A novel macrocyclic organotin carboxylate containing nona-nuclear long ladder

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Synthesis of ligand L

L was prepared by a standard method reported in the literature.^{8e} The synthesis of L was shown in Scheme S1. 3,4,9,10-Perylenetetracarboxylic aciddianhydride (3.92 g, 0.01 mol) and Amino-acetic acid (1.50g, 0.02 mol) were added into a three-neck flask with 40ml DMF in it. The reaction mixture was stirred for 8h in an oil-bath at 90°C. After stand overnight, the mixture was filtrated to get the bright red powder. After washed with ethanol, the powder was dried. Yield: 69.1%. Mp: > 300°C. ¹H NMR (CDCl₃): δ 11.94 (s, 2H, COOH), 7.99 (d, 4H, *J* = 7.5 Hz, Ar-H), 7.35 (d, 4H, *J* = 7.5 Hz, Ar-H), 4.49 (s, 4H, -CH₂-). ¹³C NMR (dimethyl sulfoxide-*d*₆): δ 171.36 (2C, COO), 168.53 (4C, C=O), 133.35 (4C, Ar-C), 132.16 (4C, Ar-C), 131.55 (2C, Ar-C), 129.46 (8C, Ar-C), 128.21 (2C, Ar-C), 49.41 (2C, -CH₂-).



Scheme S1 Synthesis of L.

Bond lengths			
Sn(1)-O(2)	2.006(5)	Sn(5)-C(51)	2.125(7)
Sn(1)-O(10)	2.169(5)	Sn(5)-C(55)	2.138(7)
Sn(1)-O(1)	2.247(5)	Sn(6)-O(6)	2.018(4)
Sn(1)-C(105)	2.091(13)	Sn(6)-O(7)	2.134(5)
Sn(1)-C(101)	2.129(9)	Sn(6)-O(5)	2.137(4)
Sn(2)-O(2)	2.039(4)	Sn(6)-C(61)	2.127(7)
Sn(2)-O(3)	2.088(4)	Sn(6)-C(65)	2.135(7)
Sn(2)-O(1)	2.168(5)	Sn(7)-O(7)	2.047(4)
Sn(2)-C(125)	2.132(8)	Sn(7)-O(6)	2.135(4)
Sn(2)-C(121)	2.138(8)	Sn(7)-O(8)	2.137(4)
Sn(3)-O(3)	2.045(4)	Sn(7)-C(75)	2.127(7)
Sn(3)-O(4)	2.112(4)	Sn(7)-C(71)	2.110(7)
Sn(3)-O(2)	2.170(5)	Sn(8)-O(8)	2.020(4)
Sn(3)-C(131)	2.122(7)	Sn(8)-O(7)	2.110(5)
Sn(3)-C(135)	2.128(7)	Sn(8)-O(9)	2.152(5)
Sn(4)-O(4)	2.024(4)	Sn(8)-C(85)	2.116(8)
Sn(4)-O(5)	2.125(4)	Sn(8)-C(81)	2.128(8)
Sn(4)-O(3)	2.163(5)	Sn(9)-O(8)	2.047(5)
Sn(4)-C(141)	2.140(7)	Sn(9)-O(9)	2.210(5)

Tab. S1 Selected bond lengths (Å) and angles (°) for complex 1.

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Sn(4)-C(145)	2.143(7)	Sn(9)-O(16)	2.233(4)
Sn(5)-O(5)	2.033(4)	Sn(9)-C(91)	2.096(9)
Sn(5)-O(6)	2.116(4)	Sn(9)-C(95)	2.131(8)
Sn(5)-O(4)	2.136(4)		
Bond angles			
O(2)-Sn(1)-O(10)	83.13(18)	C(51)-Sn(5)-O(4)	96.6(2)
O(2)-Sn(1)-O(1)	72.00(18)	O(5)-Sn(5)-C(55)	124.5(2)
O(10)-Sn(1)-O(1)	155.07(19)	O(6)-Sn(5)-C(55)	97.7(2)
O(2)-Sn(1)-C(105)	116.9(4)	O(4)-Sn(5)-C(55)	96.8(2)
O(2)-Sn(1)-C(101)	108.8(4)	C(51)-Sn(5)-C(55)	118.7(3)
C(105)-Sn(1)-O(10)	98.8(3)	O(6)-Sn(6)-O(7)	75.84(17)
C(101)-Sn(1)-O(10)	100.7(3)	O(6)-Sn(6)-O(5)	75.56(17)
C(105)-Sn(1)-O(1)	91.1(3)	O(7)-Sn(6)-O(5)	151.35(16)
C(101)-Sn(1)-O(1)	89.2(3)	O(6)-Sn(6)-C(61)	121.0(2)
C(105)-Sn(1)-C(101)	131.9(5)	C(61)-Sn(6)-O(7)	98.9(2)
O(2)-Sn(2)-O(3)	75.99(18)	O(6)-Sn(6)-C(65)	121.9(2)
O(2)-Sn(2)-O(1)	73.11(18)	O(7)-Sn(6)-C(65)	97.3(3)
O(3)-Sn(2)-O(1)	149.01(19)	C(61)-Sn(6)-O(5)	97.2(2)
O(2)-Sn(2)-C(125)	120.9(3)	C(65)-Sn(6)-O(5)	96.4(2)
O(3)-Sn(2)-C(125)	99.1(3)	C(61)-Sn(6)-C(65)	117.1(3)
O(2)-Sn(2)-C(121)	119.0(3)	O(7)-Sn(7)-O(6)	75.21(17)
O(3)-Sn(2)-C(121)	100.2(3)	O(7)-Sn(7)-O(8)	74.51(17)
C(125)-Sn(2)-O(1)	94.8(3)	O(6)-Sn(7)-O(8)	149.70(17)
C(121)-Sn(2)-O(1)	96.7(3)	O(7)-Sn(7)-C(71)	117.3(2)
C(125)-Sn(2)-C(121)	119.8(3)	O(7)-Sn(7)-C(75)	123.0(2)
O(3)-Sn(3)-O(4)	76.02(17)	C(71)-Sn(7)-O(6)	97.4(2)
O(3)-Sn(3)-O(2)	74.06(17)	C(75)-Sn(7)-O(6)	97.4(2)
O(4)-Sn(3)-O(2)	149.91(17)	C(71)-Sn(7)-O(8)	97.2(2)
O(3)-Sn(3)-C(131)	115.7(2)	C(75)-Sn(7)-O(8)	98.2(2)
O(4)-Sn(3)-C(131)	99.5(2)	C(71)-Sn(7)-C(75)	119.7(3)
O(3)-Sn(3)-C(135)	123.3(2)	O(8)-Sn(8)-O(7)	75.65(17)
O(4)-Sn(3)-C(135)	98.2(2)	O(8)-Sn(8)-O(9)	73.08(18)
C(131)-Sn(3)-O(2)	96.2(2)	O(7)-Sn(8)-O(9)	148.50(18)
C(135)-Sn(3)-O(2)	95.4(2)	O(8)-Sn(8)-C(85)	123.5(3)
C(131)-Sn(3)-C(135)	120.9(3)	O(7)-Sn(8)-C(85)	98.3(3)
O(4)-Sn(4)-O(5)	76.11(16)	O(8)-Sn(8)-C(81)	119.1(3)
O(4)-Sn(4)-O(3)	75.33(16)	O(7)-Sn(8)-C(81)	98.8(3)
O(5)-Sn(4)-O(3)	151.36(16)	C(85)-Sn(8)-O(9)	95.7(3)
O(4)-Sn(4)-C(141)	120.2(2)	C(81)-Sn(8)-O(9)	99.5(3)
O(5)-Sn(4)-C(141)	99.5(3)	C(85)-Sn(8)-C(81)	117.4(3)
O(4)-Sn(4)-C(145)	121.8(2)	O(8)-Sn(9)-O(9)	71.34(18)
O(5)-Sn(4)-C(145)	97.6(3)	O(8)-Sn(9)-O(16)	82.36(17)
C(141)-Sn(4)-O(3)	96.6(2)	O(9)-Sn(9)-O(16)	153.40(19)
C(145)-Sn(4)-O(3)	95.5(3)	O(8)-Sn(9)-C(91)	108.6(3)
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C(141)-Sn(4)-C(145)	118.0(3)	O(8)-Sn(9)-C(95)	102.8(3)
O(5)-Sn(5)-O(6)	75.71(16)	C(95)-Sn(9)-O(16)	92.6(3)
O(5)-Sn(5)-O(4)	75.66(17)	C(91)-Sn(9)-O(9)	92.8(3)
O(6)-Sn(5)-O(4)	151.30(16)	C(95)-Sn(9)-O(9)	96.9(3)
O(5)-Sn(5)-C(51)	116.8(2)	C(91)-Sn(9)-O(16)	91.8(3)
O(6)-Sn(5)-C(51)	97.9(2)	C(91)-Sn(9)-C(95)	148.7(3)
Sn(2)-O(1)-Sn(1)	100.32(19)	Sn(5)-O(5)-Sn(6)	103.65(18)
Sn(1)-O(2)-Sn(2)	113.9(2)	Sn(6)-O(6)-Sn(5)	104.93(19)
Sn(2)-O(2)-Sn(3)	103.6(2)	Sn(6)-O(6)-Sn(7)	104.83(19)
Sn(3)-O(3)-Sn(2)	106.3(2)	Sn(7)-O(7)-Sn(6)	103.89(19)
Sn(3)-O(3)-Sn(4)	102.94(18)	Sn(7)-O(7)-Sn(8)	104.9(2)
Sn(4)-O(4)-Sn(3)	105.52(18)	Sn(8)-O(8)-Sn(7)	104.9(2)
Sn(4)-O(4)-Sn(5)	104.03(18)	Sn(8)-O(8)-Sn(9)	113.3(2)
Sn(5)-O(5)-Sn(4)	104.08(18)	Sn(8)-O(9)-Sn(9)	102.3(2)



Fig. S1 IR spectrum of 1.



Fig. S2 ¹H NMR spectrum of **1**.





Fig. S4 UV-Vis spectrum of 1.



Fig. S5 Fluorescence excitation spectrum of 1.



Fig. S6 Fluorescence emission spectra of 1 and ligand.