Electronic Supporting Information

Organostannoxane-Supported Nucleobase Arrays: Synthesis and Supramolecular Structures of Polymeric and Molecular Organotin Complexes Containing Guanine, Uracil and 2-Aminopurine

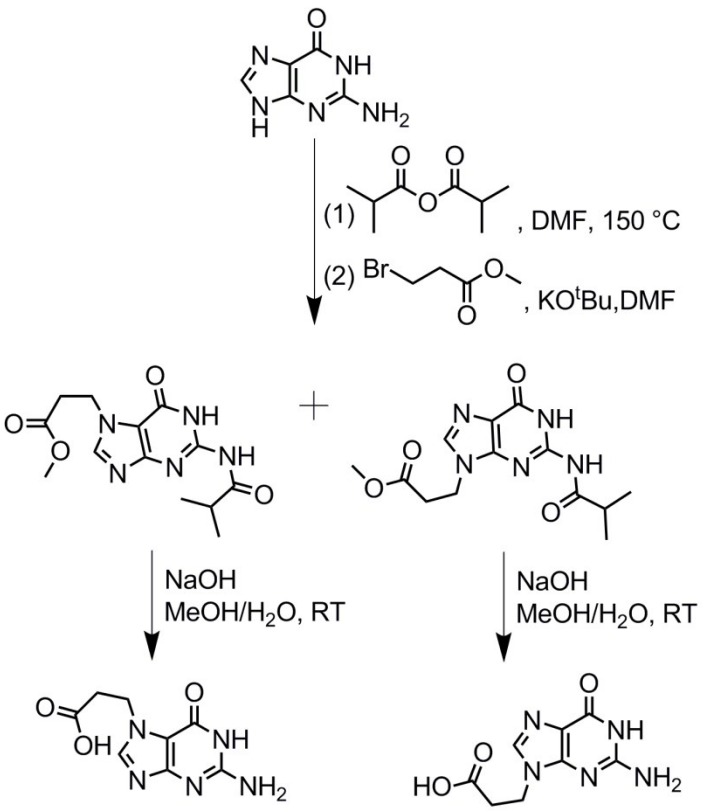
Subrata Kundu,[a] *N. Nagapradeep,*[a] *Balaram Mohapatra,*[a] *Sourav Biswas,*[a] *Sandeep Verma*[a] *and Vadapalli Chandrasekhar**[a,b]

[a] Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur-208016, India.

[b]National Institute of Science Education and Research, Institute of Physics Campus, Sachivalaya Marg, PO: Sainik School, Bhubaneswar - 751 005, India.

*E-mail: vc@iitk.ac.in; vc@niser.ac.in; Phone: (+91) 512-259-7259. Fax: (+91)521-259-0007/7436.

Scheme S1. Synthetic procedure of L1H and L2H.[1]



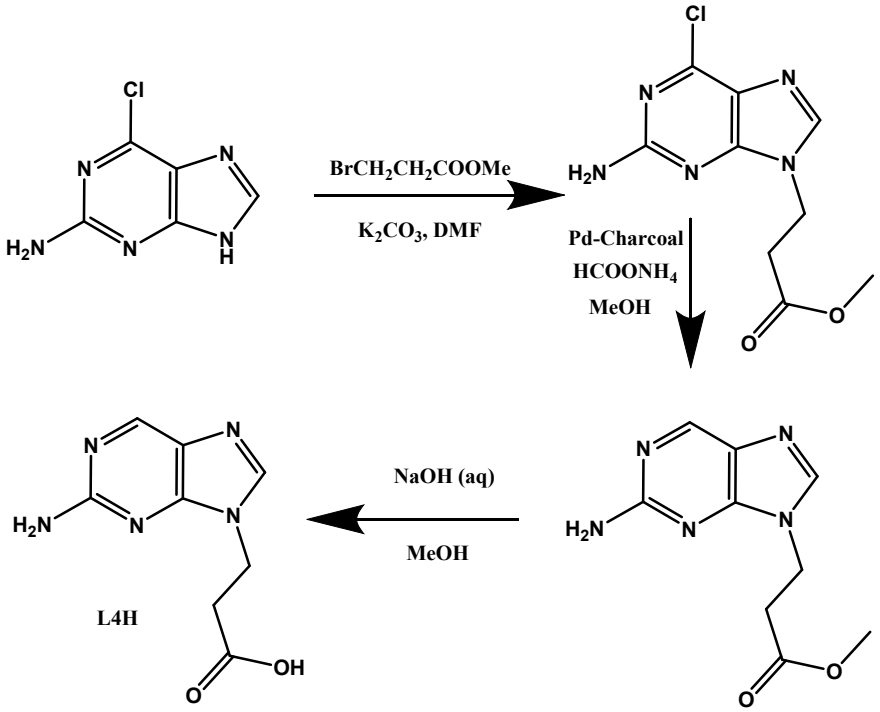
Synthesis of 3-(N9-guaninyl)propionic acid and 3-(N7-guaninyl)propionic acid: Compounds and were synthesized according to our previous report[1] by using KO^{t}Bu and methyl-3-bromopropionate.

3-(N9-guaninyl)propionic acid: (1.786 g, 16% Overall Yield). HRMS: $(M-H)^-$ calculated: 222.0633, found: 222.0626; ^{1}H NMR (500 MHz, DMSO-d_6, 25 °C, TMS): δ (ppm) 2.73 (s, 2H, CH_2), 4.09 (s, 2H, CH_2), 6.43 (s, 2H, NH_2), 7.59 (s, 1H, C8-H), 10.52 (s, 1H, N1-H); ^{13}C NMR (125 MHz, DMSO-d_6, 25 °C, TMS): δ (ppm) 34.25, 116.99, 138.06, 151.60, 154.05, 157.31, 172.64 (one peak merged with solvent).

3-(N7-guaninyl)propionic acid: (2.122 g, 19% Overall Yield). HRMS: $(M+H)^+$ calculated: 224.0784, found: 224.0786; ^{1}H NMR (500 MHz, DMSO-d_6, 25 °C, TMS): δ (ppm) 2.89 (s,

2H, CH_2), 4.43 (s, 2H, CH_2), 7.55 (s, 2H, NH_2), 8.83 (s, 1H, C8-H), 12.02 (s, 1H, N1-H); ^{13}C NMR (125 MHz, DMSO-d_6, 25 °C, TMS): δ (ppm) 34.18, 44.32, 107.60, 140.09, 150.28, 153.48, 155.08, 172.22.

Scheme S2. Synthetic procedure of L4H.[2]



3-{N9-(2-aminopurinyl)}propanoic acid (L4H): L4H synthesized according to our previous report.[2]

Referencess :

1. N. Nagapradeep, S. Sharma and S. Verma, *Cryst. Growth Des.,* 2013, **13**, 455–459.

2. S. Kundu, B. Mohapatra, C. Mohapatra, S. Verma, and V. Chandrasekhar, *Cryst. Growth Des.,* 2015, **15**, 247−256.

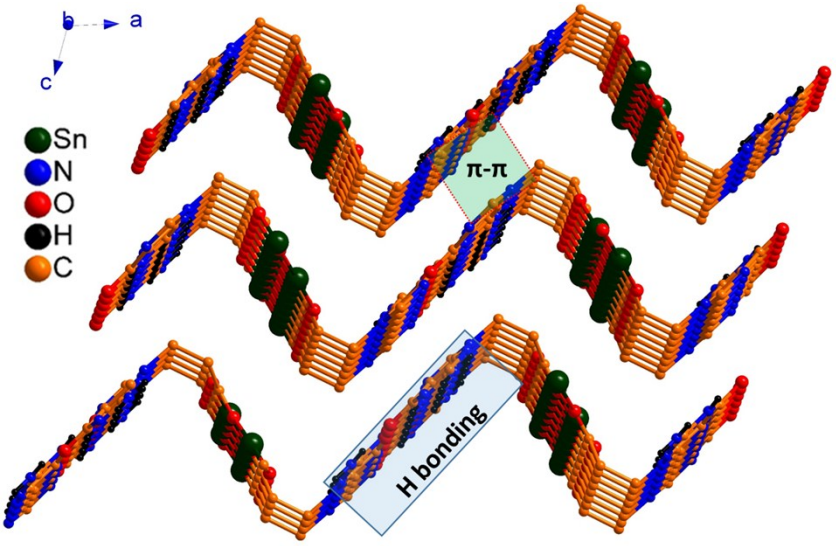


Figure S1. 3D packing of complex **1**.

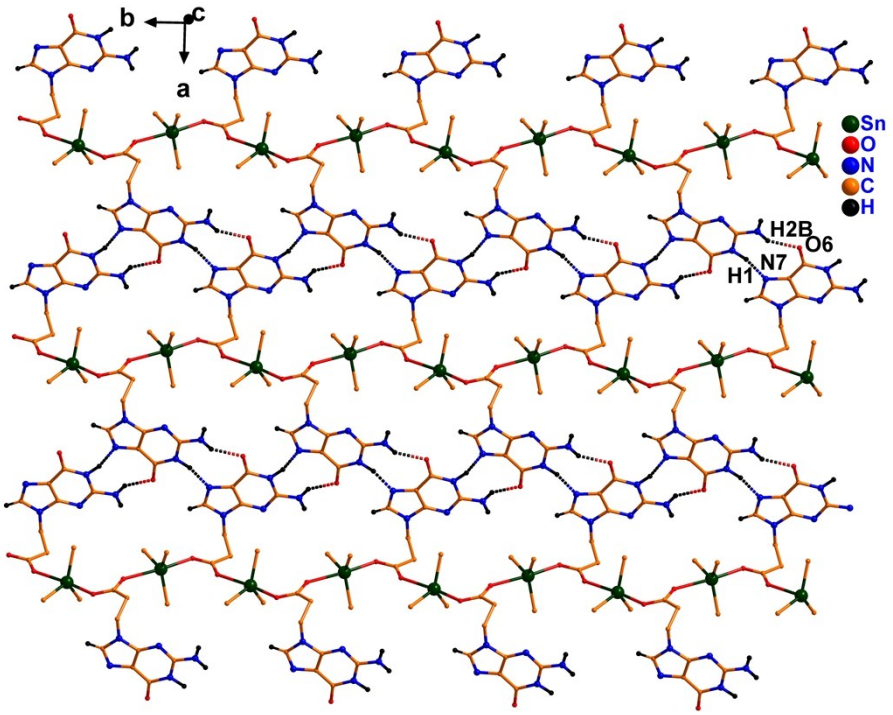


Figure S2. Hydrogen bonding of **2** (methyl groups on tin atom have been omitted for clarity).

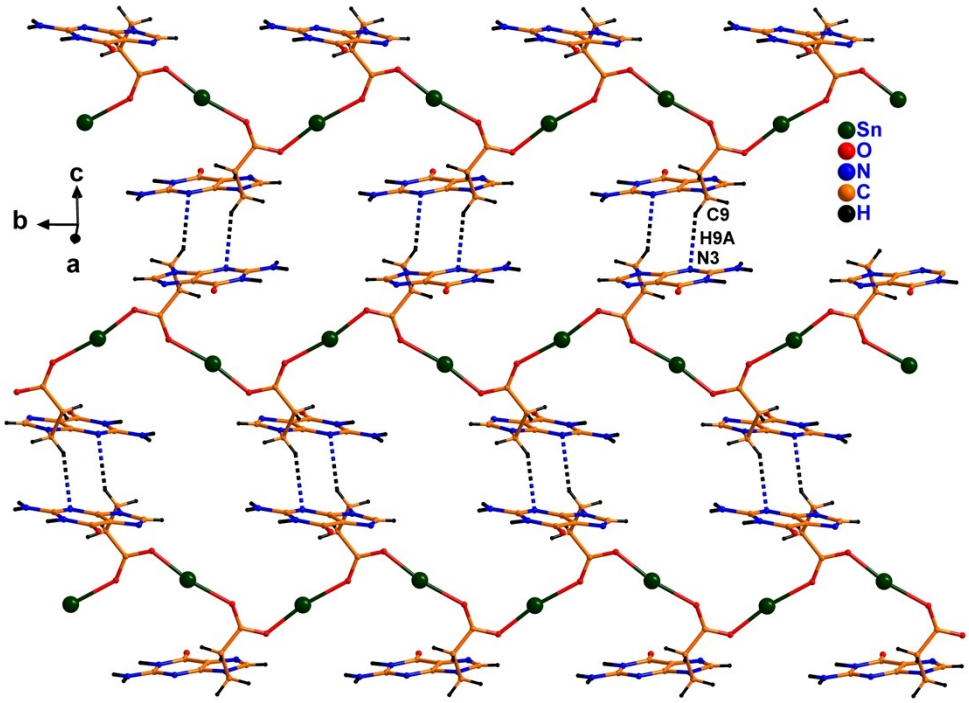


Figure S3. C-H···N interaction of **2**.

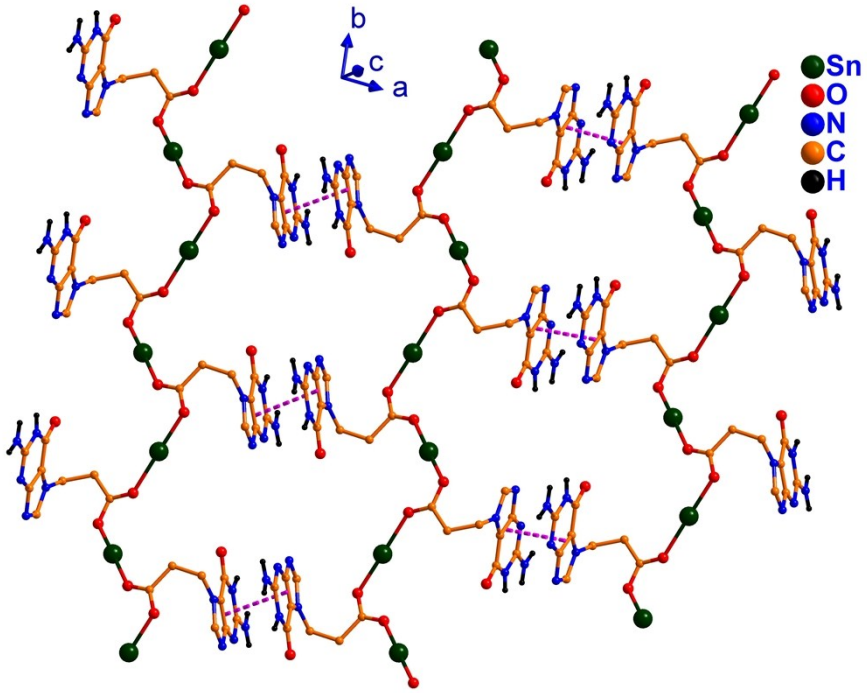


Figure S4. π···π stacking between the two polymer of **3**.

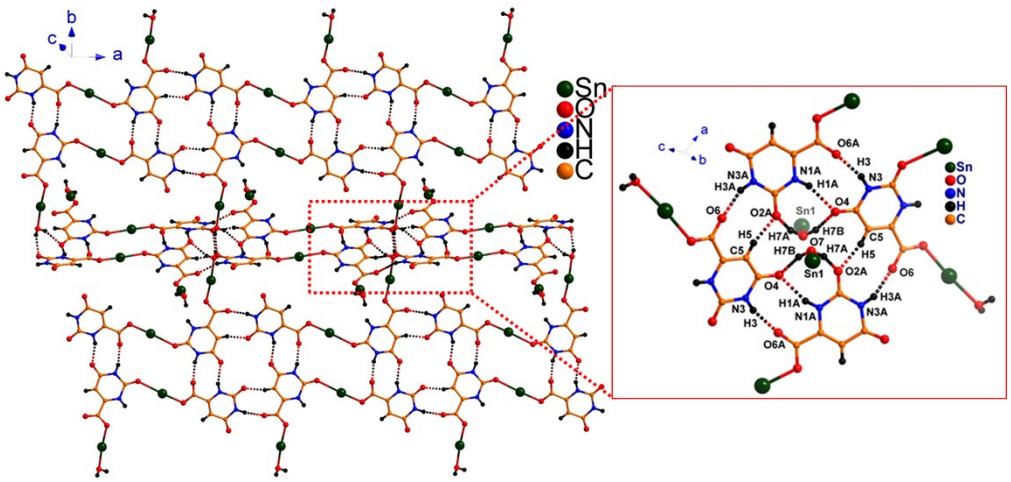


Figure S5. 3D hydrogen bonding of complex **4.**

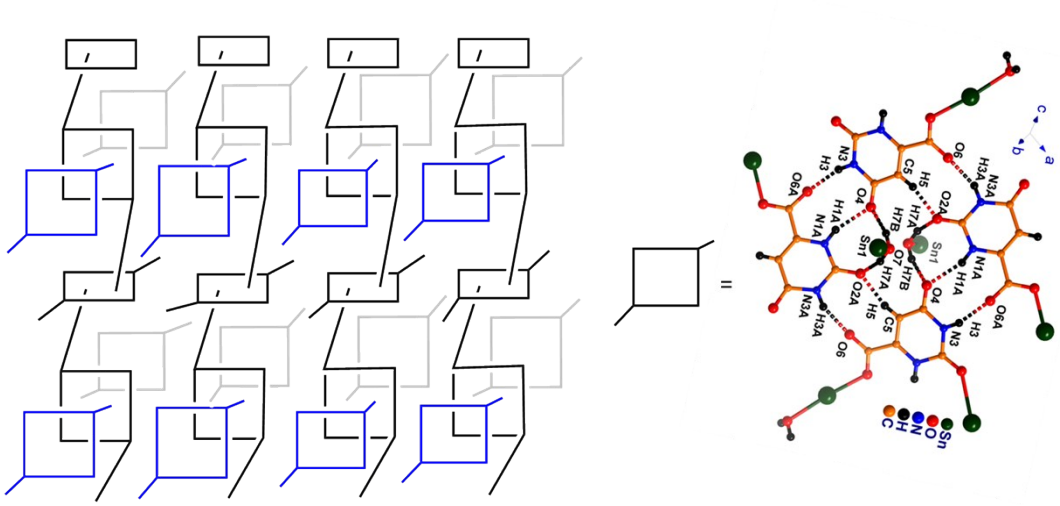


Figure S6. 3D hydrogen bonding of complex **4** (schematic representation).

Table S1. Bond lengths [Å] and angles [°] for complex **1**.

Sn(01)-C(14)	2.101(4)	N(3)-C(4)-C(5)	129.0(3)
Sn(01)-C(13)	2.107(4)	N(3)-C(4)-N(9)	125.1(3)
Sn(01)-C(12)	2.109(4)	C(5)-C(4)-N(9)	105.9(3)
Sn(01)-O(2)#1	2.190(2)	C(4)-C(5)-N(7)	110.6(3)
Sn(01)-O(1)	2.440(3)	C(4)-C(5)-C(6)	118.8(3)
N(3)-C(2)	1.325(4)	N(7)-C(5)-C(6)	130.6(4)
N(3)-C(4)	1.348(5)	C(8)-N(9)-C(4)	105.6(3)
O(6)-C(6)	1.230(4)	C(8)-N(9)-C(9)	128.1(3)
N(1)-C(2)	1.368(5)	C(4)-N(9)-C(9)	126.3(3)
N(1)-C(6)	1.375(4)	C(2)-N(2)-H(2A)	120.0
N(1)-H(1)	0.8600	C(2)-N(2)-H(2B)	120.0
C(4)-C(5)	1.368(5)	H(2A)-N(2)-H(2B)	120.0
C(4)-N(9)	1.374(4)	N(3)-C(2)-N(2)	119.3(3)
C(5)-N(7)	1.380(4)	N(3)-C(2)-N(1)	124.0(3)
C(5)-C(6)	1.413(5)	N(2)-C(2)-N(1)	116.7(3)
N(9)-C(8)	1.367(4)	C(8)-N(7)-C(5)	104.3(3)
N(9)-C(9)	1.448(4)	C(11)-C(10)-C(9)	113.9(3)
N(2)-C(2)	1.330(4)	C(11)-C(10)-H(10A)	108.8
N(2)-H(2A)	0.8600	C(9)-C(10)-H(10A)	108.8
N(2)-H(2B)	0.8600	C(11)-C(10)-H(10B)	108.8
N(7)-C(8)	1.303(4)	C(9)-C(10)-H(10B)	108.8
C(10)-C(11)	1.509(5)	H(10A)-C(10)-H(10B)	107.7
C(10)-C(9)	1.515(5)	O(6)-C(6)-N(1)	120.3(3)
C(10)-H(10A)	0.9700	O(6)-C(6)-C(5)	128.0(4)
C(10)-H(10B)	0.9700	N(1)-C(6)-C(5)	111.7(3)
C(9)-H(9A)	0.9700	N(9)-C(9)-C(10)	111.5(3)
C(9)-H(9B)	0.9700	N(9)-C(9)-H(9A)	109.3
C(8)-H(8)	0.9300	C(10)-C(9)-H(9A)	109.3
C(13)-H(13A)	0.9600	N(9)-C(9)-H(9B)	109.3
C(13)-H(13B)	0.9600	C(10)-C(9)-H(9B)	109.3
C(13)-H(13C)	0.9600	H(9A)-C(9)-H(9B)	108.0
C(14)-H(14A)	0.9600	N(7)-C(8)-N(9)	113.4(3)
C(14)-H(14B)	0.9600	N(7)-C(8)-H(8)	123.3
C(14)-H(14C)	0.9600	N(9)-C(8)-H(8)	123.3
C(12)-H(12A)	0.9600	Sn(01)-C(13)-H(13A)	109.5
C(12)-H(12B)	0.9600	Sn(01)-C(13)-H(13B)	109.5

C(12)-H(12C)	0.9600	H(13A)-C(13)-H(13B)	109.5
O(2)-C(11)	1.272(4)	Sn(01)-C(13)-H(13C)	109.5
O(2)-Sn(01)#2	2.190(2)	H(13A)-C(13)-H(13C)	109.5
C(11)-O(1)	1.229(4)	H(13B)-C(13)-H(13C)	109.5
C(14)-Sn(01)-C(13)	125.2(2)	Sn(01)-C(14)-H(14A)	109.5
C(14)-Sn(01)-C(12)	116.01(17)	Sn(01)-C(14)-H(14B)	109.5
C(13)-Sn(01)-C(12)	118.32(19)	H(14A)-C(14)-H(14B)	109.5
C(14)-Sn(01)-O(2)#1	93.93(14)	Sn(01)-C(14)-H(14C)	109.5
C(13)-Sn(01)-O(2)#1	93.68(15)	H(14A)-C(14)-H(14C)	109.5
C(12)-Sn(01)-O(2)#1	89.07(14)	H(14B)-C(14)-H(14C)	109.5
C(14)-Sn(01)-O(1)	88.23(13)	Sn(01)-C(12)-H(12A)	109.5
C(13)-Sn(01)-O(1)	89.63(14)	Sn(01)-C(12)-H(12B)	109.5
C(12)-Sn(01)-O(1)	84.96(12)	H(12A)-C(12)-H(12B)	109.5
O(2)#1-Sn(01)-O(1)	174.00(9)	Sn(01)-C(12)-H(12C)	109.5
C(2)-N(3)-C(4)	111.2(3)	H(12A)-C(12)-H(12C)	109.5
C(2)-N(1)-C(6)	125.3(3)	H(12B)-C(12)-H(12C)	109.5
C(2)-N(1)-H(1)	117.4	C(11)-O(2)-Sn(01)#2	125.9(3)
C(6)-N(1)-H(1)	117.4	O(1)-C(11)-O(2)	124.0(4)
		O(1)-C(11)-C(10)	120.7(3)
		O(2)-C(11)-C(10)	115.2(4)
		C(11)-O(1)-Sn(01)	137.9(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y-1/2,-z+3/2 #2 -x,y+1/2,-z+3/2

Table S2. Bond lengths [Å] and angles [°] for complex **2**.

Sn(1)-C(16)	2.115(7)	C(11)-C(10)-H(10A)	108.9
Sn(1)-C(12)	2.137(7)	C(9)-C(10)-H(10A)	108.9
Sn(1)-C(20)	2.137(5)	C(11)-C(10)-H(10B)	108.9
Sn(1)-O(1)	2.202(3)	C(9)-C(10)-H(10B)	108.9
Sn(1)-O(2)#1	2.420(4)	H(10A)-C(10)-H(10B)	107.8
O(1)-C(11)	1.262(5)	N(9)-C(9)-C(10)	111.6(4)
N(9)-C(8)	1.369(6)	N(9)-C(9)-H(9A)	109.3
N(9)-C(4)	1.373(5)	C(10)-C(9)-H(9A)	109.3

N(9)-C(9)	1.454(6)	N(9)-C(9)-H(9B)	109.3
O(2)-C(11)	1.237(5)	C(10)-C(9)-H(9B)	109.3
O(2)-Sn(1)#2	2.420(4)	H(9A)-C(9)-H(9B)	108.0
N(1)-C(2)	1.354(6)	N(3)-C(2)-N(2)	118.4(5)
N(1)-C(6)	1.395(7)	N(3)-C(2)-N(1)	124.5(4)
N(1)-H(1)	1.02(8)	N(2)-C(2)-N(1)	117.1(4)
N(3)-C(2)	1.321(6)	N(7)-C(8)-N(9)	113.5(4)
N(3)-C(4)	1.366(6)	N(7)-C(8)-H(8)	123.3
C(5)-C(4)	1.369(7)	N(9)-C(8)-H(8)	123.3
C(5)-N(7)	1.395(6)	C(21)-C(20)-Sn(1)	113.6(4)
C(5)-C(6)	1.413(7)	C(21)-C(20)-H(20A)	108.8
N(7)-C(8)	1.302(7)	Sn(1)-C(20)-H(20A)	108.8
O(6)-C(6)	1.240(7)	C(21)-C(20)-H(20B)	108.8
N(2)-C(2)	1.347(6)	Sn(1)-C(20)-H(20B)	108.8
N(2)-H(2A)	0.8600	H(20A)-C(20)-H(20B)	107.7
N(2)-H(2B)	0.8600	C(13)-C(12)-Sn(1)	120.5(6)
C(11)-C(10)	1.518(7)	C(13)-C(12)-H(12A)	107.2
C(10)-C(9)	1.532(7)	Sn(1)-C(12)-H(12A)	107.2
C(10)-H(10A)	0.9700	C(13)-C(12)-H(12B)	107.2
C(10)-H(10B)	0.9700	Sn(1)-C(12)-H(12B)	107.2
C(9)-H(9A)	0.9700	H(12A)-C(12)-H(12B)	106.8
C(9)-H(9B)	0.9700	C(17)-C(16)-Sn(1)	117.6(6)
C(8)-H(8)	0.9300	C(17)-C(16)-H(16A)	107.9
C(20)-C(21)	1.530(11)	Sn(1)-C(16)-H(16A)	107.9
C(20)-H(20A)	0.9700	C(17)-C(16)-H(16B)	107.9
C(20)-H(20B)	0.9700	Sn(1)-C(16)-H(16B)	107.9
C(12)-C(13)	1.410(10)	H(16A)-C(16)-H(16B)	107.2
C(12)-H(12A)	0.9700	C(21)-C(22)-C(23)	104.8(9)
C(12)-H(12B)	0.9700	C(21)-C(22)-H(22A)	110.8
C(16)-C(17)	1.467(11)	C(23)-C(22)-H(22A)	110.8
C(16)-H(16A)	0.9700	C(21)-C(22)-H(22B)	110.8
C(16)-H(16B)	0.9700	C(23)-C(22)-H(22B)	110.8
C(22)-C(21)	1.486(11)	H(22A)-C(22)-H(22B)	108.9
C(22)-C(23)	1.555(16)	C(15)-C(14)-C(13)	117.8(11)
C(22)-H(22A)	0.9700	C(15)-C(14)-H(14A)	107.9
C(22)-H(22B)	0.9700	C(13)-C(14)-H(14A)	107.9
C(14)-C(15)	1.452(15)	C(15)-C(14)-H(14B)	107.9
C(14)-C(13)	1.537(13)	C(13)-C(14)-H(14B)	107.9

C(14)-H(14A)	0.9700	H(14A)-C(14)-H(14B)	107.2
C(14)-H(14B)	0.9700	C(12)-C(13)-C(14)	119.0(8)
C(13)-H(13A)	0.9700	C(12)-C(13)-H(13A)	107.6
C(13)-H(13B)	0.9700	C(14)-C(13)-H(13A)	107.6
C(15)-H(15A)	0.9600	C(12)-C(13)-H(13B)	107.6
C(15)-H(15B)	0.9600	C(14)-C(13)-H(13B)	107.6
C(15)-H(15C)	0.9600	H(13A)-C(13)-H(13B)	107.0
C(21)-H(21A)	0.9700	C(14)-C(15)-H(15A)	109.5
C(21)-H(21B)	0.9700	C(14)-C(15)-H(15B)	109.5
C(17)-C(18)	1.604(15)	H(15A)-C(15)-H(15B)	109.5
C(17)-H(17A)	0.9700	C(14)-C(15)-H(15C)	109.5
C(17)-H(17B)	0.9700	H(15A)-C(15)-H(15C)	109.5
C(18)-C(19)	1.408(17)	H(15B)-C(15)-H(15C)	109.5
C(18)-H(18A)	0.9700	C(22)-C(21)-C(20)	116.4(7)
C(18)-H(18B)	0.9700	C(22)-C(21)-H(21A)	108.2
C(23)-H(23A)	0.9600	C(20)-C(21)-H(21A)	108.2
C(23)-H(23B)	0.9600	C(22)-C(21)-H(21B)	108.2
C(23)-H(23C)	0.9600	C(20)-C(21)-H(21B)	108.2
C(19)-H(19A)	0.9600	H(21A)-C(21)-H(21B)	107.3
C(19)-H(19B)	0.9600	C(16)-C(17)-C(18)	114.8(9)
C(19)-H(19C)	0.9600	C(16)-C(17)-H(17A)	108.6
		C(18)-C(17)-H(17A)	108.6
C(16)-Sn(1)-C(12)	119.1(3)	C(16)-C(17)-H(17B)	108.6
C(16)-Sn(1)-C(20)	122.3(3)	C(18)-C(17)-H(17B)	108.6
C(12)-Sn(1)-C(20)	117.8(3)	H(17A)-C(17)-H(17B)	107.6
C(16)-Sn(1)-O(1)	95.7(2)	C(19)-C(18)-C(17)	112.3(12)
C(12)-Sn(1)-O(1)	96.4(2)	C(19)-C(18)-H(18A)	109.2
C(20)-Sn(1)-O(1)	86.75(18)	C(17)-C(18)-H(18A)	109.2
C(16)-Sn(1)-O(2)#1	87.1(2)	C(19)-C(18)-H(18B)	109.2
C(12)-Sn(1)-O(2)#1	90.4(2)	C(17)-C(18)-H(18B)	109.2
C(20)-Sn(1)-O(2)#1	83.76(17)	H(18A)-C(18)-H(18B)	107.9
O(1)-Sn(1)-O(2)#1	170.14(12)	C(22)-C(23)-H(23A)	109.5
C(11)-O(1)-Sn(1)	128.8(3)	C(22)-C(23)-H(23B)	109.5
C(8)-N(9)-C(4)	105.7(4)	H(23A)-C(23)-H(23B)	109.5
C(8)-N(9)-C(9)	128.6(4)	C(22)-C(23)-H(23C)	109.5
C(4)-N(9)-C(9)	125.8(4)	H(23A)-C(23)-H(23C)	109.5
C(11)-O(2)-Sn(1)#2	139.1(3)	H(23B)-C(23)-H(23C)	109.5
C(2)-N(1)-C(6)	125.5(4)	C(18)-C(19)-H(19A)	109.5

C(2)-N(1)-H(1)	113(4)	C(18)-C(19)-H(19B)	109.5
C(6)-N(1)-H(1)	122(4)	H(19A)-C(19)-H(19B)	109.5
C(2)-N(3)-C(4)	111.2(4)	C(18)-C(19)-H(19C)	109.5
C(4)-C(5)-N(7)	109.8(4)	H(19A)-C(19)-H(19C)	109.5
C(4)-C(5)-C(6)	119.3(4)	H(19B)-C(19)-H(19C)	109.5
N(7)-C(5)-C(6)	130.9(5)		
C(8)-N(7)-C(5)	104.5(4)		
C(2)-N(2)-H(2A)	120.0	Symmetry transformations used to generate equivalent atoms:	
C(2)-N(2)-H(2B)	120.0		
H(2A)-N(2)-H(2B)	120.0	#1 -x+3/2,y+1/2,-z+3/2 #2 -x+3/2,y-1/2,-z+3/2	
O(6)-C(6)-N(1)	120.3(5)		
O(6)-C(6)-C(5)	128.7(5)		
N(1)-C(6)-C(5)	111.1(5)		
N(3)-C(4)-C(5)	128.4(4)		
N(3)-C(4)-N(9)	125.0(4)		
C(5)-C(4)-N(9)	106.6(4)		
O(2)-C(11)-O(1)	123.6(5)		
O(2)-C(11)-C(10)	119.8(4)		
O(1)-C(11)-C(10)	116.5(4)		
C(11)-C(10)-C(9)	113.2(4)		

Table S3. Bond lengths [Å] and angles [°] for complex **3**.

Sn(1)-C(13)	2.112(5)	C(6)-N(1)-H(1)	114(4)
Sn(1)-C(12)	2.116(6)	O(1)-C(11)-O(2)#2	122.3(4)
Sn(1)-C(14)	2.118(5)	O(1)-C(11)-C(10)	119.1(4)
Sn(1)-O(2)	2.235(3)	O(2)#2-C(11)-C(10)	118.5(4)
Sn(1)-O(1)	2.348(3)	C(8)-N(7)-C(5)	105.5(4)
O(2)-C(11)#1	1.268(5)	C(8)-N(7)-C(9)	125.3(4)
O(1)-C(11)	1.239(6)	C(5)-N(7)-C(9)	128.0(4)
N(1)-C(2)	1.381(7)	O(6)-C(6)-N(1)	121.4(5)
N(1)-C(6)	1.393(7)	O(6)-C(6)-C(5)	127.8(5)
N(1)-H(1)	0.82(6)	N(1)-C(6)-C(5)	110.8(4)
O(6)-C(6)	1.224(6)	C(2)-N(3)-C(4)	114.4(4)
C(11)-O(2)#2	1.268(5)	C(11)-C(10)-C(9)	115.0(4)
C(11)-C(10)	1.518(7)	C(11)-C(10)-H(10A)	108.5
N(7)-C(8)	1.353(6)	C(9)-C(10)-H(10A)	108.5

N(7)-C(5)	1.384(6)	C(11)-C(10)-H(10B)	108.5
N(7)-C(9)	1.457(6)	C(9)-C(10)-H(10B)	108.5
C(6)-C(5)	1.418(7)	H(10A)-C(10)-H(10B)	107.5
N(3)-C(2)	1.319(7)	C(8)-N(9)-C(4)	104.0(4)
N(3)-C(4)	1.364(6)	C(4)-C(5)-N(7)	105.7(4)
C(10)-C(9)	1.520(7)	C(4)-C(5)-C(6)	120.8(5)
C(10)-H(10A)	0.9700	N(7)-C(5)-C(6)	133.4(5)
C(10)-H(10B)	0.9700	N(3)-C(2)-N(2)	120.0(5)
N(9)-C(8)	1.319(7)	N(3)-C(2)-N(1)	122.3(5)
N(9)-C(4)	1.371(7)	N(2)-C(2)-N(1)	117.7(5)
C(5)-C(4)	1.381(7)	N(7)-C(9)-C(10)	112.2(4)
C(2)-N(2)	1.330(7)	N(7)-C(9)-H(9A)	109.2
C(9)-H(9A)	0.9700	C(10)-C(9)-H(9A)	109.2
C(9)-H(9B)	0.9700	N(7)-C(9)-H(9B)	109.2
C(8)-H(8)	0.9300	C(10)-C(9)-H(9B)	109.2
N(2)-H(2A)	0.8600	H(9A)-C(9)-H(9B)	107.9
N(2)-H(2B)	0.8600	N(9)-C(8)-N(7)	114.1(5)
C(13)-H(13A)	0.9600	N(9)-C(8)-H(8)	122.9
C(13)-H(13B)	0.9600	N(7)-C(8)-H(8)	122.9
C(13)-H(13C)	0.9600	N(3)-C(4)-N(9)	123.5(4)
C(14)-H(14A)	0.9600	N(3)-C(4)-C(5)	125.7(5)
C(14)-H(14B)	0.9600	N(9)-C(4)-C(5)	110.7(5)
C(14)-H(14C)	0.9600	C(2)-N(2)-H(2A)	120.0
C(12)-H(12A)	0.9600	C(2)-N(2)-H(2B)	120.0
C(12)-H(12B)	0.9600	H(2A)-N(2)-H(2B)	120.0
C(12)-H(12C)	0.9600	Sn(1)-C(13)-H(13A)	109.5
C(13)-Sn(1)-C(12)	127.9(3)	Sn(1)-C(13)-H(13B)	109.5
C(13)-Sn(1)-C(14)	116.8(3)	H(13A)-C(13)-H(13B)	109.5
C(12)-Sn(1)-C(14)	115.0(2)	Sn(1)-C(13)-H(13C)	109.5
C(13)-Sn(1)-O(2)	91.87(18)	H(13A)-C(13)-H(13C)	109.5
C(12)-Sn(1)-O(2)	92.69(17)	H(13B)-C(13)-H(13C)	109.5
C(14)-Sn(1)-O(2)	91.33(19)	Sn(1)-C(14)-H(14A)	109.5
C(13)-Sn(1)-O(1)	88.10(19)	Sn(1)-C(14)-H(14B)	109.5
C(12)-Sn(1)-O(1)	87.91(18)	H(14A)-C(14)-H(14B)	109.5
C(14)-Sn(1)-O(1)	88.03(19)	Sn(1)-C(14)-H(14C)	109.5
O(2)-Sn(1)-O(1)	179.27(13)	H(14A)-C(14)-H(14C)	109.5
C(11)#1-O(2)-Sn(1)	117.8(3)	H(14B)-C(14)-H(14C)	109.5
C(11)-O(1)-Sn(1)	137.7(3)	Sn(1)-C(12)-H(12A)	109.5

C(2)-N(1)-C(6)	126.0(5)	Sn(1)-C(12)-H(12B)	109.5
C(2)-N(1)-H(1)	119(4)	H(12A)-C(12)-H(12B)	109.5
		Sn(1)-C(12)-H(12C)	109.5
		H(12A)-C(12)-H(12C)	109.5
		H(12B)-C(12)-H(12C)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,y-1/2,-z+3/2 #2 -x+2,y+1/2,-z+3/2

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

Sn(1)-C(12)	2.131(4)	C(13)-C(12)-H(12B)	108.1
Sn(1)-C(8)	2.133(4)	Sn(1)-C(12)-H(12B)	108.1
Sn(1)-C(16)	2.152(3)	H(12A)-C(12)-H(12B)	107.3
Sn(1)-O(5)	2.206(2)	C(12)-C(13)-C(14)	113.3(4)
Sn(1)-O(7)	2.302(3)	C(12)-C(13)-H(13A)	108.9
Sn(2)-C(20)	2.135(4)	C(14)-C(13)-H(13A)	108.9
Sn(2)-C(28)	2.139(3)	C(12)-C(13)-H(13B)	108.9
Sn(2)-C(24)	2.148(3)	C(14)-C(13)-H(13B)	108.9
Sn(2)-O(5A)	2.168(2)	H(13A)-C(13)-H(13B)	107.7
O(5)-C(7)	1.270(4)	C(13)-C(14)-C(15)	112.4(4)
O(6)-C(7)	1.226(4)	C(13)-C(14)-H(14A)	109.1
O(2)-C(2)	1.223(4)	C(15)-C(14)-H(14A)	109.1
O(4)-C(4)	1.229(4)	C(13)-C(14)-H(14B)	109.1
O(5A)-C(7A)	1.280(4)	C(15)-C(14)-H(14B)	109.1
O(6A)-C(7A)	1.228(4)	H(14A)-C(14)-H(14B)	107.9
O(2A)-C(2A)	1.233(5)	C(14)-C(15)-H(15A)	109.5
O(4A)-C(4A)	1.212(5)	C(14)-C(15)-H(15B)	109.5
N(1)-C(6)	1.350(4)	H(15A)-C(15)-H(15B)	109.5
N(1)-C(2)	1.441(4)	C(14)-C(15)-H(15C)	109.5
N(1)-H(1)	0.8600	H(15A)-C(15)-H(15C)	109.5
N(3)-C(4)	1.371(4)	H(15B)-C(15)-H(15C)	109.5
N(3)-C(2)	1.380(4)		
N(3)-H(3)	0.8600		

O(7)-H(7A)	0.8505	O(6)-C(7)-O(5)	127.7(3)
O(7)-H(7B)	0.8504	O(6)-C(7)-C(6)	118.2(3)
N(1A)-C(2A)	1.363(4)	O(5)-C(7)-C(6)	114.1(3)
N(1A)-C(6A)	1.380(4)	N(1)-C(6)-C(5)	121.4(3)
N(1A)-H(1A)	0.8600	N(1)-C(6)-C(7)	122.1(3)
C(16)-C(17)	1.538(6)	C(5)-C(6)-C(7)	116.5(3)
C(16)-H(16A)	0.9700	O(2)-C(2)-N(3)	120.0(3)
C(16)-H(16B)	0.9700	O(2)-C(2)-N(1)	125.9(3)
C(17)-C(18)	1.498(6)	N(3)-C(2)-N(1)	114.2(3)
C(17)-H(17A)	0.9700	O(4)-C(4)-C(5)	123.2(3)
C(17)-H(17B)	0.9700	O(4)-C(4)-N(3)	121.2(3)
C(18)-C(19)	1.523(7)	C(5)-C(4)-N(3)	115.6(3)
C(18)-H(18A)	0.9700	C(4)-C(5)-C(6)	122.4(3)
C(18)-H(18B)	0.9700	C(4)-C(5)-H(5)	118.8
C(19)-H(19A)	0.9600	C(6)-C(5)-H(5)	118.8
C(19)-H(19B)	0.9600	C(9)-C(8)-Sn(1)	115.2(3)
C(19)-H(19C)	0.9600	C(9)-C(8)-H(8A)	108.5
C(12)-C(13)	1.509(5)	Sn(1)-C(8)-H(8A)	108.5
C(12)-H(12A)	0.9700	C(9)-C(8)-H(8B)	108.5
C(12)-H(12B)	0.9700	Sn(1)-C(8)-H(8B)	108.5
C(13)-C(14)	1.525(6)	H(8A)-C(8)-H(8B)	107.5
C(13)-H(13A)	0.9700	C(8)-C(9)-C(10)	114.0(4)
C(13)-H(13B)	0.9700	C(8)-C(9)-H(9A)	108.7
C(14)-C(15)	1.546(6)	C(10)-C(9)-H(9A)	108.7
C(14)-H(14A)	0.9700	C(8)-C(9)-H(9B)	108.7
C(14)-H(14B)	0.9700	C(10)-C(9)-H(9B)	108.7
C(15)-H(15A)	0.9600	H(9A)-C(9)-H(9B)	107.6
C(15)-H(15B)	0.9600	C(11)-C(10)-C(9)	114.0(4)
C(15)-H(15C)	0.9600	C(11)-C(10)-H(10A)	108.8
C(7)-C(6)	1.510(5)	C(9)-C(10)-H(10A)	108.8
C(6)-C(5)	1.371(5)	C(11)-C(10)-H(10B)	108.8
C(4)-C(5)	1.351(5)	C(9)-C(10)-H(10B)	108.8
C(5)-H(5)	0.9300	H(10A)-C(10)-H(10B)	107.7
C(8)-C(9)	1.522(5)	C(10)-C(11)-H(11A)	109.5
C(8)-H(8A)	0.9700	C(10)-C(11)-H(11B)	109.5
C(8)-H(8B)	0.9700	H(11A)-C(11)-H(11B)	109.5
C(9)-C(10)	1.535(6)	C(10)-C(11)-H(11C)	109.5
C(9)-H(9A)	0.9700	H(11A)-C(11)-H(11C)	109.5

C(9)-H(9B)	0.9700	H(11B)-C(11)-H(11C)	109.5
C(10)-C(11)	1.495(7)	C(29)-C(28)-Sn(2)	117.7(2)
C(10)-H(10A)	0.9700	C(29)-C(28)-H(28A)	107.9
C(10)-H(10B)	0.9700	Sn(2)-C(28)-H(28A)	107.9
C(11)-H(11A)	0.9600	C(29)-C(28)-H(28B)	107.9
C(11)-H(11B)	0.9600	Sn(2)-C(28)-H(28B)	107.9
C(11)-H(11C)	0.9600	H(28A)-C(28)-H(28B)	107.2
C(28)-C(29)	1.527(5)	C(30)-C(29)-C(28)	113.6(3)
C(28)-H(28A)	0.9700	C(30)-C(29)-H(29A)	108.9
C(28)-H(28B)	0.9700	C(28)-C(29)-H(29A)	108.9
C(29)-C(30)	1.527(5)	C(30)-C(29)-H(29B)	108.9
C(29)-H(29A)	0.9700	C(28)-C(29)-H(29B)	108.9
C(29)-H(29B)	0.9700	H(29A)-C(29)-H(29B)	107.7
C(30)-C(31)	1.518(6)	C(31)-C(30)-C(29)	114.4(3)
C(30)-H(30A)	0.9700	C(31)-C(30)-H(30A)	108.7
C(30)-H(30B)	0.9700	C(29)-C(30)-H(30A)	108.7
C(31)-H(31A)	0.9600	C(31)-C(30)-H(30B)	108.7
C(31)-H(31B)	0.9600	C(29)-C(30)-H(30B)	108.7
C(31)-H(31C)	0.9600	H(30A)-C(30)-H(30B)	107.6
C(20)-C(21)	1.529(5)	C(30)-C(31)-H(31A)	109.5
C(20)-H(20A)	0.9700	C(30)-C(31)-H(31B)	109.5
C(20)-H(20B)	0.9700	H(31A)-C(31)-H(31B)	109.5
C(21)-C(22)	1.509(5)	C(30)-C(31)-H(31C)	109.5
C(21)-H(21A)	0.9700	H(31A)-C(31)-H(31C)	109.5
C(21)-H(21B)	0.9700	H(31B)-C(31)-H(31C)	109.5
C(22)-C(23)	1.535(6)	C(21)-C(20)-Sn(2)	117.1(3)
C(22)-H(22A)	0.9700	C(21)-C(20)-H(20A)	108.0
C(22)-H(22B)	0.9700	Sn(2)-C(20)-H(20A)	108.0
C(23)-H(23A)	0.9600	C(21)-C(20)-H(20B)	108.0
C(23)-H(23B)	0.9600	Sn(2)-C(20)-H(20B)	108.0
C(23)-H(23C)	0.9600	H(20A)-C(20)-H(20B)	107.3
C(7A)-C(6A)	1.504(4)	C(22)-C(21)-C(20)	113.3(3)
C(6A)-C(5A)	1.336(5)	C(22)-C(21)-H(21A)	108.9
C(2A)-N(3A)	1.357(5)	C(20)-C(21)-H(21A)	108.9
N(3A)-C(4A)	1.413(5)	C(22)-C(21)-H(21B)	108.9
N(3A)-H(3A)	0.8600	C(20)-C(21)-H(21B)	108.9
C(4A)-C(5A)	1.454(5)	H(21A)-C(21)-H(21B)	107.7
C(5A)-H(5A)	0.9300	C(21)-C(22)-C(23)	112.1(3)

C(24)-C(25)	1.531(5)	C(21)-C(22)-H(22A)	109.2
C(24)-H(24A)	0.9700	C(23)-C(22)-H(22A)	109.2
C(24)-H(24B)	0.9700	C(21)-C(22)-H(22B)	109.2
C(25)-C(26)	1.521(5)	C(23)-C(22)-H(22B)	109.2
C(25)-H(25A)	0.9700	H(22A)-C(22)-H(22B)	107.9
C(25)-H(25B)	0.9700	C(22)-C(23)-H(23A)	109.5
C(26)-C(27)	1.529(6)	C(22)-C(23)-H(23B)	109.5
C(26)-H(26A)	0.9700	H(23A)-C(23)-H(23B)	109.5
C(26)-H(26B)	0.9700	C(22)-C(23)-H(23C)	109.5
C(27)-H(27A)	0.9600	H(23A)-C(23)-H(23C)	109.5
C(27)-H(27B)	0.9600	H(23B)-C(23)-H(23C)	109.5
C(27)-H(27C)	0.9600	O(6A)-C(7A)-O(5A)	126.1(3)
		O(6A)-C(7A)-C(6A)	118.9(3)
C(12)-Sn(1)-C(8)	124.05(14)	O(5A)-C(7A)-C(6A)	115.0(3)
C(12)-Sn(1)-C(16)	118.92(15)	C(5A)-C(6A)-N(1A)	121.7(3)
C(8)-Sn(1)-C(16)	116.33(15)	C(5A)-C(6A)-C(7A)	124.1(3)
C(12)-Sn(1)-O(5)	99.06(13)	N(1A)-C(6A)-C(7A)	114.1(3)
C(8)-Sn(1)-O(5)	91.86(13)	O(2A)-C(2A)-N(3A)	122.7(3)
C(16)-Sn(1)-O(5)	86.90(12)	O(2A)-C(2A)-N(1A)	121.8(3)
C(12)-Sn(1)-O(7)	86.30(14)	N(3A)-C(2A)-N(1A)	115.4(3)
C(8)-Sn(1)-O(7)	86.38(14)	C(2A)-N(3A)-C(4A)	127.2(3)
C(16)-Sn(1)-O(7)	89.13(12)	C(2A)-N(3A)-H(3A)	116.4
O(5)-Sn(1)-O(7)	174.41(10)	C(4A)-N(3A)-H(3A)	116.4
C(20)-Sn(2)-C(28)	121.43(14)	O(4A)-C(4A)-N(3A)	120.9(3)
C(20)-Sn(2)-C(24)	122.03(15)	O(4A)-C(4A)-C(5A)	126.3(3)
C(28)-Sn(2)-C(24)	113.29(15)	N(3A)-C(4A)-C(5A)	112.8(3)
C(20)-Sn(2)-O(5A)	98.31(12)	C(6A)-C(5A)-C(4A)	120.4(3)
C(28)-Sn(2)-O(5A)	98.68(11)	C(6A)-C(5A)-H(5A)	119.8
C(24)-Sn(2)-O(5A)	90.80(11)	C(4A)-C(5A)-H(5A)	119.8
C(7)-O(5)-Sn(1)	117.7(2)	C(25)-C(24)-Sn(2)	113.2(2)
C(7A)-O(5A)-Sn(2)	114.4(2)	C(25)-C(24)-H(24A)	108.9
C(6)-N(1)-C(2)	119.8(3)	Sn(2)-C(24)-H(24A)	108.9
C(6)-N(1)-H(1)	120.1	C(25)-C(24)-H(24B)	108.9
C(2)-N(1)-H(1)	120.1	Sn(2)-C(24)-H(24B)	108.9
C(4)-N(3)-C(2)	126.6(3)	H(24A)-C(24)-H(24B)	107.7
C(4)-N(3)-H(3)	116.7	C(26)-C(25)-C(24)	114.2(3)
C(2)-N(3)-H(3)	116.7	C(26)-C(25)-H(25A)	108.7
Sn(1)-O(7)-H(7A)	109.2	C(24)-C(25)-H(25A)	108.7

Sn(1)-O(7)-H(7B)	109.4	C(26)-C(25)-H(25B)	108.7
H(7A)-O(7)-H(7B)	109.5	C(24)-C(25)-H(25B)	108.7
C(2A)-N(1A)-C(6A)	122.2(3)	H(25A)-C(25)-H(25B)	107.6
C(2A)-N(1A)-H(1A)	118.9	C(25)-C(26)-C(27)	112.3(4)
C(6A)-N(1A)-H(1A)	118.9	C(25)-C(26)-H(26A)	109.1
C(17)-C(16)-Sn(1)	114.8(2)	C(27)-C(26)-H(26A)	109.1
C(17)-C(16)-H(16A)	108.6	C(25)-C(26)-H(26B)	109.1
Sn(1)-C(16)-H(16A)	108.6	C(27)-C(26)-H(26B)	109.1
C(17)-C(16)-H(16B)	108.6	H(26A)-C(26)-H(26B)	107.9
Sn(1)-C(16)-H(16B)	108.6	C(26)-C(27)-H(27A)	109.5
H(16A)-C(16)-H(16B)	107.5	C(26)-C(27)-H(27B)	109.5
C(18)-C(17)-C(16)	114.2(3)	H(27A)-C(27)-H(27B)	109.5
C(18)-C(17)-H(17A)	108.7	C(26)-C(27)-H(27C)	109.5
C(16)-C(17)-H(17A)	108.7	H(27A)-C(27)-H(27C)	109.5
C(18)-C(17)-H(17B)	108.7	H(27B)-C(27)-H(27C)	109.5
C(16)-C(17)-H(17B)	108.7		
H(17A)-C(17)-H(17B)	107.6		
C(17)-C(18)-C(19)	114.1(4)		
C(17)-C(18)-H(18A)	108.7		
C(19)-C(18)-H(18A)	108.7		
C(17)-C(18)-H(18B)	108.7		
C(19)-C(18)-H(18B)	108.7		
H(18A)-C(18)-H(18B)	107.6		
C(18)-C(19)-H(19A)	109.5		
C(18)-C(19)-H(19B)	109.5		
H(19A)-C(19)-H(19B)	109.5		
C(18)-C(19)-H(19C)	109.5		
H(19A)-C(19)-H(19C)	109.5		
H(19B)-C(19)-H(19C)	109.5		
C(13)-C(12)-Sn(1)	117.0(3)		
C(13)-C(12)-H(12A)	108.1		
Sn(1)-C(12)-H(12A)	108.1		

Table S5. Bond lengths [Å] and angles [°] for complex **5**.			
Sn(1)-C(12)	2.119(3)	C(6)-N(1)-C(2)	118.2(2)

Sn(1)-C(13)	2.120(3)	Sn(1)-C(12)-H(12A)	109.5
Sn(1)-C(14)	2.121(3)	Sn(1)-C(12)-H(12B)	109.5
Sn(1)-O(1)	2.1848(18)	H(12A)-C(12)-H(12B)	109.5
Sn(1)-O(3)	2.343(2)	Sn(1)-C(12)-H(12C)	109.5
O(3)-H(3A)	0.86(4)	H(12A)-C(12)-H(12C)	109.5
O(3)-H(3B)	0.87(4)	H(12B)-C(12)-H(12C)	109.5
O(1)-C(11)	1.289(3)	Sn(1)-C(14)-H(14A)	109.5
O(2)-C(11)	1.240(3)	Sn(1)-C(14)-H(14B)	109.5
N(9)-C(8)	1.369(3)	H(14A)-C(14)-H(14B)	109.5
N(9)-C(4)	1.372(3)	Sn(1)-C(14)-H(14C)	109.5
N(9)-C(9)	1.460(3)	H(14A)-C(14)-H(14C)	109.5
N(3)-C(4)	1.328(3)	H(14B)-C(14)-H(14C)	109.5
N(3)-C(2)	1.349(3)	Sn(1)-C(13)-H(13A)	109.5
N(1)-C(6)	1.330(4)	Sn(1)-C(13)-H(13B)	109.5
N(1)-C(2)	1.365(3)	H(13A)-C(13)-H(13B)	109.5
C(12)-H(12A)	0.9600	Sn(1)-C(13)-H(13C)	109.5
C(12)-H(12B)	0.9600	H(13A)-C(13)-H(13C)	109.5
C(12)-H(12C)	0.9600	H(13B)-C(13)-H(13C)	109.5
C(14)-H(14A)	0.9600	O(2)-C(11)-O(1)	125.4(3)
C(14)-H(14B)	0.9600	O(2)-C(11)-C(10)	119.4(2)
C(14)-H(14C)	0.9600	O(1)-C(11)-C(10)	115.3(2)
C(13)-H(13A)	0.9600	C(11)-C(10)-C(9)	116.1(2)
C(13)-H(13B)	0.9600	C(11)-C(10)-H(10A)	108.3
C(13)-H(13C)	0.9600	C(9)-C(10)-H(10A)	108.3
C(11)-C(10)	1.513(4)	C(11)-C(10)-H(10B)	108.3
C(10)-C(9)	1.514(3)	C(9)-C(10)-H(10B)	108.3
C(10)-H(10A)	0.9700	H(10A)-C(10)-H(10B)	107.4
C(10)-H(10B)	0.9700	N(9)-C(9)-C(10)	112.6(2)
C(9)-H(9A)	0.9700	N(9)-C(9)-H(9A)	109.1
C(9)-H(9B)	0.9700	C(10)-C(9)-H(9A)	109.1
C(8)-N(7)	1.310(4)	N(9)-C(9)-H(9B)	109.1
C(8)-H(8)	0.9300	C(10)-C(9)-H(9B)	109.1
N(7)-C(5)	1.396(4)	H(9A)-C(9)-H(9B)	107.8
C(5)-C(6)	1.385(4)	N(7)-C(8)-N(9)	113.8(2)
C(5)-C(4)	1.395(3)	N(7)-C(8)-H(8)	123.1
C(2)-N(2)	1.346(4)	N(9)-C(8)-H(8)	123.1
C(6)-H(6)	0.9300	C(8)-N(7)-C(5)	104.2(2)
N(2)-H(2B)	0.86(3)	C(6)-C(5)-C(4)	115.4(2)

N(2)-H(2A)	0.80(4)	C(6)-C(5)-N(7)	134.7(2)
C(12)-Sn(1)-C(13)	114.76(12)	C(4)-C(5)-N(7)	109.9(2)
C(12)-Sn(1)-C(14)	129.34(12)	N(3)-C(4)-N(9)	127.2(2)
C(13)-Sn(1)-C(14)	115.08(12)	N(3)-C(4)-C(5)	126.9(2)
C(12)-Sn(1)-O(1)	91.82(11)	N(9)-C(4)-C(5)	105.9(2)
C(13)-Sn(1)-O(1)	91.80(10)	N(2)-C(2)-N(3)	117.1(2)
C(14)-Sn(1)-O(1)	95.16(9)	N(2)-C(2)-N(1)	116.5(2)
C(12)-Sn(1)-O(3)	89.01(11)	N(3)-C(2)-N(1)	126.3(2)
C(13)-Sn(1)-O(3)	89.36(10)	N(1)-C(6)-C(5)	120.7(2)
C(14)-Sn(1)-O(3)	83.03(10)	N(1)-C(6)-H(6)	119.6
O(1)-Sn(1)-O(3)	178.13(7)	C(5)-C(6)-H(6)	119.6
Sn(1)-O(3)-H(3A)	123(3)	C(2)-N(2)-H(2B)	118(2)
Sn(1)-O(3)-H(3B)	123(3)	C(2)-N(2)-H(2A)	118(2)
H(3A)-O(3)-H(3B)	106(4)	H(2B)-N(2)-H(2A)	117(3)
C(11)-O(1)-Sn(1)	121.79(17)		
C(8)-N(9)-C(4)	106.2(2)		
C(8)-N(9)-C(9)	129.0(2)		
C(4)-N(9)-C(9)	124.8(2)		
C(4)-N(3)-C(2)	112.4(2)		