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Supporting Information

Supplementary Tables for:

Ti-Sn, Zr-Sn and Hf-Sn Heterodimetallic Complexes: Stabilizing Unsupported Group 4-Group 14 Metal-Metal Bonds

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Tables S1-S6: Crystallographic data, atomic coordinates, bond lengths, bond angles, anisotropic displacement parameters, hydrogen coordinates and isotropic displacement parameters and torsion angles for structure 1 (**1**).

Tables S7-S12: Crystallographic data, atomic coordinates, bond lengths, bond angles, anisotropic displacement parameters, hydrogen coordinates and isotropic displacement parameters and torsion angles for structure 2 (**2**).

Figure S1: ORTEP drawing of structure 1.

Figure S2: ORTEP drawing of Structure 2.

Table S1. Crystal data and structure refinement for structure 1.

Identification code	Structure 1
Empirical formula	C44 H52 Cl D6 N3 Si4 Sn Zr
Formula weight	992.69
Temperature	150(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P 21 21 21
Unit cell dimensions	a = 12.32520(10) A alpha = 90 deg.
	b = 17.58540(10) A beta = 90 deg.
	c = 21.0750(2) A gamma = 90 deg.
Volume	4567.87(6) A^3
Z, Calculated density	4, 1.443 Mg/m^3
Absorption coefficient	0.972 mm^-1
F(000)	2024
Crystal size	0.40 x 0.30 x 0.30 mm
Theta range for data collection	3.61 to 27.48 deg.
Limiting indices	-16<=h<=16, -22<=k<=22, -27<=l<=27
Reflections collected / unique	55527 / 10432 [R(int) = 0.0282]
Completeness to theta = 27.48	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.2685 and 0.2249
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10432 / 0 / 498
Goodness-of-fit on F^2	1.075
Final R indices [I>2sigma(I)]	R1 = 0.0174, wR2 = 0.0430
R indices (all data)	R1 = 0.0185, wR2 = 0.0436
Absolute structure parameter	0.459(8)
Largest diff. peak and hole	0.456 and -0.297 e.A^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for structure 1. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Sn(1)	3481(1)	10037(1)	4835(1)	14(1)
Zr(1)	5775(1)	10036(1)	4329(1)	17(1)
Cl(1)	5387(1)	10042(1)	3211(1)	28(1)
Si(1)	1462(1)	8853(1)	5274(1)	17(1)
Si(2)	791(1)	10061(1)	5514(1)	17(1)
Si(3)	2132(1)	10598(1)	6154(1)	20(1)
Si(4)	971(1)	10736(1)	4562(1)	19(1)
N(1)	2582(1)	9026(1)	4787(1)	18(1)
N(2)	3324(1)	10293(1)	5797(1)	21(1)
N(3)	2368(1)	10830(1)	4484(1)	20(1)
C(1)	3803(2)	6904(1)	2823(1)	34(1)
C(2)	3499(2)	7467(1)	3336(1)	23(1)
C(3)	3428(2)	8242(1)	3217(1)	22(1)
C(4)	3105(2)	8750(1)	3686(1)	21(1)
C(5)	2875(1)	8508(1)	4303(1)	18(1)
C(6)	2949(2)	7726(1)	4419(1)	22(1)
C(7)	3241(2)	7221(1)	3945(1)	23(1)
C(8)	1804(2)	8308(1)	6012(1)	27(1)
C(9)	401(2)	8310(1)	4823(1)	25(1)
C(10)	-613(1)	10048(1)	5891(1)	29(1)
C(11)	2070(2)	10211(1)	6985(1)	31(1)
C(12)	2003(2)	11661(1)	6205(1)	29(1)
C(13)	4253(1)	10202(1)	6193(1)	21(1)
C(14)	4671(2)	9487(1)	6331(1)	27(1)

C(15)	5539(2)	9400(1)	6746(1)	32(1)
C(16)	6021(1)	10024(2)	7035(1)	31(1)
C(17)	6946(2)	9933(2)	7501(1)	45(1)
C(18)	5614(2)	10741(1)	6891(1)	33(1)
C(19)	4745(2)	10826(1)	6476(1)	30(1)
C(20)	351(2)	10248(1)	3855(1)	30(1)
C(21)	306(2)	11696(1)	4637(1)	28(1)
C(22)	2779(2)	11395(1)	4062(1)	18(1)
C(23)	3104(2)	11220(1)	3448(1)	22(1)
C(24)	3482(2)	11779(1)	3036(1)	24(1)
C(25)	3536(2)	12539(1)	3220(1)	26(1)
C(26)	3220(2)	12712(1)	3836(1)	30(1)
C(27)	2862(2)	12157(1)	4254(1)	26(1)
C(28)	6521(2)	9114(1)	5112(1)	31(1)
C(29)	5574(2)	8765(1)	4868(1)	29(1)
C(30)	5746(2)	8609(1)	4220(1)	29(1)
C(31)	6803(2)	8845(1)	4065(1)	29(1)
C(32)	7281(2)	9161(1)	4614(1)	30(1)
C(33)	6421(2)	10957(1)	5143(1)	32(1)
C(34)	7213(2)	10937(1)	4659(1)	36(1)
C(35)	6761(2)	11252(1)	4111(1)	36(1)
C(36)	5684(2)	11465(1)	4245(1)	31(1)
C(37)	5480(2)	11289(1)	4884(1)	30(1)
C(38)	3885(2)	13150(1)	2763(1)	41(1)
C(39)	3993(2)	2396(1)	7547(1)	33(1)
C(40)	5717(2)	2868(1)	7209(1)	32(1)
C(41)	4626(2)	2733(1)	7088(1)	31(1)
C(42)	6161(2)	2672(1)	7788(1)	34(1)
C(43)	4431(2)	2196(1)	8125(1)	38(1)
C(44)	5519(2)	2337(1)	8248(1)	36(1)

Table S3. Bond lengths [A] and angles [deg] for structure 1.

Sn(1)-N(2)	2.0846(14)
Sn(1)-N(3)	2.0913(14)
Sn(1)-N(1)	2.0973(14)
Sn(1)-Zr(1)	3.02313(17)
Zr(1)-Cl(1)	2.4043(4)
Zr(1)-C(34)	2.476(2)
Zr(1)-C(32)	2.484(2)
Zr(1)-C(33)	2.489(2)
Zr(1)-C(28)	2.4895(19)
Zr(1)-C(35)	2.501(2)
Zr(1)-C(31)	2.510(2)
Zr(1)-C(29)	2.5206(19)
Zr(1)-C(30)	2.5209(19)
Zr(1)-C(36)	2.5216(19)
Zr(1)-C(37)	2.522(2)
Si(1)-N(1)	1.7469(15)
Si(1)-C(8)	1.875(2)
Si(1)-C(9)	1.877(2)
Si(1)-Si(2)	2.3342(7)
Si(2)-C(10)	1.9038(17)
Si(2)-Si(3)	2.3331(7)
Si(2)-Si(4)	2.3413(6)
Si(3)-N(2)	1.7350(16)
Si(3)-C(12)	1.880(2)
Si(3)-C(11)	1.8814(19)
Si(4)-N(3)	1.7381(15)
Si(4)-C(20)	1.882(2)

Si(4)-C(21)	1.883(2)
N(1)-C(5)	1.416(2)
N(2)-C(13)	1.427(2)
N(3)-C(22)	1.426(2)
C(1)-C(2)	1.513(3)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-C(3)	1.389(3)
C(2)-C(7)	1.392(3)
C(3)-C(4)	1.390(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.396(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.399(2)
C(6)-C(7)	1.385(3)
C(6)-H(6)	0.9500
C(7)-H(7)	0.9500
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.389(3)
C(13)-C(19)	1.389(3)
C(14)-C(15)	1.390(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.390(3)
C(15)-H(15)	0.9500
C(16)-C(18)	1.390(3)
C(16)-C(17)	1.512(2)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-C(19)	1.391(3)
C(18)-H(18)	0.9500
C(19)-H(19)	0.9500
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(23)	1.390(3)
C(22)-C(27)	1.404(3)
C(23)-C(24)	1.391(3)
C(23)-H(23)	0.9500
C(24)-C(25)	1.393(3)
C(24)-H(24)	0.9500
C(25)-C(26)	1.390(3)
C(25)-C(38)	1.504(3)
C(26)-C(27)	1.387(3)
C(26)-H(26)	0.9500
C(27)-H(27)	0.9500
C(28)-C(32)	1.409(3)

C(28)-C(29)	1.416(3)
C(28)-H(28)	0.9500
C(29)-C(30)	1.407(4)
C(29)-H(29)	0.9500
C(30)-C(31)	1.406(3)
C(30)-H(30)	0.9500
C(31)-C(32)	1.412(3)
C(31)-H(31)	0.9500
C(32)-H(32)	0.9500
C(33)-C(37)	1.409(3)
C(33)-C(34)	1.412(3)
C(33)-H(33)	0.9500
C(34)-C(35)	1.397(4)
C(34)-H(34)	0.9500
C(35)-C(36)	1.408(3)
C(35)-H(35)	0.9500
C(36)-C(37)	1.405(4)
C(36)-H(36)	0.9500
C(37)-H(37)	0.9500
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-C(41)	1.377(3)
C(39)-C(43)	1.378(3)
C(39)-D(39)	0.9500
C(40)-C(42)	1.382(3)
C(40)-C(41)	1.389(3)
C(40)-D(40)	0.9500
C(41)-D(41)	0.9500
C(42)-C(44)	1.383(3)
C(42)-D(42)	0.9500
C(43)-C(44)	1.389(3)
C(43)-D(43)	0.9500
C(44)-D(44)	0.9500

N(2)-Sn(1)-N(3)	98.00(6)
N(2)-Sn(1)-N(1)	100.43(6)
N(3)-Sn(1)-N(1)	101.65(6)
N(2)-Sn(1)-Zr(1)	115.48(4)
N(3)-Sn(1)-Zr(1)	119.25(4)
N(1)-Sn(1)-Zr(1)	118.48(4)
Cl(1)-Zr(1)-C(34)	114.52(6)
Cl(1)-Zr(1)-C(32)	112.85(6)
C(34)-Zr(1)-C(32)	78.10(6)
Cl(1)-Zr(1)-C(33)	137.41(6)
C(34)-Zr(1)-C(33)	33.04(8)
C(32)-Zr(1)-C(33)	89.84(7)
Cl(1)-Zr(1)-C(28)	136.55(5)
C(34)-Zr(1)-C(28)	88.07(8)
C(32)-Zr(1)-C(28)	32.91(7)
C(33)-Zr(1)-C(28)	81.29(6)
Cl(1)-Zr(1)-C(35)	85.02(6)
C(34)-Zr(1)-C(35)	32.59(8)
C(32)-Zr(1)-C(35)	102.19(8)
C(33)-Zr(1)-C(35)	54.23(8)
C(28)-Zr(1)-C(35)	119.95(8)
Cl(1)-Zr(1)-C(31)	83.50(5)
C(34)-Zr(1)-C(31)	103.58(7)
C(32)-Zr(1)-C(31)	32.85(7)
C(33)-Zr(1)-C(31)	122.27(7)
C(28)-Zr(1)-C(31)	54.35(7)
C(35)-Zr(1)-C(31)	115.31(7)
Cl(1)-Zr(1)-C(29)	115.20(6)
C(34)-Zr(1)-C(29)	120.76(8)
C(32)-Zr(1)-C(29)	54.21(7)

C(33)-Zr(1)-C(29)	107.33(8)
C(28)-Zr(1)-C(29)	32.83(7)
C(35)-Zr(1)-C(29)	152.74(8)
C(31)-Zr(1)-C(29)	53.80(7)
Cl(1)-Zr(1)-C(30)	85.00(6)
C(34)-Zr(1)-C(30)	132.27(7)
C(32)-Zr(1)-C(30)	54.25(7)
C(33)-Zr(1)-C(30)	135.59(8)
C(28)-Zr(1)-C(30)	54.31(7)
C(35)-Zr(1)-C(30)	147.30(8)
C(31)-Zr(1)-C(30)	32.47(7)
C(29)-Zr(1)-C(30)	32.42(8)
Cl(1)-Zr(1)-C(36)	85.30(6)
C(34)-Zr(1)-C(36)	54.15(8)
C(32)-Zr(1)-C(36)	131.89(7)
C(33)-Zr(1)-C(36)	54.18(8)
C(28)-Zr(1)-C(36)	135.41(8)
C(35)-Zr(1)-C(36)	32.55(8)
C(31)-Zr(1)-C(36)	146.99(8)
C(29)-Zr(1)-C(36)	155.69(8)
C(30)-Zr(1)-C(36)	170.19(6)
Cl(1)-Zr(1)-C(37)	115.00(6)
C(34)-Zr(1)-C(37)	54.13(7)
C(32)-Zr(1)-C(37)	122.47(7)
C(33)-Zr(1)-C(37)	32.65(7)
C(28)-Zr(1)-C(37)	108.34(8)
C(35)-Zr(1)-C(37)	53.73(8)
C(31)-Zr(1)-C(37)	154.81(7)
C(29)-Zr(1)-C(37)	123.49(6)
C(30)-Zr(1)-C(37)	155.51(8)
C(36)-Zr(1)-C(37)	32.36(8)
Cl(1)-Zr(1)-Sn(1)	99.197(11)
C(34)-Zr(1)-Sn(1)	124.75(6)
C(32)-Zr(1)-Sn(1)	127.85(5)
C(33)-Zr(1)-Sn(1)	93.19(5)
C(28)-Zr(1)-Sn(1)	96.40(5)
C(35)-Zr(1)-Sn(1)	121.25(6)
C(31)-Zr(1)-Sn(1)	123.42(5)
C(29)-Zr(1)-Sn(1)	75.46(5)
C(30)-Zr(1)-Sn(1)	91.08(5)
C(36)-Zr(1)-Sn(1)	88.99(5)
C(37)-Zr(1)-Sn(1)	72.58(5)
N(1)-Si(1)-C(8)	113.49(9)
N(1)-Si(1)-C(9)	109.95(8)
C(8)-Si(1)-C(9)	108.45(9)
N(1)-Si(1)-Si(2)	104.38(5)
C(8)-Si(1)-Si(2)	111.45(7)
C(9)-Si(1)-Si(2)	109.02(6)
C(10)-Si(2)-Si(3)	114.02(7)
C(10)-Si(2)-Si(1)	113.68(8)
Si(3)-Si(2)-Si(1)	104.01(2)
C(10)-Si(2)-Si(4)	116.73(7)
Si(3)-Si(2)-Si(4)	102.86(2)
Si(1)-Si(2)-Si(4)	104.06(2)
N(2)-Si(3)-C(12)	113.81(9)
N(2)-Si(3)-C(11)	109.08(8)
C(12)-Si(3)-C(11)	107.57(9)
N(2)-Si(3)-Si(2)	102.96(5)
C(12)-Si(3)-Si(2)	112.09(7)
C(11)-Si(3)-Si(2)	111.32(7)
N(3)-Si(4)-C(20)	111.76(9)
N(3)-Si(4)-C(21)	110.70(8)
C(20)-Si(4)-C(21)	107.35(10)
N(3)-Si(4)-Si(2)	102.92(5)
C(20)-Si(4)-Si(2)	114.11(7)

C(21)-Si(4)-Si(2)	110.00(7)
C(5)-N(1)-Si(1)	120.91(11)
C(5)-N(1)-Sn(1)	116.44(11)
Si(1)-N(1)-Sn(1)	122.47(8)
C(13)-N(2)-Si(3)	117.42(11)
C(13)-N(2)-Sn(1)	118.05(11)
Si(3)-N(2)-Sn(1)	124.52(8)
C(22)-N(3)-Si(4)	118.53(12)
C(22)-N(3)-Sn(1)	116.90(11)
Si(4)-N(3)-Sn(1)	123.54(8)
C(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(3)-C(2)-C(7)	117.15(17)
C(3)-C(2)-C(1)	122.00(19)
C(7)-C(2)-C(1)	120.81(18)
C(2)-C(3)-C(4)	121.40(17)
C(2)-C(3)-H(3)	119.3
C(4)-C(3)-H(3)	119.3
C(3)-C(4)-C(5)	121.60(17)
C(3)-C(4)-H(4)	119.2
C(5)-C(4)-H(4)	119.2
C(4)-C(5)-C(6)	116.69(17)
C(4)-C(5)-N(1)	121.82(16)
C(6)-C(5)-N(1)	121.49(16)
C(7)-C(6)-C(5)	121.41(18)
C(7)-C(6)-H(6)	119.3
C(5)-C(6)-H(6)	119.3
C(6)-C(7)-C(2)	121.69(17)
C(6)-C(7)-H(7)	119.2
C(2)-C(7)-H(7)	119.2
Si(1)-C(8)-H(8A)	109.5
Si(1)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
Si(1)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
Si(1)-C(9)-H(9A)	109.5
Si(1)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
Si(1)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
Si(2)-C(10)-H(10A)	109.5
Si(2)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
Si(2)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
Si(3)-C(11)-H(11A)	109.5
Si(3)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
Si(3)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
Si(3)-C(12)-H(12A)	109.5
Si(3)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
Si(3)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(19)	117.62(16)

C(14)-C(13)-N(2)	121.50(16)
C(19)-C(13)-N(2)	120.83(16)
C(13)-C(14)-C(15)	121.14(18)
C(13)-C(14)-H(14)	119.4
C(15)-C(14)-H(14)	119.4
C(14)-C(15)-C(16)	121.18(19)
C(14)-C(15)-H(15)	119.4
C(16)-C(15)-H(15)	119.4
C(18)-C(16)-C(15)	117.80(17)
C(18)-C(16)-C(17)	120.6(2)
C(15)-C(16)-C(17)	121.6(2)
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-C(19)	120.9(2)
C(16)-C(18)-H(18)	119.6
C(19)-C(18)-H(18)	119.6
C(13)-C(19)-C(18)	121.38(19)
C(13)-C(19)-H(19)	119.3
C(18)-C(19)-H(19)	119.3
Si(4)-C(20)-H(20A)	109.5
Si(4)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
Si(4)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
Si(4)-C(21)-H(21A)	109.5
Si(4)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
Si(4)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(23)-C(22)-C(27)	117.32(17)
C(23)-C(22)-N(3)	121.93(17)
C(27)-C(22)-N(3)	120.76(17)
C(22)-C(23)-C(24)	121.41(18)
C(22)-C(23)-H(23)	119.3
C(24)-C(23)-H(23)	119.3
C(23)-C(24)-C(25)	121.39(19)
C(23)-C(24)-H(24)	119.3
C(25)-C(24)-H(24)	119.3
C(26)-C(25)-C(24)	117.12(18)
C(26)-C(25)-C(38)	121.4(2)
C(24)-C(25)-C(38)	121.4(2)
C(27)-C(26)-C(25)	121.96(19)
C(27)-C(26)-H(26)	119.0
C(25)-C(26)-H(26)	119.0
C(26)-C(27)-C(22)	120.76(19)
C(26)-C(27)-H(27)	119.6
C(22)-C(27)-H(27)	119.6
C(32)-C(28)-C(29)	107.6(2)
C(32)-C(28)-Zr(1)	73.34(12)
C(29)-C(28)-Zr(1)	74.79(11)
C(32)-C(28)-H(28)	126.2
C(29)-C(28)-H(28)	126.2
Zr(1)-C(28)-H(28)	117.7
C(30)-C(29)-C(28)	108.2(2)
C(30)-C(29)-Zr(1)	73.80(12)
C(28)-C(29)-Zr(1)	72.38(11)
C(30)-C(29)-H(29)	125.9
C(28)-C(29)-H(29)	125.9
Zr(1)-C(29)-H(29)	119.7

C(31)-C(30)-C(29)	108.0(2)
C(31)-C(30)-Zr(1)	73.33(11)
C(29)-C(30)-Zr(1)	73.78(11)
C(31)-C(30)-H(30)	126.0
C(29)-C(30)-H(30)	126.0
Zr(1)-C(30)-H(30)	118.8
C(30)-C(31)-C(32)	108.1(2)
C(30)-C(31)-Zr(1)	74.20(11)
C(32)-C(31)-Zr(1)	72.58(12)
C(30)-C(31)-H(31)	125.9
C(32)-C(31)-H(31)	125.9
Zr(1)-C(31)-H(31)	119.1
C(28)-C(32)-C(31)	108.06(19)
C(28)-C(32)-Zr(1)	73.74(11)
C(31)-C(32)-Zr(1)	74.57(12)
C(28)-C(32)-H(32)	126.0
C(31)-C(32)-H(32)	126.0
Zr(1)-C(32)-H(32)	117.7
C(37)-C(33)-C(34)	107.5(2)
C(37)-C(33)-Zr(1)	74.96(12)
C(34)-C(33)-Zr(1)	72.97(12)
C(37)-C(33)-H(33)	126.3
C(34)-C(33)-H(33)	126.3
Zr(1)-C(33)-H(33)	117.8
C(35)-C(34)-C(33)	108.2(2)
C(35)-C(34)-Zr(1)	74.70(13)
C(33)-C(34)-Zr(1)	73.99(12)
C(35)-C(34)-H(34)	125.9
C(33)-C(34)-H(34)	125.9
Zr(1)-C(34)-H(34)	117.4
C(34)-C(35)-C(36)	108.4(2)
C(34)-C(35)-Zr(1)	72.71(12)
C(36)-C(35)-Zr(1)	74.53(11)
C(34)-C(35)-H(35)	125.8
C(36)-C(35)-H(35)	125.8
Zr(1)-C(35)-H(35)	118.8
C(37)-C(36)-C(35)	107.6(2)
C(37)-C(36)-Zr(1)	73.83(11)
C(35)-C(36)-Zr(1)	72.92(12)
C(37)-C(36)-H(36)	126.2
C(35)-C(36)-H(36)	126.2
Zr(1)-C(36)-H(36)	119.0
C(36)-C(37)-C(33)	108.3(2)
C(36)-C(37)-Zr(1)	73.81(12)
C(33)-C(37)-Zr(1)	72.39(11)
C(36)-C(37)-H(37)	125.8
C(33)-C(37)-H(37)	125.8
Zr(1)-C(37)-H(37)	119.8
C(25)-C(38)-H(38A)	109.5
C(25)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(25)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(41)-C(39)-C(43)	120.5(2)
C(41)-C(39)-D(39)	119.7
C(43)-C(39)-D(39)	119.7
C(42)-C(40)-C(41)	120.17(19)
C(42)-C(40)-D(40)	119.9
C(41)-C(40)-D(40)	119.9
C(39)-C(41)-C(40)	119.6(2)
C(39)-C(41)-D(41)	120.2
C(40)-C(41)-D(41)	120.2
C(40)-C(42)-C(44)	119.9(2)
C(40)-C(42)-D(42)	120.0

C(44)-C(42)-D(42)	120.0
C(39)-C(43)-C(44)	119.9(2)
C(39)-C(43)-D(43)	120.1
C(44)-C(43)-D(43)	120.1
C(42)-C(44)-C(43)	119.9(2)
C(42)-C(44)-D(44)	120.1
C(43)-C(44)-D(44)	120.1

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters (A^2 x 10^3) for structure 1. 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
Sn(1)	14(1)	13(1)	15(1)	0(1)	-1(1)	-1(1)
Zr(1)	14(1)	16(1)	21(1)	0(1)	0(1)	-1(1)
Cl(1)	26(1)	37(1)	22(1)	1(1)	1(1)	3(1)
Si(1)	19(1)	16(1)	17(1)	0(1)	1(1)	-2(1)
Si(2)	18(1)	17(1)	17(1)	0(1)	1(1)	0(1)
Si(3)	23(1)	19(1)	17(1)	-2(1)	-1(1)	0(1)
Si(4)	19(1)	19(1)	20(1)	2(1)	-1(1)	0(1)
N(1)	21(1)	14(1)	21(1)	-4(1)	2(1)	-3(1)
N(2)	22(1)	24(1)	17(1)	-3(1)	-4(1)	3(1)
N(3)	17(1)	18(1)	23(1)	9(1)	1(1)	0(1)
C(1)	35(1)	30(1)	37(1)	-13(1)	4(1)	2(1)
C(2)	18(1)	23(1)	28(1)	-9(1)	-2(1)	0(1)
C(3)	20(1)	27(1)	20(1)	0(1)	0(1)	-3(1)
C(4)	21(1)	16(1)	26(1)	1(1)	1(1)	-1(1)
C(5)	12(1)	18(1)	23(1)	-4(1)	-1(1)	-2(1)
C(6)	25(1)	17(1)	24(1)	1(1)	2(1)	-1(1)
C(7)	26(1)	14(1)	30(1)	-2(1)	1(1)	1(1)
C(8)	35(1)	20(1)	25(1)	4(1)	0(1)	-3(1)
C(9)	24(1)	23(1)	27(1)	-3(1)	3(1)	-7(1)
C(10)	22(1)	33(1)	33(1)	4(1)	6(1)	-1(1)
C(11)	39(1)	33(1)	20(1)	-1(1)	4(1)	2(1)
C(12)	34(1)	23(1)	30(1)	-6(1)	-3(1)	2(1)
C(13)	20(1)	27(1)	16(1)	-2(1)	-1(1)	0(1)
C(14)	30(1)	23(1)	27(1)	-1(1)	-6(1)	-4(1)
C(15)	34(1)	27(1)	34(1)	8(1)	-6(1)	4(1)
C(16)	27(1)	40(1)	26(1)	1(1)	-8(1)	3(1)
C(17)	37(1)	55(1)	42(1)	1(1)	-21(1)	5(1)
C(18)	31(1)	32(1)	37(1)	-8(1)	-13(1)	0(1)
C(19)	33(1)	25(1)	31(1)	-5(1)	-10(1)	5(1)
C(20)	32(1)	32(1)	27(1)	0(1)	-6(1)	-5(1)
C(21)	24(1)	24(1)	35(1)	5(1)	0(1)	5(1)
C(22)	15(1)	17(1)	23(1)	6(1)	-2(1)	0(1)
C(23)	20(1)	19(1)	25(1)	1(1)	0(1)	2(1)
C(24)	18(1)	31(1)	24(1)	4(1)	1(1)	3(1)
C(25)	22(1)	26(1)	30(1)	11(1)	3(1)	1(1)
C(26)	34(1)	18(1)	39(1)	4(1)	4(1)	-3(1)
C(27)	31(1)	22(1)	26(1)	0(1)	4(1)	-1(1)
C(28)	32(1)	29(1)	32(1)	6(1)	-12(1)	7(1)
C(29)	26(1)	18(1)	44(1)	11(1)	4(1)	3(1)
C(30)	28(1)	17(1)	43(1)	-3(1)	-5(1)	1(1)
C(31)	27(1)	26(1)	35(1)	-2(1)	2(1)	1(1)
C(32)	20(1)	25(1)	45(1)	1(1)	-5(1)	3(1)

C(33)	33(1)	28(1)	36(1)	-8(1)	-5(1)	-8(1)
C(34)	20(1)	26(1)	61(2)	-5(1)	-7(1)	-7(1)
C(35)	33(1)	24(1)	51(1)	5(1)	7(1)	-12(1)
C(36)	30(1)	15(1)	50(1)	4(1)	-5(1)	-5(1)
C(37)	28(1)	20(1)	43(1)	-11(1)	1(1)	-7(1)
C(38)	40(1)	36(1)	46(1)	19(1)	11(1)	1(1)
C(39)	24(1)	46(1)	29(1)	-6(1)	3(1)	-9(1)
C(40)	31(1)	37(1)	29(1)	0(1)	7(1)	-9(1)
C(41)	33(1)	34(1)	24(1)	0(1)	3(1)	-2(1)
C(42)	26(1)	44(1)	31(1)	-4(1)	3(1)	-10(1)
C(43)	34(1)	51(1)	28(1)	2(1)	6(1)	-12(1)
C(44)	33(1)	51(1)	24(1)	4(1)	1(1)	-7(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for structure 1.

	x	y	z	U(eq)
H(1A)	4170	7171	2476	51
H(1B)	3146	6657	2661	51
H(1C)	4291	6518	3000	51
H(3)	3604	8429	2807	26
H(4)	3038	9274	3585	25
H(6)	2796	7538	4832	26
H(7)	3266	6693	4038	28
H(8A)	2345	8590	6258	40
H(8B)	2099	7809	5896	40
H(8C)	1148	8239	6268	40
H(9A)	700	7819	4688	37
H(9B)	180	8602	4449	37
H(9C)	-230	8224	5097	37
H(10A)	-886	10570	5926	44
H(10B)	-567	9820	6315	44
H(10C)	-1107	9748	5627	44
H(11A)	2627	10457	7246	46
H(11B)	2198	9661	6977	46
H(11C)	1352	10313	7166	46
H(12A)	2084	11882	5781	43
H(12B)	2569	11862	6485	43
H(12C)	1288	11793	6376	43
H(14)	4359	9050	6138	32
H(15)	5808	8904	6833	38
H(17A)	6958	10369	7790	67
H(17B)	7634	9907	7269	67
H(17C)	6844	9465	7745	67
H(18)	5933	11178	7079	40
H(19)	4483	11322	6384	35
H(20A)	694	9751	3795	45
H(20B)	464	10561	3476	45
H(20C)	-429	10179	3926	45
H(21A)	529	12018	4281	42
H(21B)	528	11934	5037	42
H(21C)	-484	11635	4632	42
H(23)	3066	10708	3306	26
H(24)	3708	11639	2621	29
H(26)	3249	13226	3975	36
H(27)	2672	12295	4676	31
H(28)	6625	9286	5535	37

H(29)	4933	8654	5100	35
H(30)	5238	8383	3938	35
H(31)	7137	8801	3660	35
H(32)	7991	9369	4642	36
H(33)	6508	10778	5565	39
H(34)	7929	10743	4699	43
H(35)	7119	11312	3715	43
H(36)	5185	11688	3955	38
H(37)	4820	11380	5105	36
H(38A)	4576	13368	2905	61
H(38B)	3332	13549	2748	61
H(38C)	3976	12930	2339	61
D(39)	3247	2300	7464	40
D(40)	6159	3095	6892	39
D(41)	4318	2873	6692	37
D(42)	6907	2767	7870	40
D(43)	3989	1962	8439	45
D(44)	5822	2204	8647	43

Table S6. Torsion angles [deg] for structure 1.

N(2)-Sn(1)-Zr(1)-Cl(1)	-165.91(5)
N(3)-Sn(1)-Zr(1)-Cl(1)	-49.58(5)
N(1)-Sn(1)-Zr(1)-Cl(1)	74.97(5)
N(2)-Sn(1)-Zr(1)-C(34)	-37.31(9)
N(3)-Sn(1)-Zr(1)-C(34)	79.03(9)
N(1)-Sn(1)-Zr(1)-C(34)	-156.42(9)
N(2)-Sn(1)-Zr(1)-C(32)	65.48(8)
N(3)-Sn(1)-Zr(1)-C(32)	-178.19(8)
N(1)-Sn(1)-Zr(1)-C(32)	-53.64(8)
N(2)-Sn(1)-Zr(1)-C(33)	-26.80(7)
N(3)-Sn(1)-Zr(1)-C(33)	89.53(7)
N(1)-Sn(1)-Zr(1)-C(33)	-145.92(7)
N(2)-Sn(1)-Zr(1)-C(28)	54.79(7)
N(3)-Sn(1)-Zr(1)-C(28)	171.12(7)
N(1)-Sn(1)-Zr(1)-C(28)	-64.33(7)
N(2)-Sn(1)-Zr(1)-C(35)	-76.18(9)
N(3)-Sn(1)-Zr(1)-C(35)	40.16(9)
N(1)-Sn(1)-Zr(1)-C(35)	164.71(9)
N(2)-Sn(1)-Zr(1)-C(31)	105.84(8)
N(3)-Sn(1)-Zr(1)-C(31)	-137.83(8)
N(1)-Sn(1)-Zr(1)-C(31)	-13.28(8)
N(2)-Sn(1)-Zr(1)-C(29)	80.28(7)
N(3)-Sn(1)-Zr(1)-C(29)	-163.39(8)
N(1)-Sn(1)-Zr(1)-C(29)	-38.84(8)
N(2)-Sn(1)-Zr(1)-C(30)	108.98(7)
N(3)-Sn(1)-Zr(1)-C(30)	-134.69(7)
N(1)-Sn(1)-Zr(1)-C(30)	-10.14(7)
N(2)-Sn(1)-Zr(1)-C(36)	-80.84(7)
N(3)-Sn(1)-Zr(1)-C(36)	35.50(8)
N(1)-Sn(1)-Zr(1)-C(36)	160.05(7)
N(2)-Sn(1)-Zr(1)-C(37)	-52.47(8)
N(3)-Sn(1)-Zr(1)-C(37)	63.86(8)
N(1)-Sn(1)-Zr(1)-C(37)	-171.59(8)
N(1)-Si(1)-Si(2)-C(10)	167.35(8)
C(8)-Si(1)-Si(2)-C(10)	-69.78(10)
C(9)-Si(1)-Si(2)-C(10)	49.90(10)
N(1)-Si(1)-Si(2)-Si(3)	-68.08(6)
C(8)-Si(1)-Si(2)-Si(3)	54.79(8)
C(9)-Si(1)-Si(2)-Si(3)	174.47(7)
N(1)-Si(1)-Si(2)-Si(4)	39.31(6)

C(8)-Si(1)-Si(2)-Si(4)	162.19(7)
C(9)-Si(1)-Si(2)-Si(4)	-78.13(7)
C(10)-Si(2)-Si(3)-N(2)	163.94(10)
Si(1)-Si(2)-Si(3)-N(2)	39.59(6)
Si(4)-Si(2)-Si(3)-N(2)	-68.70(6)
C(10)-Si(2)-Si(3)-C(12)	-73.34(11)
Si(1)-Si(2)-Si(3)-C(12)	162.31(8)
Si(4)-Si(2)-Si(3)-C(12)	54.02(8)
C(10)-Si(2)-Si(3)-C(11)	47.20(11)
Si(1)-Si(2)-Si(3)-C(11)	-77.15(7)
Si(4)-Si(2)-Si(3)-C(11)	174.56(7)
C(10)-Si(2)-Si(4)-N(3)	164.90(10)
Si(3)-Si(2)-Si(4)-N(3)	39.28(6)
Si(1)-Si(2)-Si(4)-N(3)	-68.97(6)
C(10)-Si(2)-Si(4)-C(20)	-73.81(11)
Si(3)-Si(2)-Si(4)-C(20)	160.57(8)
Si(1)-Si(2)-Si(4)-C(20)	52.32(8)
C(10)-Si(2)-Si(4)-C(21)	46.89(11)
Si(3)-Si(2)-Si(4)-C(21)	-78.72(7)
Si(1)-Si(2)-Si(4)-C(21)	173.02(7)
C(8)-Si(1)-N(1)-C(5)	90.50(15)
C(9)-Si(1)-N(1)-C(5)	-31.16(16)
Si(2)-Si(1)-N(1)-C(5)	-147.96(12)
C(8)-Si(1)-N(1)-Sn(1)	-94.48(11)
C(9)-Si(1)-N(1)-Sn(1)	143.86(9)
Si(2)-Si(1)-N(1)-Sn(1)	27.06(10)
N(2)-Sn(1)-N(1)-C(5)	-152.81(12)
N(3)-Sn(1)-N(1)-C(5)	106.67(12)
Zr(1)-Sn(1)-N(1)-C(5)	-26.13(14)
N(2)-Sn(1)-N(1)-Si(1)	31.96(10)
N(3)-Sn(1)-N(1)-Si(1)	-68.56(11)
Zr(1)-Sn(1)-N(1)-Si(1)	158.64(7)
C(12)-Si(3)-N(2)-C(13)	87.21(15)
C(11)-Si(3)-N(2)-C(13)	-32.92(16)
Si(2)-Si(3)-N(2)-C(13)	-151.23(12)
C(12)-Si(3)-N(2)-Sn(1)	-93.82(12)
C(11)-Si(3)-N(2)-Sn(1)	146.05(10)
Si(2)-Si(3)-N(2)-Sn(1)	27.73(10)
N(3)-Sn(1)-N(2)-C(13)	-148.28(13)
N(1)-Sn(1)-N(2)-C(13)	108.23(13)
Zr(1)-Sn(1)-N(2)-C(13)	-20.43(14)
N(3)-Sn(1)-N(2)-Si(3)	32.76(11)
N(1)-Sn(1)-N(2)-Si(3)	-70.73(10)
Zr(1)-Sn(1)-N(2)-Si(3)	160.60(7)
C(20)-Si(4)-N(3)-C(22)	75.17(16)
C(21)-Si(4)-N(3)-C(22)	-44.44(16)
Si(2)-Si(4)-N(3)-C(22)	-161.94(13)
C(20)-Si(4)-N(3)-Sn(1)	-92.80(11)
C(21)-Si(4)-N(3)-Sn(1)	147.59(10)
Si(2)-Si(4)-N(3)-Sn(1)	30.08(10)
N(2)-Sn(1)-N(3)-C(22)	118.79(13)
N(1)-Sn(1)-N(3)-C(22)	-138.76(13)
Zr(1)-Sn(1)-N(3)-C(22)	-6.42(15)
N(2)-Sn(1)-N(3)-Si(4)	-73.06(11)
N(1)-Sn(1)-N(3)-Si(4)	29.39(12)
Zr(1)-Sn(1)-N(3)-Si(4)	161.73(7)
C(7)-C(2)-C(3)-C(4)	-0.5(3)
C(1)-C(2)-C(3)-C(4)	177.4(2)
C(2)-C(3)-C(4)-C(5)	2.4(3)
C(3)-C(4)-C(5)-C(6)	-2.2(3)
C(3)-C(4)-C(5)-N(1)	177.81(17)
Si(1)-N(1)-C(5)-C(4)	132.16(16)
Sn(1)-N(1)-C(5)-C(4)	-43.2(2)
Si(1)-N(1)-C(5)-C(6)	-47.8(2)
Sn(1)-N(1)-C(5)-C(6)	136.87(15)

C(4)-C(5)-C(6)-C(7)	0.3(3)
N(1)-C(5)-C(6)-C(7)	-179.73(18)
C(5)-C(6)-C(7)-C(2)	1.5(3)
C(3)-C(2)-C(7)-C(6)	-1.4(3)
C(1)-C(2)-C(7)-C(6)	-179.3(2)
Si(3)-N(2)-C(13)-C(14)	110.25(18)
Sn(1)-N(2)-C(13)-C(14)	-68.8(2)
Si(3)-N(2)-C(13)-C(19)	-67.1(2)
Sn(1)-N(2)-C(13)-C(19)	113.86(17)
C(19)-C(13)-C(14)-C(15)	1.1(3)
N(2)-C(13)-C(14)-C(15)	-176.36(18)
C(13)-C(14)-C(15)-C(16)	-0.2(3)
C(14)-C(15)-C(16)-C(18)	-0.7(3)
C(14)-C(15)-C(16)-C(17)	178.3(2)
C(15)-C(16)-C(18)-C(19)	0.6(3)
C(17)-C(16)-C(18)-C(19)	-178.3(2)
C(14)-C(13)-C(19)-C(18)	-1.1(3)
N(2)-C(13)-C(19)-C(18)	176.36(19)
C(16)-C(18)-C(19)-C(13)	0.2(4)
Si(4)-N(3)-C(22)-C(23)	-97.71(19)
Sn(1)-N(3)-C(22)-C(23)	71.1(2)
Si(4)-N(3)-C(22)-C(27)	81.8(2)
Sn(1)-N(3)-C(22)-C(27)	-109.46(18)
C(27)-C(22)-C(23)-C(24)	-0.9(3)
N(3)-C(22)-C(23)-C(24)	178.62(18)
C(22)-C(23)-C(24)-C(25)	-0.9(3)
C(23)-C(24)-C(25)-C(26)	1.4(3)
C(23)-C(24)-C(25)-C(38)	-176.5(2)
C(24)-C(25)-C(26)-C(27)	-0.1(3)
C(38)-C(25)-C(26)-C(27)	177.8(2)
C(25)-C(26)-C(27)-C(22)	-1.8(3)
C(23)-C(22)-C(27)-C(26)	2.2(3)
N(3)-C(22)-C(27)-C(26)	-177.31(19)
Cl(1)-Zr(1)-C(28)-C(32)	53.74(15)
C(34)-Zr(1)-C(28)-C(32)	-70.88(13)
C(33)-Zr(1)-C(28)-C(32)	-103.38(14)
C(35)-Zr(1)-C(28)-C(32)	-63.80(15)
C(31)-Zr(1)-C(28)-C(32)	37.39(12)
C(29)-Zr(1)-C(28)-C(32)	114.15(19)
C(30)-Zr(1)-C(28)-C(32)	77.64(14)
C(36)-Zr(1)-C(28)-C(32)	-100.55(15)
C(37)-Zr(1)-C(28)-C(32)	-121.91(13)
Sn(1)-Zr(1)-C(28)-C(32)	164.36(12)
Cl(1)-Zr(1)-C(28)-C(29)	-60.41(16)
C(34)-Zr(1)-C(28)-C(29)	174.97(14)
C(32)-Zr(1)-C(28)-C(29)	-114.15(19)
C(33)-Zr(1)-C(28)-C(29)	142.47(15)
C(35)-Zr(1)-C(28)-C(29)	-177.95(13)
C(31)-Zr(1)-C(28)-C(29)	-76.76(14)
C(30)-Zr(1)-C(28)-C(29)	-36.51(13)
C(36)-Zr(1)-C(28)-C(29)	145.30(13)
C(37)-Zr(1)-C(28)-C(29)	123.94(12)
Sn(1)-Zr(1)-C(28)-C(29)	50.22(13)
C(32)-C(28)-C(29)-C(30)	-0.9(2)
Zr(1)-C(28)-C(29)-C(30)	65.65(14)
C(32)-C(28)-C(29)-Zr(1)	-66.54(14)
Cl(1)-Zr(1)-C(29)-C(30)	22.95(14)
C(34)-Zr(1)-C(29)-C(30)	-121.52(14)
C(32)-Zr(1)-C(29)-C(30)	-77.99(14)
C(33)-Zr(1)-C(29)-C(30)	-154.78(13)
C(28)-Zr(1)-C(29)-C(30)	-115.67(19)
C(35)-Zr(1)-C(29)-C(30)	-111.8(2)
C(31)-Zr(1)-C(29)-C(30)	-37.08(13)
C(36)-Zr(1)-C(29)-C(30)	168.23(13)
C(37)-Zr(1)-C(29)-C(30)	173.56(13)

Sn(1)-Zr(1)-C(29)-C(30)	116.41(13)
Cl(1)-Zr(1)-C(29)-C(28)	138.62(12)
C(34)-Zr(1)-C(29)-C(28)	-5.85(16)
C(32)-Zr(1)-C(29)-C(28)	37.68(13)
C(33)-Zr(1)-C(29)-C(28)	-39.10(15)
C(35)-Zr(1)-C(29)-C(28)	3.9(2)
C(31)-Zr(1)-C(29)-C(28)	78.59(14)
C(30)-Zr(1)-C(29)-C(28)	115.67(19)
C(36)-Zr(1)-C(29)-C(28)	-76.1(2)
C(37)-Zr(1)-C(29)-C(28)	-70.77(14)
Sn(1)-Zr(1)-C(29)-C(28)	-127.91(13)
C(28)-C(29)-C(30)-C(31)	1.2(2)
Zr(1)-C(29)-C(30)-C(31)	65.89(14)
C(28)-C(29)-C(30)-Zr(1)	-64.71(13)
Cl(1)-Zr(1)-C(30)-C(31)	85.74(13)
C(34)-Zr(1)-C(30)-C(31)	-33.16(18)
C(32)-Zr(1)-C(30)-C(31)	-37.16(13)
C(33)-Zr(1)-C(30)-C(31)	-79.45(17)
C(28)-Zr(1)-C(30)-C(31)	-78.01(14)
C(35)-Zr(1)-C(30)-C(31)	13.1(2)
C(29)-Zr(1)-C(30)-C(31)	-115.0(2)
C(36)-Zr(1)-C(30)-C(31)	94.5(4)
C(37)-Zr(1)-C(30)-C(31)	-128.04(18)
Sn(1)-Zr(1)-C(30)-C(31)	-175.12(13)
Cl(1)-Zr(1)-C(30)-C(29)	-159.26(13)
C(34)-Zr(1)-C(30)-C(29)	81.83(16)
C(32)-Zr(1)-C(30)-C(29)	77.83(14)
C(33)-Zr(1)-C(30)-C(29)	35.54(18)
C(28)-Zr(1)-C(30)-C(29)	36.99(13)
C(35)-Zr(1)-C(30)-C(29)	128.06(16)
C(31)-Zr(1)-C(30)-C(29)	115.0(2)
C(36)-Zr(1)-C(30)-C(29)	-150.5(3)
C(37)-Zr(1)-C(30)-C(29)	-13.0(3)
Sn(1)-Zr(1)-C(30)-C(29)	-60.12(12)
C(29)-C(30)-C(31)-C(32)	-1.0(2)
Zr(1)-C(30)-C(31)-C(32)	65.16(14)
C(29)-C(30)-C(31)-Zr(1)	-66.19(13)
Cl(1)-Zr(1)-C(31)-C(30)	-90.90(13)
C(34)-Zr(1)-C(31)-C(30)	155.39(14)
C(32)-Zr(1)-C(31)-C(30)	115.3(2)
C(33)-Zr(1)-C(31)-C(30)	125.55(14)
C(28)-Zr(1)-C(31)-C(30)	77.86(15)
C(35)-Zr(1)-C(31)-C(30)	-172.24(15)
C(29)-Zr(1)-C(31)-C(30)	37.02(13)
C(36)-Zr(1)-C(31)-C(30)	-161.83(12)
C(37)-Zr(1)-C(31)-C(30)	129.90(19)
Sn(1)-Zr(1)-C(31)-C(30)	5.85(15)
Cl(1)-Zr(1)-C(31)-C(32)	153.77(13)
C(34)-Zr(1)-C(31)-C(32)	40.06(15)
C(33)-Zr(1)-C(31)-C(32)	10.22(16)
C(28)-Zr(1)-C(31)-C(32)	-37.47(13)
C(35)-Zr(1)-C(31)-C(32)	72.43(14)
C(29)-Zr(1)-C(31)-C(32)	-78.31(15)
C(30)-Zr(1)-C(31)-C(32)	-115.3(2)
C(36)-Zr(1)-C(31)-C(32)	82.84(19)
C(37)-Zr(1)-C(31)-C(32)	14.6(2)
Sn(1)-Zr(1)-C(31)-C(32)	-109.48(12)
C(29)-C(28)-C(32)-C(31)	0.3(2)
Zr(1)-C(28)-C(32)-C(31)	-67.26(14)
C(29)-C(28)-C(32)-Zr(1)	67.51(13)
C(30)-C(31)-C(32)-C(28)	0.5(2)
Zr(1)-C(31)-C(32)-C(28)	66.71(14)
C(30)-C(31)-C(32)-Zr(1)	-66.23(14)
Cl(1)-Zr(1)-C(32)-C(28)	-143.00(11)
C(34)-Zr(1)-C(32)-C(28)	105.20(14)

C(33)-Zr(1)-C(32)-C(28)	74.08(13)
C(35)-Zr(1)-C(32)-C(28)	127.31(13)
C(31)-Zr(1)-C(32)-C(28)	-114.54(19)
C(29)-Zr(1)-C(32)-C(28)	-37.58(13)
C(30)-Zr(1)-C(32)-C(28)	-77.83(14)
C(36)-Zr(1)-C(32)-C(28)	112.02(14)
C(37)-Zr(1)-C(32)-C(28)	72.75(14)
Sn(1)-Zr(1)-C(32)-C(28)	-19.83(15)
Cl(1)-Zr(1)-C(32)-C(31)	-28.46(14)
C(34)-Zr(1)-C(32)-C(31)	-140.26(15)
C(33)-Zr(1)-C(32)-C(31)	-171.37(14)
C(28)-Zr(1)-C(32)-C(31)	114.54(19)
C(35)-Zr(1)-C(32)-C(31)	-118.15(13)
C(29)-Zr(1)-C(32)-C(31)	76.96(14)
C(30)-Zr(1)-C(32)-C(31)	36.72(13)
C(36)-Zr(1)-C(32)-C(31)	-133.44(13)
C(37)-Zr(1)-C(32)-C(31)	-172.71(12)
Sn(1)-Zr(1)-C(32)-C(31)	94.72(13)
Cl(1)-Zr(1)-C(33)-C(37)	57.28(16)
C(34)-Zr(1)-C(33)-C(37)	114.04(19)
C(32)-Zr(1)-C(33)-C(37)	-177.91(14)
C(28)-Zr(1)-C(33)-C(37)	-146.00(15)
C(35)-Zr(1)-C(33)-C(37)	76.88(14)
C(31)-Zr(1)-C(33)-C(37)	176.56(13)
C(29)-Zr(1)-C(33)-C(37)	-125.76(12)
C(30)-Zr(1)-C(33)-C(37)	-144.82(13)
C(36)-Zr(1)-C(33)-C(37)	36.45(13)
Sn(1)-Zr(1)-C(33)-C(37)	-50.01(13)
Cl(1)-Zr(1)-C(33)-C(34)	-56.77(16)
C(32)-Zr(1)-C(33)-C(34)	68.04(14)
C(28)-Zr(1)-C(33)-C(34)	99.96(14)
C(35)-Zr(1)-C(33)-C(34)	-37.16(13)
C(31)-Zr(1)-C(33)-C(34)	62.52(15)
C(29)-Zr(1)-C(33)-C(34)	120.19(13)
C(30)-Zr(1)-C(33)-C(34)	101.14(15)
C(36)-Zr(1)-C(33)-C(34)	-77.60(14)
C(37)-Zr(1)-C(33)-C(34)	-114.04(19)
Sn(1)-Zr(1)-C(33)-C(34)	-164.05(13)
C(37)-C(33)-C(34)-C(35)	-0.1(2)
Zr(1)-C(33)-C(34)-C(35)	67.48(15)
C(37)-C(33)-C(34)-Zr(1)	-67.60(14)
Cl(1)-Zr(1)-C(34)-C(35)	27.04(15)
C(32)-Zr(1)-C(34)-C(35)	136.92(16)
C(33)-Zr(1)-C(34)-C(35)	-114.5(2)
C(28)-Zr(1)-C(34)-C(35)	168.56(15)
C(31)-Zr(1)-C(34)-C(35)	116.01(14)
C(29)-Zr(1)-C(34)-C(35)	171.73(13)
C(30)-Zr(1)-C(34)-C(35)	133.60(14)
C(36)-Zr(1)-C(34)-C(35)	-36.82(14)
C(37)-Zr(1)-C(34)-C(35)	-77.05(15)
Sn(1)-Zr(1)-C(34)-C(35)	-94.99(15)
Cl(1)-Zr(1)-C(34)-C(33)	141.53(12)
C(32)-Zr(1)-C(34)-C(33)	-108.59(15)
C(28)-Zr(1)-C(34)-C(33)	-76.94(14)
C(35)-Zr(1)-C(34)-C(33)	114.5(2)
C(31)-Zr(1)-C(34)-C(33)	-129.49(13)
C(29)-Zr(1)-C(34)-C(33)	-73.77(15)
C(30)-Zr(1)-C(34)-C(33)	-111.91(14)
C(36)-Zr(1)-C(34)-C(33)	77.67(14)
C(37)-Zr(1)-C(34)-C(33)	37.45(13)
Sn(1)-Zr(1)-C(34)-C(33)	19.51(16)
C(33)-C(34)-C(35)-C(36)	-0.5(2)
Zr(1)-C(34)-C(35)-C(36)	66.53(15)
C(33)-C(34)-C(35)-Zr(1)	-67.01(14)
Cl(1)-Zr(1)-C(35)-C(34)	-155.47(14)

C(32)-Zr(1)-C(35)-C(34)	-43.14(16)
C(33)-Zr(1)-C(35)-C(34)	37.70(14)
C(28)-Zr(1)-C(35)-C(34)	-13.22(17)
C(31)-Zr(1)-C(35)-C(34)	-75.08(15)
C(29)-Zr(1)-C(35)-C(34)	-15.6(3)
C(30)-Zr(1)-C(35)-C(34)	-82.8(2)
C(36)-Zr(1)-C(35)-C(34)	115.5(2)
C(37)-Zr(1)-C(35)-C(34)	78.37(16)
Sn(1)-Zr(1)-C(35)-C(34)	106.78(13)
Cl(1)-Zr(1)-C(35)-C(36)	89.07(14)
C(34)-Zr(1)-C(35)-C(36)	-115.5(2)
C(32)-Zr(1)-C(35)-C(36)	-158.60(15)
C(33)-Zr(1)-C(35)-C(36)	-77.76(16)
C(28)-Zr(1)-C(35)-C(36)	-128.68(15)
C(31)-Zr(1)-C(35)-C(36)	169.46(15)
C(29)-Zr(1)-C(35)-C(36)	-131.11(18)
C(30)-Zr(1)-C(35)-C(36)	161.75(12)
C(37)-Zr(1)-C(35)-C(36)	-37.09(14)
Sn(1)-Zr(1)-C(35)-C(36)	-8.68(17)
C(34)-C(35)-C(36)-C(37)	0.9(2)
Zr(1)-C(35)-C(36)-C(37)	66.24(14)
C(34)-C(35)-C(36)-Zr(1)	-65.33(15)
Cl(1)-Zr(1)-C(36)-C(37)	157.19(13)
C(34)-Zr(1)-C(36)-C(37)	-77.85(15)
C(32)-Zr(1)-C(36)-C(37)	-86.09(16)
C(33)-Zr(1)-C(36)-C(37)	-36.78(13)
C(28)-Zr(1)-C(36)-C(37)	-40.23(18)
C(35)-Zr(1)-C(36)-C(37)	-114.7(2)
C(31)-Zr(1)-C(36)-C(37)	-132.39(15)
C(29)-Zr(1)-C(36)-C(37)	8.3(3)
C(30)-Zr(1)-C(36)-C(37)	148.4(3)
Sn(1)-Zr(1)-C(36)-C(37)	57.87(13)
Cl(1)-Zr(1)-C(36)-C(35)	-88.10(15)
C(34)-Zr(1)-C(36)-C(35)	36.86(15)
C(32)-Zr(1)-C(36)-C(35)	28.63(19)
C(33)-Zr(1)-C(36)-C(35)	77.93(16)
C(28)-Zr(1)-C(36)-C(35)	74.48(18)
C(31)-Zr(1)-C(36)-C(35)	-17.7(2)
C(29)-Zr(1)-C(36)-C(35)	123.0(2)
C(30)-Zr(1)-C(36)-C(35)	-96.9(4)
C(37)-Zr(1)-C(36)-C(35)	114.7(2)
Sn(1)-Zr(1)-C(36)-C(35)	172.59(15)
C(35)-C(36)-C(37)-C(33)	-1.0(2)
Zr(1)-C(36)-C(37)-C(33)	64.65(13)
C(35)-C(36)-C(37)-Zr(1)	-65.63(14)
C(34)-C(33)-C(37)-C(36)	0.7(2)
Zr(1)-C(33)-C(37)-C(36)	-65.58(14)
C(34)-C(33)-C(37)-Zr(1)	66.26(14)
Cl(1)-Zr(1)-C(37)-C(36)	-25.24(14)
C(34)-Zr(1)-C(37)-C(36)	77.94(15)
C(32)-Zr(1)-C(37)-C(36)	118.32(14)
C(33)-Zr(1)-C(37)-C(36)	115.85(19)
C(28)-Zr(1)-C(37)-C(36)	151.46(14)
C(35)-Zr(1)-C(37)-C(36)	37.32(14)
C(31)-Zr(1)-C(37)-C(36)	109.0(2)
C(29)-Zr(1)-C(37)-C(36)	-175.90(13)
C(30)-Zr(1)-C(37)-C(36)	-167.56(13)
Sn(1)-Zr(1)-C(37)-C(36)	-117.44(14)
Cl(1)-Zr(1)-C(37)-C(33)	-141.09(12)
C(34)-Zr(1)-C(37)-C(33)	-37.91(13)
C(32)-Zr(1)-C(37)-C(33)	2.47(16)
C(28)-Zr(1)-C(37)-C(33)	35.61(15)
C(35)-Zr(1)-C(37)-C(33)	-78.53(15)
C(31)-Zr(1)-C(37)-C(33)	-6.8(3)
C(29)-Zr(1)-C(37)-C(33)	68.25(14)

C(30)-Zr(1)-C(37)-C(33)	76.6(2)
C(36)-Zr(1)-C(37)-C(33)	-115.85(19)
Sn(1)-Zr(1)-C(37)-C(33)	126.71(14)
C(43)-C(39)-C(41)-C(40)	0.5(3)
C(42)-C(40)-C(41)-C(39)	-0.7(3)
C(41)-C(40)-C(42)-C(44)	0.4(3)
C(41)-C(39)-C(43)-C(44)	0.2(4)
C(40)-C(42)-C(44)-C(43)	0.3(4)
C(39)-C(43)-C(44)-C(42)	-0.5(4)

Symmetry transformations used to generate equivalent atoms:

Table S7. Crystal data and structure refinement for structure 2.

Identification code	Structure 2
Empirical formula	C44 H52 Cl D6 Hf N3 Si4 Sn
Formula weight	1079.96
Temperature	150(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P 21 21 21
Unit cell dimensions	a = 12.30500(10) A alpha = 90 deg. b = 17.56460(10) A beta = 90 deg. c = 21.0887(2) A gamma = 90 deg.
Volume	4557.95(6) A^3
Z, Calculated density	4, 1.574 Mg/m^3
Absorption coefficient	3.021 mm^-1
F(000)	2152
Crystal size	0.20 x 0.20 x 0.10 mm
Theta range for data collection	2.24 to 25.17 deg.
Limiting indices	-14<=h<=14, -21<=k<=20, -25<=l<=25
Reflections collected / unique	45411 / 8152 [R(int) = 0.0438]
Completeness to theta = 25.17	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.26797 and 0.23070
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8152 / 0 / 498
Goodness-of-fit on F^2	1.076
Final R indices [I>2sigma(I)]	R1 = 0.0227, wR2 = 0.0448
R indices (all data)	R1 = 0.0288, wR2 = 0.0472
Absolute structure parameter	0.240(5)
Largest diff. peak and hole	0.418 and -0.662 e.A^-3

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for structure 2.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Hf(1)	4220(1)	5036(1)	660(1)	19(1)
Sn(1)	6504(1)	5038(1)	168(1)	14(1)
Cl(1)	4624(1)	5040(1)	1764(1)	28(1)
Si(1)	8526(1)	3852(1)	-272(1)	18(1)
Si(2)	9200(1)	5062(1)	-511(1)	17(1)
Si(3)	7856(1)	5600(1)	-1147(1)	20(1)
Si(4)	9019(1)	5735(1)	441(1)	19(1)
N(1)	7407(3)	4027(2)	209(2)	17(1)
N(2)	6664(3)	5300(2)	-790(2)	20(1)
N(3)	7616(3)	5826(2)	519(2)	19(1)
C(1)	6190(5)	1903(3)	2181(3)	33(1)
C(2)	6493(4)	2469(3)	1667(2)	21(1)
C(3)	6572(4)	3238(2)	1786(2)	21(1)
C(4)	6895(4)	3750(2)	1309(2)	19(1)
C(5)	7110(4)	3505(2)	698(2)	17(1)
C(6)	7037(4)	2726(2)	577(2)	20(1)
C(7)	6749(4)	2223(2)	1058(2)	22(1)
C(8)	8198(4)	3302(2)	-1005(2)	28(1)
C(9)	9588(4)	3311(3)	179(2)	25(1)
C(10)	10609(3)	5055(3)	-887(2)	30(1)
C(11)	7917(4)	5211(2)	-1978(2)	32(1)
C(12)	7991(5)	6665(2)	-1197(2)	29(1)

C(13)	5734(4)	5203(2)	-1187(2)	21(1)
C(14)	5321(4)	4489(2)	-1337(2)	24(1)
C(15)	4463(5)	4400(3)	-1745(2)	32(1)
C(16)	3979(3)	5036(3)	-2035(2)	28(1)
C(17)	3047(4)	4933(4)	-2503(2)	46(1)
C(18)	4379(5)	5735(3)	-1892(2)	34(1)
C(19)	5242(4)	5829(2)	-1474(2)	29(1)
C(20)	9638(3)	5249(2)	1146(2)	29(1)
C(21)	9681(4)	6696(3)	370(2)	27(1)
C(22)	7215(4)	6401(2)	937(2)	18(1)
C(23)	6899(4)	6223(2)	1554(2)	21(1)
C(24)	6524(4)	6778(3)	1971(2)	24(1)
C(25)	6463(5)	7541(3)	1789(3)	27(1)
C(26)	6757(5)	7710(3)	1174(3)	31(1)
C(27)	7118(4)	7154(2)	752(2)	24(1)
C(28)	3473(5)	4117(3)	-108(3)	30(1)
C(29)	4428(5)	3781(2)	129(3)	27(1)
C(30)	4247(5)	3617(2)	780(3)	26(1)
C(31)	3202(5)	3861(3)	933(3)	28(1)
C(32)	2708(5)	4175(3)	388(3)	29(1)
C(33)	3568(5)	5960(3)	-143(3)	33(1)
C(34)	2782(5)	5931(3)	334(3)	35(1)
C(35)	3224(5)	6243(3)	886(3)	34(2)
C(36)	4305(5)	6452(2)	749(3)	31(1)
C(37)	4501(5)	6291(2)	114(3)	30(1)
C(38)	6117(5)	8154(3)	2242(3)	43(2)
C(39)	10708(5)	2127(3)	2787(2)	32(1)
C(40)	9628(4)	2266(3)	2910(2)	28(1)
C(41)	9000(4)	2609(3)	2452(2)	33(1)
C(42)	9428(4)	2806(3)	1875(2)	37(1)
C(43)	10515(4)	2661(3)	1753(2)	35(1)
C(44)	11153(4)	2330(3)	2211(2)	36(1)

Table S9. Bond lengths [A] and angles [deg] for structure 2.

Hf(1)-Cl(1)	2.3807(9)
Hf(1)-C(28)	2.464(5)
Hf(1)-C(32)	2.465(5)
Hf(1)-C(34)	2.466(5)
Hf(1)-C(33)	2.479(5)
Hf(1)-C(31)	2.481(5)
Hf(1)-C(29)	2.485(4)
Hf(1)-C(35)	2.495(5)
Hf(1)-C(36)	2.497(4)
Hf(1)-C(30)	2.505(4)
Hf(1)-C(37)	2.511(5)
Hf(1)-Sn(1)	2.9956(3)
Sn(1)-N(2)	2.081(3)
Sn(1)-N(3)	2.082(3)
Sn(1)-N(1)	2.096(3)
Si(1)-N(1)	1.738(3)
Si(1)-C(8)	1.866(5)
Si(1)-C(9)	1.875(5)
Si(1)-Si(2)	2.3362(15)
Si(2)-C(10)	1.907(4)
Si(2)-Si(3)	2.3301(15)
Si(2)-Si(4)	2.3399(15)
Si(3)-N(2)	1.731(3)

Si(3)-C(11)	1.881(4)
Si(3)-C(12)	1.881(4)
Si(4)-N(3)	1.742(4)
Si(4)-C(20)	1.876(4)
Si(4)-C(21)	1.879(5)
N(1)-C(5)	1.427(5)
N(2)-C(13)	1.429(5)
N(3)-C(22)	1.429(5)
C(1)-C(2)	1.519(7)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-C(3)	1.376(6)
C(2)-C(7)	1.390(7)
C(3)-C(4)	1.407(6)
C(3)-H(3)	0.9500
C(4)-C(5)	1.384(6)
C(4)-H(4)	0.9500
C(5)-C(6)	1.394(6)
C(6)-C(7)	1.391(6)
C(6)-H(6)	0.9500
C(7)-H(7)	0.9500
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.389(6)
C(13)-C(19)	1.393(6)
C(14)-C(15)	1.371(7)
C(14)-H(14)	0.9500
C(15)-C(16)	1.406(7)
C(15)-H(15)	0.9500
C(16)-C(18)	1.357(7)
C(16)-C(17)	1.525(5)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-C(19)	1.389(7)
C(18)-H(18)	0.9500
C(19)-H(19)	0.9500
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(27)	1.384(6)
C(22)-C(23)	1.393(6)
C(23)-C(24)	1.392(6)
C(23)-H(23)	0.9500
C(24)-C(25)	1.395(7)
C(24)-H(24)	0.9500
C(25)-C(26)	1.380(8)
C(25)-C(38)	1.501(7)

C(26)-C(27)	1.393(7)
C(26)-H(26)	0.9500
C(27)-H(27)	0.9500
C(28)-C(29)	1.406(8)
C(28)-C(32)	1.410(8)
C(28)-H(28)	0.9500
C(29)-C(30)	1.418(8)
C(29)-H(29)	0.9500
C(30)-C(31)	1.393(8)
C(30)-H(30)	0.9500
C(31)-C(32)	1.413(7)
C(31)-H(31)	0.9500
C(32)-H(32)	0.9500
C(33)-C(37)	1.396(8)
C(33)-C(34)	1.397(8)
C(33)-H(33)	0.9500
C(34)-C(35)	1.395(8)
C(34)-H(34)	0.9500
C(35)-C(36)	1.409(9)
C(35)-H(35)	0.9500
C(36)-C(37)	1.390(9)
C(36)-H(36)	0.9500
C(37)-H(37)	0.9500
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-C(40)	1.376(7)
C(39)-C(44)	1.381(7)
C(39)-D(39)	0.9500
C(40)-C(41)	1.376(7)
C(40)-D(40)	0.9500
C(41)-C(42)	1.371(7)
C(41)-D(41)	0.9500
C(42)-C(43)	1.386(7)
C(42)-D(42)	0.9500
C(43)-C(44)	1.373(7)
C(43)-D(43)	0.9500
C(44)-D(44)	0.9500
Cl(1)-Hf(1)-C(28)	136.27(13)
Cl(1)-Hf(1)-C(32)	112.78(13)
C(28)-Hf(1)-C(32)	33.26(18)
Cl(1)-Hf(1)-C(34)	114.83(15)
C(28)-Hf(1)-C(34)	88.12(19)
C(32)-Hf(1)-C(34)	77.55(13)
Cl(1)-Hf(1)-C(33)	137.16(14)
C(28)-Hf(1)-C(33)	81.92(13)
C(32)-Hf(1)-C(33)	89.89(19)
C(34)-Hf(1)-C(33)	32.82(19)
Cl(1)-Hf(1)-C(31)	83.17(13)
C(28)-Hf(1)-C(31)	54.52(18)
C(32)-Hf(1)-C(31)	33.20(17)
C(34)-Hf(1)-C(31)	103.46(18)
C(33)-Hf(1)-C(31)	122.66(19)
Cl(1)-Hf(1)-C(29)	114.95(14)
C(28)-Hf(1)-C(29)	33.01(18)
C(32)-Hf(1)-C(29)	55.17(19)
C(34)-Hf(1)-C(29)	120.95(19)
C(33)-Hf(1)-C(29)	107.86(18)
C(31)-Hf(1)-C(29)	54.46(18)
Cl(1)-Hf(1)-C(35)	85.01(14)
C(28)-Hf(1)-C(35)	119.9(2)
C(32)-Hf(1)-C(35)	101.21(18)
C(34)-Hf(1)-C(35)	32.67(18)
C(33)-Hf(1)-C(35)	54.18(19)
C(31)-Hf(1)-C(35)	114.47(13)

C(29)-Hf(1)-C(35)	152.9(2)
Cl(1)-Hf(1)-C(36)	85.08(14)
C(28)-Hf(1)-C(36)	135.86(19)
C(32)-Hf(1)-C(36)	131.3(2)
C(34)-Hf(1)-C(36)	54.2(2)
C(33)-Hf(1)-C(36)	54.02(19)
C(31)-Hf(1)-C(36)	146.3(2)
C(29)-Hf(1)-C(36)	155.99(19)
C(35)-Hf(1)-C(36)	32.8(2)
Cl(1)-Hf(1)-C(30)	84.38(13)
C(28)-Hf(1)-C(30)	54.51(18)
C(32)-Hf(1)-C(30)	54.80(19)
C(34)-Hf(1)-C(30)	132.25(19)
C(33)-Hf(1)-C(30)	136.43(18)
C(31)-Hf(1)-C(30)	32.45(19)
C(29)-Hf(1)-C(30)	33.02(18)
C(35)-Hf(1)-C(30)	146.4(2)
C(36)-Hf(1)-C(30)	169.41(13)
Cl(1)-Hf(1)-C(37)	114.63(15)
C(28)-Hf(1)-C(37)	108.98(18)
C(32)-Hf(1)-C(37)	122.37(18)
C(34)-Hf(1)-C(37)	53.89(19)
C(33)-Hf(1)-C(37)	32.48(18)
C(31)-Hf(1)-C(37)	154.93(19)
C(29)-Hf(1)-C(37)	123.95(13)
C(35)-Hf(1)-C(37)	53.76(18)
C(36)-Hf(1)-C(37)	32.23(19)
C(30)-Hf(1)-C(37)	156.6(2)
Cl(1)-Hf(1)-Sn(1)	98.21(2)
C(28)-Hf(1)-Sn(1)	97.08(14)
C(32)-Hf(1)-Sn(1)	128.93(13)
C(34)-Hf(1)-Sn(1)	125.20(14)
C(33)-Hf(1)-Sn(1)	93.82(14)
C(31)-Hf(1)-Sn(1)	123.70(13)
C(29)-Hf(1)-Sn(1)	75.46(13)
C(35)-Hf(1)-Sn(1)	121.75(14)
C(36)-Hf(1)-Sn(1)	89.20(15)
C(30)-Hf(1)-Sn(1)	91.35(14)
C(37)-Hf(1)-Sn(1)	73.23(13)
N(2)-Sn(1)-N(3)	97.80(13)
N(2)-Sn(1)-N(1)	100.20(13)
N(3)-Sn(1)-N(1)	101.60(14)
N(2)-Sn(1)-Hf(1)	115.14(9)
N(3)-Sn(1)-Hf(1)	119.60(9)
N(1)-Sn(1)-Hf(1)	118.81(9)
N(1)-Si(1)-C(8)	113.7(2)
N(1)-Si(1)-C(9)	110.2(2)
C(8)-Si(1)-C(9)	108.0(2)
N(1)-Si(1)-Si(2)	104.28(11)
C(8)-Si(1)-Si(2)	111.67(16)
C(9)-Si(1)-Si(2)	108.87(15)
C(10)-Si(2)-Si(3)	114.11(14)
C(10)-Si(2)-Si(1)	113.96(17)
Si(3)-Si(2)-Si(1)	103.97(5)
C(10)-Si(2)-Si(4)	116.52(14)
Si(3)-Si(2)-Si(4)	102.81(6)
Si(1)-Si(2)-Si(4)	103.96(5)
N(2)-Si(3)-C(11)	109.19(18)
N(2)-Si(3)-C(12)	113.7(2)
C(11)-Si(3)-C(12)	107.8(2)
N(2)-Si(3)-Si(2)	103.11(11)
C(11)-Si(3)-Si(2)	111.13(15)
C(12)-Si(3)-Si(2)	111.86(17)
N(3)-Si(4)-C(20)	111.63(19)
N(3)-Si(4)-C(21)	110.8(2)

C(20)-Si(4)-C(21)	107.2(2)
N(3)-Si(4)-Si(2)	102.80(12)
C(20)-Si(4)-Si(2)	114.28(14)
C(21)-Si(4)-Si(2)	110.12(17)
C(5)-N(1)-Si(1)	120.7(3)
C(5)-N(1)-Sn(1)	116.0(3)
Si(1)-N(1)-Sn(1)	123.05(17)
C(13)-N(2)-Si(3)	117.4(2)
C(13)-N(2)-Sn(1)	117.8(2)
Si(3)-N(2)-Sn(1)	124.76(17)
C(22)-N(3)-Si(4)	117.8(3)
C(22)-N(3)-Sn(1)	117.5(3)
Si(4)-N(3)-Sn(1)	123.83(17)
C(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(3)-C(2)-C(7)	117.2(4)
C(3)-C(2)-C(1)	122.0(4)
C(7)-C(2)-C(1)	120.7(4)
C(2)-C(3)-C(4)	121.1(4)
C(2)-C(3)-H(3)	119.5
C(4)-C(3)-H(3)	119.5
C(5)-C(4)-C(3)	121.4(4)
C(5)-C(4)-H(4)	119.3
C(3)-C(4)-H(4)	119.3
C(4)-C(5)-C(6)	117.5(4)
C(4)-C(5)-N(1)	121.4(4)
C(6)-C(5)-N(1)	121.0(4)
C(7)-C(6)-C(5)	120.4(4)
C(7)-C(6)-H(6)	119.8
C(5)-C(6)-H(6)	119.8
C(2)-C(7)-C(6)	122.2(4)
C(2)-C(7)-H(7)	118.9
C(6)-C(7)-H(7)	118.9
Si(1)-C(8)-H(8A)	109.5
Si(1)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
Si(1)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
Si(1)-C(9)-H(9A)	109.5
Si(1)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
Si(1)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
Si(2)-C(10)-H(10A)	109.5
Si(2)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
Si(2)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
Si(3)-C(11)-H(11A)	109.5
Si(3)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
Si(3)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
Si(3)-C(12)-H(12A)	109.5
Si(3)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
Si(3)-C(12)-H(12C)	109.5

H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(19)	117.1(4)
C(14)-C(13)-N(2)	122.2(3)
C(19)-C(13)-N(2)	120.6(4)
C(15)-C(14)-C(13)	121.9(4)
C(15)-C(14)-H(14)	119.1
C(13)-C(14)-H(14)	119.1
C(14)-C(15)-C(16)	120.5(4)
C(14)-C(15)-H(15)	119.8
C(16)-C(15)-H(15)	119.8
C(18)-C(16)-C(15)	118.0(4)
C(18)-C(16)-C(17)	121.6(5)
C(15)-C(16)-C(17)	120.4(5)
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-C(19)	121.7(4)
C(16)-C(18)-H(18)	119.1
C(19)-C(18)-H(18)	119.1
C(18)-C(19)-C(13)	120.9(4)
C(18)-C(19)-H(19)	119.6
C(13)-C(19)-H(19)	119.6
Si(4)-C(20)-H(20A)	109.5
Si(4)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
Si(4)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
Si(4)-C(21)-H(21A)	109.5
Si(4)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
Si(4)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(27)-C(22)-C(23)	117.0(4)
C(27)-C(22)-N(3)	122.1(4)
C(23)-C(22)-N(3)	120.9(4)
C(24)-C(23)-C(22)	121.7(4)
C(24)-C(23)-H(23)	119.2
C(22)-C(23)-H(23)	119.2
C(23)-C(24)-C(25)	121.1(5)
C(23)-C(24)-H(24)	119.4
C(25)-C(24)-H(24)	119.4
C(26)-C(25)-C(24)	116.8(5)
C(26)-C(25)-C(38)	121.2(5)
C(24)-C(25)-C(38)	122.0(5)
C(25)-C(26)-C(27)	122.2(5)
C(25)-C(26)-H(26)	118.9
C(27)-C(26)-H(26)	118.9
C(22)-C(27)-C(26)	121.1(5)
C(22)-C(27)-H(27)	119.4
C(26)-C(27)-H(27)	119.4
C(29)-C(28)-C(32)	108.9(5)
C(29)-C(28)-Hf(1)	74.3(3)
C(32)-C(28)-Hf(1)	73.4(3)
C(29)-C(28)-H(28)	125.5
C(32)-C(28)-H(28)	125.5
Hf(1)-C(28)-H(28)	118.5
C(28)-C(29)-C(30)	107.4(5)

C(28)-C(29)-Hf(1)	72.7(3)
C(30)-C(29)-Hf(1)	74.3(3)
C(28)-C(29)-H(29)	126.3
C(30)-C(29)-H(29)	126.3
Hf(1)-C(29)-H(29)	118.7
C(31)-C(30)-C(29)	107.8(5)
C(31)-C(30)-Hf(1)	72.8(3)
C(29)-C(30)-Hf(1)	72.7(2)
C(31)-C(30)-H(30)	126.1
C(29)-C(30)-H(30)	126.1
Hf(1)-C(30)-H(30)	120.2
C(30)-C(31)-C(32)	109.2(5)
C(30)-C(31)-Hf(1)	74.7(3)
C(32)-C(31)-Hf(1)	72.8(3)
C(30)-C(31)-H(31)	125.4
C(32)-C(31)-H(31)	125.4
Hf(1)-C(31)-H(31)	118.9
C(28)-C(32)-C(31)	106.7(5)
C(28)-C(32)-Hf(1)	73.3(3)
C(31)-C(32)-Hf(1)	74.0(3)
C(28)-C(32)-H(32)	126.7
C(31)-C(32)-H(32)	126.7
Hf(1)-C(32)-H(32)	118.1
C(37)-C(33)-C(34)	107.7(5)
C(37)-C(33)-Hf(1)	75.0(3)
C(34)-C(33)-Hf(1)	73.1(3)
C(37)-C(33)-H(33)	126.1
C(34)-C(33)-H(33)	126.1
Hf(1)-C(33)-H(33)	117.8
C(35)-C(34)-C(33)	108.4(5)
C(35)-C(34)-Hf(1)	74.8(3)
C(33)-C(34)-Hf(1)	74.1(3)
C(35)-C(34)-H(34)	125.8
C(33)-C(34)-H(34)	125.8
Hf(1)-C(34)-H(34)	117.3
C(34)-C(35)-C(36)	107.5(5)
C(34)-C(35)-Hf(1)	72.5(3)
C(36)-C(35)-Hf(1)	73.7(3)
C(34)-C(35)-H(35)	126.3
C(36)-C(35)-H(35)	126.3
Hf(1)-C(35)-H(35)	119.4
C(37)-C(36)-C(35)	107.9(5)
C(37)-C(36)-Hf(1)	74.4(3)
C(35)-C(36)-Hf(1)	73.5(3)
C(37)-C(36)-H(36)	126.0
C(35)-C(36)-H(36)	126.0
Hf(1)-C(36)-H(36)	118.0
C(36)-C(37)-C(33)	108.4(6)
C(36)-C(37)-Hf(1)	73.3(3)
C(33)-C(37)-Hf(1)	72.5(3)
C(36)-C(37)-H(37)	125.8
C(33)-C(37)-H(37)	125.8
Hf(1)-C(37)-H(37)	120.2
C(25)-C(38)-H(38A)	109.5
C(25)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(25)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(40)-C(39)-C(44)	120.2(5)
C(40)-C(39)-D(39)	119.9
C(44)-C(39)-D(39)	119.9
C(39)-C(40)-C(41)	119.3(5)
C(39)-C(40)-D(40)	120.4
C(41)-C(40)-D(40)	120.4

C(42)-C(41)-C(40)	121.2(5)
C(42)-C(41)-D(41)	119.4
C(40)-C(41)-D(41)	119.4
C(41)-C(42)-C(43)	119.3(5)
C(41)-C(42)-D(42)	120.4
C(43)-C(42)-D(42)	120.4
C(44)-C(43)-C(42)	120.0(5)
C(44)-C(43)-D(43)	120.0
C(42)-C(43)-D(43)	120.0
C(43)-C(44)-C(39)	120.1(5)
C(43)-C(44)-D(44)	119.9
C(39)-C(44)-D(44)	119.9

Symmetry transformations used to generate equivalent atoms:

Table S10. Anisotropic displacement parameters (A^2 x 10^3) for structure 2. 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
Hf(1)	16(1)	18(1)	24(1)	0(1)	0(1)	1(1)
Sn(1)	14(1)	13(1)	16(1)	0(1)	-1(1)	1(1)
Cl(1)	26(1)	37(1)	23(1)	-3(1)	1(1)	-4(1)
Si(1)	19(1)	16(1)	18(1)	-1(1)	1(1)	2(1)
Si(2)	17(1)	16(1)	18(1)	1(1)	0(1)	0(1)
Si(3)	21(1)	20(1)	17(1)	2(1)	-1(1)	-1(1)
Si(4)	18(1)	19(1)	20(1)	-3(1)	-1(1)	0(1)
N(1)	20(2)	13(2)	18(2)	1(2)	7(2)	3(1)
N(2)	19(2)	23(2)	19(2)	2(1)	-3(2)	-3(1)
N(3)	20(2)	18(2)	19(2)	-6(2)	4(2)	3(1)
C(1)	34(4)	30(3)	36(3)	10(2)	8(3)	1(2)
C(2)	15(3)	25(2)	22(3)	9(2)	-1(2)	-4(2)
C(3)	19(3)	27(2)	18(3)	-1(2)	-2(2)	4(2)
C(4)	16(2)	12(2)	30(3)	-1(2)	-4(2)	-1(2)
C(5)	12(2)	22(2)	18(2)	4(2)	0(2)	6(2)
C(6)	26(3)	17(2)	18(3)	1(2)	4(2)	0(2)
C(7)	24(3)	15(2)	27(3)	0(2)	-3(2)	-1(2)
C(8)	35(3)	20(2)	30(3)	-5(2)	1(2)	-1(2)
C(9)	22(3)	27(2)	24(3)	2(2)	5(2)	2(2)
C(10)	28(2)	28(2)	34(2)	-4(2)	4(2)	2(3)
C(11)	46(3)	36(3)	15(2)	3(2)	6(2)	-1(2)
C(12)	31(3)	23(2)	33(3)	10(2)	-3(2)	-4(2)
C(13)	20(2)	27(2)	16(2)	3(2)	3(2)	-1(2)
C(14)	29(3)	20(2)	22(3)	6(2)	-4(2)	8(2)
C(15)	34(3)	25(2)	37(3)	-3(2)	-9(3)	3(2)
C(16)	28(2)	34(2)	24(2)	2(3)	-3(2)	-5(3)
C(17)	43(3)	52(3)	43(2)	-1(3)	-23(2)	-11(4)
C(18)	30(3)	35(3)	35(3)	12(2)	-15(3)	4(2)
C(19)	30(3)	19(2)	38(3)	6(2)	-5(2)	-6(2)
C(20)	28(3)	31(2)	27(2)	0(2)	-8(2)	5(2)
C(21)	24(3)	25(2)	33(3)	-7(2)	1(2)	-5(2)
C(22)	12(2)	21(2)	21(3)	-6(2)	-1(2)	-2(2)
C(23)	17(3)	18(2)	27(3)	0(2)	-1(2)	-3(2)
C(24)	14(3)	33(3)	25(3)	-9(2)	1(2)	-3(2)
C(25)	22(3)	26(2)	33(3)	-14(2)	1(2)	-7(2)

C(26)	34(4)	16(2)	44(3)	-3(2)	3(3)	1(2)
C(27)	29(3)	23(2)	20(3)	3(2)	3(2)	-1(2)
C(28)	34(3)	26(2)	29(3)	-5(2)	-13(3)	-13(2)
C(29)	25(3)	15(2)	40(3)	-14(2)	2(3)	-3(2)
C(30)	21(3)	12(2)	46(4)	2(2)	-5(3)	-7(2)
C(31)	28(3)	24(2)	31(3)	1(2)	3(3)	-17(2)
C(32)	19(3)	26(3)	42(3)	-1(2)	-2(3)	-9(2)
C(33)	36(4)	31(3)	33(3)	13(2)	-6(3)	6(2)
C(34)	18(3)	25(3)	61(4)	4(3)	-10(3)	5(2)
C(35)	32(4)	18(2)	53(4)	-1(2)	10(3)	14(2)
C(36)	36(4)	11(2)	48(4)	-2(2)	-4(4)	2(2)
C(37)	27(3)	16(2)	48(4)	14(2)	4(3)	5(2)
C(38)	43(4)	38(3)	49(4)	-22(3)	11(3)	-3(3)
C(39)	37(3)	31(2)	28(3)	2(2)	-8(3)	8(2)
C(40)	29(3)	35(3)	20(2)	0(2)	0(2)	2(2)
C(41)	20(3)	47(3)	34(3)	-8(2)	-5(2)	8(2)
C(42)	36(3)	50(3)	24(3)	2(2)	-5(3)	15(2)
C(43)	32(3)	51(3)	22(3)	4(2)	4(2)	7(2)
C(44)	29(3)	40(3)	39(3)	-3(3)	3(3)	8(2)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for structure 2.

	x	y	z	U(eq)
H(1A)	6852	1672	2355	50
H(1B)	5727	1504	2000	50
H(1C)	5796	2166	2520	50
H(3)	6405	3426	2197	25
H(4)	6968	4275	1408	23
H(6)	7186	2537	164	25
H(7)	6726	1693	968	26
H(8A)	7896	2806	-887	42
H(8B)	8861	3228	-1255	42
H(8C)	7663	3584	-1257	42
H(9A)	9831	3614	542	37
H(9B)	10208	3206	-99	37
H(9C)	9280	2829	330	37
H(10A)	10558	4859	-1321	45
H(10B)	11093	4728	-638	45
H(10C)	10900	5574	-895	45
H(11A)	7833	4657	-1966	48
H(11B)	8619	5341	-2169	48
H(11C)	7330	5434	-2231	48
H(12A)	7431	6868	-1480	43
H(12B)	8711	6797	-1362	43
H(12C)	7901	6886	-773	43
H(14)	5641	4051	-1151	29
H(15)	4194	3904	-1833	39
H(17A)	2361	5077	-2300	69
H(17B)	3012	4400	-2637	69
H(17C)	3171	5258	-2875	69
H(18)	4061	6172	-2082	40
H(19)	5501	6327	-1383	35
H(20A)	9526	5563	1525	43
H(20B)	10418	5178	1074	43
H(20C)	9291	4752	1207	43
H(21A)	9449	6939	-26	41

H(21B)	10473	6635	367	41
H(21C)	9467	7014	730	41
H(23)	6940	5710	1693	25
H(24)	6306	6635	2386	29
H(26)	6712	8223	1033	38
H(27)	7302	7295	331	28
H(28)	3362	4279	-533	36
H(29)	5074	3681	-103	32
H(30)	4750	3383	1060	31
H(31)	2875	3823	1339	34
H(32)	1998	4385	360	35
H(33)	3483	5785	-567	40
H(34)	2067	5734	291	42
H(35)	2863	6303	1281	41
H(36)	4810	6666	1040	38
H(37)	5158	6390	-108	36
H(38A)	6665	8559	2248	65
H(38B)	6043	7939	2668	65
H(38C)	5418	8365	2105	65
D(39)	11149	1891	3100	38
D(40)	9319	2126	3306	34
D(41)	8256	2711	2537	40
D(42)	8984	3040	1562	44
D(43)	10818	2789	1353	42
D(44)	11902	2242	2130	44

Table S12. Torsion angles [deg] for structure 2.

Cl(1)-Hf(1)-Sn(1)-N(2)	-165.67(10)
C(28)-Hf(1)-Sn(1)-N(2)	55.42(15)
C(32)-Hf(1)-Sn(1)-N(2)	66.06(18)
C(34)-Hf(1)-Sn(1)-N(2)	-37.28(19)
C(33)-Hf(1)-Sn(1)-N(2)	-26.90(16)
C(31)-Hf(1)-Sn(1)-N(2)	107.09(18)
C(29)-Hf(1)-Sn(1)-N(2)	80.58(16)
C(35)-Hf(1)-Sn(1)-N(2)	-76.48(19)
C(36)-Hf(1)-Sn(1)-N(2)	-80.75(17)
C(30)-Hf(1)-Sn(1)-N(2)	109.82(16)
C(37)-Hf(1)-Sn(1)-N(2)	-52.32(17)
Cl(1)-Hf(1)-Sn(1)-N(3)	-49.63(12)
C(28)-Hf(1)-Sn(1)-N(3)	171.47(16)
C(32)-Hf(1)-Sn(1)-N(3)	-177.90(19)
C(34)-Hf(1)-Sn(1)-N(3)	78.8(2)
C(33)-Hf(1)-Sn(1)-N(3)	89.15(17)
C(31)-Hf(1)-Sn(1)-N(3)	-136.87(19)
C(29)-Hf(1)-Sn(1)-N(3)	-163.38(17)
C(35)-Hf(1)-Sn(1)-N(3)	39.6(2)
C(36)-Hf(1)-Sn(1)-N(3)	35.29(18)
C(30)-Hf(1)-Sn(1)-N(3)	-134.14(17)
C(37)-Hf(1)-Sn(1)-N(3)	63.72(18)
Cl(1)-Hf(1)-Sn(1)-N(1)	75.56(12)
C(28)-Hf(1)-Sn(1)-N(1)	-63.35(16)
C(32)-Hf(1)-Sn(1)-N(1)	-52.7(2)
C(34)-Hf(1)-Sn(1)-N(1)	-156.1(2)
C(33)-Hf(1)-Sn(1)-N(1)	-145.67(17)
C(31)-Hf(1)-Sn(1)-N(1)	-11.68(18)
C(29)-Hf(1)-Sn(1)-N(1)	-38.19(18)
C(35)-Hf(1)-Sn(1)-N(1)	164.8(2)
C(36)-Hf(1)-Sn(1)-N(1)	160.47(18)
C(30)-Hf(1)-Sn(1)-N(1)	-8.95(17)

C(37)-Hf(1)-Sn(1)-N(1)	-171.10(19)
N(1)-Si(1)-Si(2)-C(10)	167.52(18)
C(8)-Si(1)-Si(2)-C(10)	-69.3(2)
C(9)-Si(1)-Si(2)-C(10)	49.9(2)
N(1)-Si(1)-Si(2)-Si(3)	-67.64(13)
C(8)-Si(1)-Si(2)-Si(3)	55.58(19)
C(9)-Si(1)-Si(2)-Si(3)	174.71(17)
N(1)-Si(1)-Si(2)-Si(4)	39.65(14)
C(8)-Si(1)-Si(2)-Si(4)	162.87(19)
C(9)-Si(1)-Si(2)-Si(4)	-78.00(18)
C(10)-Si(2)-Si(3)-N(2)	164.5(2)
Si(1)-Si(2)-Si(3)-N(2)	39.79(12)
Si(4)-Si(2)-Si(3)-N(2)	-68.36(12)
C(10)-Si(2)-Si(3)-C(11)	47.7(2)
Si(1)-Si(2)-Si(3)-C(11)	-77.07(16)
Si(4)-Si(2)-Si(3)-C(11)	174.78(15)
C(10)-Si(2)-Si(3)-C(12)	-72.9(3)
Si(1)-Si(2)-Si(3)-C(12)	162.35(19)
Si(4)-Si(2)-Si(3)-C(12)	54.2(2)
C(10)-Si(2)-Si(4)-N(3)	164.9(2)
Si(3)-Si(2)-Si(4)-N(3)	39.36(13)
Si(1)-Si(2)-Si(4)-N(3)	-68.79(13)
C(10)-Si(2)-Si(4)-C(20)	-73.9(2)
Si(3)-Si(2)-Si(4)-C(20)	160.49(16)
Si(1)-Si(2)-Si(4)-C(20)	52.34(16)
C(10)-Si(2)-Si(4)-C(21)	46.8(3)
Si(3)-Si(2)-Si(4)-C(21)	-78.75(18)
Si(1)-Si(2)-Si(4)-C(21)	173.10(17)
C(8)-Si(1)-N(1)-C(5)	90.3(4)
C(9)-Si(1)-N(1)-C(5)	-31.1(4)
Si(2)-Si(1)-N(1)-C(5)	-147.8(3)
C(8)-Si(1)-N(1)-Sn(1)	-95.3(2)
C(9)-Si(1)-N(1)-Sn(1)	143.3(2)
Si(2)-Si(1)-N(1)-Sn(1)	26.6(2)
N(2)-Sn(1)-N(1)-C(5)	-153.3(3)
N(3)-Sn(1)-N(1)-C(5)	106.5(3)
Hf(1)-Sn(1)-N(1)-C(5)	-27.0(3)
N(2)-Sn(1)-N(1)-Si(1)	32.1(2)
N(3)-Sn(1)-N(1)-Si(1)	-68.1(3)
Hf(1)-Sn(1)-N(1)-Si(1)	158.38(16)
C(11)-Si(3)-N(2)-C(13)	-32.4(3)
C(12)-Si(3)-N(2)-C(13)	88.0(3)
Si(2)-Si(3)-N(2)-C(13)	-150.7(2)
C(11)-Si(3)-N(2)-Sn(1)	145.5(2)
C(12)-Si(3)-N(2)-Sn(1)	-94.0(3)
Si(2)-Si(3)-N(2)-Sn(1)	27.3(2)
N(3)-Sn(1)-N(2)-C(13)	-148.9(3)
N(1)-Sn(1)-N(2)-C(13)	107.7(3)
Hf(1)-Sn(1)-N(2)-C(13)	-21.0(3)
N(3)-Sn(1)-N(2)-Si(3)	33.1(2)
N(1)-Sn(1)-N(2)-Si(3)	-70.2(2)
Hf(1)-Sn(1)-N(2)-Si(3)	161.08(15)
C(20)-Si(4)-N(3)-C(22)	76.0(4)
C(21)-Si(4)-N(3)-C(22)	-43.4(4)
Si(2)-Si(4)-N(3)-C(22)	-161.0(3)
C(20)-Si(4)-N(3)-Sn(1)	-93.0(2)
C(21)-Si(4)-N(3)-Sn(1)	147.6(2)
Si(2)-Si(4)-N(3)-Sn(1)	30.0(2)
N(2)-Sn(1)-N(3)-C(22)	118.0(3)
N(1)-Sn(1)-N(3)-C(22)	-139.8(3)
Hf(1)-Sn(1)-N(3)-C(22)	-6.8(3)
N(2)-Sn(1)-N(3)-Si(4)	-73.0(2)
N(1)-Sn(1)-N(3)-Si(4)	29.2(3)
Hf(1)-Sn(1)-N(3)-Si(4)	162.20(16)
C(7)-C(2)-C(3)-C(4)	0.1(6)

C(1)-C(2)-C(3)-C(4)	177.5(5)
C(2)-C(3)-C(4)-C(5)	2.3(8)
C(3)-C(4)-C(5)-C(6)	-2.6(7)
C(3)-C(4)-C(5)-N(1)	178.1(4)
Si(1)-N(1)-C(5)-C(4)	131.2(4)
Sn(1)-N(1)-C(5)-C(4)	-43.6(5)
Si(1)-N(1)-C(5)-C(6)	-48.2(5)
Sn(1)-N(1)-C(5)-C(6)	137.1(4)
C(4)-C(5)-C(6)-C(7)	0.6(7)
N(1)-C(5)-C(6)-C(7)	179.9(4)
C(3)-C(2)-C(7)-C(6)	-2.2(8)
C(1)-C(2)-C(7)-C(6)	-179.5(5)
C(5)-C(6)-C(7)-C(2)	1.9(8)
Si(3)-N(2)-C(13)-C(14)	108.7(4)
Sn(1)-N(2)-C(13)-C(14)	-69.4(5)
Si(3)-N(2)-C(13)-C(19)	-67.2(5)
Sn(1)-N(2)-C(13)-C(19)	114.7(4)
C(19)-C(13)-C(14)-C(15)	-0.4(7)
N(2)-C(13)-C(14)-C(15)	-176.5(4)
C(13)-C(14)-C(15)-C(16)	0.8(8)
C(14)-C(15)-C(16)-C(18)	-0.7(6)
C(14)-C(15)-C(16)-C(17)	178.2(4)
C(15)-C(16)-C(18)-C(19)	0.1(7)
C(17)-C(16)-C(18)-C(19)	-178.7(5)
C(16)-C(18)-C(19)-C(13)	0.2(8)
C(14)-C(13)-C(19)-C(18)	-0.1(7)
N(2)-C(13)-C(19)-C(18)	176.0(4)
Si(4)-N(3)-C(22)-C(27)	82.2(5)
Sn(1)-N(3)-C(22)-C(27)	-108.1(4)
Si(4)-N(3)-C(22)-C(23)	-98.0(5)
Sn(1)-N(3)-C(22)-C(23)	71.7(5)
C(27)-C(22)-C(23)-C(24)	-1.3(7)
N(3)-C(22)-C(23)-C(24)	178.9(4)
C(22)-C(23)-C(24)-C(25)	-0.8(8)
C(23)-C(24)-C(25)-C(26)	2.0(8)
C(23)-C(24)-C(25)-C(38)	-176.7(5)
C(24)-C(25)-C(26)-C(27)	-1.1(9)
C(38)-C(25)-C(26)-C(27)	177.6(5)
C(23)-C(22)-C(27)-C(26)	2.2(7)
N(3)-C(22)-C(27)-C(26)	-178.0(5)
C(25)-C(26)-C(27)-C(22)	-1.0(8)
Cl(1)-Hf(1)-C(28)-C(29)	-60.7(4)
C(32)-Hf(1)-C(28)-C(29)	-115.8(5)
C(34)-Hf(1)-C(28)-C(29)	174.3(4)
C(33)-Hf(1)-C(28)-C(29)	141.9(4)
C(31)-Hf(1)-C(28)-C(29)	-77.7(3)
C(35)-Hf(1)-C(28)-C(29)	-177.9(3)
C(36)-Hf(1)-C(28)-C(29)	145.2(3)
C(30)-Hf(1)-C(28)-C(29)	-37.6(3)
C(37)-Hf(1)-C(28)-C(29)	123.7(3)
Sn(1)-Hf(1)-C(28)-C(29)	49.0(3)
Cl(1)-Hf(1)-C(28)-C(32)	55.1(4)
C(34)-Hf(1)-C(28)-C(32)	-69.9(3)
C(33)-Hf(1)-C(28)-C(32)	-102.3(3)
C(31)-Hf(1)-C(28)-C(32)	38.1(3)
C(29)-Hf(1)-C(28)-C(32)	115.8(5)
C(35)-Hf(1)-C(28)-C(32)	-62.1(4)
C(36)-Hf(1)-C(28)-C(32)	-99.0(4)
C(30)-Hf(1)-C(28)-C(32)	78.2(3)
C(37)-Hf(1)-C(28)-C(32)	-120.5(3)
Sn(1)-Hf(1)-C(28)-C(32)	164.8(3)
C(32)-C(28)-C(29)-C(30)	0.9(5)
Hf(1)-C(28)-C(29)-C(30)	66.7(3)
C(32)-C(28)-C(29)-Hf(1)	-65.8(3)
Cl(1)-Hf(1)-C(29)-C(28)	138.3(3)

C(32)-Hf(1)-C(29)-C(28)	37.0(3)
C(34)-Hf(1)-C(29)-C(28)	-6.7(4)
C(33)-Hf(1)-C(29)-C(28)	-39.9(4)
C(31)-Hf(1)-C(29)-C(28)	77.9(4)
C(35)-Hf(1)-C(29)-C(28)	4.0(6)
C(36)-Hf(1)-C(29)-C(28)	-77.4(6)
C(30)-Hf(1)-C(29)-C(28)	114.4(5)
C(37)-Hf(1)-C(29)-C(28)	-71.5(3)
Sn(1)-Hf(1)-C(29)-C(28)	-129.3(3)
Cl(1)-Hf(1)-C(29)-C(30)	23.9(4)
C(28)-Hf(1)-C(29)-C(30)	-114.4(5)
C(32)-Hf(1)-C(29)-C(30)	-77.4(4)
C(34)-Hf(1)-C(29)-C(30)	-121.1(4)
C(33)-Hf(1)-C(29)-C(30)	-154.3(4)
C(31)-Hf(1)-C(29)-C(30)	-36.5(3)
C(35)-Hf(1)-C(29)-C(30)	-110.3(5)
C(36)-Hf(1)-C(29)-C(30)	168.2(3)
C(37)-Hf(1)-C(29)-C(30)	174.1(4)
Sn(1)-Hf(1)-C(29)-C(30)	116.3(4)
C(28)-C(29)-C(30)-C(31)	-0.7(5)
Hf(1)-C(29)-C(30)-C(31)	64.9(3)
C(28)-C(29)-C(30)-Hf(1)	-65.6(3)
Cl(1)-Hf(1)-C(30)-C(31)	86.1(3)
C(28)-Hf(1)-C(30)-C(31)	-78.0(4)
C(32)-Hf(1)-C(30)-C(31)	-37.0(3)
C(34)-Hf(1)-C(30)-C(31)	-32.6(5)
C(33)-Hf(1)-C(30)-C(31)	-78.8(4)
C(29)-Hf(1)-C(30)-C(31)	-115.6(5)
C(35)-Hf(1)-C(30)-C(31)	13.9(6)
C(36)-Hf(1)-C(30)-C(31)	91.3(8)
C(37)-Hf(1)-C(30)-C(31)	-128.0(5)
Sn(1)-Hf(1)-C(30)-C(31)	-175.8(3)
Cl(1)-Hf(1)-C(30)-C(29)	-158.3(4)
C(28)-Hf(1)-C(30)-C(29)	37.5(3)
C(32)-Hf(1)-C(30)-C(29)	78.6(4)
C(34)-Hf(1)-C(30)-C(29)	83.0(4)
C(33)-Hf(1)-C(30)-C(29)	36.8(5)
C(31)-Hf(1)-C(30)-C(29)	115.6(5)
C(35)-Hf(1)-C(30)-C(29)	129.5(4)
C(36)-Hf(1)-C(30)-C(29)	-153.1(7)
C(37)-Hf(1)-C(30)-C(29)	-12.5(8)
Sn(1)-Hf(1)-C(30)-C(29)	-60.2(3)
C(29)-C(30)-C(31)-C(32)	0.3(5)
Hf(1)-C(30)-C(31)-C(32)	65.1(3)
C(29)-C(30)-C(31)-Hf(1)	-64.8(3)
Cl(1)-Hf(1)-C(31)-C(30)	-90.3(3)
C(28)-Hf(1)-C(31)-C(30)	78.0(4)
C(32)-Hf(1)-C(31)-C(30)	116.2(5)
C(34)-Hf(1)-C(31)-C(30)	155.8(3)
C(33)-Hf(1)-C(31)-C(30)	126.6(3)
C(29)-Hf(1)-C(31)-C(30)	37.2(3)
C(35)-Hf(1)-C(31)-C(30)	-171.6(4)
C(36)-Hf(1)-C(31)-C(30)	-160.7(3)
C(37)-Hf(1)-C(31)-C(30)	132.5(5)
Sn(1)-Hf(1)-C(31)-C(30)	5.1(4)
Cl(1)-Hf(1)-C(31)-C(32)	153.6(3)
C(28)-Hf(1)-C(31)-C(32)	-38.2(3)
C(34)-Hf(1)-C(31)-C(32)	39.6(4)
C(33)-Hf(1)-C(31)-C(32)	10.4(4)
C(29)-Hf(1)-C(31)-C(32)	-79.0(3)
C(35)-Hf(1)-C(31)-C(32)	72.2(3)
C(36)-Hf(1)-C(31)-C(32)	83.1(4)
C(30)-Hf(1)-C(31)-C(32)	-116.2(5)
C(37)-Hf(1)-C(31)-C(32)	16.3(6)
Sn(1)-Hf(1)-C(31)-C(32)	-111.1(3)

C(29)-C(28)-C(32)-C(31)	-0.6(5)
Hf(1)-C(28)-C(32)-C(31)	-67.1(3)
C(29)-C(28)-C(32)-Hf(1)	66.4(3)
C(30)-C(31)-C(32)-C(28)	0.2(5)
Hf(1)-C(31)-C(32)-C(28)	66.6(3)
C(30)-C(31)-C(32)-Hf(1)	-66.4(3)
Cl(1)-Hf(1)-C(32)-C(28)	-142.1(3)
C(34)-Hf(1)-C(32)-C(28)	106.0(4)
C(33)-Hf(1)-C(32)-C(28)	75.3(3)
C(31)-Hf(1)-C(32)-C(28)	-113.4(4)
C(29)-Hf(1)-C(32)-C(28)	-36.7(3)
C(35)-Hf(1)-C(32)-C(28)	128.7(3)
C(36)-Hf(1)-C(32)-C(28)	113.7(3)
C(30)-Hf(1)-C(32)-C(28)	-77.3(3)
C(37)-Hf(1)-C(32)-C(28)	74.7(4)
Sn(1)-Hf(1)-C(32)-C(28)	-19.5(4)
Cl(1)-Hf(1)-C(32)-C(31)	-28.7(3)
C(28)-Hf(1)-C(32)-C(31)	113.4(4)
C(34)-Hf(1)-C(32)-C(31)	-140.6(4)
C(33)-Hf(1)-C(32)-C(31)	-171.3(3)
C(29)-Hf(1)-C(32)-C(31)	76.7(3)
C(35)-Hf(1)-C(32)-C(31)	-117.9(3)
C(36)-Hf(1)-C(32)-C(31)	-132.8(3)
C(30)-Hf(1)-C(32)-C(31)	36.1(3)
C(37)-Hf(1)-C(32)-C(31)	-171.9(3)
Sn(1)-Hf(1)-C(32)-C(31)	93.9(3)
Cl(1)-Hf(1)-C(33)-C(37)	56.4(4)
C(28)-Hf(1)-C(33)-C(37)	-146.6(4)
C(32)-Hf(1)-C(33)-C(37)	-179.0(4)
C(34)-Hf(1)-C(33)-C(37)	114.3(5)
C(31)-Hf(1)-C(33)-C(37)	175.4(3)
C(29)-Hf(1)-C(33)-C(37)	-125.9(3)
C(35)-Hf(1)-C(33)-C(37)	77.1(4)
C(36)-Hf(1)-C(33)-C(37)	36.3(3)
C(30)-Hf(1)-C(33)-C(37)	-146.0(3)
Sn(1)-Hf(1)-C(33)-C(37)	-50.0(3)
Cl(1)-Hf(1)-C(33)-C(34)	-57.8(4)
C(28)-Hf(1)-C(33)-C(34)	99.1(4)
C(32)-Hf(1)-C(33)-C(34)	66.7(3)
C(31)-Hf(1)-C(33)-C(34)	61.1(4)
C(29)-Hf(1)-C(33)-C(34)	119.8(3)
C(35)-Hf(1)-C(33)-C(34)	-37.2(3)
C(36)-Hf(1)-C(33)-C(34)	-78.0(4)
C(30)-Hf(1)-C(33)-C(34)	99.8(4)
C(37)-Hf(1)-C(33)-C(34)	-114.3(5)
Sn(1)-Hf(1)-C(33)-C(34)	-164.2(3)
C(37)-C(33)-C(34)-C(35)	-0.1(6)
Hf(1)-C(33)-C(34)-C(35)	67.6(4)
C(37)-C(33)-C(34)-Hf(1)	-67.6(3)
Cl(1)-Hf(1)-C(34)-C(35)	25.9(4)
C(28)-Hf(1)-C(34)-C(35)	167.3(4)
C(32)-Hf(1)-C(34)-C(35)	135.5(4)
C(33)-Hf(1)-C(34)-C(35)	-114.7(5)
C(31)-Hf(1)-C(34)-C(35)	114.6(3)
C(29)-Hf(1)-C(34)-C(35)	171.0(3)
C(36)-Hf(1)-C(34)-C(35)	-37.3(3)
C(30)-Hf(1)-C(34)-C(35)	131.9(3)
C(37)-Hf(1)-C(34)-C(35)	-77.4(4)
Sn(1)-Hf(1)-C(34)-C(35)	-95.3(3)
Cl(1)-Hf(1)-C(34)-C(33)	140.6(3)
C(28)-Hf(1)-C(34)-C(33)	-78.0(3)
C(32)-Hf(1)-C(34)-C(33)	-109.8(4)
C(31)-Hf(1)-C(34)-C(33)	-130.7(3)
C(29)-Hf(1)-C(34)-C(33)	-74.3(4)
C(35)-Hf(1)-C(34)-C(33)	114.7(5)

C(36)-Hf(1)-C(34)-C(33)	77.4(4)
C(30)-Hf(1)-C(34)-C(33)	-113.4(4)
C(37)-Hf(1)-C(34)-C(33)	37.3(3)
Sn(1)-Hf(1)-C(34)-C(33)	19.4(4)
C(33)-C(34)-C(35)-C(36)	-1.1(6)
Hf(1)-C(34)-C(35)-C(36)	65.9(3)
C(33)-C(34)-C(35)-Hf(1)	-67.1(4)
Cl(1)-Hf(1)-C(35)-C(34)	-156.5(3)
C(28)-Hf(1)-C(35)-C(34)	-14.6(4)
C(32)-Hf(1)-C(35)-C(34)	-44.2(4)
C(33)-Hf(1)-C(35)-C(34)	37.4(3)
C(31)-Hf(1)-C(35)-C(34)	-76.4(4)
C(29)-Hf(1)-C(35)-C(34)	-17.2(6)
C(36)-Hf(1)-C(35)-C(34)	114.8(5)
C(30)-Hf(1)-C(35)-C(34)	-84.5(5)
C(37)-Hf(1)-C(35)-C(34)	77.8(4)
Sn(1)-Hf(1)-C(35)-C(34)	106.9(3)
Cl(1)-Hf(1)-C(35)-C(36)	88.7(3)
C(28)-Hf(1)-C(35)-C(36)	-129.5(4)
C(32)-Hf(1)-C(35)-C(36)	-159.1(4)
C(34)-Hf(1)-C(35)-C(36)	-114.8(5)
C(33)-Hf(1)-C(35)-C(36)	-77.4(4)
C(31)-Hf(1)-C(35)-C(36)	168.8(4)
C(29)-Hf(1)-C(35)-C(36)	-132.0(4)
C(30)-Hf(1)-C(35)-C(36)	160.7(2)
C(37)-Hf(1)-C(35)-C(36)	-37.0(3)
Sn(1)-Hf(1)-C(35)-C(36)	-7.9(4)
C(34)-C(35)-C(36)-C(37)	1.9(5)
Hf(1)-C(35)-C(36)-C(37)	67.1(3)
C(34)-C(35)-C(36)-Hf(1)	-65.2(3)
Cl(1)-Hf(1)-C(36)-C(37)	157.0(4)
C(28)-Hf(1)-C(36)-C(37)	-40.6(5)
C(32)-Hf(1)-C(36)-C(37)	-86.7(4)
C(34)-Hf(1)-C(36)-C(37)	-77.4(4)
C(33)-Hf(1)-C(36)-C(37)	-36.6(3)
C(31)-Hf(1)-C(36)-C(37)	-133.1(4)
C(29)-Hf(1)-C(36)-C(37)	9.2(8)
C(35)-Hf(1)-C(36)-C(37)	-114.5(5)
C(30)-Hf(1)-C(36)-C(37)	151.8(7)
Sn(1)-Hf(1)-C(36)-C(37)	58.7(4)
Cl(1)-Hf(1)-C(36)-C(35)	-88.4(3)
C(28)-Hf(1)-C(36)-C(35)	73.9(4)
C(32)-Hf(1)-C(36)-C(35)	27.8(5)
C(34)-Hf(1)-C(36)-C(35)	37.2(3)
C(33)-Hf(1)-C(36)-C(35)	78.0(4)
C(31)-Hf(1)-C(36)-C(35)	-18.5(6)
C(29)-Hf(1)-C(36)-C(35)	123.7(5)
C(30)-Hf(1)-C(36)-C(35)	-93.6(8)
C(37)-Hf(1)-C(36)-C(35)	114.5(5)
Sn(1)-Hf(1)-C(36)-C(35)	173.3(3)
C(35)-C(36)-C(37)-C(33)	-2.0(5)
Hf(1)-C(36)-C(37)-C(33)	64.5(3)
C(35)-C(36)-C(37)-Hf(1)	-66.4(3)
C(34)-C(33)-C(37)-C(36)	1.3(5)
Hf(1)-C(33)-C(37)-C(36)	-65.0(3)
C(34)-C(33)-C(37)-Hf(1)	66.3(3)
Cl(1)-Hf(1)-C(37)-C(36)	-25.3(4)
C(28)-Hf(1)-C(37)-C(36)	151.3(4)
C(32)-Hf(1)-C(37)-C(36)	117.3(4)
C(34)-Hf(1)-C(37)-C(36)	78.4(4)
C(33)-Hf(1)-C(37)-C(36)	116.1(5)
C(31)-Hf(1)-C(37)-C(36)	106.9(5)
C(29)-Hf(1)-C(37)-C(36)	-175.5(4)
C(35)-Hf(1)-C(37)-C(36)	37.7(4)
C(30)-Hf(1)-C(37)-C(36)	-167.4(3)

Sn(1)-Hf(1)-C(37)-C(36)	-116.8(4)
Cl(1)-Hf(1)-C(37)-C(33)	-141.4(3)
C(28)-Hf(1)-C(37)-C(33)	35.2(4)
C(32)-Hf(1)-C(37)-C(33)	1.2(4)
C(34)-Hf(1)-C(37)-C(33)	-37.7(3)
C(31)-Hf(1)-C(37)-C(33)	-9.3(6)
C(29)-Hf(1)-C(37)-C(33)	68.3(4)
C(35)-Hf(1)-C(37)-C(33)	-78.5(4)
C(36)-Hf(1)-C(37)-C(33)	-116.1(5)
C(30)-Hf(1)-C(37)-C(33)	76.5(6)
Sn(1)-Hf(1)-C(37)-C(33)	127.1(4)
C(44)-C(39)-C(40)-C(41)	-0.1(7)
C(39)-C(40)-C(41)-C(42)	0.8(7)
C(40)-C(41)-C(42)-C(43)	-0.4(8)
C(41)-C(42)-C(43)-C(44)	-0.8(8)
C(42)-C(43)-C(44)-C(39)	1.5(7)
C(40)-C(39)-C(44)-C(43)	-1.1(7)

Symmetry transformations used to generate equivalent atoms:

Figure S1.

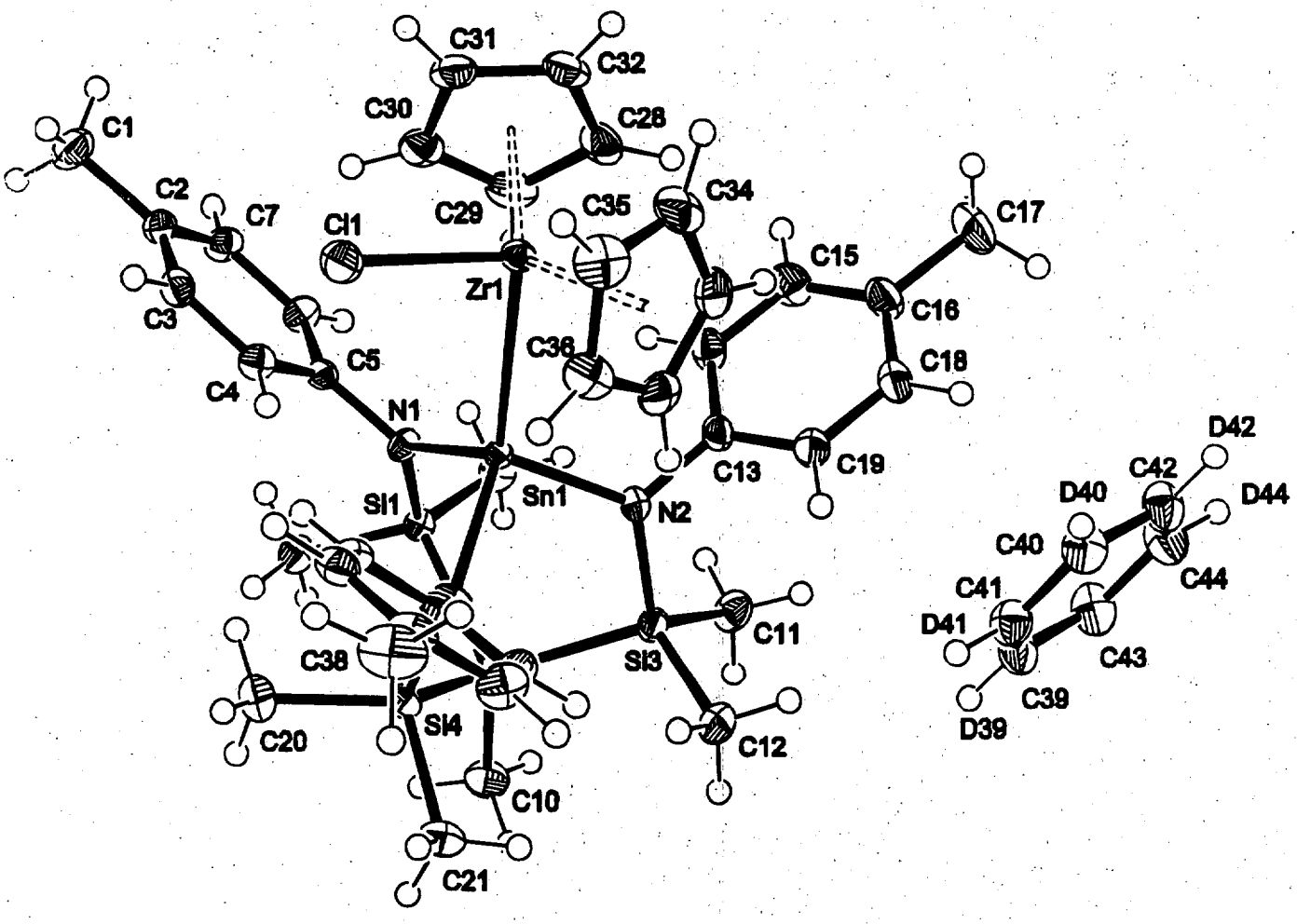
C31
C32
C30
C28
C1
C29
C35
C34
C2
C7
Cl1
C17
C15
Zr1
C3
C16
C36
C18
C5
C4
N1
C13
C19
D42
C42
D40
D44
Sn1
Si1
N2
C40
C44
C41
C11
D41
C43
C38
Si3
C39
Si4
C20
C12
D39
C10
C21

Figure S2.