Two novel macrocyclic organotin(IV) carboxylates based on amide carboxylic acids

Xiao Xiao,[a] Lisong Yan,[b] Zemin Mei,[c] Dongsheng Zhu*[a] and Lin Xu[a]

a Northeast Normal University, Department of Chemistry, Changchun, China. Fax: 86 0431 85684009; Tel: 86 0431 85098620; E-mail: zhuds206@nenu.edu.cn

b Changchun Institute of Optics Fine Mechanics and Physics Chinese Academy of Sciences, Key Laboratory of Optical System Advanced Manufacturing Technology, Changchun, China.

c Baicheng Normal University, Department of Chemistry, Baicheng, China.

Antitumor activity test

The inhibitory actions against tumour of **1**, **2**, L^1 and L^2 were detected by MTT method. Mouse sarcoma cells S180 were routinely grown in the abdomen, after that the mice were executed by snapping neck. In aseptic conditions, peritoneal fluid was taken out of the mouse, and washed with physiological saline three times. After resuspended in 1640 culture medium, cells were diluted and added into 96-well plates (1×10^5 cells/ hole, 100 μL/ hole). Added 100 μL sample into the hole (the final concentration is 0.5 mg/ml), and cultured the cells in an incubator (37˚C, 5% CO_2) for 48h. Each hole was added with 20 μL MTT staining solution (the final concentration is 0.5mg/ml). After 4h, 100 μL 20% SDS was added into them. And the cells were cultured for 16h additionally. Absorption values at 570nm were measured by ELIASA to get the survival rate of the cells.

Table S1

Selected bond lengths (Å) and angles (˚) for **1** and **2**.

Complex **1**			
Bond lengths			
Sn(1)-C(2)	2.668(3)	Sn(1)-O(1)	2.503(2)
Sn(1)-C(21)	2.114(3)	Sn(1)-O(2)	2.507(2)
Sn(1)-C(31)	2.118(3)	Sn(1)-O(3)	2.152(2)
		Sn(1)-O(4)	2.118(2)
Bond angles			
O(4)-Sn(1)-O(1)	139.26(8)	O(4)-Sn(1)-O(2)	56.15(8)
O(3)-Sn(1)-O(1)	55.57(7)	O(3)-Sn(1)-O(2)	139.38(7)
O(4)-Sn(1)-O(3)	83.75(8)	O(1)-Sn(1)-O(2)	164.32(7)
C(21)-Sn(1)-C(31)	144.86(13)	C(21)-Sn(1)-C(2)	93.30(11)
C(21)-Sn(1)-O(4)	102.92(10)	C(31)-Sn(1)-C(2)	98.51(11)
C(31)-Sn(1)-O(4)	103.20(10)	O(4)-Sn(1)-C(2)	28.62(9)
C(21)-Sn(1)-O(3)	100.60(10)	O(3)-Sn(1)-C(2)	112.09(9)
C(31)-Sn(1)-O(3)	105.24(11)	O(1)-Sn(1)-C(2)	167.58(9)
C(21)-Sn(1)-O(1)	88.14(10)	O(2)-Sn(1)-C(2)	27.54(8)
C(31)-Sn(1)-O(1)	87.22(10)	C(21)-Sn(1)-O(2)	84.08(10)
C(31)-Sn(1)-O(2)	91.33(10)		
Complex **2**			
Bond lengths			
Sn(1)-C(31)	2.108(10)	Sn(1)-O(5)	2.170(5)

Sn(1)-C(41)	2.107(10)	Sn(1)-O(2)	2.173(5)
Sn(1)-C(1)	2.624(8)	Sn(1)-O(1)	2.390(5)
Sn(2)-C(51)	2.090(13)	Sn(2)-O(3)	2.107(6)
Bond angles			
O(5)-Sn(1)-O(2)	83.71(19)	O(1)-Sn(1)-C(1)	28.5(2)
O(5)-Sn(1)-O(1)	140.94(19)	C(31)-Sn(1)-O(2)	97.7(3)
O(2)-Sn(1)-O(1)	57.49(18)	C(41)-Sn(1)-O(1)	89.9(3)
O(3#)-Sn(2)-O(3)	83.0(3)	C(31)-Sn(1)-O(1)	91.0(3)
C(41)-Sn(1)-C(31)	160.8(4)	O(5)-Sn(1)-C(1)	112.6(2)
C(41)-Sn(1)-C(1)	95.5(3)	O(2)-Sn(1)-C(1)	29.0(2)
C(31)-Sn(1)-C(1)	94.3(3)	C(51)-Sn(2)-O(3)	102.3(4)
C(51#) -Sn(2)-C(51)	141.2(8)	C(51#)-Sn(2)-O(3#)	102.3(4)
C(41)-Sn(1)-O(5)	92.0(3)	C(51)-Sn(2)-O(3#)	106.6(4)
C(31)-Sn(1)-O(5)	99.3(3)	C(51#)-Sn(2)-O(3)	106.6(4)
C(41)-Sn(1)-O(2)	98.9(3)		

Table S2

Crystal data and structure refinement parameters for **1** and **2**.

	1	**2**
Empirical formula	$C_{53}H_{61}N_2O_{10}Sn_2$	$C_{72}H_7N_3O_{19}Sn_3$
M	1123.42	1644.44
Crystal system	Monoclinic	Monoclinic
Space group	*P2(1)/n*	*C2/c*
a (Å)	14.530(2)	12.5992(12)
b (Å)	9.0116(13)	30.212(3)
c (Å)	19.199(3)	19.9730(19)
α (˚)	90.00	90.00
β (˚)	96.039(2)	92.320(2)
γ (˚)	90.00	90.00
V (Å^3)	7131.7(12)	7596.5(13)
Z	2	4
μ (mm^{-1})	1.059	1.047
Reflections collected	14449	22385
Independent reflections	4402	6703
R_{int}	0.0270	0.0754
Goodness-of-fit on F^2	1.024	1.036
R_1, wR_2 [$I>2\sigma(I)$]	0.0292, 0.0711	0.0647, 0.1624
R_1, wR_2 (all data)	0.0416, 0.0775	0.1112, 0.1892

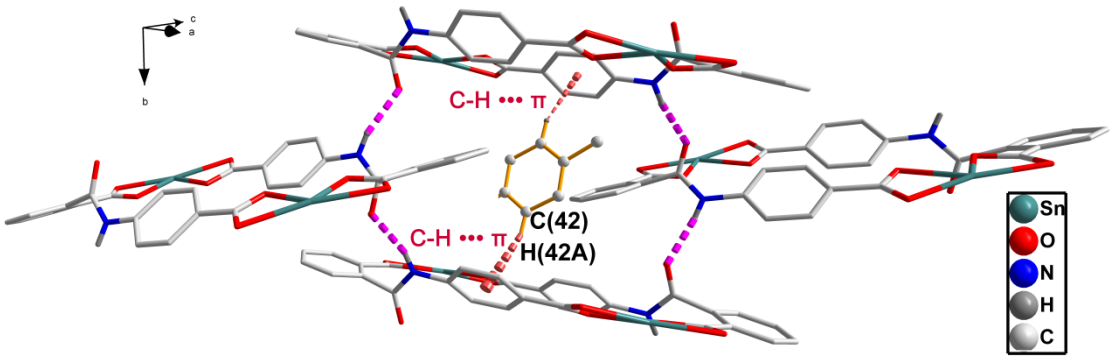

Fig. S1 Toluene interacts with intermolecular channel with C-H···π interactions

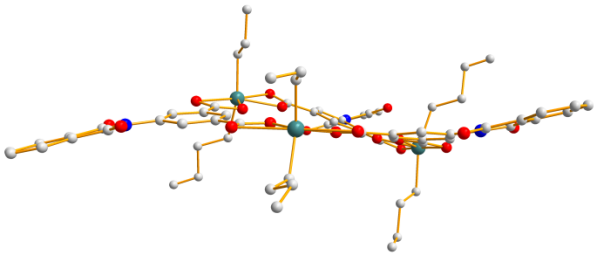

Fig. S2 Distorted molecular macrocycle of **2**.

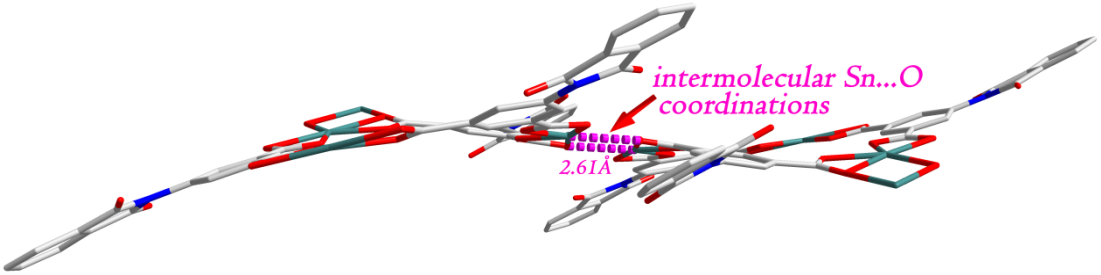

Fig. S3 Distorted molecular macrocycle of **2** caused by intermolecular Sn···O coordinations.

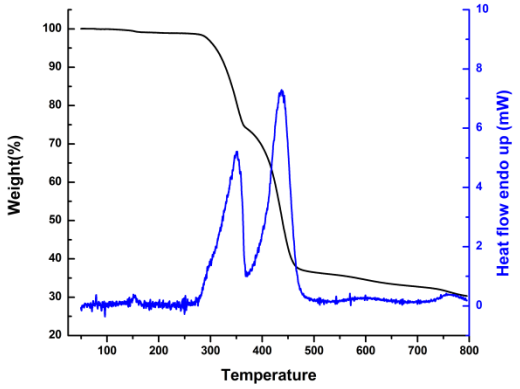

Fig. S4 TGA - DTG curves of **1**.

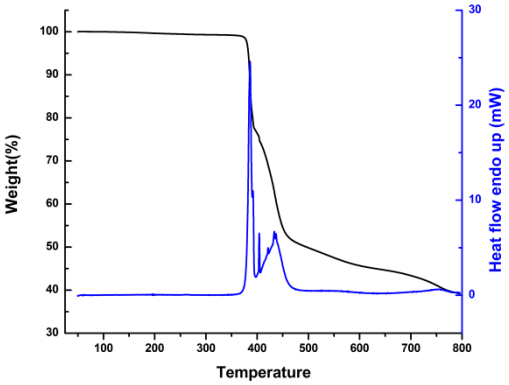

Fig. S5 TGA - DTG curves of **2**.

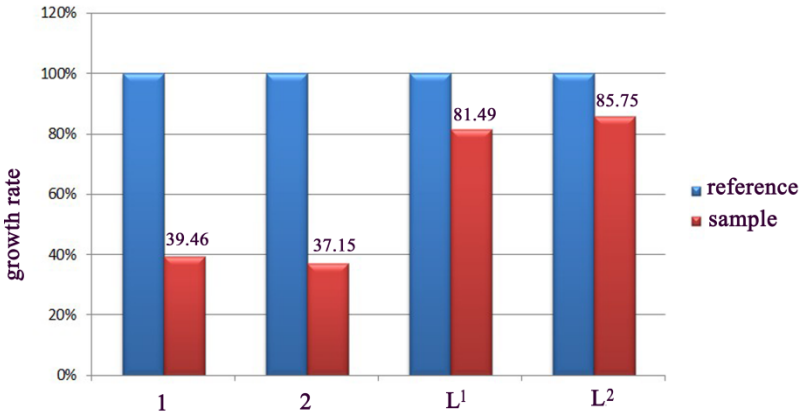

Fig. S6 The inhibition effects of **1**, **2**, L^1 and L^2 against S180.