Supporting information

Table S1 Crystallographic data for compounds $\mathbf{C_1}$ and $\mathbf{C_2}$.

Compound reference	$\mathbf{C_1}$	$\mathbf{C_2}$
Chemical formula	$C_{35}H_{30}ClN_2OPSn$	$C_{35}H_{30}ClN_2OPSn{\bullet}C_{17}H_{15}N_2OP$
Formula Mass	679.78	974.00
Crystal system	Monoclinic	Triclinic
a/Å	57.264(2)	9.9181(6)
b/Å	9.8858(2)	14.7686(9)
c/Å	22.2965(8)	16.9564(10)
α/°	90.00	82.955(5)
β/°	93.908(3)	81.181(5)
γ/°	90.00	74.541(5)
Unit cell volume/Å^3	12592.6(7)	2356.8(2)
Temperature/K	292(2)	292(2)
Space group	$C2/n$	$P\bar{1}$
No. of formula units per unit cell, Z	16	2
No. of reflections measured	39843	46955
No. of independent reflections	11829	12706
R_{int}	0.0235	0.0480
Final R_1 values ($I > 2\sigma(I)$)	0.0252	0.0491
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.0561	0.1275
Final R_1 values (all data)	0.0377	0.0699
Final $wR(F^2)$ values (all data)	0.0602	0.1557
Goodness of fit on F^2	1.021	1.048
Flack parameter		
Rogers parameter		
CCDC number	978396	978395

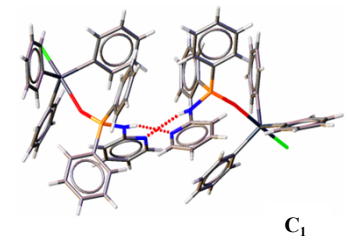
Table S2 Selected bond lengths (Å) and angles (°) for compound $\mathbf{C_1}$.

Bond length (Å)			
Sn(1)-Cl(1)	2.4693(8)	P(1)-C(1)	1.789(2)
Sn(1)-O(1)	2.4637(15)	P(1)-C(7)	1.788(2)
Sn(1)-C(16A)	2.133(4)	P(2)-O(2)	1.4848(15)
Sn(1)-C(22)	2.137(2)	P(2)-N(4)	1.6493(18)
Sn(1)-C(28)	2.132(3)	P(2)-C(63)	1.800(2)
Sn(2)-Cl(2)	2.4820(6)	P(2)-C(81)	1.790(2)
Sn(2)-O(2)	2.4031(14)	N(1)-C(45)	1.328(3)
Sn(2)-C(51)	2.132(2)	N(1)-C(49)	1.341(3)
Sn(2)-C(57)	2.127(2)	N(2)-C(45)	1.395(3)
Sn(2)-C(72A)	2.140(3)	N(3)-C(91)	1.332(3)
P(1)-O(1)	1.4894(15)	N(3)-C(95)	1.342(3)
P(1)-N(2)	1.6663(18)	N(4)-C(91)	1.402(3)
Bond angles (º)			
Cl(1)-Sn(1)-O(1)	178.21(5)	O(2)-Sn(2)-C(72A)	88.0(3)
Cl(1)-Sn(1)-C(16A)	93.4(6)	C(51)-Sn(2)-C(57)	118.76(9)
Cl(1)-Sn(1)-C(22)	94.80(7)	C(51)-Sn(2)-C(72A)	117.8(3)
Cl(1)-Sn(1)-C(28)	93.04(7)	C(57)-Sn(2)-C(72A)	121.6(3)
O(1)-Sn(1)-C(16A)	87.0(6)	Sn(2)-O(2)-P(2)	154.60(9)
O(1)-Sn(1)-C(22)	86.44(7)	Sn(2)-C(51)-C(52)	121.06(17)
O(1)-Sn(1)-C(28)	85.22(7)	Sn(2)-C(51)-C(56)	120.95(17)
C(16A)-Sn(1)-C(22)	125.3(6)	Sn(2)-C(57)-C(58)	121.9(2)
C(16A)-Sn(1)-C(28)	114.3(6)	Sn(2)-C(57)-C(62)	119.7(2)
C(22)-Sn(1)-C(28)	119.06(9)	P(1)-C(1)-C(2)	120.9(2)
Sn(1)-O(1)-P(1)	145.44(9)	P(1)-C(1)-C(6)	120.06(19)
Sn(1)-C(16A)-C(17A)	120.0(8)	N(1)-C(45)-N(2)	115.14(19)
Sn(1)-C(16A)-C(21A)	118.0(9)	O(2)-P(2)-N(4)	113.85(9)
Sn(1)-C(22)-C(23)	121.98(18)	O(2)-P(2)-C(63)	109.88(9)
Sn(1)-C(22)-C(27)	119.89(18)	O(2)-P(2)-C(81)	114.30(10)
Cl(2)-Sn(2)-O(2)	176.99(4)	N(4)-P(2)-C(63)	108.65(10)
Cl(2)-Sn(2)-C(51)	94.20(6)	N(4)-P(2)-C(81)	101.66(10)
Cl(2)-Sn(2)-C(57)	94.99(6)	C(63)-P(2)-C(81)	108.05(11)
Cl(2)-Sn(2)-C(72A)	94.2(3)	P(2)-N(4)-C(91)	127.85(15)
O(2)-Sn(2)-C(51)	86.56(7)	P(2)-C(63)-C(64)	120.22(17)
O(2)-Sn(2)-C(57)	82.10(7)	P(2)-C(81)-C(82)	118.67(18)
Sn(2)-C(72A)-C(73A)	122.4(8)	N(1)-C(45)-C(46)	122.3(2)
Sn(2)-C(72A)-C(77A)	119.7(8)	N(2)-C(45)-C(46)	122.5(2)
O(1)-P(1)-N(2)	114.26(9)	N(1)-C(49)-C(48)	124.5(2)
O(1)-P(1)-C(1)	114.01(10)	N(1)-C(49)-H(49)	117.7
O(1)-P(1)-C(7)	110.91(10)	N(3)-C(91)-N(4)	114.1(9)
N(2)-P(1)-C(1)	103.27(10)	N(3)-C(91)-C(92)	123.5(2)
N(2)-P(1)-C(7)	105.90(11)	N(4)-C(91)-C(92)	122.4(2)
C(1)-P(1)-C(7)	107.83(10)	N(3)-C(95)-C(94)	124.5(2)
P(1)-N(2)-C(45)	124.93(15)	N(3)-C(95)-H(95)	117.8

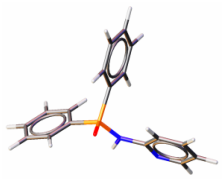
Table S3 Selected bond lengths (Å) and angles (°) for compound $\mathbf{C_2}$.

Bond length (Å)			
Sn(1)-Cl(1)	2.5029(9)	P(2)-N(4)	1.658(3)
Sn(1)-N(1)	2.553(3)	P(2)-C(51)	1.799(3)
Sn(1)-C(16)	2.125(3)	P(2)-C(71)	1.799(3)
Sn(1)-C(22)	2.135(3)	N(1)-C(45)	1.332(4)
Sn(1)-C(28)	2.125(3)	N(1)-C(49)	1.329(5)
P(1)-O(1)	1.480(2)	N(2)-C(47)	1.393(4)
P(1)- N(2)	1.668(3)	N(3)-C(61)	1.327(7)
P(1)-C(1)	1.798(4)	N(3)-C(65)	1.322(7)
P(1)-C(7)	1.792(3)	N(4)-C(63)	1.391(4)
P(2)-O(2)	1.484(2)		
Bond angles (º)			
Cl(1)-Sn(1)-N(1)	175.82(7)	P(1)-N(2)-C(47)	125.2(2)
Cl(1)-Sn(1)-C(16)	92.54(9)	P(1)-C(1)-C(2)	124.7(3)
Cl(1)-Sn(1)-C(22)	93.34(9)	P(1)-C(7)-C(8)	122.3(3)
Cl(1)-Sn(1)-C(28)	94.72(9)	P(2)-N(4)-H(44)	114(3)
N(1)-Sn(1)-C(16)	85.01(11)	P(2)-N(4)-C(63)	125.7(3)
N(1)-Sn(1)-C(22)	90.80(11)	P(2)-C(51)-C(56)	121.7(3)
N(1)-Sn(1)-C(28)	83.78(11)	N(2)-P(1)-C(1)	107.66(17)
C(16)-Sn(1)-C(22)	117.71(13)	N(2)-P(1)-C(7)	101.33(15)
C(16)-Sn(1)-C(28)	122.28(15)	N(1)-C(45)-H(45)	117.9
C(22)-Sn(1)-C(28)	118.87(14)	N(1)-C(45)-C(46)	124.2(3)
Sn(1)-N(1)-C(45)	120.3(2)	N(2)-C(47)-C(46)	120.7(3)
Sn(1)-N(1)-C(49)	123.9(2)	N(2)-C(47)-C(48)	122.6(3)
Sn(1)-C(28)-C(29)	122.8(3)	N(3)-C(61)-H(61)	117.6
O(1)-P(1)-N(2)	114.26(15)	N(3)-C(61)-C(62)	124.8(5)
O(1)-P(1)-C(1)	110.95(16)	N(3)-C(65)-C(64)	125.2(5)
O(1)-P(1)-C(7)	113.07(16)	N(4)-P(2)-C(51)	101.93(15)
O(2)-P(2)-N(4)	114.41(16)	N(4)-P(2)-C(71)	106.99(16)
O(2)-P(2)-C(51)	113.05(16)	N(4)-C(63)-C(62)	119.4(3)
O(2)-P(2)-C(71)	111.09(15)	N(4)-C(63)-C(64)	122.9(4)
P(1)-N(2)-H(22)	117(3)		

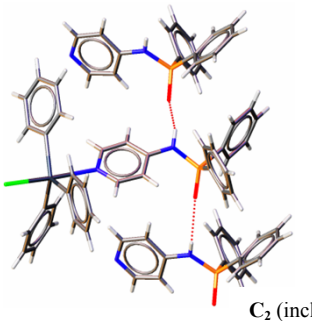
Figure S1. Representation of the fully optimized ligands and Binuclear complex and the H-bonded systems of $\mathbf{C_1}$ and $\mathbf{C_2}$ (including $\mathbf{L_2'}$).



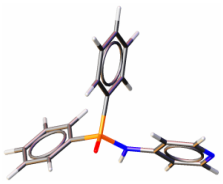
$\mathbf{C_1}$



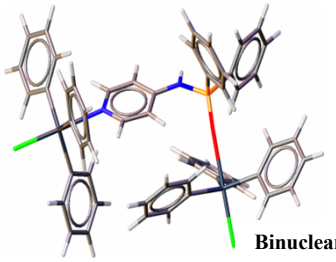
$\mathbf{L_1}$



$\mathbf{C_2}$ (including $\mathbf{L_2'}$)



$\mathbf{L_2}$



Binuclear model