164.1(7)
C(27)-Si(4)-N(4)-Zr(1)	-80.5(7)
N(2)-Zr(1)-N(4)-C(18)	-73.9(4)
N(3)-Zr(1)-N(4)-C(18)	-2.4(3)
N(1)-Zr(1)-N(4)-C(18)	11.9(8)
Cl(1)-Zr(1)-N(4)-C(18)	101.6(4)
Cl(2)-Zr(1)-N(4)-C(18)	-162.4(4)
C(4)-Zr(1)-N(4)-C(18)	-57.7(6)
N(2)-Zr(1)-N(4)-Si(4)	113.4(5)
N(3)-Zr(1)-N(4)-Si(4)	-175.1(6)
N(1)-Zr(1)-N(4)-Si(4)	-160.8(4)
Cl(1)-Zr(1)-N(4)-Si(4)	-71.1(5)
Cl(2)-Zr(1)-N(4)-Si(4)	24.9(5)
C(4)-Zr(1)-N(4)-Si(4)	129.7(5)
C(18)-Zr(1)-N(4)-Si(4)	-172.7(8)
Si(2)-N(2)-C(4)-N(1)	-175.8(4)

Zr(1)-N(2)-C(4)-N(1)	-15.2(5)
Si(2)-N(2)-C(4)-C(5)	-0.2(9)
Zr(1)-N(2)-C(4)-C(5)	160.4(5)
Si(2)-N(2)-C(4)-Zr(1)	-160.6(6)
Si(1)-N(1)-C(4)-N(2)	176.6(4)
Zr(1)-N(1)-C(4)-N(2)	14.8(5)
Si(1)-N(1)-C(4)-C(5)	1.0(9)
Zr(1)-N(1)-C(4)-C(5)	-160.8(5)
Si(1)-N(1)-C(4)-Zr(1)	161.7(6)
N(3)-Zr(1)-C(4)-N(2)	-75.1(4)
N(4)-Zr(1)-C(4)-N(2)	-28.3(6)
N(1)-Zr(1)-C(4)-N(2)	-164.4(6)
Cl(1)-Zr(1)-C(4)-N(2)	175.3(3)
Cl(2)-Zr(1)-C(4)-N(2)	75.2(4)
C(18)-Zr(1)-C(4)-N(2)	-60.3(4)
N(2)-Zr(1)-C(4)-N(1)	164.4(6)
N(3)-Zr(1)-C(4)-N(1)	89.3(4)
N(4)-Zr(1)-C(4)-N(1)	136.1(5)
Cl(1)-Zr(1)-C(4)-N(1)	-20.4(4)
Cl(2)-Zr(1)-C(4)-N(1)	-120.4(3)
C(18)-Zr(1)-C(4)-N(1)	104.0(4)
N(2)-Zr(1)-C(4)-C(5)	-95.5(19)
N(3)-Zr(1)-C(4)-C(5)	-170.6(19)
N(4)-Zr(1)-C(4)-C(5)	-123.8(18)
N(1)-Zr(1)-C(4)-C(5)	100.1(19)
Cl(1)-Zr(1)-C(4)-C(5)	79.8(19)
Cl(2)-Zr(1)-C(4)-C(5)	-20.3(19)
C(18)-Zr(1)-C(4)-C(5)	-155.8(18)
N(2)-C(4)-C(5)-C(6)	88.7(9)
N(1)-C(4)-C(5)-C(6)	-96.0(8)
Zr(1)-C(4)-C(5)-C(6)	173.7(15)
N(2)-C(4)-C(5)-C(10)	-93.9(8)
N(1)-C(4)-C(5)-C(10)	81.5(8)
Zr(1)-C(4)-C(5)-C(10)	-9(2)
C(10)-C(5)-C(6)-C(7)	-0.7(11)
C(4)-C(5)-C(6)-C(7)	176.7(7)
C(5)-C(6)-C(7)-C(8)	-0.2(13)
C(6)-C(7)-C(8)-C(9)	1.9(14)
C(7)-C(8)-C(9)-C(10)	-2.7(13)
C(8)-C(9)-C(10)-O(1)	-179.1(7)
C(8)-C(9)-C(10)-C(5)	1.7(12)
C(11)-O(1)-C(10)-C(9)	-6.6(11)
C(11)-O(1)-C(10)-C(5)	172.6(7)
C(6)-C(5)-C(10)-C(9)	-0.1(11)
C(4)-C(5)-C(10)-C(9)	-177.7(7)
C(6)-C(5)-C(10)-O(1)	-179.4(6)
C(4)-C(5)-C(10)-O(1)	3.1(9)
Si(4)-N(4)-C(18)-N(3)	177.0(6)
Zr(1)-N(4)-C(18)-N(3)	4.0(6)
Si(4)-N(4)-C(18)-C(19)	5.4(9)
Zr(1)-N(4)-C(18)-C(19)	-167.61(13)
Si(4)-N(4)-C(18)-Zr(1)	173.1(8)
Si(3)-N(3)-C(18)-N(4)	171.7(5)
Zr(1)-N(3)-C(18)-N(4)	-4.0(6)
Si(3)-N(3)-C(18)-C(19)	-16.6(7)
Zr(1)-N(3)-C(18)-C(19)	167.63(13)
Si(3)-N(3)-C(18)-Zr(1)	175.7(7)
N(2)-Zr(1)-C(18)-N(4)	118.4(4)
N(3)-Zr(1)-C(18)-N(4)	175.9(6)
N(1)-Zr(1)-C(18)-N(4)	-174.3(4)
Cl(1)-Zr(1)-C(18)-N(4)	-81.2(4)
Cl(2)-Zr(1)-C(18)-N(4)	20.6(4)
C(4)-Zr(1)-C(18)-N(4)	146.4(4)
N(2)-Zr(1)-C(18)-N(3)	-57.5(4)
N(4)-Zr(1)-C(18)-N(3)	-175.9(6)
N(1)-Zr(1)-C(18)-N(3)	9.8(4)
Cl(1)-Zr(1)-C(18)-N(3)	102.9(4)
Cl(2)-Zr(1)-C(18)-N(3)	-155.3(4)

C(4)-Zr(1)-C(18)-N(3)	-29.5(5)
N(2)-Zr(1)-C(18)-C(19)	-148.2(4)
N(3)-Zr(1)-C(18)-C(19)	-90.7(6)
N(4)-Zr(1)-C(18)-C(19)	93.4(5)
N(1)-Zr(1)-C(18)-C(19)	-80.8(4)
Cl(1)-Zr(1)-C(18)-C(19)	12.2(4)
Cl(2)-Zr(1)-C(18)-C(19)	114.0(4)
C(4)-Zr(1)-C(18)-C(19)	-120.2(4)
N(4)-C(18)-C(19)-C(20)	95.4(4)
N(3)-C(18)-C(19)-C(20)	-75.9(4)
Zr(1)-C(18)-C(19)-C(20)	8.4(4)
N(4)-C(18)-C(19)-C(24)	-84.4(4)
N(3)-C(18)-C(19)-C(24)	104.3(4)
Zr(1)-C(18)-C(19)-C(24)	-171.4(4)
C(24)-C(19)-C(20)-C(21)	0.0
C(18)-C(19)-C(20)-C(21)	-179.8
C(19)-C(20)-C(21)-C(22)	0.0
C(20)-C(21)-C(22)-C(23)	0.0
C(21)-C(22)-C(23)-C(24)	0.0
C(25)-O(2)-C(24)-C(23)	5.8(8)
C(25)-O(2)-C(24)-C(19)	-174.7(6)
C(22)-C(23)-C(24)-O(2)	179.5(4)
C(22)-C(23)-C(24)-C(19)	0.0
C(20)-C(19)-C(24)-O(2)	-179.6(4)
C(18)-C(19)-C(24)-O(2)	0.3(4)
C(20)-C(19)-C(24)-C(23)	0.0
C(18)-C(19)-C(24)-C(23)	179.8

Symmetry transformations used to generate equivalent atoms:

5. Crystal data for complex 13

Table 1. Crystal data and structure refinement for complex 13.

Identification code	zrmmtxdim
Empirical formula	C28 H50 Cl2 N4 O2 Si4 Zr
Formula weight	749.20
Temperature	230.0(1) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 11.7290(4) A alpha = 90 deg. b = 17.8860(6) A beta = 92.6470(13) deg. c = 18.8940(7) A gamma = 90 deg.
Volume	3959.4(2) A^3
Z, Calculated density	4, 1.257 Mg/m^3
Absorption coefficient	0.562 mm^-1
F(000)	1568
Crystal size	0.27 x 0.24 x 0.18 mm
Theta range for data collection	1.57 to 23.00 deg.
Limiting indices	0<=h<=12, 0<=k<=19, -20<=l<=20

Reflections collected / unique	5500 / 5500 [R(int) = 0.0000]
Completeness to theta = 23.00	99.8 %
Absorption correction	None
Max. and min. transmission	0.9056 and 0.8631
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5500 / 0 / 370
Goodness-of-fit on F^2	1.043
Final R indices [I>2sigma(I)]	R1 = 0.0392, wR2 = 0.0819
R indices (all data)	R1 = 0.0620, wR2 = 0.0887
Largest diff. peak and hole	0.312 and -0.275 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for complex 13.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Zr(1)	6470(1)	-1345(1)	2500(1)	41(1)
Cl(1)	7844(1)	-2008(1)	3261(1)	80(1)
Cl(2)	5953(1)	-2359(1)	1704(1)	93(1)
Si(1)	5061(1)	-1903(1)	4140(1)	49(1)
Si(2)	4022(1)	-469(1)	1540(1)	55(1)
Si(3)	8539(1)	-1207(1)	1093(1)	49(1)
Si(4)	6995(1)	526(1)	3339(1)	48(1)
O(1)	982(2)	45(2)	3861(2)	69(1)
O(2)	8509(2)	1750(2)	501(2)	67(1)
N(1)	5192(2)	-1405(2)	3343(2)	41(1)
N(2)	4769(2)	-853(2)	2287(2)	44(1)
N(3)	7710(2)	-866(2)	1781(2)	42(1)
N(4)	7160(2)	-201(2)	2724(2)	42(1)
C(1)	6223(4)	-1587(3)	4759(2)	74(1)
C(2)	5170(5)	-2913(2)	3945(3)	89(2)
C(3)	3701(4)	-1735(3)	4587(2)	82(2)
C(4)	4399(3)	-1118(2)	2891(2)	39(1)
C(5)	3145(3)	-1110(2)	3033(2)	41(1)
C(6)	2456(3)	-1680(2)	2781(2)	54(1)
C(7)	1295(3)	-1669(2)	2899(2)	61(1)
C(8)	836(3)	-1089(2)	3261(2)	60(1)
C(9)	1514(3)	-511(2)	3513(2)	49(1)
C(10)	2683(3)	-516(2)	3402(2)	44(1)
C(11)	1629(4)	667(3)	4097(3)	89(2)
C(12)	2953(4)	239(3)	1778(2)	82(2)
C(13)	5138(4)	2(3)	1051(2)	67(1)
C(14)	3341(5)	-1226(3)	988(3)	99(2)
C(15)	7685(4)	-1139(3)	246(2)	94(2)
C(16)	9924(4)	-719(3)	1015(3)	83(2)
C(17)	8879(4)	-2197(2)	1312(3)	77(1)
C(18)	7785(3)	-227(2)	2149(2)	40(1)
C(19)	8514(3)	409(2)	1932(2)	40(1)
C(20)	9496(3)	604(2)	2327(2)	49(1)
C(21)	10166(3)	1182(2)	2100(2)	57(1)
C(22)	9874(3)	1578(2)	1494(2)	53(1)
C(23)	8887(3)	1393(2)	1108(2)	48(1)
C(24)	8212(3)	805(2)	1320(2)	44(1)
C(25)	9139(4)	2370(2)	262(2)	74(1)
C(26)	5534(4)	456(2)	3668(3)	72(1)
C(27)	7125(5)	1470(2)	2970(3)	93(2)
C(28)	8055(4)	370(3)	4088(2)	94(2)

Table 3. Bond lengths [A] and angles [deg] for complex 13.

Zr(1)-N(2)	2.200(3)
Zr(1)-N(3)	2.208(3)
Zr(1)-N(4)	2.234(3)
Zr(1)-N(1)	2.239(3)
Zr(1)-Cl(2)	2.4164(12)
Zr(1)-Cl(1)	2.4202(12)
Zr(1)-C(4)	2.602(3)
Zr(1)-C(18)	2.629(3)
Si(1)-N(1)	1.763(3)
Si(1)-C(1)	1.843(4)
Si(1)-C(2)	1.850(5)
Si(1)-C(3)	1.862(4)

Si(2)-N(2)	1.767(3)
Si(2)-C(13)	1.841(4)
Si(2)-C(12)	1.852(4)
Si(2)-C(14)	1.864(5)
Si(3)-N(3)	1.767(3)
Si(3)-C(15)	1.853(5)
Si(3)-C(16)	1.856(4)
Si(3)-C(17)	1.857(4)
Si(4)-N(4)	1.760(3)
Si(4)-C(27)	1.836(4)
Si(4)-C(26)	1.854(4)
Si(4)-C(28)	1.862(5)
O(1)-C(9)	1.361(5)
O(1)-C(11)	1.407(5)
O(2)-C(23)	1.369(4)
O(2)-C(25)	1.418(5)
N(1)-C(4)	1.336(4)
N(2)-C(4)	1.326(4)
N(3)-C(18)	1.338(4)
N(4)-C(18)	1.338(4)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(1)-H(1C)	0.9700
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(2)-H(2C)	0.9700
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(3)-H(3C)	0.9700
C(4)-C(5)	1.508(5)
C(5)-C(6)	1.372(5)
C(5)-C(10)	1.394(5)
C(6)-C(7)	1.390(5)
C(6)-H(6)	0.9400
C(7)-C(8)	1.367(6)
C(7)-H(7)	0.9400
C(8)-C(9)	1.377(5)
C(8)-H(8)	0.9400
C(9)-C(10)	1.396(5)
C(10)-H(10)	0.9400
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(11)-H(11C)	0.9700
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(12)-H(12C)	0.9700
C(13)-H(13A)	0.9700
C(13)-H(13B)	0.9700
C(13)-H(13C)	0.9700
C(14)-H(14A)	0.9700
C(14)-H(14B)	0.9700
C(14)-H(14C)	0.9700
C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700
C(15)-H(15C)	0.9700
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(16)-H(16C)	0.9700
C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700
C(17)-H(17C)	0.9700
C(18)-C(19)	1.493(5)
C(19)-C(20)	1.388(5)
C(19)-C(24)	1.388(5)
C(20)-C(21)	1.380(5)
C(20)-H(20)	0.9400
C(21)-C(22)	1.376(6)
C(21)-H(21)	0.9400

C(22)-C(23)	1.379(5)
C(22)-H(22)	0.9400
C(23)-C(24)	1.387(5)
C(24)-H(24)	0.9400
C(25)-H(25A)	0.9700
C(25)-H(25B)	0.9700
C(25)-H(25C)	0.9700
C(26)-H(26A)	0.9700
C(26)-H(26B)	0.9700
C(26)-H(26C)	0.9700
C(27)-H(27A)	0.9700
C(27)-H(27B)	0.9700
C(27)-H(27C)	0.9700
C(28)-H(28A)	0.9700
C(28)-H(28B)	0.9700
C(28)-H(28C)	0.9700

N(2)-Zr(1)-N(3)	110.47(11)
N(2)-Zr(1)-N(4)	89.23(11)
N(3)-Zr(1)-N(4)	61.16(10)
N(2)-Zr(1)-N(1)	61.20(10)
N(3)-Zr(1)-N(1)	159.69(10)
N(4)-Zr(1)-N(1)	99.16(10)
N(2)-Zr(1)-Cl(2)	89.23(8)
N(3)-Zr(1)-Cl(2)	93.50(8)
N(4)-Zr(1)-Cl(2)	152.08(8)
N(1)-Zr(1)-Cl(2)	104.44(8)
N(2)-Zr(1)-Cl(1)	151.39(8)
N(3)-Zr(1)-Cl(1)	96.68(8)
N(4)-Zr(1)-Cl(1)	96.41(8)
N(1)-Zr(1)-Cl(1)	90.20(8)
Cl(2)-Zr(1)-Cl(1)	98.19(5)
N(2)-Zr(1)-C(4)	30.62(10)
N(3)-Zr(1)-C(4)	139.80(11)
N(4)-Zr(1)-C(4)	98.01(10)
N(1)-Zr(1)-C(4)	30.89(10)
Cl(2)-Zr(1)-C(4)	94.73(8)
Cl(1)-Zr(1)-C(4)	120.84(9)
N(2)-Zr(1)-C(18)	100.80(11)
N(3)-Zr(1)-C(18)	30.57(10)
N(4)-Zr(1)-C(18)	30.59(10)
N(1)-Zr(1)-C(18)	129.53(11)
Cl(2)-Zr(1)-C(18)	123.14(8)
Cl(1)-Zr(1)-C(18)	98.11(8)
C(4)-Zr(1)-C(18)	121.30(10)
N(1)-Si(1)-C(1)	107.27(17)
N(1)-Si(1)-C(2)	108.23(19)
C(1)-Si(1)-C(2)	111.7(2)
N(1)-Si(1)-C(3)	114.61(18)
C(1)-Si(1)-C(3)	106.7(2)
C(2)-Si(1)-C(3)	108.5(2)
N(2)-Si(2)-C(13)	103.94(17)
N(2)-Si(2)-C(12)	112.83(18)
C(13)-Si(2)-C(12)	108.3(2)
N(2)-Si(2)-C(14)	110.4(2)
C(13)-Si(2)-C(14)	110.4(2)
C(12)-Si(2)-C(14)	110.8(3)
N(3)-Si(3)-C(15)	108.62(18)
N(3)-Si(3)-C(16)	114.20(17)
C(15)-Si(3)-C(16)	109.9(3)
N(3)-Si(3)-C(17)	106.54(17)
C(15)-Si(3)-C(17)	110.9(2)
C(16)-Si(3)-C(17)	106.6(2)
N(4)-Si(4)-C(27)	114.52(19)
N(4)-Si(4)-C(26)	107.68(17)
C(27)-Si(4)-C(26)	106.4(2)
N(4)-Si(4)-C(28)	107.55(19)
C(27)-Si(4)-C(28)	111.2(3)

C(26)-Si(4)-C(28)	109.3(2)
C(9)-O(1)-C(11)	118.5(3)
C(23)-O(2)-C(25)	118.6(3)
C(4)-N(1)-Si(1)	130.9(2)
C(4)-N(1)-Zr(1)	89.7(2)
Si(1)-N(1)-Zr(1)	136.04(15)
C(4)-N(2)-Si(2)	131.0(3)
C(4)-N(2)-Zr(1)	91.7(2)
Si(2)-N(2)-Zr(1)	135.56(16)
C(18)-N(3)-Si(3)	130.6(2)
C(18)-N(3)-Zr(1)	92.4(2)
Si(3)-N(3)-Zr(1)	136.00(15)
C(18)-N(4)-Si(4)	130.0(2)
C(18)-N(4)-Zr(1)	91.3(2)
Si(4)-N(4)-Zr(1)	138.66(16)
Si(1)-C(1)-H(1A)	109.5
Si(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
Si(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
Si(1)-C(2)-H(2A)	109.5
Si(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
Si(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
Si(1)-C(3)-H(3A)	109.5
Si(1)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
Si(1)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
N(2)-C(4)-N(1)	116.2(3)
N(2)-C(4)-C(5)	120.7(3)
N(1)-C(4)-C(5)	123.1(3)
N(2)-C(4)-Zr(1)	57.67(18)
N(1)-C(4)-Zr(1)	59.37(17)
C(5)-C(4)-Zr(1)	169.5(2)
C(6)-C(5)-C(10)	120.2(3)
C(6)-C(5)-C(4)	119.6(3)
C(10)-C(5)-C(4)	120.1(3)
C(5)-C(6)-C(7)	120.0(4)
C(5)-C(6)-H(6)	120.0
C(7)-C(6)-H(6)	120.0
C(8)-C(7)-C(6)	120.1(4)
C(8)-C(7)-H(7)	120.0
C(6)-C(7)-H(7)	120.0
C(7)-C(8)-C(9)	120.6(4)
C(7)-C(8)-H(8)	119.7
C(9)-C(8)-H(8)	119.7
O(1)-C(9)-C(8)	116.5(4)
O(1)-C(9)-C(10)	123.6(4)
C(8)-C(9)-C(10)	119.9(4)
C(5)-C(10)-C(9)	119.1(4)
C(5)-C(10)-H(10)	120.4
C(9)-C(10)-H(10)	120.4
O(1)-C(11)-H(11A)	109.5
O(1)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
O(1)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
Si(2)-C(12)-H(12A)	109.5
Si(2)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
Si(2)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5

H(12B)-C(12)-H(12C)	109.5
Si(2)-C(13)-H(13A)	109.5
Si(2)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
Si(2)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
Si(2)-C(14)-H(14A)	109.5
Si(2)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
Si(2)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
Si(3)-C(15)-H(15A)	109.5
Si(3)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
Si(3)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
Si(3)-C(16)-H(16A)	109.5
Si(3)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
Si(3)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
Si(3)-C(17)-H(17A)	109.5
Si(3)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
Si(3)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
N(4)-C(18)-N(3)	115.2(3)
N(4)-C(18)-C(19)	122.6(3)
N(3)-C(18)-C(19)	122.2(3)
N(4)-C(18)-Zr(1)	58.15(17)
N(3)-C(18)-Zr(1)	57.07(17)
C(19)-C(18)-Zr(1)	178.6(3)
C(20)-C(19)-C(24)	119.7(3)
C(20)-C(19)-C(18)	121.0(3)
C(24)-C(19)-C(18)	119.3(3)
C(21)-C(20)-C(19)	119.4(4)
C(21)-C(20)-H(20)	120.3
C(19)-C(20)-H(20)	120.3
C(22)-C(21)-C(20)	121.4(4)
C(22)-C(21)-H(21)	119.3
C(20)-C(21)-H(21)	119.3
C(21)-C(22)-C(23)	119.2(4)
C(21)-C(22)-H(22)	120.4
C(23)-C(22)-H(22)	120.4
O(2)-C(23)-C(22)	124.2(3)
O(2)-C(23)-C(24)	115.3(3)
C(22)-C(23)-C(24)	120.4(4)
C(23)-C(24)-C(19)	120.0(3)
C(23)-C(24)-H(24)	120.0
C(19)-C(24)-H(24)	120.0
O(2)-C(25)-H(25A)	109.5
O(2)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
O(2)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
Si(4)-C(26)-H(26A)	109.5
Si(4)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
Si(4)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
Si(4)-C(27)-H(27A)	109.5

Si(4)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
Si(4)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
Si(4)-C(28)-H(28A)	109.5
Si(4)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
Si(4)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for complex 13.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Zr(1)	37(1)	38(1)	50(1)	-1(1)	8(1)	2(1)
Cl(1)	57(1)	90(1)	95(1)	37(1)	17(1)	30(1)
Cl(2)	80(1)	83(1)	117(1)	-54(1)	28(1)	-21(1)
Si(1)	48(1)	51(1)	47(1)	6(1)	2(1)	-1(1)
Si(2)	45(1)	69(1)	50(1)	10(1)	-3(1)	4(1)
Si(3)	49(1)	50(1)	48(1)	-7(1)	12(1)	1(1)
Si(4)	47(1)	43(1)	54(1)	-10(1)	10(1)	-1(1)
O(1)	44(2)	84(2)	79(2)	-18(2)	7(2)	13(2)
O(2)	74(2)	65(2)	63(2)	16(2)	4(2)	-14(2)
N(1)	37(2)	43(2)	44(2)	4(1)	1(1)	5(1)
N(2)	40(2)	48(2)	44(2)	5(1)	1(1)	2(1)
N(3)	43(2)	39(2)	43(2)	-4(1)	8(1)	0(1)
N(4)	42(2)	40(2)	44(2)	-4(1)	9(2)	3(1)
C(1)	71(3)	96(4)	55(3)	11(2)	-5(2)	-7(3)
C(2)	130(5)	54(3)	84(4)	12(3)	9(3)	-6(3)
C(3)	63(3)	121(4)	63(3)	26(3)	18(2)	10(3)
C(4)	39(2)	31(2)	48(2)	-6(2)	2(2)	-1(2)
C(5)	35(2)	42(2)	47(2)	5(2)	1(2)	0(2)
C(6)	52(3)	41(2)	68(3)	-3(2)	3(2)	-2(2)
C(7)	49(3)	58(3)	76(3)	6(2)	-3(2)	-20(2)
C(8)	39(2)	68(3)	72(3)	14(2)	0(2)	-6(2)
C(9)	38(2)	59(3)	51(2)	1(2)	1(2)	5(2)
C(10)	35(2)	45(2)	52(2)	-1(2)	-2(2)	-2(2)
C(11)	79(4)	90(4)	100(4)	-38(3)	7(3)	20(3)
C(12)	62(3)	113(4)	72(3)	31(3)	8(2)	37(3)
C(13)	61(3)	82(3)	58(3)	19(2)	8(2)	17(2)
C(14)	108(4)	109(4)	76(4)	-4(3)	-32(3)	-18(4)
C(15)	96(4)	137(5)	49(3)	-27(3)	-2(3)	37(3)
C(16)	66(3)	80(3)	107(4)	-27(3)	45(3)	-6(3)
C(17)	84(3)	63(3)	88(4)	-4(3)	40(3)	15(3)
C(18)	34(2)	40(2)	46(2)	0(2)	0(2)	1(2)
C(19)	38(2)	38(2)	44(2)	-6(2)	6(2)	-1(2)
C(20)	45(2)	48(2)	55(2)	2(2)	-2(2)	1(2)
C(21)	38(2)	59(3)	73(3)	-12(2)	-3(2)	-5(2)
C(22)	45(2)	46(2)	71(3)	-7(2)	17(2)	-9(2)
C(23)	50(2)	47(2)	47(2)	0(2)	8(2)	-1(2)
C(24)	40(2)	46(2)	46(2)	-4(2)	3(2)	-5(2)
C(25)	90(4)	61(3)	73(3)	10(2)	34(3)	-4(3)
C(26)	66(3)	64(3)	87(3)	-29(2)	28(3)	-3(2)
C(27)	130(5)	44(3)	110(4)	-8(3)	54(4)	5(3)
C(28)	71(3)	146(5)	66(3)	-35(3)	-2(3)	25(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic

displacement parameters (A^2 x 10^3) for complex 13.

	x	y	z	U(eq)
H(1A)	6140	-1056	4849	111
H(1B)	6952	-1679	4553	111
H(1C)	6189	-1860	5202	111
H(2A)	4545	-3060	3621	134
H(2B)	5133	-3195	4382	134
H(2C)	5891	-3013	3731	134
H(3A)	3063	-1891	4278	122
H(3B)	3630	-1207	4693	122
H(3C)	3703	-2020	5024	122
H(6)	2770	-2078	2530	64
H(7)	824	-2061	2728	74
H(8)	51	-1085	3339	72
H(10)	3152	-124	3573	53
H(11A)	1140	1016	4334	134
H(11B)	1954	911	3695	134
H(11C)	2237	502	4426	134
H(12A)	2355	1	2034	123
H(12B)	2625	468	1350	123
H(12C)	3321	620	2074	123
H(13A)	5706	-362	921	100
H(13B)	5498	384	1348	100
H(13C)	4798	230	626	100
H(14A)	2754	-1468	1252	149
H(14B)	3913	-1591	870	149
H(14C)	3001	-1012	556	149
H(15A)	6965	-1398	289	141
H(15B)	8103	-1367	-130	141
H(15C)	7540	-618	134	141
H(16A)	10367	-757	1460	125
H(16B)	9787	-196	904	125
H(16C)	10342	-948	641	125
H(17A)	9328	-2218	1756	116
H(17B)	9311	-2414	938	116
H(17C)	8176	-2474	1357	116
H(20)	9702	344	2746	59
H(21)	10837	1309	2365	68
H(22)	10342	1969	1344	64
H(24)	7549	675	1048	53
H(25A)	8778	2562	-173	110
H(25B)	9912	2213	174	110
H(25C)	9159	2758	620	110
H(26A)	5427	-35	3871	108
H(26B)	4980	532	3277	108
H(26C)	5432	835	4026	108
H(27A)	7880	1534	2791	140
H(27B)	7006	1837	3338	140
H(27C)	6555	1538	2587	140
H(28A)	7965	-131	4274	142
H(28B)	7932	732	4459	142
H(28C)	8820	428	3922	142

Table 6. Torsion angles [deg] for complex 13.

C(1)-Si(1)-N(1)-C(4)	-141.7(3)
C(2)-Si(1)-N(1)-C(4)	97.6(4)
C(3)-Si(1)-N(1)-C(4)	-23.5(4)
C(1)-Si(1)-N(1)-Zr(1)	65.3(3)
C(2)-Si(1)-N(1)-Zr(1)	-55.4(3)
C(3)-Si(1)-N(1)-Zr(1)	-176.5(2)
N(2)-Zr(1)-N(1)-C(4)	6.28(18)
N(3)-Zr(1)-N(1)-C(4)	76.7(4)
N(4)-Zr(1)-N(1)-C(4)	90.3(2)
Cl(2)-Zr(1)-N(1)-C(4)	-74.66(19)
Cl(1)-Zr(1)-N(1)-C(4)	-173.17(19)
C(18)-Zr(1)-N(1)-C(4)	86.1(2)
N(2)-Zr(1)-N(1)-Si(1)	166.2(3)
N(3)-Zr(1)-N(1)-Si(1)	-123.4(3)
N(4)-Zr(1)-N(1)-Si(1)	-109.7(2)
Cl(2)-Zr(1)-N(1)-Si(1)	85.3(2)
Cl(1)-Zr(1)-N(1)-Si(1)	-13.2(2)
C(4)-Zr(1)-N(1)-Si(1)	160.0(4)
C(18)-Zr(1)-N(1)-Si(1)	-113.9(2)
C(13)-Si(2)-N(2)-C(4)	164.5(3)
C(12)-Si(2)-N(2)-C(4)	47.4(4)
C(14)-Si(2)-N(2)-C(4)	-77.2(4)
C(13)-Si(2)-N(2)-Zr(1)	-34.9(3)
C(12)-Si(2)-N(2)-Zr(1)	-152.0(3)
C(14)-Si(2)-N(2)-Zr(1)	83.4(3)
N(3)-Zr(1)-N(2)-C(4)	-165.90(19)
N(4)-Zr(1)-N(2)-C(4)	-107.2(2)
N(1)-Zr(1)-N(2)-C(4)	-6.34(19)
Cl(2)-Zr(1)-N(2)-C(4)	100.65(19)
Cl(1)-Zr(1)-N(2)-C(4)	-5.2(3)
C(18)-Zr(1)-N(2)-C(4)	-135.7(2)
N(3)-Zr(1)-N(2)-Si(2)	28.6(3)
N(4)-Zr(1)-N(2)-Si(2)	87.3(2)
N(1)-Zr(1)-N(2)-Si(2)	-171.8(3)
Cl(2)-Zr(1)-N(2)-Si(2)	-64.9(2)
Cl(1)-Zr(1)-N(2)-Si(2)	-170.69(12)
C(4)-Zr(1)-N(2)-Si(2)	-165.5(4)
C(18)-Zr(1)-N(2)-Si(2)	58.8(2)
C(15)-Si(3)-N(3)-C(18)	-106.5(4)
C(16)-Si(3)-N(3)-C(18)	16.5(4)
C(17)-Si(3)-N(3)-C(18)	134.0(3)
C(15)-Si(3)-N(3)-Zr(1)	88.5(3)
C(16)-Si(3)-N(3)-Zr(1)	-148.5(3)
C(17)-Si(3)-N(3)-Zr(1)	-31.0(3)
N(2)-Zr(1)-N(3)-C(18)	76.2(2)
N(4)-Zr(1)-N(3)-C(18)	-0.98(19)
N(1)-Zr(1)-N(3)-C(18)	14.4(4)
Cl(2)-Zr(1)-N(3)-C(18)	166.7(2)
Cl(1)-Zr(1)-N(3)-C(18)	-94.6(2)
C(4)-Zr(1)-N(3)-C(18)	65.1(3)
N(2)-Zr(1)-N(3)-Si(3)	-115.2(2)
N(4)-Zr(1)-N(3)-Si(3)	167.7(3)
N(1)-Zr(1)-N(3)-Si(3)	-176.9(2)
Cl(2)-Zr(1)-N(3)-Si(3)	-24.7(2)
Cl(1)-Zr(1)-N(3)-Si(3)	74.0(2)
C(4)-Zr(1)-N(3)-Si(3)	-126.2(2)
C(18)-Zr(1)-N(3)-Si(3)	168.7(4)
C(27)-Si(4)-N(4)-C(18)	30.5(4)
C(26)-Si(4)-N(4)-C(18)	148.6(3)
C(28)-Si(4)-N(4)-C(18)	-93.7(4)
C(27)-Si(4)-N(4)-Zr(1)	-145.5(3)
C(26)-Si(4)-N(4)-Zr(1)	-27.3(3)
C(28)-Si(4)-N(4)-Zr(1)	90.3(3)
N(2)-Zr(1)-N(4)-C(18)	-113.0(2)
N(3)-Zr(1)-N(4)-C(18)	0.98(19)

N(1)-Zr(1)-N(4)-C(18)	-173.67(19)
Cl(2)-Zr(1)-N(4)-C(18)	-26.1(3)
Cl(1)-Zr(1)-N(4)-C(18)	95.09(19)
C(4)-Zr(1)-N(4)-C(18)	-142.4(2)
N(2)-Zr(1)-N(4)-Si(4)	63.9(2)
N(3)-Zr(1)-N(4)-Si(4)	177.9(3)
N(1)-Zr(1)-N(4)-Si(4)	3.2(3)
Cl(2)-Zr(1)-N(4)-Si(4)	150.80(16)
Cl(1)-Zr(1)-N(4)-Si(4)	-88.0(2)
C(4)-Zr(1)-N(4)-Si(4)	34.5(3)
C(18)-Zr(1)-N(4)-Si(4)	176.9(4)
Si(2)-N(2)-C(4)-N(1)	177.0(2)
Zr(1)-N(2)-C(4)-N(1)	10.4(3)
Si(2)-N(2)-C(4)-C(5)	-1.3(5)
Zr(1)-N(2)-C(4)-C(5)	-167.8(3)
Si(2)-N(2)-C(4)-Zr(1)	166.6(3)
Si(1)-N(1)-C(4)-N(2)	-171.9(2)
Zr(1)-N(1)-C(4)-N(2)	-10.2(3)
Si(1)-N(1)-C(4)-C(5)	6.3(5)
Zr(1)-N(1)-C(4)-C(5)	168.0(3)
Si(1)-N(1)-C(4)-Zr(1)	-161.6(3)
N(3)-Zr(1)-C(4)-N(2)	20.7(3)
N(4)-Zr(1)-C(4)-N(2)	74.7(2)
N(1)-Zr(1)-C(4)-N(2)	169.1(3)
Cl(2)-Zr(1)-C(4)-N(2)	-80.4(2)
Cl(1)-Zr(1)-C(4)-N(2)	177.11(17)
C(18)-Zr(1)-C(4)-N(2)	53.4(2)
N(2)-Zr(1)-C(4)-N(1)	-169.1(3)
N(3)-Zr(1)-C(4)-N(1)	-148.44(19)
N(4)-Zr(1)-C(4)-N(1)	-94.5(2)
Cl(2)-Zr(1)-C(4)-N(1)	110.44(19)
Cl(1)-Zr(1)-C(4)-N(1)	8.0(2)
C(18)-Zr(1)-C(4)-N(1)	-115.8(2)
N(2)-Zr(1)-C(4)-C(5)	84.2(14)
N(3)-Zr(1)-C(4)-C(5)	104.9(14)
N(4)-Zr(1)-C(4)-C(5)	158.8(14)
N(1)-Zr(1)-C(4)-C(5)	-106.7(15)
Cl(2)-Zr(1)-C(4)-C(5)	3.8(14)
Cl(1)-Zr(1)-C(4)-C(5)	-98.7(14)
C(18)-Zr(1)-C(4)-C(5)	137.6(14)
N(2)-C(4)-C(5)-C(6)	84.4(4)
N(1)-C(4)-C(5)-C(6)	-93.7(4)
Zr(1)-C(4)-C(5)-C(6)	6.6(16)
N(2)-C(4)-C(5)-C(10)	-94.0(4)
N(1)-C(4)-C(5)-C(10)	87.9(4)
Zr(1)-C(4)-C(5)-C(10)	-171.8(12)
C(10)-C(5)-C(6)-C(7)	-0.4(6)
C(4)-C(5)-C(6)-C(7)	-178.8(4)
C(5)-C(6)-C(7)-C(8)	0.3(6)
C(6)-C(7)-C(8)-C(9)	0.1(6)
C(11)-O(1)-C(9)-C(8)	-176.9(4)
C(11)-O(1)-C(9)-C(10)	2.8(6)
C(7)-C(8)-C(9)-O(1)	179.4(4)
C(7)-C(8)-C(9)-C(10)	-0.3(6)
C(6)-C(5)-C(10)-C(9)	0.1(5)
C(4)-C(5)-C(10)-C(9)	178.5(3)
O(1)-C(9)-C(10)-C(5)	-179.4(3)
C(8)-C(9)-C(10)-C(5)	0.2(6)
Si(4)-N(4)-C(18)-N(3)	-178.9(3)
Zr(1)-N(4)-C(18)-N(3)	-1.6(3)
Si(4)-N(4)-C(18)-C(19)	1.2(5)
Zr(1)-N(4)-C(18)-C(19)	178.5(3)
Si(4)-N(4)-C(18)-Zr(1)	-177.3(3)
Si(3)-N(3)-C(18)-N(4)	-168.0(2)
Zr(1)-N(3)-C(18)-N(4)	1.6(3)
Si(3)-N(3)-C(18)-C(19)	11.9(5)
Zr(1)-N(3)-C(18)-C(19)	-178.5(3)
Si(3)-N(3)-C(18)-Zr(1)	-169.6(3)

N(2)-Zr(1)-C(18)-N(4)	69.5(2)
N(3)-Zr(1)-C(18)-N(4)	-178.3(3)
N(1)-Zr(1)-C(18)-N(4)	8.1(2)
Cl(2)-Zr(1)-C(18)-N(4)	165.75(17)
Cl(1)-Zr(1)-C(18)-N(4)	-88.90(19)
C(4)-Zr(1)-C(18)-N(4)	44.9(2)
N(2)-Zr(1)-C(18)-N(3)	-112.2(2)
N(4)-Zr(1)-C(18)-N(3)	178.3(3)
N(1)-Zr(1)-C(18)-N(3)	-173.57(19)
Cl(2)-Zr(1)-C(18)-N(3)	-15.9(2)
Cl(1)-Zr(1)-C(18)-N(3)	89.4(2)
C(4)-Zr(1)-C(18)-N(3)	-136.7(2)
N(4)-C(18)-C(19)-C(20)	69.6(5)
N(3)-C(18)-C(19)-C(20)	-110.3(4)
N(4)-C(18)-C(19)-C(24)	-111.2(4)
N(3)-C(18)-C(19)-C(24)	68.9(5)
C(24)-C(19)-C(20)-C(21)	-0.9(5)
C(18)-C(19)-C(20)-C(21)	178.3(3)
C(19)-C(20)-C(21)-C(22)	0.9(6)
C(20)-C(21)-C(22)-C(23)	0.4(6)
C(25)-O(2)-C(23)-C(22)	-2.7(6)
C(25)-O(2)-C(23)-C(24)	178.4(3)
C(21)-C(22)-C(23)-O(2)	179.6(4)
C(21)-C(22)-C(23)-C(24)	-1.6(6)
O(2)-C(23)-C(24)-C(19)	-179.6(3)
C(22)-C(23)-C(24)-C(19)	1.5(5)
C(20)-C(19)-C(24)-C(23)	-0.3(5)
C(18)-C(19)-C(24)-C(23)	-179.4(3)

Symmetry transformations used to generate equivalent atoms: