Supplementary Data For Pd-catalyzed Reactions of Alkynes with Model Distannanes and Poly[di-(*n*-butyl)]stannanes

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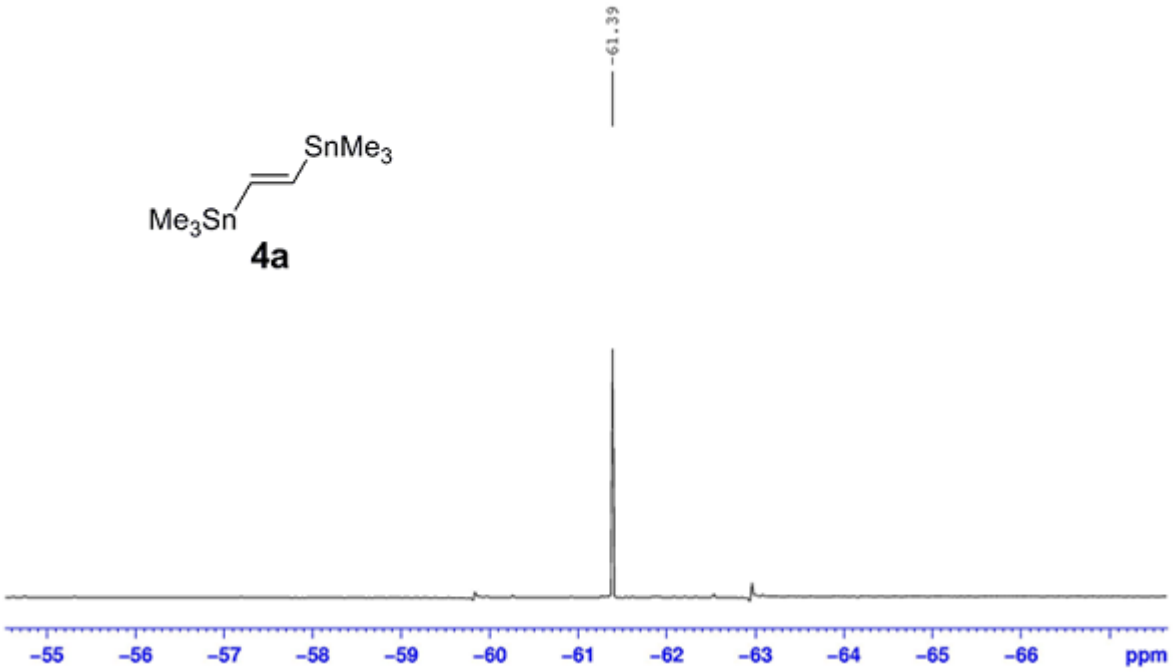

Figure S1: ^{119}Sn NMR of **4a**

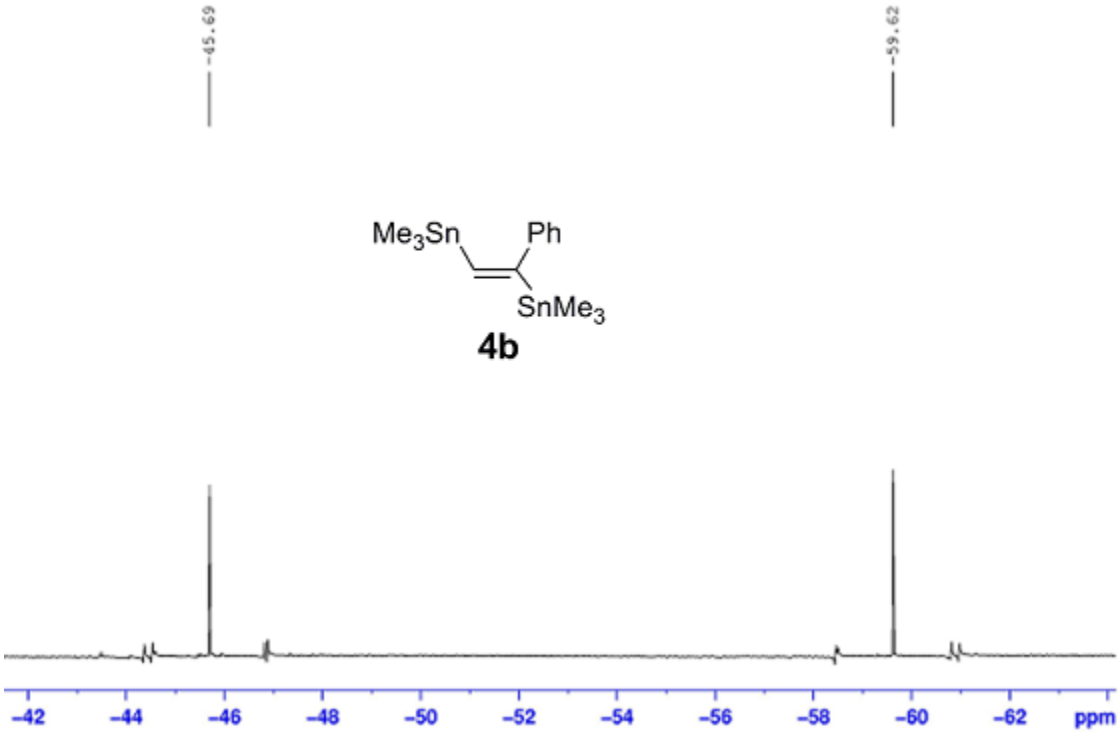

Figure S2: ^{119}Sn NMR of **4b**

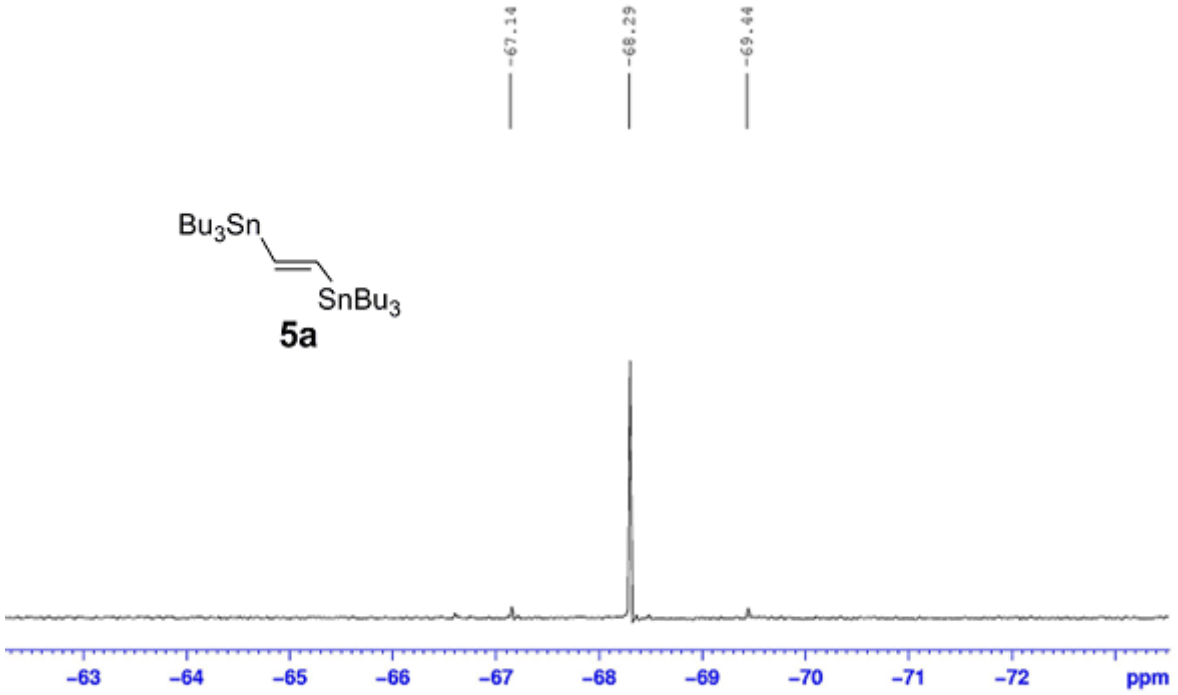

Figure S3: ^{119}Sn NMR of **5a**

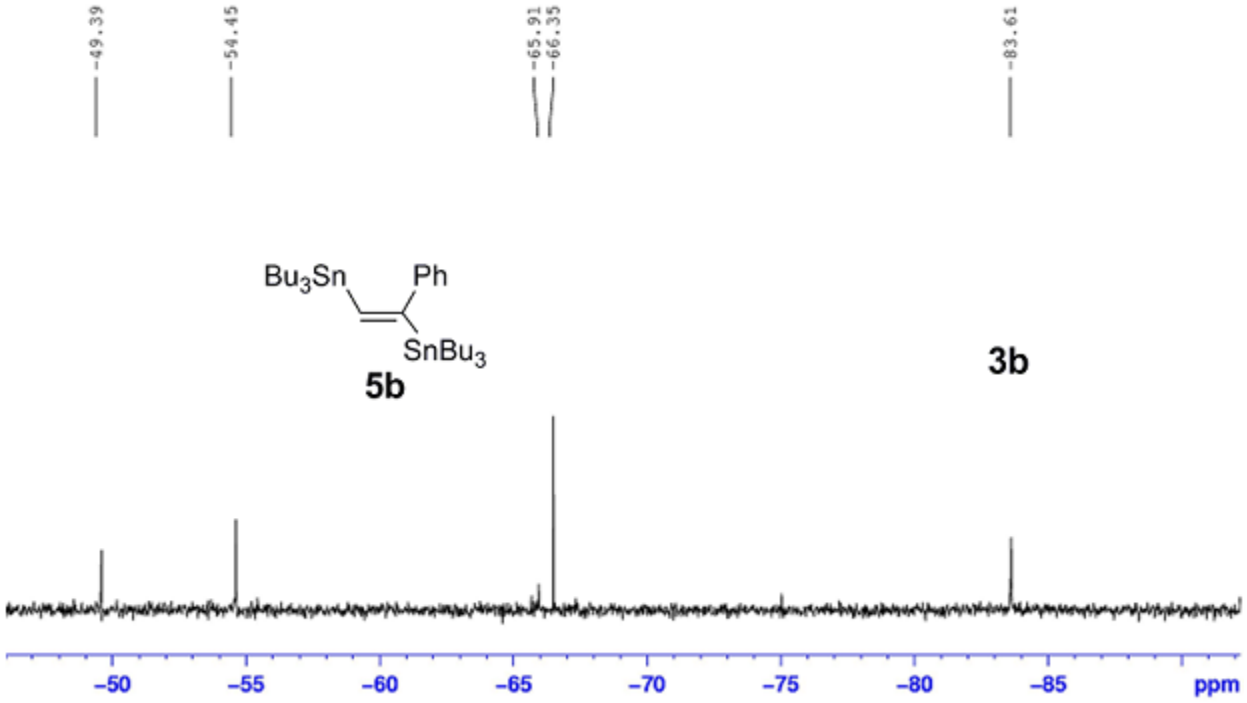

Figure S4: ^{119}Sn NMR of **5b**

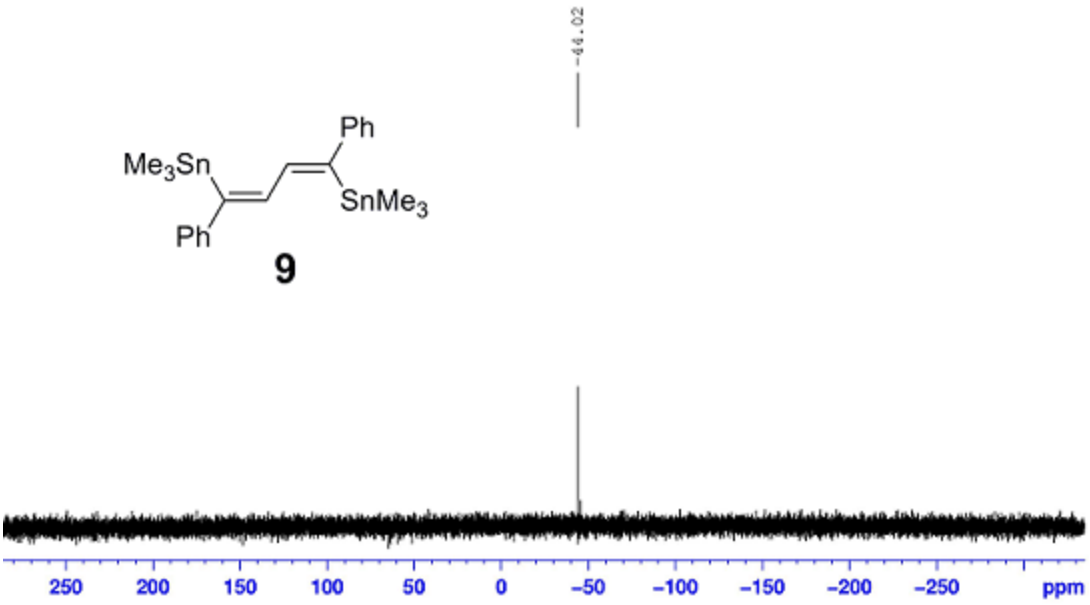

Figure S5: ^{119}Sn NMR of **9**

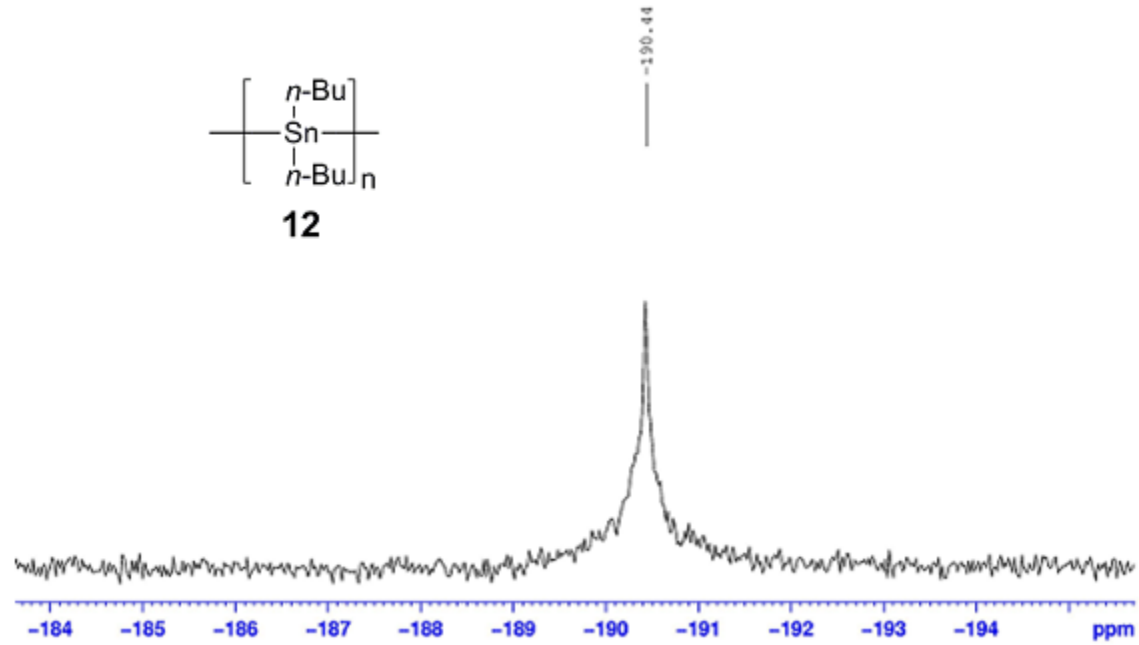

Figure S6: ^{119}Sn NMR of **12**

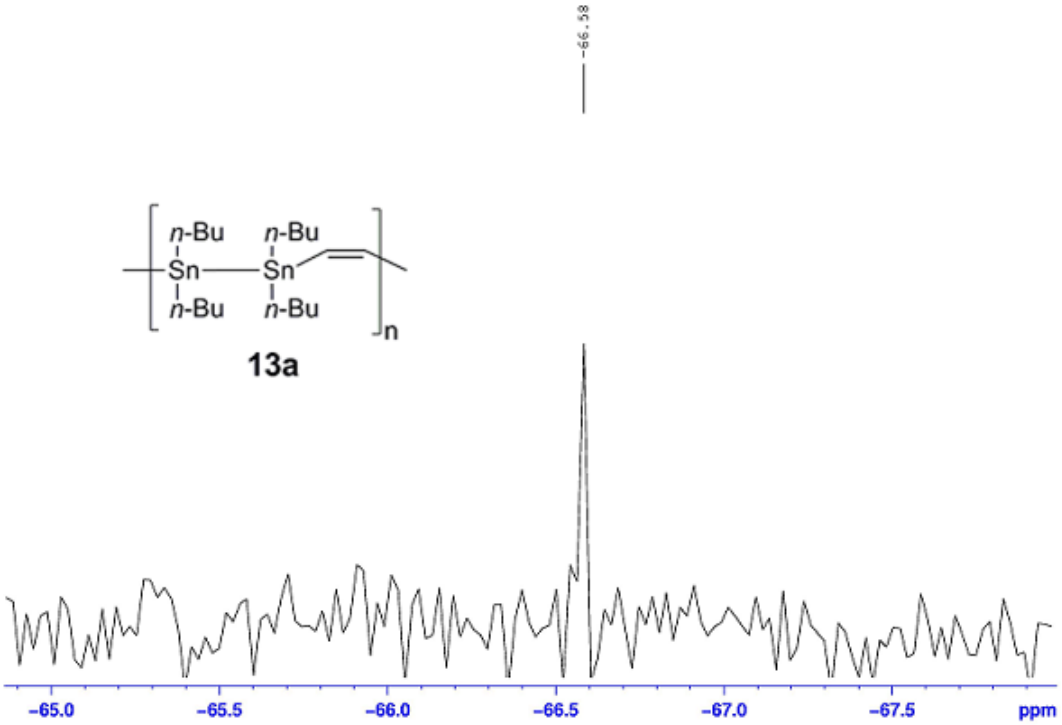

Figure S7: ^{119}Sn NMR of **13a**

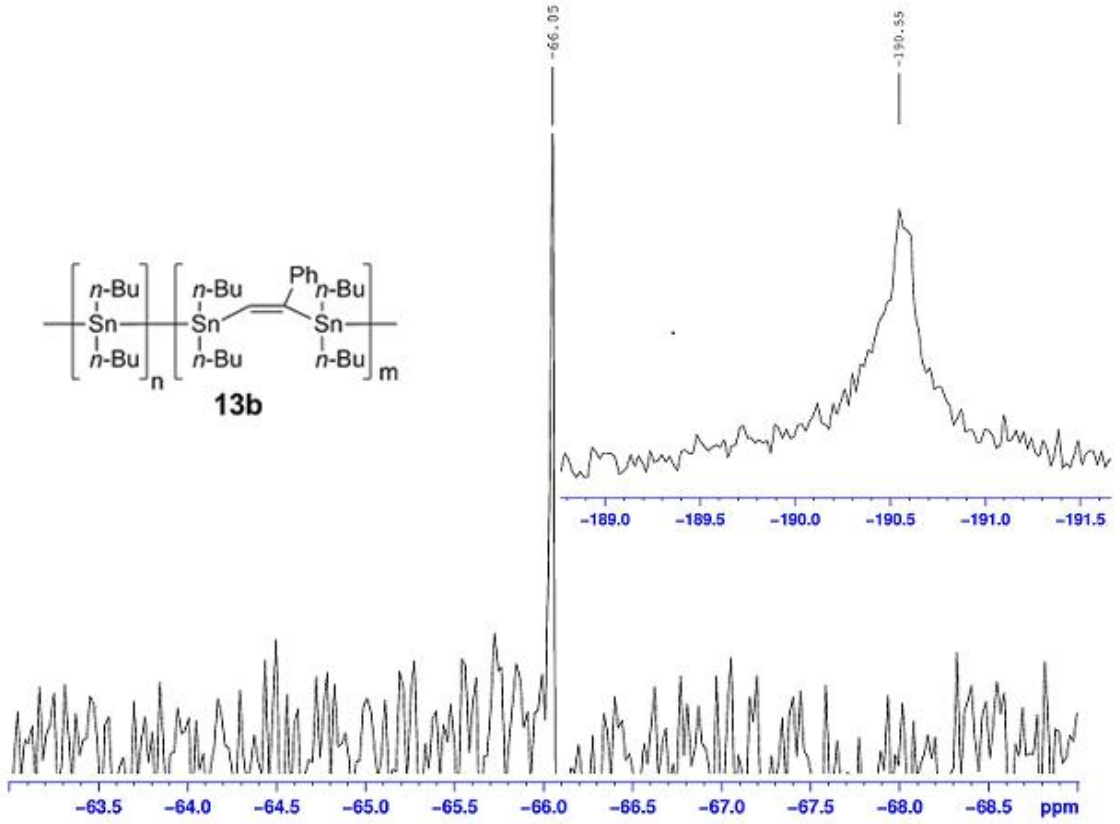

Figure S8: ^{119}Sn NMR of **13b**

	X-ray	DFT (B3LYP 6-31G*)
Sn(1)-C(4)	2.189(13)	2.172
Sn(2)-C(1)	2.148(14)	2.171
C(1)-C(2)	1.37(2)	1.359
C(1)-C(5)	1.481(19)	1.485
C(2)-C(3)	1.445(18)	1.449
C(3)-C(4)	1.343(19)	1.359
C(4)-C(11)	1.501(18)	1.485
C(3)-C(4)-Sn(1)	120.4(10)	124.3
C(1)-C(2)-C(3)	125.2(12)	127.02
C(4)-C(3)-C(2)	128.0(12)	127.0

Table S1: Selected bond lenghts (A) and bond angles (^{o}) for **9** as measured (X-ray) and calculated. In parentheses estimated standard deviations are given.

Compound	HOMO (eV)	LUMO (eV)	Difference (eV)
3a	-6.22	0.44	5.18
3b	-5.93	0.41	5.52
4a	-6.43	-0.14	6.29
4b	-6.02	-0.45	5.57
5a	-6.23	-0.15	6.08
5b	-5.91	-0.56	5.35
9	-5.45	-1.38	4.07

Table S2: Calculated HOMO/LUMO energies for Tin containing compounds

Crystal data of 9:

Table S3. Crystal data and structure refinement for **9**.

Identification code	k1059a	
Empirical formula	C22 H30 Sn2	
Formula weight	531.84	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P c a 21	
Unit cell dimensions	a = 16.1862(3) Å	a= 90°.
	b = 6.2126(6) Å	b= 90°.
	c = 22.2214(11) Å	g = 90°.
Volume	2234.5(2) $Å^3$	
Z	4	
Density (calculated)	1.581 Mg/m^3	
Absorption coefficient	2.236 mm^{-1}	
F(000)	1048	
Crystal size	0.16 × 0.10 × 0.10 mm^3	
Theta range for data collection	2.68 to 27.46°.	
Index ranges	-20<=h<=21, -8<=k<=8, -22<=l<=28	
Reflections collected	13220	
Independent reflections	4024 [R(int) = 0.0906]	
Completeness to theta = 27.46°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.767 and 0.658	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4024 / 1 / 222	
Goodness-of-fit on F^2	1.036	
Final R indices [I>2sigma(I)]	R1 = 0.0590, wR2 = 0.1328	
R indices (all data)	R1 = 0.1033, wR2 = 0.1620	
Absolute structure parameter	0.58(9)	
Largest diff. peak and hole	2.028 and -1.675 $e.Å^{-3}$	

Table S4. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **9**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Sn(1)	5647(1)	8269(1)	2090(1)	36(1)
Sn(2)	3243(1)	7029(1)	4328(1)	36(1)
C(1)	4436(8)	6250(20)	3967(7)	31(3)
C(2)	4697(8)	6970(20)	3417(6)	34(3)
C(3)	4244(8)	8440(20)	3034(6)	36(3)
C(4)	4468(8)	9210(20)	2494(6)	35(3)
C(5)	4979(8)	4780(20)	4311(8)	38(3)
C(6)	5209(8)	2800(20)	4123(8)	44(4)
C(7)	5696(7)	1350(20)	4400(8)	41(4)
C(8)	5952(9)	1890(30)	4972(7)	46(4)
C(9)	5727(10)	3910(30)	5218(8)	48(4)
C(10)	5245(9)	5330(30)	4892(7)	49(4)
C(11)	3921(7)	10756(18)	2160(7)	30(3)
C(12)	3660(9)	10380(30)	1577(7)	49(4)
C(13)	3151(9)	11810(30)	1282(7)	47(4)
C(14)	2928(9)	13690(30)	1572(8)	51(4)
C(15)	3194(7)	14180(20)	2142(8)	41(3)
C(16)	3690(7)	12640(20)	2445(6)	32(3)
C(17)	5756(9)	9590(30)	1216(9)	51(5)
C(18)	6587(9)	9530(30)	2665(8)	52(4)
C(19)	5716(7)	4910(20)	2047(9)	45(4)
C(20)	3077(10)	10399(19)	4405(12)	64(6)
C(21)	2347(9)	5620(30)	3740(7)	48(4)
C(22)	3135(10)	5700(30)	5223(7)	51(4)

Table S5. Bond lengths [Å] and angles [°] for **9**.

Sn(1)-C(19)	2.090(14)
Sn(1)-C(17)	2.115(19)
Sn(1)-C(18)	2.135(16)
Sn(1)-C(4)	2.189(13)
Sn(2)-C(20)	2.117(12)
Sn(2)-C(21)	2.140(15)
Sn(2)-C(1)	2.148(14)
Sn(2)-C(22)	2.160(15)
C(1)-C(2)	1.37(2)
C(1)-C(5)	1.481(19)
C(2)-C(3)	1.445(18)
C(3)-C(4)	1.343(19)
C(4)-C(11)	1.501(18)
C(5)-C(6)	1.354(18)
C(5)-C(10)	1.40(2)
C(6)-C(7)	1.342(19)
C(7)-C(8)	1.38(2)
C(8)-C(9)	1.41(2)
C(9)-C(10)	1.38(2)
C(11)-C(12)	1.38(2)
C(11)-C(16)	1.385(18)
C(12)-C(13)	1.38(2)
C(13)-C(14)	1.38(2)
C(14)-C(15)	1.37(2)
C(15)-C(16)	1.416(19)

C(19)-Sn(1)-C(17)	109.8(7)
C(19)-Sn(1)-C(18)	110.9(7)
C(17)-Sn(1)-C(18)	110.4(6)
C(19)-Sn(1)-C(4)	109.4(5)
C(17)-Sn(1)-C(4)	110.2(5)
C(18)-Sn(1)-C(4)	106.1(6)
C(20)-Sn(2)-C(21)	111.6(8)
C(20)-Sn(2)-C(1)	111.5(6)

C(21)-Sn(2)-C(1)	106.8(6)
C(20)-Sn(2)-C(22)	107.2(9)
C(21)-Sn(2)-C(22)	110.5(6)
C(1)-Sn(2)-C(22)	109.3(6)
C(2)-C(1)-C(5)	118.8(13)
C(2)-C(1)-Sn(2)	122.5(10)
C(5)-C(1)-Sn(2)	118.7(10)
C(1)-C(2)-C(3)	125.2(12)
C(4)-C(3)-C(2)	128.0(12)
C(3)-C(4)-C(11)	120.8(12)
C(3)-C(4)-Sn(1)	120.4(10)
C(11)-C(4)-Sn(1)	118.8(9)
C(6)-C(5)-C(10)	114.9(13)
C(6)-C(5)-C(1)	124.3(15)
C(10)-C(5)-C(1)	120.6(13)
C(7)-C(6)-C(5)	128.9(16)
C(6)-C(7)-C(8)	116.0(14)
C(7)-C(8)-C(9)	119.5(13)
C(10)-C(9)-C(8)	120.6(16)
C(9)-C(10)-C(5)	120.0(15)
C(12)-C(11)-C(16)	119.2(12)
C(12)-C(11)-C(4)	122.4(13)
C(16)-C(11)-C(4)	118.4(13)
C(13)-C(12)-C(11)	121.5(15)
C(12)-C(13)-C(14)	118.6(15)
C(15)-C(14)-C(13)	122.3(14)
C(14)-C(15)-C(16)	118.0(13)
C(11)-C(16)-C(15)	120.3(13)

Symmetry transformations used to generate equivalent atoms:

Table S6. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **9**. The anisotropic displacement factor exponent takes the form: $-2p^2[\, h^2 a^{*2} U^{11} + \ldots + 2\, h\, k\, a^*\, b^*\, U^{12}\,]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Sn(1)	35(1)	35(1)	38(1)	-1(1)	4(1)	1(1)
Sn(2)	36(1)	37(1)	36(1)	1(1)	3(1)	2(1)
C(1)	32(8)	36(7)	27(8)	3(6)	2(6)	-5(6)
C(2)	26(7)	45(8)	30(7)	-6(6)	1(6)	5(6)
C(3)	37(7)	34(7)	38(8)	3(6)	15(7)	1(6)
C(4)	29(7)	44(8)	31(8)	-3(7)	14(6)	5(6)
C(5)	41(7)	35(7)	39(8)	12(9)	-4(9)	4(5)
C(6)	38(7)	17(6)	75(13)	4(7)	5(7)	-6(6)
C(7)	26(7)	38(7)	58(11)	3(8)	-2(8)	8(5)
C(8)	42(8)	58(10)	37(9)	29(8)	-10(7)	-7(7)
C(9)	56(11)	51(10)	36(10)	2(8)	-17(8)	2(8)
C(10)	63(10)	55(10)	28(9)	-3(8)	-2(8)	-5(8)
C(11)	24(6)	24(6)	41(8)	16(7)	-7(7)	-4(5)
C(12)	43(8)	61(11)	44(10)	-3(9)	7(8)	9(8)
C(13)	55(10)	69(11)	18(7)	-9(7)	-6(7)	28(9)
C(14)	39(8)	66(11)	47(10)	13(9)	-5(8)	12(7)
C(15)	48(8)	27(6)	47(9)	1(7)	15(9)	3(5)
C(16)	23(6)	54(9)	21(7)	7(6)	0(5)	7(6)
C(17)	40(9)	43(9)	69(13)	-5(8)	11(8)	-4(7)
C(18)	41(9)	69(12)	48(10)	-1(9)	3(8)	8(8)
C(19)	35(7)	67(10)	33(9)	6(10)	9(8)	-16(7)
C(20)	78(11)	14(6)	100(16)	7(10)	28(13)	7(6)
C(21)	44(9)	58(10)	41(9)	4(8)	5(8)	-14(7)
C(22)	70(12)	64(11)	18(8)	13(7)	-12(8)	4(9)

Table S7.Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2× 10^3)for **9**.

	x	y	z	U(eq)
H(2A)	5218	6478	3277	41
H(3A)	3724	8906	3182	44
H(6A)	4997	2366	3743	52
H(7A)	5854	42	4212	49
H(8A)	6278	913	5200	55
H(9A)	5908	4289	5610	57
H(10A)	5094	6677	5061	58
H(12A)	3837	9117	1375	59
H(13A)	2957	11509	888	57
H(14A)	2579	14680	1369	61
H(15A)	3049	15501	2328	49
H(16A)	3866	12913	2846	39
H(17A)	6330	10016	1144	76
H(17B)	5396	10847	1180	76
H(17C)	5593	8504	918	76
H(18A)	6357	9779	3067	79
H(18B)	6790	10895	2500	79
H(18C)	7043	8501	2692	79
H(19A)	5913	4349	2432	67
H(19B)	6100	4492	1726	67
H(19C)	5167	4324	1960	67
H(20A)	3094	11052	4003	96
H(20B)	3520	11006	4653	96
H(20C)	2542	10697	4592	96
H(21A)	2193	6662	3428	72
H(21B)	1855	5219	3972	72
H(21C)	2581	4334	3550	72
H(22A)	3461	6564	5504	76
H(22B)	3342	4214	5223	76
H(22C)	2554	5705	5346	76