Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supporting Information

Cyclophosphazene-Organostannoxane Hybrid Motifs in Polymeric and Molecular Systems

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Experimental Section:

Solvents were distilled and dried prior to use according to standard procedures. [*n*-$Bu_2SnO]_n$, 3,5-dinitrosalicylic acid, 2,2′-biphenol and 4-hydroxy pyridine (all from Aldrich) were used as such. Hexachlorocyclotriphosphazene (Nippon Soda, Japan) was recrystallized from *n*-hexane before use. Melting points were measured using a JSGW melting point apparatus and are uncorrected. Elemental analyses were carried out using a Thermoquest CE instruments model EA/110 CHNS-O elemental analyzer. Infrared spectra were recorded as KBr pellets on a FT-IR Bruker-Vector Model. ^{1}H,^{31}P and ^{119}Sn NMR spectra were obtained on a JEOL-DELTA2 500 model spectrometer using $CDCl_3$ as solvent. Chemical shifts were referenced with respect to tetramethylsilane (for ^{1}H NMR), phosphoric acid (for ^{31}P NMR) and tetramethyltin (for ^{119}Sn NMR) respectively. ^{119}Sn NMR spectra were recorded under broad-band decoupled conditions.

Synthesis:

Compound **1**[1] and **L**[2] were synthesized according to literature procedure and purity was checked by ^{1}H, ^{119}Sn and ^{31}P NMR (given below).

[*n*-Bu_2Sn-OOR(O)$H_2O]_n$ (1):

^{1}H NMR ($CDCl_3$): δ (ppm) = 0.84-1.94, (m, 18H, n-Bu); 8.62 (d, 1H, ArH); 8.86 (d, 1H, ArH).

^{119}Sn NMR ($CDCl_3$): δ (ppm) = -47.5

gem-**[$N_3P_3(O_2C_{12}H_8)_2(OC_5H_4N$-4)] (L):**

^{1}H NMR($CDCl_3$): δ (ppm) = 7.7 (d, 4H); 7.20-7.52 (m, 16H); 8.63 (d, 4H). ^{31}P NMR: δ (ppm) = 9.15(t), 25.20 (d){^{2}J(P–N–P) = 93.83 Hz}.

Synthesis of 2 and 3:

Polymer **1** (200 mg, 0.42 mmol) and **L** [*gem*-{$N_3P_3(O_2C_{12}H_8)_2(OC_5H_4N\text{-}4)_2$](145mg, 0.21 mmol) were heated to reflux for 24h in 40 mL methanol. Then the methanol was concentrated to 5mL under reduced pressure to get a yellow precipitate. The yellow solid product was re-dissolved in 15mL of (1:1) CH_3OH-$CHCl_3$ solvent mixture. Slow evaporation of the solvent mixture yielded compound **2** and **3** as a crystalline form.

Compounds **2** and **3** were separated by recrystallization from $CHCl_3$ solution. The polymer **2** was collected from chloroform solution (filtrate) and compound **3**was collected as an insoluble crystalline material.

[*gem*-{N_3P_3-$(O_2C_{12}H_8)_2(OC_5H_4N\text{-}4)_2$}{*n*-$Bu_2Sn$-OOCR(O)}$_2$]$_n$ (2), R= [3,5-$(NO_2)_2C_6H_2$]:Yield: 216mg(63 %, with respect to tin).M.p.: 141 °C.Elemental Analysis: Calcd. (%)for $C_{64}H_{64}N_9O_{20}P_3Sn_2$: C, 47.76; H, 4.01; N, 7.83.Found: C, 47.26; H,4.08; N, 7.89; ^{1}H NMR[DMSO-d^6]: δ (ppm) = 0.73 (t, 12H, *n*-Bu); 1.19 (m, 8H, *n*-Bu); 1.33 (m, 8H, *n*-Bu); 1.42 (m, 8H, *n*-Bu); 7.16-7.51 (m, 16H, biphenol); 7.64 (d, 4H, Pyridyl); 8.57 (d, 2H , Ar- salicylate); 8.70 (d, 4H, Pyridyl); 8.79 (d, 2H, Ar- salicylate). ^{31}P NMR[DMSO-d^6]: δ (ppm) = δ ppm = 25.22 (d, P($O_2C_{12}H_8$), 9.59 (t, P(O-C_5H_4N-3)$_2$, {^{2}J(P–N–P) = 95.52 Hz}];^{119}Sn NMR [DMSO-d^6]: δ (ppm) = -347 ppm. IR (KBr, ν/cm−1): 3092 (m), 2956 (m, br), 2927 (m), 2869 (s), 1635 (s), 2605 (m), 1528 (s), 1436 (s), 1338 (s), 1228 (s), 1174 (m), 1092 (m), 889 (m), 719 (s), 609 (m), 522 (m). ESI-MS: m/z (%) 355.0531 [(*n*-$Bu_2Sn)_2OOCR(O)]^{2+}$ (100); 693.1010 $[LH]^+$ (58).

[*gem*-{N_3P_3-$(O_2C_{12}H_8)_2$}(O)(*n*-$Bu_2Sn)_2$(μ$_3$-O)(μ-OMe)]$_2$.MeOH(3):Yield: 29.8mg (13%, with respect to tin). M.p.: 189 °C.Elemental Analysis: Calcd. (%) for $C_{64}H_{64}N_9O_{20}P_3Sn_2$: C, 47.15; H, 5.71; N, 3.84.Found: C, 46.96; H, 5.78; N, 3.81. IR (KBr, ν/cm−1): 3571 (m), 3422 (m, br),

3069(m, br), 2926 (s), 2957 (s), 2856 (m), 1635 (s), 1603 (s), 1500 (s), 1437 (s), 1227 (m), 1171(s), 1093 (s), 776 (s), 609 (s), 533 (m).

References

1. L.Tian, F. Li, X.Zheng, Y.Sun, D.Yan and L. Tu, *Synth. React. Inorg. Met.-Org. Nano-Metal Chem.,* 2011, **41**, 454.
2. G. A. Carriedo, F. J. G. Alonso, J. L. García, R. J. Carbajo and F. L. Ortiz, *Inorg. Chem.,*1999**,6**, 1015.

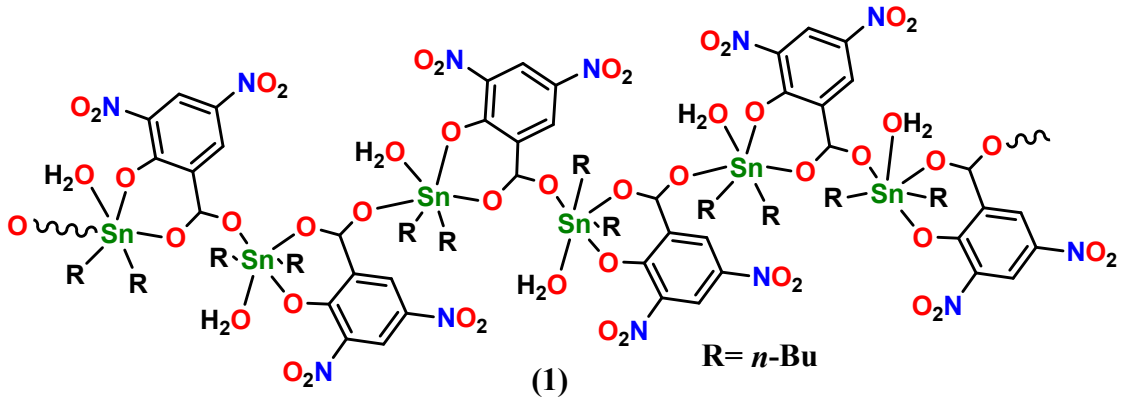


Figure S1: 1-D coordination polymer (**1**)

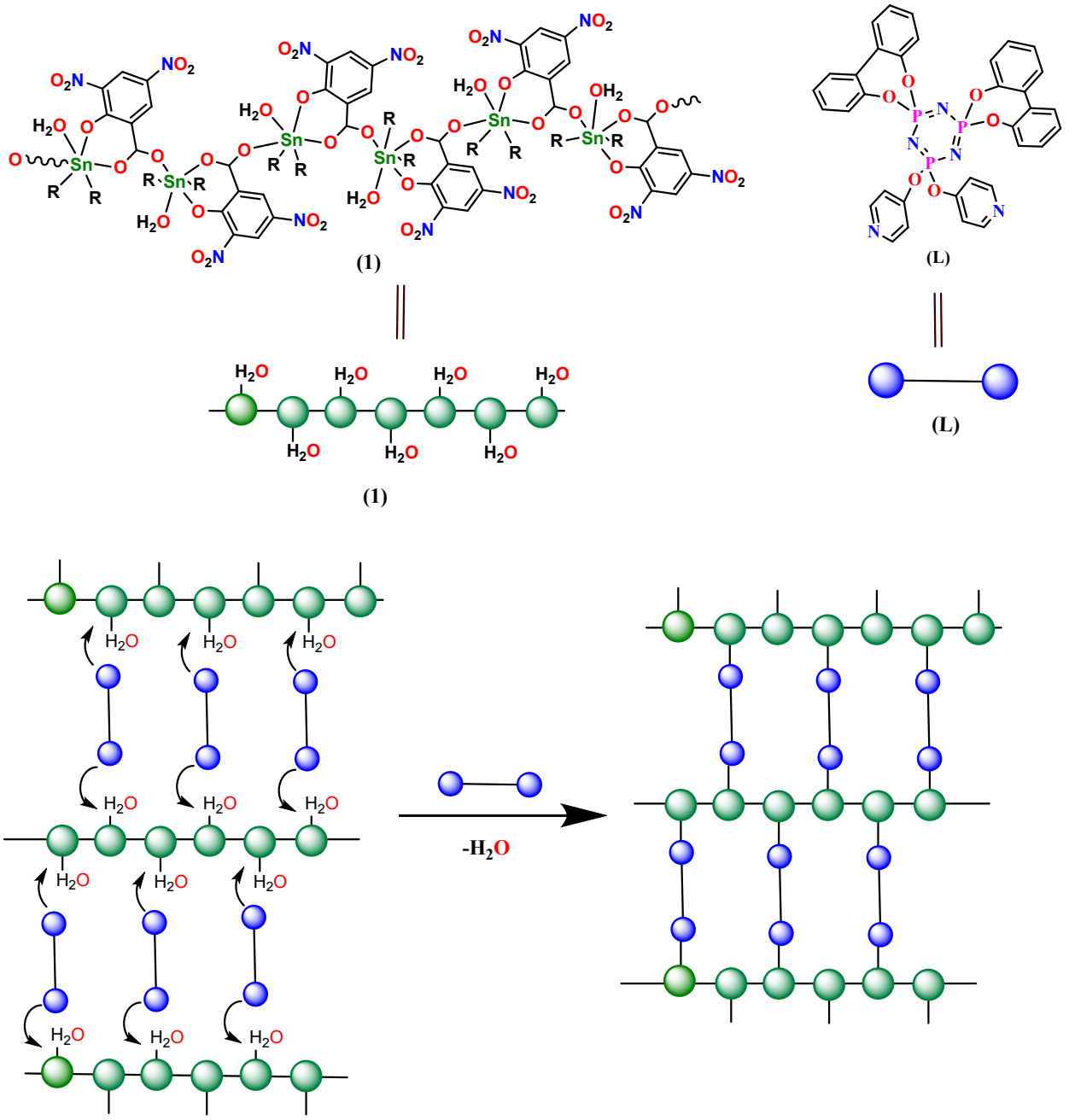
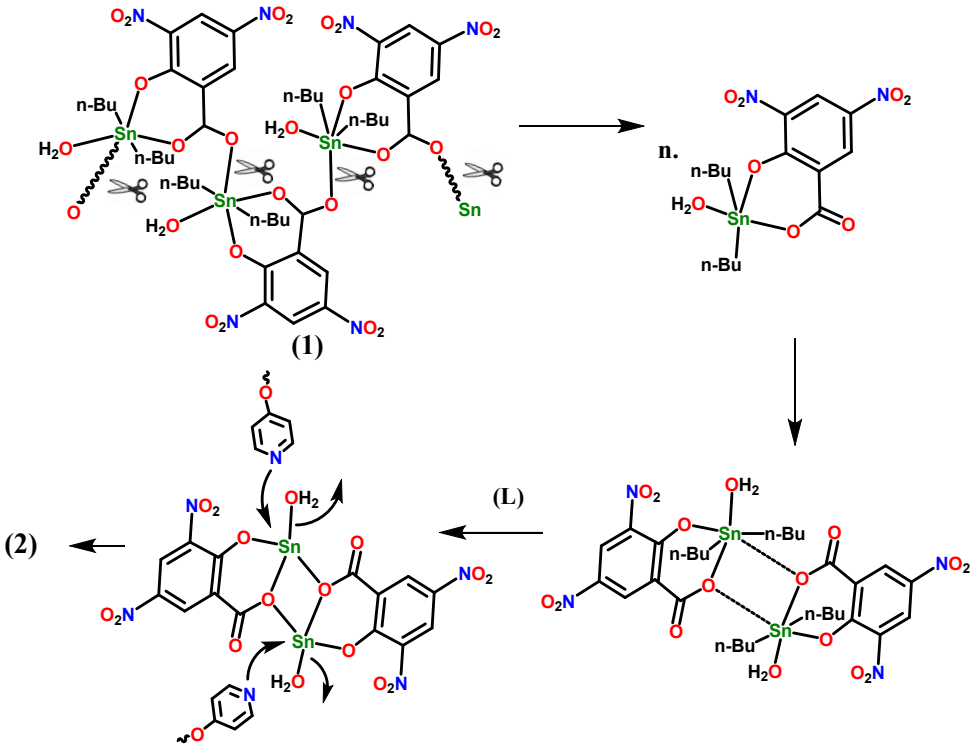


Figure S2: Schematic representation of the expected 2-D polymer in the reaction between **1** and L



Scheme S1: Formation of **2** from **1**.

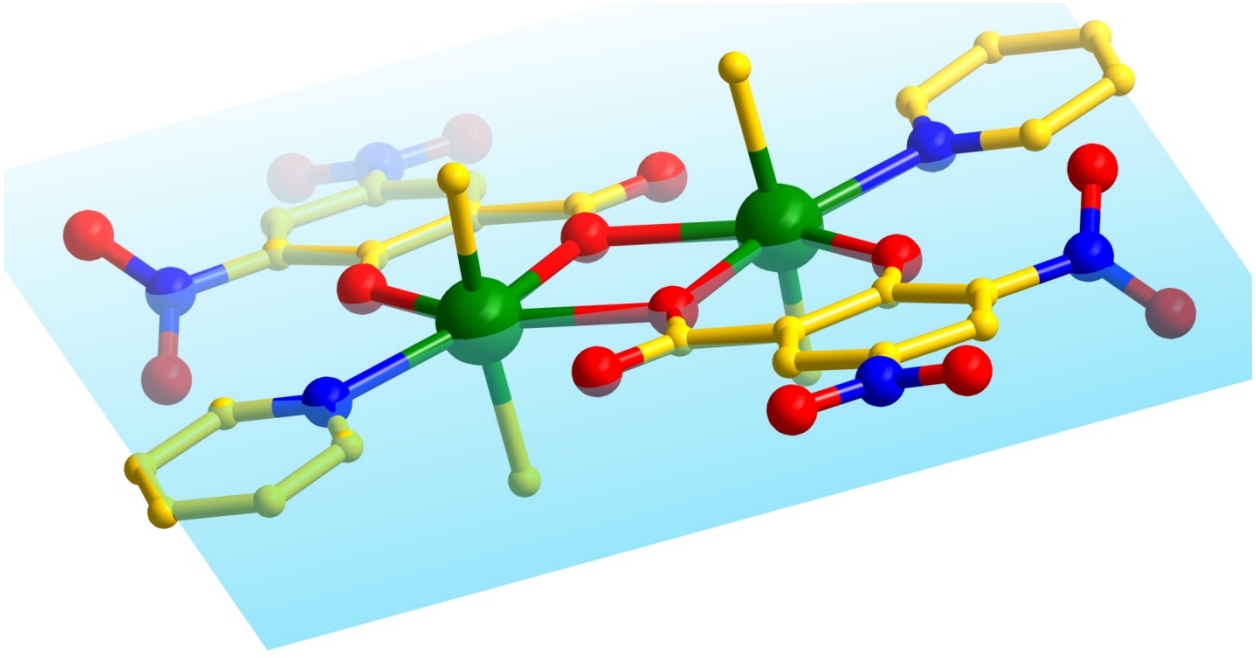


Figure S3: The core of polymer **1** lying in a plane.

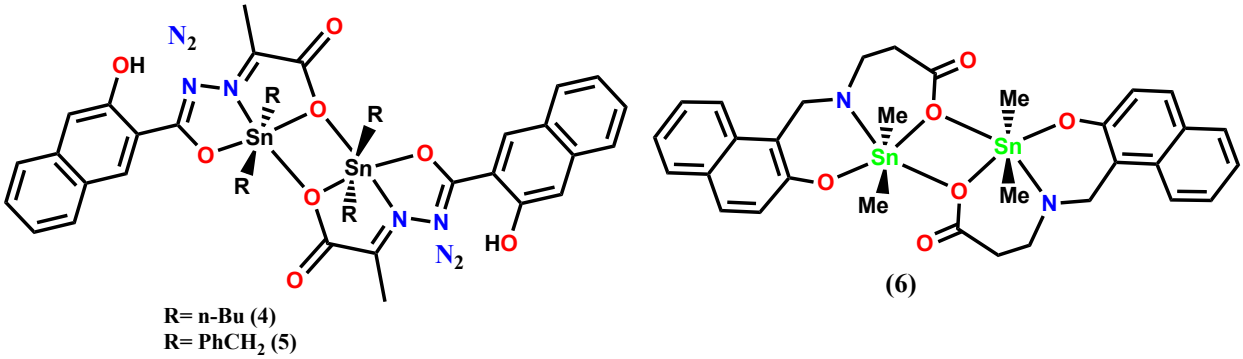
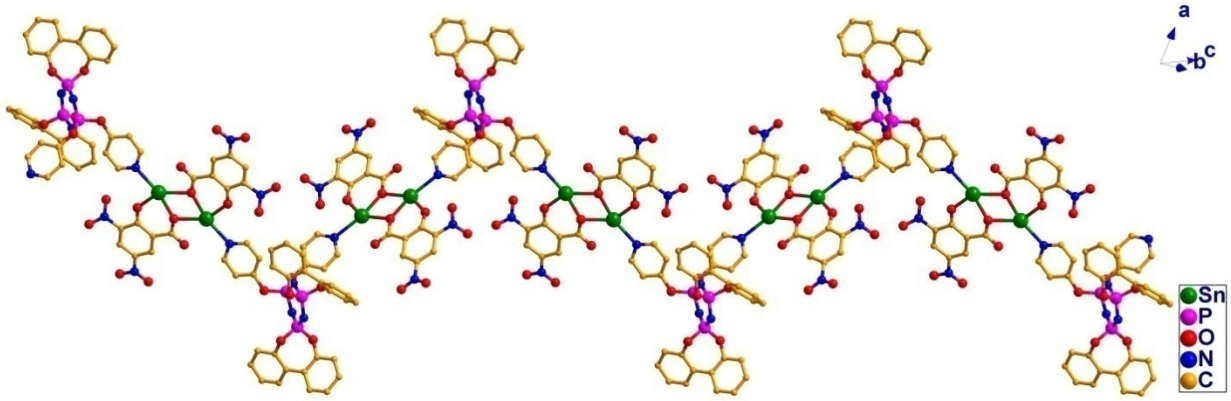


Chart S1: Carboxylate-bridged dimer



FigureS4: Zig-zag coordination polymer (**2**)**.**

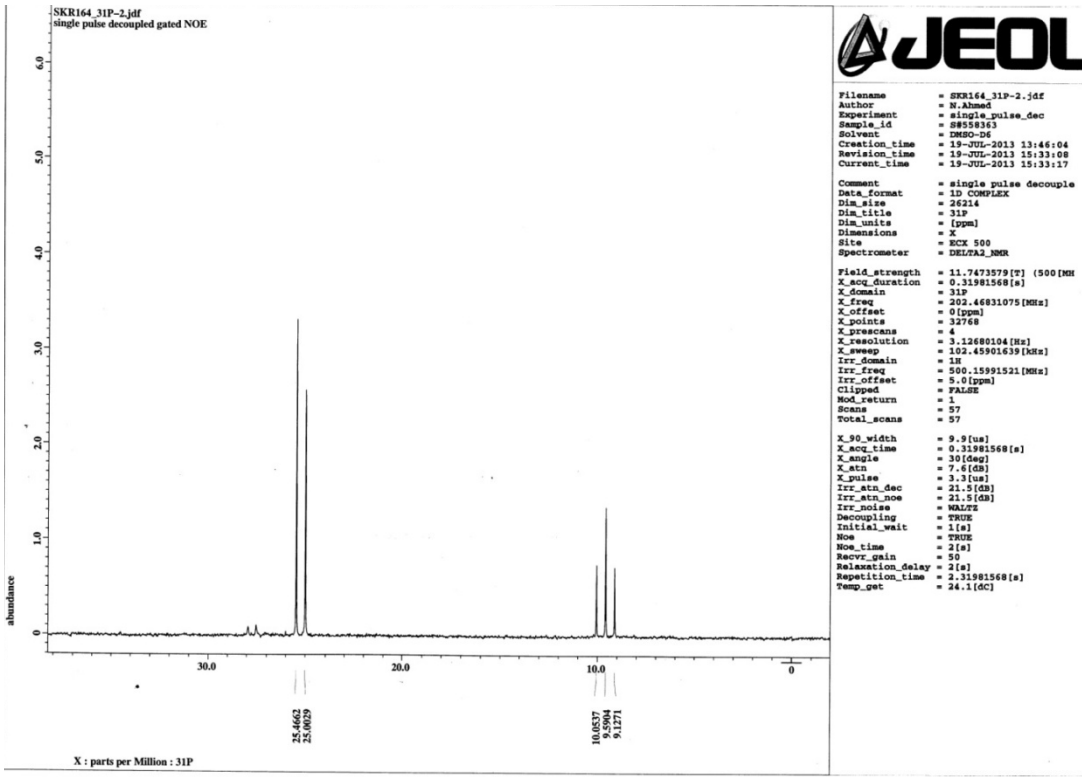


Figure S5: ^{31}P NMR of **2**.

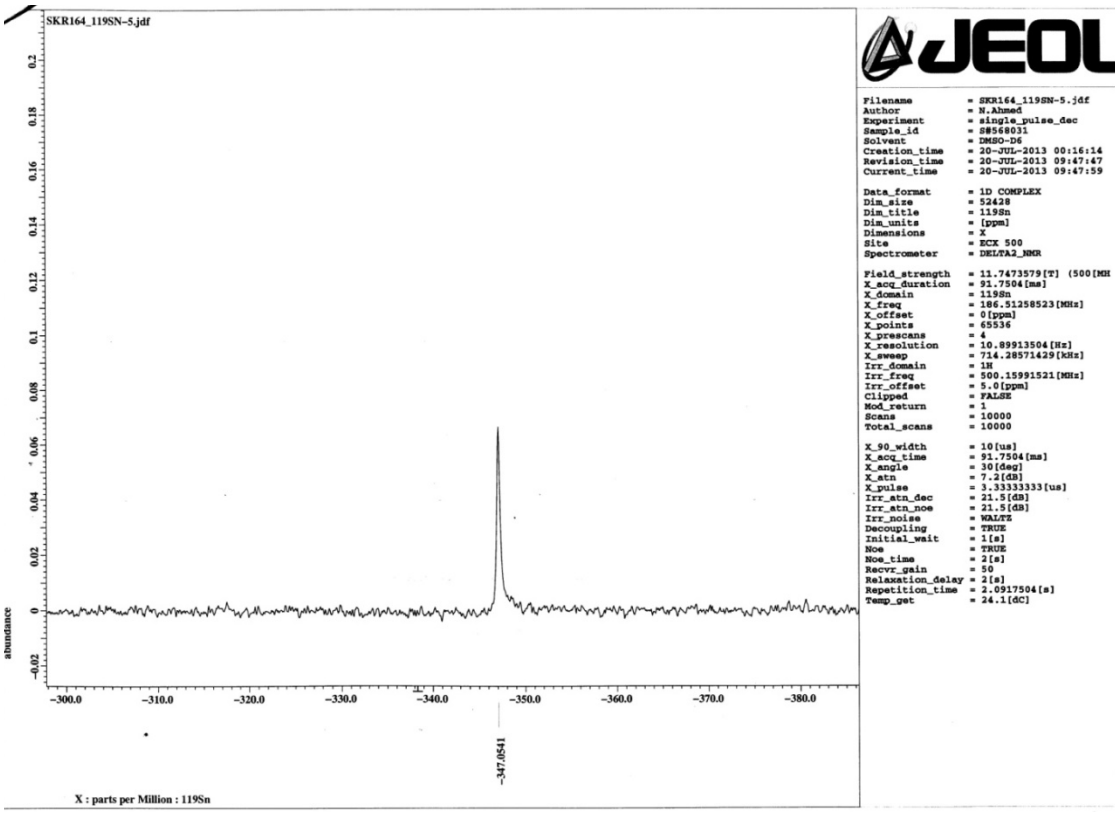


Figure S6: ^{119}Sn NMR of **2.**

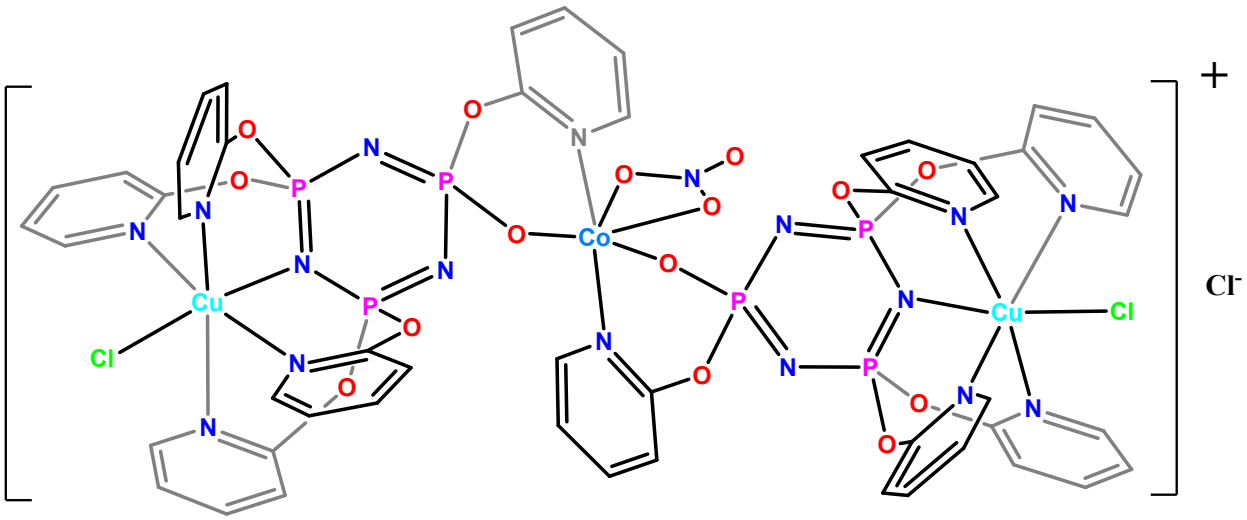


Figure S7: Co(II)-mediated hydrolysis product [{(LCuCl)$_2$(Co(NO$_3$)}Cl] where (L)= $N_3P_3(OC_5H_4N)_5(O)$ (Reference: V. Chandrasekhar, B. M. Pandian and R. Azhakar, *Inorg. Chem*. 2006, **45**, 3510)

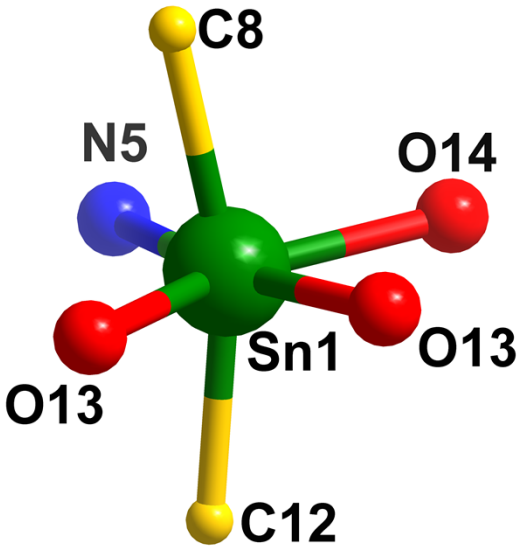


Figure S8: Coordination environment around the tin atomsof **2**(distorted octahedral geometry)

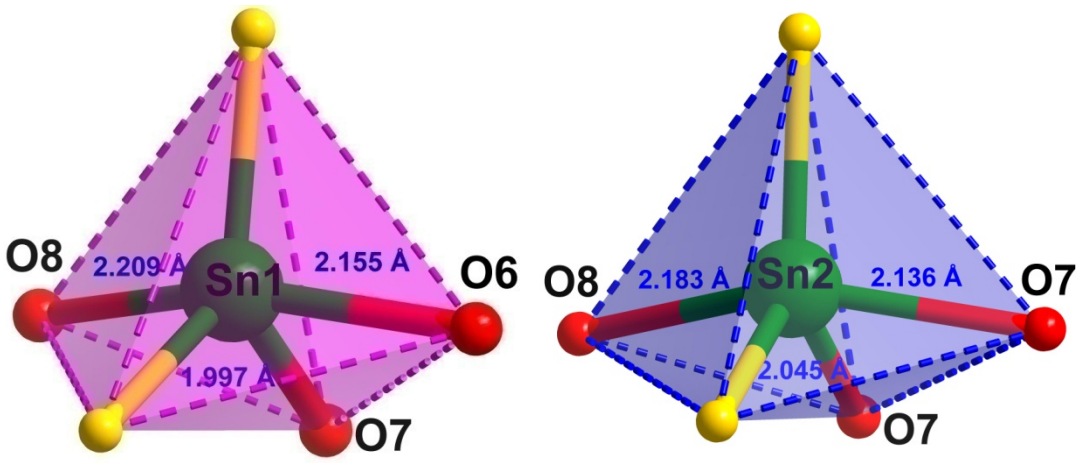


Figure S9:(a) Coordination environment around terminal tin(Sn1) atoms[distorted rectangular pyramidal geometry (τ = 0.41, cf. the τ values for theidealized geometries are τ = 0, rectangular pyramidal; τ= 1, trigonalbipyramidal))][3] (b) around central tin atoms [distorted rectangular pyramidal geometry (τ = 0.31)]

Reference:

3.A. W.Addison, T. N.Rao, J.Reedijk, J.van Rijn and G. C. Verschoor, *J. Chem. Soc., Dalton Trans.***1984**, 1349.

X-ray Crystallographic Study: The crystal data for compounds**2**and **3**were collected on a BrukerD8 QUESTDiffractrometer. SMART software package (version 5.628) was used for collecting data frames, SAINT software package (version 6.45) for integration of the intensity and scaling and SADABS was used for absorption correction. The structures were solved and refined by full-matrix least squares on F^2 using SHELXTL software package.[1]Non-hydrogen atoms were refined with anisotropic displacement parameters. Figures and their bonding parameters were obtained from DIAMOND 3.1f software package.[2]

Reference:

(1) G. M. Sheldrick, SHELXTL version 6.14; Bruker AXS Inc.:Madison, WI, **2003**.

(2) (a) K.Brandenburg, Diamond, Ver. 3.1eM; Crystal Impact GbR: Bonn, Germany, **2005**.(b) DIAMOND version 3.1f; Crystal Impact GbR: Bonn, Germany, **2004**.

Table S1.Crystal data and structure refinement parameters of compound **2** (ccdc 971483) and **3** (ccdc971484).

Parameters	**2**	**3**
Empirical formula	$C_{64}H_{64}N_9O_{20}P_3Sn_2$	$C_{86}H_{124}N_6O_{18}P_6Sn_4$
Formula weight	1609.58	2190.58
Temperature	100(2) K	100(2) K
Wavelength	0.71069 Å	0.71069 Å
Crystal system, space group	Triclinic	Monoclinic
Unit cell dimensions	a = 11.378(5) Å b = 14.319(5) Å c = 23.323(5) Å α = 82.037(5)°. β = 79.189(5)°. γ = 68.015(5)°.	a = 18.805(5) Å b = 12.506(5) Å c = 21.511(5) Å α= 90 β= 110.835(5)°. γ = 90
Volume	3451(2) $Å^3$	4728(3) $Å^3$
Z, Calculated density	2, 1.549 Mg/m^3	2, 1.539 Mg/m^3
Absorption coefficient	0.872 mm^{-1}	1.213 mm^{-1}
F(000)	2264	2640
Crystal size	0.20 x 0.18 x 0.15 mm^3	0.14 x 0.13 x 0.10 mm^3
θ range for data collection	1.83 to 25.50°	2.00 to 25.00°
Limiting indices	-13<=h<=13, -17<=k<=15, -28<=l<=28	-22<=h<=20, -13<=k<=14, -24<=l<=25
Reflections collected / unique	18859/12631 [R(int) = 0.0290]	31227/8327 [R(int) = 0.0684]
Completeness to theta	98.2 %	99.8 %
Data / restraints / parameters	12631 / 0 / 887	8327 / 24 / 549
Goodness-of-fit on F^2	1.043	1.080
Final R indices [I >2σ(I)]	R1 = 0.0483, wR2 = 0.1294	R1 = 0.0702, wR2 = 0.1586
R indices (all data)	R1 = 0.0590, wR2 = 0.1544	R1 = 0.1185, wR2 = 0.1789
Largest diff. peak and hole	2.206 and -0.963 e.$Å^{-3}$	1.840 and -1.059 e.$Å^{-3}$

Table S2: Bond parameters of polymer **2:**

Bond lengths (Å)		Bond angles (°)	
Sn(1)-C(8)	2.128(4)	C(8)-Sn(1)-C(12)	163.61(18)
Sn(1)-C(12)	2.128(4)	C(8)-Sn(1)-O(14)	95.63(14)
Sn(1)-O(14)	2.132(3)	C(12)-Sn(1)-O(14)	99.63(15)
Sn(1)-O(13)	2.195(3)	C(8)-Sn(1)-O(13)	92.87(15)
Sn(1)-O(13)#1	2.426(3)	C(12)-Sn(1)-O(13)	95.58(16)
Sn(1)-N(5)	2.429(4)	O(14)-Sn(1)-O(13)	80.14(11)
Sn(2)-O(7)	2.105(3)	C(8)-Sn(1)-O(13)#1	83.16(14)
Sn(2)-C(30)	2.128(5)	C(12)-Sn(1)-O(13)#1	87.67(14)
Sn(2)-C(26)	2.131(5)	O(14)-Sn(1)-O(13)#1	145.16(11)
Sn(2)-O(6)	2.173(3)	O(13)-Sn(1)-O(13)#1	65.20(12)
Sn(2)-O(6)#2	2.440(3)	C(8)-Sn(1)-N(5)	89.48(15)
Sn(2)-N(4)	2.486(4)	C(12)-Sn(1)-N(5)	85.73(16)
P(2)-N(1)	1.574(4)	O(14)-Sn(1)-N(5)	85.86(13)
P(2)-N(3)	1.579(4)	O(13)-Sn(1)-N(5)	165.96(12)
P(2)-O(8)	1.593(3)	O(13)#1-Sn(1)-N(5)	128.84(12)
P(2)-O(9)	1.606(3)	O(7)-Sn(2)-C(30)	100.18(16)
P(3)-N(2)	1.568(4)	O(7)-Sn(2)-C(26)	98.75(16)
P(3)-N(3)	1.586(4)	C(30)-Sn(2)-C(26)	157.99(19)
P(3)-O(17)	1.588(3)	O(7)-Sn(2)-O(6)	80.95(12)
P(3)-O(18)	1.591(3)	C(30)-Sn(2)-O(6)	99.70(16)
P(1)-N(2)	1.577(4)	C(26)-Sn(2)-O(6)	94.26(16)
P(1)-O(19)	1.581(3)	O(7)-Sn(2)-O(6)#2	146.44(11)
P(1)-O(20)	1.591(3)	C(30)-Sn(2)-O(6)#2	85.65(15)
P(1)-N(1)	1.596(4)	C(26)-Sn(2)-O(6)#2	84.76(15)
O(18)-C(53)	1.406(5)	O(6)-Sn(2)-O(6)#2	65.49(13)
O(9)-C(18)	1.375(5)	O(7)-Sn(2)-N(4)	84.22(13)
O(20)-C(52)	1.402(5)	C(30)-Sn(2)-N(4)	84.58(16)
O(8)-C(21)	1.396(5)	C(26)-Sn(2)-N(4)	86.26(16)
O(19)-C(41)	1.414(5)	O(6)-Sn(2)-N(4)	165.07(12)
O(6)-C(34)	1.313(6)	O(6)#2-Sn(2)-N(4)	129.33(12)

O(6)-Sn(2)#2	2.440(3)	N(1)-P(2)-N(3)	118.8(2)
O(13)-C(65)	1.298(5)	N(1)-P(2)-O(8)	111.10(18)
O(13)-Sn(1)#1	2.426(3)	N(3)-P(2)-O(8)	109.38(18)
O(17)-C(60)	1.405(5)	N(1)-P(2)-O(9)	105.69(18)
O(10)-N(7)	1.229(5)	N(3)-P(2)-O(9)	111.82(18)
O(7)-C(36)	1.298(5)	O(8)-P(2)-O(9)	97.99(16)
O(3)-N(8)	1.208(6)	N(2)-P(3)-N(3)	117.71(19)
N(4)-C(24)	1.332(6)	N(2)-P(3)-O(17)	107.23(19)
N(4)-C(23)	1.332(6)	N(3)-P(3)-O(17)	110.19(19)
O(1)-N(9)	1.224(6)	N(2)-P(3)-O(18)	112.52(19)
O(11)-N(7)	1.235(5)	N(3)-P(3)-O(18)	104.59(18)
N(5)-C(16)	1.336(6)	O(17)-P(3)-O(18)	103.76(16)
N(5)-C(20)	1.349(6)	N(2)-P(1)-O(19)	112.63(19)
O(12)-C(65)	1.225(5)	N(2)-P(1)-O(20)	106.03(19)
O(5)-C(34)	1.220(6)	O(19)-P(1)-O(20)	103.39(17)
O(14)-C(1)	1.296(5)	N(2)-P(1)-N(1)	117.5(2)
N(10)-O(15)	1.234(5)	O(19)-P(1)-N(1)	104.19(18)
N(10)-O(16)	1.237(5)	O(20)-P(1)-N(1)	112.32(18)
N(10)-C(6)	1.465(6)	C(53)-O(18)-P(3)	121.3(3)
C(58)-C(57)	1.398(6)	C(18)-O(9)-P(2)	125.0(3)
C(58)-C(53)	1.405(6)	C(52)-O(20)-P(1)	119.8(3)
C(58)-C(59)	1.480(7)	C(21)-O(8)-P(2)	125.5(3)
N(8)-O(4)	1.243(6)	C(41)-O(19)-P(1)	119.9(3)
N(8)-C(37)	1.475(6)	C(34)-O(6)-Sn(2)	137.0(3)
C(6)-C(5)	1.370(6)	C(34)-O(6)-Sn(2)#2	108.5(3)
C(6)-C(1)	1.423(6)	Sn(2)-O(6)-Sn(2)#2	114.50(13)
N(9)-O(2)	1.226(6)	C(65)-O(13)-Sn(1)	136.8(3)
N(9)-C(39)	1.456(6)	C(65)-O(13)-Sn(1)#1	106.9(3)
C(3)-C(4)	1.387(6)	Sn(1)-O(13)-Sn(1)#1	114.80(12)
C(3)-C(2)	1.387(6)	C(60)-O(17)-P(3)	118.1(3)
C(2)-C(1)	1.429(6)	C(36)-O(7)-Sn(2)	133.1(3)
C(2)-C(65)	1.497(6)	C(24)-N(4)-C(23)	117.0(4)
N(7)-C(4)	1.456(6)	C(24)-N(4)-Sn(2)	114.4(3)
C(41)-C(46)	1.387(6)	C(23)-N(4)-Sn(2)	128.6(3)
C(41)-C(42)	1.391(6)	P(2)-N(3)-P(3)	120.9(2)

C(53)-C(54)	1.372(6)	C(16)-N(5)-C(20)	117.4(4)
C(4)-C(5)	1.375(6)	C(16)-N(5)-Sn(1)	118.3(3)
C(40)-C(39)	1.366(7)	C(20)-N(5)-Sn(1)	124.0(3)
C(40)-C(35)	1.403(6)	P(2)-N(1)-P(1)	119.0(2)
C(36)-C(35)	1.415(6)	C(1)-O(14)-Sn(1)	132.6(3)
C(36)-C(37)	1.435(6)	P(3)-N(2)-P(1)	122.5(2)
C(64)-C(63)	1.389(7)	O(15)-N(10)-O(16)	122.9(4)
C(64)-C(59)	1.395(7)	O(15)-N(10)-C(6)	118.1(4)
C(17)-C(16)	1.376(6)	O(16)-N(10)-C(6)	119.0(4)
C(17)-C(18)	1.392(6)	C(57)-C(58)-C(53)	116.7(4)
C(23)-C(22)	1.367(7)	C(57)-C(58)-C(59)	121.5(4)
C(18)-C(19)	1.361(7)	C(53)-C(58)-C(59)	121.8(4)
C(38)-C(37)	1.363(7)	O(3)-N(8)-O(4)	125.4(5)
C(38)-C(39)	1.402(7)	O(3)-N(8)-C(37)	119.4(5)
C(59)-C(60)	1.404(6)	O(4)-N(8)-C(37)	115.2(5)
C(46)-C(45)	1.417(6)	C(5)-C(6)-C(1)	125.0(4)
C(46)-C(47)	1.480(6)	C(5)-C(6)-N(10)	114.8(4)
C(52)-C(51)	1.371(6)	C(1)-C(6)-N(10)	120.1(4)
C(52)-C(47)	1.400(6)	O(1)-N(9)-O(2)	123.3(4)
C(35)-C(34)	1.494(6)	O(1)-N(9)-C(39)	118.4(4)
C(10)-C(11)	1.520(7)	O(2)-N(9)-C(39)	118.3(4)
C(10)-C(9)	1.521(6)	C(4)-C(3)-C(2)	121.1(4)
C(42)-C(43)	1.392(7)	C(3)-C(2)-C(1)	121.1(4)
C(21)-C(22)	1.376(7)	C(3)-C(2)-C(65)	115.2(4)
C(21)-C(25)	1.382(6)	C(1)-C(2)-C(65)	123.6(4)
C(20)-C(19)	1.396(7)	O(10)-N(7)-O(11)	124.1(4)
C(61)-C(62)	1.364(7)	O(10)-N(7)-C(4)	118.7(4)
C(61)-C(60)	1.385(7)	O(11)-N(7)-C(4)	117.2(4)
C(56)-C(55)	1.368(7)	C(46)-C(41)-C(42)	123.1(4)
C(56)-C(57)	1.396(7)	C(46)-C(41)-O(19)	119.1(4)
C(24)-C(25)	1.386(6)	C(42)-C(41)-O(19)	117.7(4)
C(48)-C(49)	1.379(6)	C(54)-C(53)-C(58)	122.4(4)
C(48)-C(47)	1.395(6)	C(54)-C(53)-O(18)	118.3(4)
C(50)-C(49)	1.398(7)	C(58)-C(53)-O(18)	119.0(4)
C(50)-C(51)	1.404(6)	C(5)-C(4)-C(3)	120.2(4)

C(30)-C(31)	1.519(7)	C(5)-C(4)-N(7)	119.7(4)
C(43)-C(44)	1.365(7)	C(3)-C(4)-N(7)	119.9(4)
C(54)-C(55)	1.382(7)	O(14)-C(1)-C(6)	119.1(4)
C(62)-C(63)	1.403(8)	O(14)-C(1)-C(2)	126.9(4)
C(44)-C(45)	1.400(7)	C(6)-C(1)-C(2)	113.9(4)
C(27)-C(28)	1.494(7)	C(39)-C(40)-C(35)	120.9(4)
C(27)-C(26)	1.531(7)	O(7)-C(36)-C(35)	126.6(4)
C(9)-C(8)	1.531(6)	O(7)-C(36)-C(37)	118.6(4)
C(32)-C(33)	1.507(8)	C(35)-C(36)-C(37)	114.8(4)
C(32)-C(31)	1.530(7)	C(63)-C(64)-C(59)	120.9(5)
C(12)-C(13)	1.509(7)	C(16)-C(17)-C(18)	117.9(4)
C(28)-C(29)	1.543(7)	N(4)-C(23)-C(22)	124.7(5)
C(13)-C(66)	1.413(11)	C(19)-C(18)-O(9)	124.9(4)
C(66)-C(67)	1.677(13)	C(19)-C(18)-C(17)	119.8(4)
		O(9)-C(18)-C(17)	115.3(4)
		C(37)-C(38)-C(39)	117.6(4)
		C(64)-C(59)-C(60)	117.8(4)
		C(64)-C(59)-C(58)	122.0(4)
		C(60)-C(59)-C(58)	120.2(4)
		C(41)-C(46)-C(45)	117.4(4)
		C(41)-C(46)-C(47)	122.1(4)
		C(45)-C(46)-C(47)	120.5(4)
		C(51)-C(52)-O(20)	117.8(4)
		C(51)-C(52)-C(47)	123.6(4)
		O(20)-C(52)-C(47)	118.5(4)
		C(40)-C(35)-C(36)	120.8(4)
		C(40)-C(35)-C(34)	114.6(4)
		C(36)-C(35)-C(34)	124.6(4)
		C(11)-C(10)-C(9)	112.7(4)
		C(43)-C(42)-C(41)	118.4(4)
		O(12)-C(65)-O(13)	120.3(4)
		O(12)-C(65)-C(2)	121.1(4)
		O(13)-C(65)-C(2)	118.6(4)
		C(22)-C(21)-C(25)	120.6(4)
		C(22)-C(21)-O(8)	117.3(4)

	C(25)-C(21)-O(8)	122.1(4)
	N(5)-C(20)-C(19)	122.4(4)
	C(23)-C(22)-C(21)	117.0(4)
	C(38)-C(37)-C(36)	124.7(4)
	C(38)-C(37)-N(8)	117.0(4)
	C(36)-C(37)-N(8)	118.3(4)
	C(6)-C(5)-C(4)	118.5(4)
	C(62)-C(61)-C(60)	119.9(5)
	C(55)-C(56)-C(57)	120.3(5)
	N(4)-C(24)-C(25)	123.4(4)
	N(5)-C(16)-C(17)	123.8(4)
	C(18)-C(19)-C(20)	118.7(4)
	C(61)-C(60)-C(59)	121.5(4)
	C(61)-C(60)-O(17)	119.0(4)
	C(59)-C(60)-O(17)	119.5(4)
	C(49)-C(48)-C(47)	121.8(4)
	C(49)-C(50)-C(51)	119.6(4)
	C(31)-C(30)-Sn(2)	115.0(3)
	C(52)-C(51)-C(50)	118.5(4)
	C(44)-C(43)-C(42)	120.3(4)
	C(53)-C(54)-C(55)	119.4(4)
	C(48)-C(49)-C(50)	120.1(4)
	C(40)-C(39)-C(38)	121.1(4)
	C(40)-C(39)-N(9)	120.1(4)
	C(38)-C(39)-N(9)	118.7(4)
	C(48)-C(47)-C(52)	116.5(4)
	C(48)-C(47)-C(46)	122.3(4)
	C(52)-C(47)-C(46)	121.2(4)
	C(56)-C(57)-C(58)	120.9(5)
	C(61)-C(62)-C(63)	120.3(5)
	C(43)-C(44)-C(45)	121.4(5)
	C(28)-C(27)-C(26)	116.0(4)
	O(5)-C(34)-O(6)	120.2(4)
	O(5)-C(34)-C(35)	122.0(4)
	O(6)-C(34)-C(35)	117.8(4)

	C(27)-C(26)-Sn(2)	117.5(3)
	C(10)-C(9)-C(8)	111.0(4)
	C(44)-C(45)-C(46)	119.4(4)
	C(21)-C(25)-C(24)	117.2(4)
	C(64)-C(63)-C(62)	119.6(5)
	C(33)-C(32)-C(31)	112.7(5)
	C(9)-C(8)-Sn(1)	118.6(3)
	C(13)-C(12)-Sn(1)	114.8(3)
	C(27)-C(28)-C(29)	112.7(5)
	C(30)-C(31)-C(32)	114.6(4)
	C(56)-C(55)-C(54)	120.3(5)
	C(66)-C(13)-C(12)	114.9(7)
	C(13)-C(66)-C(67)	105.0(8)
	Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+2,-z+2 #2 -x+1,-y+1,-z+1	

Table S3: Bond parameters of complex **3.**

Bond lengths (Å)		Bond angles (°)	
Sn(1)-O(7)	1.996(11)	O(7)-Sn(1)-C(27)	116.1(7)
Sn(1)-C(27)	2.09(2)	O(7)-Sn(1)-C(31)	113.6(7)
Sn(1)-C(31)	2.14(2)	C(27)-Sn(1)-C(31)	129.9(7)
Sn(1)-O(6)	2.157(10)	O(7)-Sn(1)-O(6)	82.7(4)
Sn(1)-O(8)	2.211(11)	C(27)-Sn(1)-O(6)	96.6(6)
Sn(2)-O(7)	2.044(10)	C(31)-Sn(1)-O(6)	95.4(6)
Sn(2)-C(35)	2.08(3)	O(7)-Sn(1)-O(8)	71.8(4)
Sn(2)-C(39)	2.12(2)	C(27)-Sn(1)-O(8)	93.8(7)
Sn(2)-O(7)#1	2.138(11)	C(31)-Sn(1)-O(8)	95.7(7)
Sn(2)-O(8)	2.183(12)	O(6)-Sn(1)-O(8)	154.4(4)
P(1)-N(1)	1.556(13)	O(7)-Sn(2)-C(35)	116.3(8)
P(1)-O(2)	1.582(11)	O(7)-Sn(2)-C(39)	117.1(8)
P(1)-N(2)	1.589(12)	C(35)-Sn(2)-C(39)	126.5(10)

P(1)-O(1)	1.590(10)	O(7)-Sn(2)-O(7)#1	73.8(5)
P(2)-N(3)	1.566(13)	C(35)-Sn(2)-O(7)#1	98.3(8)
P(2)-N(2)	1.584(13)	C(39)-Sn(2)-O(7)#1	97.8(8)
P(2)-O(5)	1.590(11)	O(7)-Sn(2)-O(8)	71.5(4)
P(2)-O(4)	1.603(10)	C(35)-Sn(2)-O(8)	95.5(8)
P(3)-O(6)	1.515(10)	C(39)-Sn(2)-O(8)	99.2(8)
P(3)-O(3)	1.573(13)	O(7)#1-Sn(2)-O(8)	145.3(4)
P(3)-N(1)	1.599(13)	N(1)-P(1)-O(2)	105.9(6)
P(3)-N(3)	1.605(12)	N(1)-P(1)-N(2)	119.5(7)
O(1)-C(12)	1.397(16)	O(2)-P(1)-N(2)	111.5(7)
O(2)-C(1)	1.396(19)	N(1)-P(1)-O(1)	113.3(7)
O(3)-C(25)	1.44(2)	O(2)-P(1)-O(1)	102.1(6)
O(4)-C(13)	1.403(18)	N(2)-P(1)-O(1)	103.5(6)
O(5)-C(24)	1.408(19)	N(3)-P(2)-N(2)	119.2(6)
O(7)-Sn(2)#1	2.138(11)	N(3)-P(2)-O(5)	107.0(6)
O(8)-C(26)	1.39(2)	N(2)-P(2)-O(5)	110.7(7)
C(1)-C(6)	1.38(2)	N(3)-P(2)-O(4)	112.1(7)
C(1)-C(5)	1.40(2)	N(2)-P(2)-O(4)	105.2(6)
C(2)-C(6)	1.36(3)	O(5)-P(2)-O(4)	101.2(5)
C(2)-C(3)	1.38(3)	O(6)-P(3)-O(3)	102.4(7)
C(3)-C(4)	1.37(3)	O(6)-P(3)-N(1)	113.0(6)
C(4)-C(5)	1.40(2)	O(3)-P(3)-N(1)	107.7(7)
C(5)-C(7)	1.48(2)	O(6)-P(3)-N(3)	110.1(6)
C(7)-C(12)	1.38(2)	O(3)-P(3)-N(3)	109.4(7)
C(7)-C(8)	1.39(2)	N(1)-P(3)-N(3)	113.5(7)
C(8)-C(9)	1.38(2)	C(12)-O(1)-P(1)	119.5(8)
C(9)-C(10)	1.38(2)	C(1)-O(2)-P(1)	124.7(9)
C(10)-C(11)	1.39(2)	C(25)-O(3)-P(3)	118.5(11)
C(11)-C(12)	1.38(2)	C(13)-O(4)-P(2)	117.3(8)
C(13)-C(14)	1.35(2)	C(24)-O(5)-P(2)	120.6(9)
C(13)-C(18)	1.39(2)	P(3)-O(6)-Sn(1)	123.2(6)
C(14)-C(15)	1.40(2)	Sn(1)-O(7)-Sn(2)	115.0(5)
C(15)-C(16)	1.38(3)	Sn(1)-O(7)-Sn(2)#1	138.7(5)
C(16)-C(17)	1.37(3)	Sn(2)-O(7)-Sn(2)#1	106.2(5)
C(17)-C(18)	1.41(2)	C(26)-O(8)-Sn(2)	127.0(11)

C(18)-C(19)	1.46(3)	C(26)-O(8)-Sn(1)	130.0(11)
C(19)-C(24)	1.39(2)	Sn(2)-O(8)-Sn(1)	101.7(5)
C(19)-C(20)	1.41(2)	P(1)-N(1)-P(3)	124.1(7)
C(20)-C(21)	1.36(3)	P(2)-N(2)-P(1)	119.0(8)
C(21)-C(22)	1.39(3)	P(2)-N(3)-P(3)	123.8(8)
C(22)-C(23)	1.39(3)	C(6)-C(1)-C(5)	121.9(16)
C(23)-C(24)	1.35(3)	C(6)-C(1)-O(2)	118.9(14)
C(27)-C(28)	1.47(3)	C(5)-C(1)-O(2)	118.8(15)
C(28)-C(29)	1.59(4)	C(6)-C(2)-C(3)	120(2)
C(29)-C(30)	1.46(4)	C(4)-C(3)-C(2)	119.8(19)
C(31)-C(32)	1.53(3)	C(3)-C(4)-C(5)	121.7(17)
C(32)-C(33)	1.57(3)	C(1)-C(5)-C(4)	116.3(16)
C(33)-C(34)	1.54(3)	C(1)-C(5)-C(7)	123.1(15)
C(35)-C(36)	1.36(4)	C(4)-C(5)-C(7)	120.6(14)
C(36)-C(37)	1.52(4)	C(2)-C(6)-C(1)	120.0(17)
C(37)-C(38)	1.46(3)	C(12)-C(7)-C(8)	117.4(16)
C(39)-C(40)	1.51(4)	C(12)-C(7)-C(5)	121.3(13)
C(40)-C(41)	1.40(5)	C(8)-C(7)-C(5)	121.2(15)
C(41)-C(42)	1.62(5)	C(9)-C(8)-C(7)	121.1(17)
O(9)-C(43)	1.38(2)	C(10)-C(9)-C(8)	120.1(16)
		C(9)-C(10)-C(11)	120.3(17)
		C(12)-C(11)-C(10)	118.2(17)
		C(7)-C(12)-C(11)	122.7(14)
		C(7)-C(12)-O(1)	120.4(14)
		C(11)-C(12)-O(1)	116.7(15)
		C(14)-C(13)-C(18)	123.7(16)
		C(14)-C(13)-O(4)	118.0(15)
		C(18)-C(13)-O(4)	118.2(17)
		C(13)-C(14)-C(15)	119.1(17)
		C(16)-C(15)-C(14)	119(2)
		C(17)-C(16)-C(15)	120.6(17)
		C(16)-C(17)-C(18)	121.2(18)
		C(13)-C(18)-C(17)	116.1(19)
		C(13)-C(18)-C(19)	121.7(15)
		C(17)-C(18)-C(19)	122.3(17)

	C(24)-C(19)-C(20)	117.4(19)
	C(24)-C(19)-C(18)	121.1(15)
	C(20)-C(19)-C(18)	121.5(16)
	C(21)-C(20)-C(19)	120.7(18)
	C(20)-C(21)-C(22)	120.1(19)
	C(23)-C(22)-C(21)	120(2)
	C(24)-C(23)-C(22)	119.9(18)
	C(23)-C(24)-C(19)	121.9(16)
	C(23)-C(24)-O(5)	119.2(15)
	C(19)-C(24)-O(5)	118.7(17)
	C(28)-C(27)-Sn(1)	115.6(15)
	C(27)-C(28)-C(29)	116(2)
	C(30)-C(29)-C(28)	113(2)
	C(32)-C(31)-Sn(1)	115.7(13)
	C(31)-C(32)-C(33)	114.4(18)
	C(34)-C(33)-C(32)	110(2)
	C(36)-C(35)-Sn(2)	124(2)
	C(35)-C(36)-C(37)	128(3)
	C(38)-C(37)-C(36)	117(3)
	C(40)-C(39)-Sn(2)	130(2)
	C(41)-C(40)-C(39)	115(4)
	C(40)-C(41)-C(42)	109(4)
	Symmetry transformations used to generate equivalent atoms: #1 -x+2,-y+1,-z+1	