

## **Tin (II) ketoacidoximates: synthesis, X-ray structures and processing to tin (II) oxide**

Jayaprakash Khanderi,<sup>a</sup> Bambar Davaasuren,<sup>a</sup> Buthainah Ameen Alshankiti<sup>a</sup> and Alexander Rothenberger<sup>a\*</sup>

<sup>a</sup>Physical Sciences and Engineering Division, 4700 King Abdullah University of Science & Technology (KAUST), Thuwal, 23955-6900, Kingdom of Saudi Arabia

\* to whom correspondence should be made

e-mail: [alexander.rothenberger@kaust.edu.sa](mailto:alexander.rothenberger@kaust.edu.sa)

Fax: +966 12 8021258

Phone: +966 12 808 0745

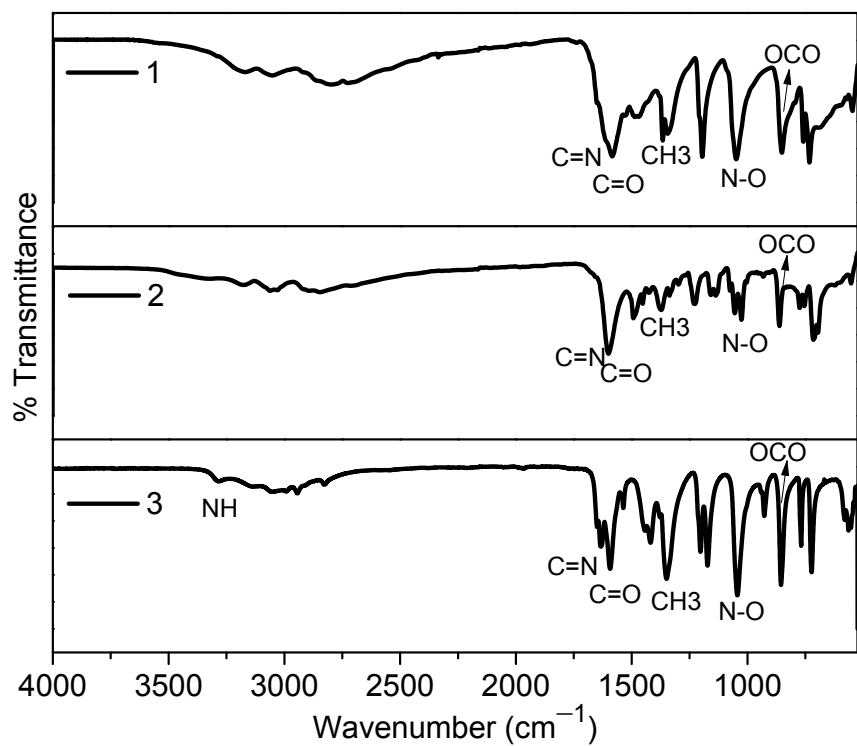


Fig. S1 IR spectra of **1**, **2** and **3**

Table S1. Atomic coordinates and equivalent isotropic displacement parameters ( $\text{\AA}^2$ ) for  $\text{C}_{12}\text{H}_{16}\text{N}_4\text{O}_{12}\text{Sn}_2$  (**1**)

Label	x	y	z	Occupancy	$U_{\text{eq}}^*$
Sn(1)	0.828203(18)	0.561736(16)	0.358643(16)	1	0.01512(5)
C(3)	0.6729(4)	0.6453(3)	0.7167(3)	1	0.0265(6)
H(3A)	0.5692	0.6090	0.7082	1	0.040
H(3B)	0.6976	0.7444	0.7676	1	0.040
H(3C)	0.7489	0.6078	0.7646	1	0.040
C(5)	0.6768(3)	0.4564(3)	0.0373(3)	1	0.0223(5)
C(1)	0.6150(3)	0.6857(2)	0.5024(3)	1	0.0180(5)
C(4)	0.6148(3)	0.3535(3)	0.0746(3)	1	0.0208(5)
C(2)	0.6775(3)	0.6069(3)	0.5799(3)	1	0.0180(5)
O(6)	0.7821(3)	0.6743(2)	0.1059(2)	1	0.0282(5)
H(6)	0.7916	0.7515	0.1676	1	0.042
N(2)	0.7273(3)	0.5756(2)	0.1365(2)	1	0.0204(4)
O(5)	0.5352(3)	0.2422(2)	-0.0196(2)	1	0.0302(5)
N(1)	0.7275(2)	0.5068(2)	0.5132(2)	1	0.0157(4)
O(3)	0.7805(2)	0.42946(19)	0.57948(19)	1	0.0203(4)
H(3)	0.7882	0.3550	0.5240	1	0.030
O(2)	0.5379(2)	0.7684(2)	0.5453(2)	1	0.0240(4)
O(4)	0.6437(2)	0.38565(19)	0.19887(19)	1	0.0205(4)
O(1)	0.6417(2)	0.66174(19)	0.39495(19)	1	0.0192(4)
C(6)	0.6720(5)	0.4171(3)	-0.1025(3)	1	0.0367(8)
H(6A)	0.5641	0.3916	-0.1648	1	0.055
H(6B)	0.7213	0.3399	-0.1295	1	0.055
H(6C)	0.7274	0.4939	-0.1054	1	0.055
Sn(2)	0.569012(19)	0.014225(16)	0.274043(17)	1	0.01660(5)
C(11)	0.7960(3)	0.1132(3)	0.1508(3)	1	0.0198(5)
C(7)	0.8244(3)	-0.0933(2)	0.4232(3)	1	0.0180(5)
C(8)	0.7882(3)	0.0007(3)	0.5420(3)	1	0.0187(5)
C(10)	0.8334(3)	0.2171(2)	0.2948(3)	1	0.0189(5)
O(12)	0.6509(3)	-0.0880(2)	-0.0179(2)	1	0.0290(5)
H(12)	0.7266	-0.1233	-0.0264	1	0.043
O(9)	0.6465(2)	0.1491(2)	0.6161(2)	1	0.0243(4)
H(9)	0.5794	0.1880	0.5877	1	0.036
N(4)	0.6912(3)	0.0094(2)	0.1129(2)	1	0.0195(4)

O(8)	0.9225(2)	-0.15949(19)	0.4408(2)	1	0.0231(4)
N(3)	0.6843(3)	0.0633(2)	0.5103(2)	1	0.0176(4)
O(11)	0.9384(2)	0.3176(2)	0.3431(2)	1	0.0256(4)
O(10)	0.7519(2)	0.19486(18)	0.35905(19)	1	0.0183(4)
O(7)	0.7465(2)	-0.10023(18)	0.30560(19)	1	0.0196(4)
C(12)	0.8780(4)	0.1357(3)	0.0673(3)	1	0.0292(6)
H(12A)	0.9740	0.1027	0.0830	1	0.044
H(12B)	0.9024	0.2328	0.0924	1	0.044
H(12C)	0.8117	0.0863	-0.0287	1	0.044
C(9)	0.8708(3)	0.0149(3)	0.6805(3)	1	0.0275(6)
H(9A)	0.9198	0.1105	0.7422	1	0.041
H(9B)	0.9502	-0.0391	0.6785	1	0.041
H(9C)	0.7968	-0.0173	0.7119	1	0.041

---

\* $U_{eq}$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

Table S2. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for  $\text{C}_{12}\text{H}_{16}\text{N}_4\text{O}_{12}\text{Sn}_2$  (**1**) at 150(2) K with estimated standard deviations in parentheses.

Label	$U_{11}$	$U_{22}$	$U_{33}$	$U_{12}$	$U_{13}$	$U_{23}$
Sn(1)	17(1)	14(1)	14(1)	4(1)	7(1)	5(1)
C(3)	34(2)	30(2)	18(2)	13(2)	14(2)	10(2)
C(5)	30(2)	20(2)	16(2)	8(1)	8(1)	6(1)
C(1)	17(2)	14(1)	20(2)	2(1)	6(1)	5(1)
C(4)	22(2)	17(2)	18(2)	7(1)	4(1)	5(1)
C(2)	15(1)	16(1)	18(2)	2(1)	5(1)	4(1)
O(6)	49(2)	15(1)	26(1)	7(1)	19(1)	11(1)
N(2)	32(2)	15(1)	20(1)	6(1)	11(1)	11(1)
O(5)	40(2)	18(1)	19(1)	-2(1)	4(1)	1(1)
N(1)	19(1)	16(1)	17(1)	4(1)	7(1)	11(1)
O(3)	30(1)	16(1)	20(1)	8(1)	11(1)	12(1)
O(2)	28(1)	23(1)	27(1)	14(1)	16(1)	12(1)
O(4)	22(1)	18(1)	16(1)	1(1)	5(1)	5(1)
O(1)	23(1)	21(1)	19(1)	9(1)	10(1)	12(1)
C(6)	61(2)	27(2)	19(2)	8(2)	16(2)	7(2)
Sn(2)	18(1)	15(1)	16(1)	4(1)	5(1)	7(1)
C(11)	22(2)	20(2)	18(2)	7(1)	8(1)	8(1)
C(7)	18(2)	12(1)	24(2)	2(1)	8(1)	8(1)
C(8)	17(2)	18(2)	19(2)	3(1)	5(1)	8(1)
C(10)	21(2)	14(1)	20(2)	6(1)	5(1)	6(1)
O(12)	44(2)	21(1)	15(1)	4(1)	12(1)	1(1)
O(9)	29(1)	27(1)	19(1)	15(1)	12(1)	8(1)
N(4)	28(2)	14(1)	14(1)	6(1)	8(1)	4(1)
O(8)	22(1)	17(1)	30(1)	7(1)	8(1)	11(1)
N(3)	20(1)	15(1)	17(1)	5(1)	9(1)	6(1)
O(11)	24(1)	22(1)	26(1)	-1(1)	6(1)	9(1)
O(10)	22(1)	13(1)	18(1)	4(1)	8(1)	6(1)
O(7)	24(1)	16(1)	19(1)	8(1)	8(1)	7(1)
C(12)	35(2)	29(2)	30(2)	6(2)	20(2)	14(2)
C(9)	25(2)	39(2)	20(2)	10(2)	7(2)	15(2)

The anisotropic displacement factor exponent takes the form:  $-2\pi^2[h^2a^{*2}U_{11} + \dots + 2hka^*b^*U_{12}]$ .

Table S3. Bond lengths [ $\text{\AA}$ ] for  $\text{C}_{12}\text{H}_{16}\text{N}_4\text{O}_{12}\text{Sn}_2$  (**1**) at 150(2) K with estimated standard deviations in parentheses.

Label	Distances
Sn(1)-O(1)	2.1776(18)
Sn(1)-O(4)	2.2038(18)
Sn(1)-N(1)	2.508(2)
Sn(1)-N(2)	2.526(2)
C(3)-C(2)	1.484(4)
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(5)-N(2)	1.281(3)
C(5)-C(6)	1.485(4)
C(5)-C(4)	1.506(4)
C(1)-O(2)	1.240(3)
C(1)-O(1)	1.272(3)
C(1)-C(2)	1.507(4)
C(4)-O(5)	1.245(3)
C(4)-O(4)	1.270(3)
C(2)-N(1)	1.280(3)
O(6)-N(2)	1.384(3)
O(6)-H(6)	0.8400
N(1)-O(3)	1.381(3)
O(3)-H(3)	0.8400
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
Sn(2)-O(7)	2.1750(18)
Sn(2)-O(10)	2.1852(18)
Sn(2)-N(3)	2.421(2)
Sn(2)-N(4)	2.455(2)
C(11)-N(4)	1.280(4)
C(11)-C(12)	1.485(4)
C(11)-C(10)	1.509(4)
C(7)-O(8)	1.225(3)
C(7)-O(7)	1.299(3)
C(7)-C(8)	1.508(4)
C(8)-N(3)	1.273(3)
C(8)-C(9)	1.487(4)

C(10)-O(11)	1.232(3)
C(10)-O(10)	1.289(3)
O(12)-N(4)	1.372(3)
O(12)-H(12)	0.8400
O(9)-N(3)	1.379(3)
O(9)-H(9)	0.8400
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800

---

Symmetry transformations used to generate equivalent atoms:

Table S4. Bond angles [°] for C<sub>12</sub>H<sub>16</sub>N<sub>4</sub>O<sub>12</sub>Sn<sub>2</sub> (**1**) at 150(2) K with estimated standard deviations in parentheses.

Label	Angles
O(1)-Sn(1)-O(4)	85.90(7)
O(1)-Sn(1)-N(1)	67.29(7)
O(4)-Sn(1)-N(1)	83.38(8)
O(1)-Sn(1)-N(2)	83.17(7)
O(4)-Sn(1)-N(2)	66.86(8)
N(1)-Sn(1)-N(2)	139.50(8)
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
N(2)-C(5)-C(6)	126.5(3)
N(2)-C(5)-C(4)	112.6(2)
C(6)-C(5)-C(4)	120.9(2)
O(2)-C(1)-O(1)	123.7(3)
O(2)-C(1)-C(2)	118.2(2)
O(1)-C(1)-C(2)	118.1(2)
O(5)-C(4)-O(4)	123.9(3)
O(5)-C(4)-C(5)	117.5(3)
O(4)-C(4)-C(5)	118.6(2)
N(1)-C(2)-C(3)	126.7(3)
N(1)-C(2)-C(1)	112.6(2)
C(3)-C(2)-C(1)	120.7(2)
N(2)-O(6)-H(6)	109.5
C(5)-N(2)-O(6)	114.6(2)
C(5)-N(2)-Sn(1)	110.46(18)
O(6)-N(2)-Sn(1)	127.12(16)
C(2)-N(1)-O(3)	114.1(2)
C(2)-N(1)-Sn(1)	109.70(18)
O(3)-N(1)-Sn(1)	128.26(15)
N(1)-O(3)-H(3)	109.5
C(4)-O(4)-Sn(1)	120.96(18)
C(1)-O(1)-Sn(1)	120.40(16)
C(5)-C(6)-H(6A)	109.5
C(5)-C(6)-H(6B)	109.5



H(6A)-C(6)-H(6B)	109.5
C(5)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
O(7)-Sn(2)-O(10)	88.80(7)
O(7)-Sn(2)-N(3)	68.74(7)
O(10)-Sn(2)-N(3)	76.53(8)
O(7)-Sn(2)-N(4)	76.42(8)
O(10)-Sn(2)-N(4)	68.16(7)
N(3)-Sn(2)-N(4)	130.23(8)
N(4)-C(11)-C(12)	126.1(2)
N(4)-C(11)-C(10)	113.3(3)
C(12)-C(11)-C(10)	120.6(2)
O(8)-C(7)-O(7)	123.5(2)
O(8)-C(7)-C(8)	119.6(2)
O(7)-C(7)-C(8)	117.0(2)
N(3)-C(8)-C(9)	125.7(2)
N(3)-C(8)-C(7)	113.4(2)
C(9)-C(8)-C(7)	120.9(2)
O(11)-C(10)-O(10)	124.3(2)
O(11)-C(10)-C(11)	118.3(3)
O(10)-C(10)-C(11)	117.4(2)
N(4)-O(12)-H(12)	109.5
N(3)-O(9)-H(9)	109.5
C(11)-N(4)-O(12)	115.9(2)
C(11)-N(4)-Sn(2)	116.92(17)
O(12)-N(4)-Sn(2)	126.92(18)
C(8)-N(3)-O(9)	115.1(2)
C(8)-N(3)-Sn(2)	117.52(17)
O(9)-N(3)-Sn(2)	127.32(15)
C(10)-O(10)-Sn(2)	124.06(16)
C(7)-O(7)-Sn(2)	123.34(16)
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5

C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5

---

Symmetry transformations used to generate equivalent atoms:

Table S5. Atomic coordinates and equivalent isotropic displacement parameters for C<sub>18</sub>H<sub>16</sub>N<sub>2</sub>O<sub>6</sub>Sn (**2**) at 150(2) K with estimated standard deviations in parentheses.

Label	x	y	z	Occupancy	U <sub>eq</sub> *
Sn(01)	0.3584(1)	1.0821(1)	0.7052(1)	1	0.022(1)
O(1)	0.3506(7)	1.0716(7)	0.8780(4)	1	0.027(2)
O(2)	0.6404(7)	1.1214(4)	0.7603(4)	1	0.032(2)
H(2)	0.6139	1.1830	0.7605	1	0.049
O(3)	0.1076(5)	0.9552(5)	0.6953(7)	1	0.035(2)
H(3)	0.1298	0.9518	0.6334	1	0.053
O(4)	0.3968(4)	0.9087(5)	0.7082(6)	1	0.028(2)
O(5)	0.2589(6)	1.0249(6)	1.0257(5)	1	0.030(2)
O(6)	0.5124(6)	0.7698(5)	0.7337(5)	1	0.030(2)
N(1)	0.5572(7)	1.0464(6)	0.7465(6)	1	0.026(2)
N(2)	0.1897(7)	0.9948(7)	0.7588(5)	1	0.022(2)
C(1)	0.1676(9)	0.9983(8)	0.8611(7)	1	0.026(2)
C(2)	0.0600(9)	0.9628(9)	0.9084(8)	1	0.031(3)
H(2A)	0.0005	0.9832	0.8601	1	0.037
H(2B)	0.0486	1.0019	0.9749	1	0.037
C(3)	0.5860(8)	0.9452(7)	0.7546(7)	1	0.027(2)
C(4)	0.7652(8)	0.8559(7)	0.6932(10)	1	0.031(2)
C(5)	-0.0375(10)	0.8045(10)	0.9936(8)	1	0.043(3)
H(5)	-0.0878	0.8540	1.0226	1	0.052
C(6)	0.0518(9)	0.8409(9)	0.9307(9)	1	0.030(2)
C(7)	0.6985(7)	0.9036(8)	0.7842(9)	1	0.032(2)
H(7A)	0.6898	0.8482	0.8388	1	0.038
H(7B)	0.7405	0.9632	0.8153	1	0.038
C(8)	0.4922(9)	0.8686(7)	0.7294(7)	1	0.028(2)
C(9)	0.2660(8)	1.0356(7)	0.9257(7)	1	0.022(2)
C(10)	0.1122(10)	0.6547(9)	0.9107(9)	1	0.049(3)
H(10)	0.1634	0.6053	0.8831	1	0.059
C(11)	-0.0495(13)	0.6928(12)	1.0117(9)	1	0.061(5)
H(11)	-0.1094	0.6683	1.0520	1	0.073
C(12)	0.8948(13)	0.7728(11)	0.5274(10)	1	0.061(5)
H(12)	0.9385	0.7454	0.4722	1	0.074
C(13)	0.8609(10)	0.7983(7)	0.7144(9)	1	0.041(2)
H(13)	0.8814	0.7847	0.7848	1	0.049
C(14)	0.1240(10)	0.7657(8)	0.8900(7)	1	0.037(3)
H(14)	0.1826	0.7892	0.8474	1	0.044

C(15)	0.9266(11)	0.7603(10)	0.6318(11)	1	0.051(3)
H(15)	0.9935	0.7258	0.6473	1	0.061
C(16)	0.7315(12)	0.8676(11)	0.5860(9)	1	0.058(4)
H(16)	0.6652	0.9030	0.5700	1	0.069
C(17)	0.0250(11)	0.6179(11)	0.9719(10)	1	0.054(4)
H(17)	0.0164	0.5439	0.9860	1	0.064
C(18)	0.7960(14)	0.8270(13)	0.5054(11)	1	0.082(6)
H(18)	0.7735	0.8357	0.4348	1	0.098

---

\* $U_{eq}$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

Table S6. Anisotropic displacement parameters for C<sub>18</sub>H<sub>16</sub>N<sub>2</sub>O<sub>6</sub>Sn (**2**) at 150(2) K with estimated standard deviations in parentheses.

Label	U <sub>11</sub>	U <sub>22</sub>	U <sub>33</sub>	U <sub>12</sub>	U <sub>13</sub>	U <sub>23</sub>
Sn(01)	0.030(1)	0.018(1)	0.018(1)	-0.001(1)	0.001(1)	0.002(1)
O(1)	0.030(4)	0.032(4)	0.018(2)	0(5)	0.004(4)	0.005(3)
O(2)	0.034(3)	0.020(3)	0.044(3)	-0.009(3)	0(4)	-0.006(2)
O(3)	0.030(4)	0.050(4)	0.026(3)	-0.011(3)	-0.007(4)	0.005(4)
O(4)	0.029(3)	0.020(2)	0.034(3)	0.002(3)	-0.007(3)	0.002(4)
O(5)	0.034(4)	0.038(4)	0.017(3)	-0.006(4)	0(3)	0(3)
O(6)	0.043(4)	0.015(3)	0.034(5)	0.004(3)	-0.005(3)	0.002(3)
N(1)	0.036(5)	0.019(4)	0.023(4)	0(3)	0.001(3)	-0.002(3)
N(2)	0.025(4)	0.020(4)	0.022(4)	-0.007(3)	-0.005(3)	0.004(3)
C(1)	0.026(7)	0.028(5)	0.023(5)	0(4)	0.003(4)	0.003(4)
C(2)	0.025(6)	0.046(6)	0.022(5)	0.001(5)	0.001(4)	0.001(4)
C(3)	0.035(5)	0.024(5)	0.021(4)	0.001(4)	0.004(4)	-0.003(3)
C(4)	0.042(6)	0.019(4)	0.032(6)	-0.002(4)	0.001(5)	-0.004(5)
C(5)	0.047(7)	0.065(8)	0.018(5)	-0.026(6)	-0.004(5)	0.003(5)
C(7)	0.041(5)	0.026(5)	0.028(5)	0.002(4)	-0.006(5)	0.004(5)
C(8)	0.043(6)	0.019(4)	0.021(6)	-0.001(4)	0.009(4)	-0.005(3)
C(9)	0.029(5)	0.014(4)	0.022(4)	0(4)	-0.002(4)	-0.005(3)
C(10)	0.057(9)	0.041(6)	0.050(7)	-0.011(6)	-0.008(6)	0.008(5)
C(11)	0.083(11)	0.077(10)	0.023(6)	-0.062(9)	-0.010(6)	0.012(6)
C(12)	0.086(13)	0.054(8)	0.044(8)	0.015(8)	0.031(7)	-0.009(6)
C(13)	0.031(4)	0.051(5)	0.040(5)	0.010(6)	0(8)	-0.019(5)
C(14)	0.042(8)	0.035(5)	0.034(5)	-0.018(5)	-0.008(5)	0.012(4)
C(15)	0.033(7)	0.046(7)	0.073(9)	0.002(6)	0.002(7)	-0.010(7)
C(16)	0.073(10)	0.062(8)	0.038(7)	0.021(7)	0.009(7)	0.011(6)
C(17)	0.068(10)	0.045(8)	0.048(8)	-0.023(7)	-0.021(7)	0.012(6)
C(18)	0.102(13)	0.096(12)	0.047(8)	0.053(10)	0.037(8)	0.010(8)

The anisotropic displacement factor exponent takes the form:  $-2\pi^2[h^2a^*U_{11} + \dots + 2hka^*b^*U_{12}]$ .

Table S7. Bond lengths [ $\text{\AA}$ ] for  $\text{C}_{18}\text{H}_{16}\text{N}_2\text{O}_6$  Sn (**2**) at 150(2) K with estimated standard deviations in parentheses.

Label	Distances
Sn(01)-O(1)	2.167(5)
Sn(01)-O(4)	2.175(6)
Sn(01)-N(2)	2.391(8)
Sn(01)-N(1)	2.487(8)
O(1)-C(9)	1.261(12)
O(2)-N(1)	1.370(9)
O(3)-N(2)	1.357(9)
O(4)-C(8)	1.278(12)
O(5)-C(9)	1.260(10)
O(6)-C(8)	1.236(10)
N(1)-C(3)	1.293(10)
N(2)-C(1)	1.308(11)
C(1)-C(2)	1.490(14)
C(1)-C(9)	1.505(14)
C(2)-C(6)	1.523(14)
C(3)-C(7)	1.494(11)
C(3)-C(8)	1.502(13)
C(4)-C(13)	1.377(15)
C(4)-C(16)	1.409(16)
C(4)-C(7)	1.511(15)
C(5)-C(11)	1.395(17)
C(5)-C(6)	1.405(14)
C(6)-C(14)	1.366(15)
C(10)-C(17)	1.375(17)
C(10)-C(14)	1.393(13)
C(11)-C(17)	1.376(19)
C(12)-C(15)	1.369(18)
C(12)-C(18)	1.390(19)
C(13)-C(15)	1.382(16)
C(16)-C(18)	1.366(16)

Table S8. Bond angles [°] for C<sub>18</sub>H<sub>16</sub>N<sub>2</sub>O<sub>6</sub>Sn (**2**) at 150(2) K with estimated standard deviations in parentheses.

Label	Angles
O(1)-Sn(01)-O(4)	86.2(3)
O(1)-Sn(01)-N(2)	70.0(3)
O(4)-Sn(01)-N(2)	74.8(2)
O(1)-Sn(01)-N(1)	79.9(3)
O(4)-Sn(01)-N(1)	67.7(2)
N(2)-Sn(01)-N(1)	132.9(3)
C(9)-O(1)-Sn(01)	121.9(6)
C(8)-O(4)-Sn(01)	124.8(5)
C(3)-N(1)-O(2)	116.0(8)
C(3)-N(1)-Sn(01)	116.3(7)
O(2)-N(1)-Sn(01)	127.8(5)
C(1)-N(2)-O(3)	115.8(9)
C(1)-N(2)-Sn(01)	115.6(7)
O(3)-N(2)-Sn(01)	127.9(5)
N(2)-C(1)-C(2)	123.8(10)
N(2)-C(1)-C(9)	112.1(9)
C(2)-C(1)-C(9)	124.1(8)
C(1)-C(2)-C(6)	114.6(9)
N(1)-C(3)-C(7)	126.1(9)
N(1)-C(3)-C(8)	112.5(9)
C(7)-C(3)-C(8)	121.4(7)
C(13)-C(4)-C(16)	118.4(11)
C(13)-C(4)-C(7)	120.0(10)
C(16)-C(4)-C(7)	121.6(10)
C(11)-C(5)-C(6)	118.8(13)
C(14)-C(6)-C(5)	118.8(10)
C(14)-C(6)-C(2)	123.5(10)
C(5)-C(6)-C(2)	117.6(10)
C(3)-C(7)-C(4)	115.3(9)
O(6)-C(8)-O(4)	124.3(9)
O(6)-C(8)-C(3)	117.1(9)
O(4)-C(8)-C(3)	118.6(8)
O(5)-C(9)-O(1)	124.2(9)
O(5)-C(9)-C(1)	116.6(8)
O(1)-C(9)-C(1)	119.2(8)
C(17)-C(10)-C(14)	120.1(12)

C(17)-C(11)-C(5)	121.9(12)
C(15)-C(12)-C(18)	118.8(11)
C(4)-C(13)-C(15)	120.5(11)
C(6)-C(14)-C(10)	121.7(11)
C(12)-C(15)-C(13)	121.0(12)
C(18)-C(16)-C(4)	120.1(13)
C(10)-C(17)-C(11)	118.7(12)
C(16)-C(18)-C(12)	121.0(13)

---



Table S9. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for  $\text{C}_{12}\text{H}_{26}\text{N}_4\text{O}_{11}$  Sn (**3**) at 150(2) K with estimated standard deviations in parentheses.

Label	x	y	z	Occupancy	$U_{\text{eq}}^*$
Sn(1)	9671(1)	3112(1)	1220(1)	1	23(1)
O(1)	10775(1)	2862(1)	1016(1)	1	29(1)
O(2)	11026(1)	4248(1)	2573(1)	1	31(1)
O(3)	11704(1)	2116(1)	730(1)	1	36(1)
O(4)	10117(1)	4589(1)	1318(1)	1	28(1)
O(5)	9106(1)	3572(1)	-18(1)	1	29(1)
O(6)	10513(1)	7376(1)	1827(1)	1	39(1)
O(7)	7263(1)	4677(1)	-2051(1)	1	34(1)
O(8)	8390(1)	2212(1)	-307(1)	1	44(1)
O(9)	9819(1)	337(1)	1209(1)	1	44(1)
N(1)	7885(1)	4338(1)	-1321(1)	1	26(1)
N(2)	10336(1)	6416(1)	1628(1)	1	26(1)
N(3)	10143(1)	1212(1)	1146(1)	1	30(1)
C(1)	11112(1)	2103(1)	900(1)	1	24(1)
C(2)	9102(2)	485(2)	1364(2)	1	68(1)
H(2A)	9298	759	1897	1	102
H(2B)	8821	-125	1337	1	102
H(2C)	8699	921	966	1	102
C(3)	10759(1)	1151(1)	973(1)	1	23(1)
C(4)	7284(2)	5701(2)	-2028(2)	1	37(1)
H(4A)	7225	5922	-1563	1	56
H(4B)	6814	5952	-2514	1	56
H(4C)	7826	5925	-1992	1	56
C(5)	11453(2)	6188(2)	3005(1)	1	37(1)

H(5A)	12021	6012	3076	1	56
H(5B)	11346	5879	3416	1	56
H(5C)	11422	6879	3049	1	56
C(6)	10647(1)	4824(1)	2032(1)	1	22(1)
C(7)	10802(1)	5874(1)	2204(1)	1	22(1)
C(8)	8495(1)	3027(1)	-482(1)	1	28(1)
C(9)	7290(2)	2780(2)	-1918(1)	1	39(1)
H(9A)	6750	2730	-1891	1	59
H(9B)	7551	2149	-1844	1	59
H(9C)	7184	3032	-2439	1	59
C(10)	11125(2)	257(2)	833(2)	1	35(1)
H(10A)	10811	-290	887	1	52
H(10B)	11725	207	1225	1	52
H(10C)	11079	266	296	1	52
C(11)	7876(1)	3432(2)	-1278(1)	1	26(1)
C(12)	9938(2)	7933(2)	1166(2)	1	52(1)
H(12A)	10026	7793	700	1	77
H(12B)	10044	8610	1298	1	77
H(12C)	9351	7778	1048	1	77
N(4)	9001(1)	5699(1)	-34(1)	1	28(1)
H(40A)	8530(10)	5871(13)	-3(11)	1	42
H(40B)	9088(12)	6081(12)	-349(10)	1	42
H(40C)	8917(12)	5106(10)	-229(11)	1	42
H(40D)	9437(10)	5671(13)	447(8)	1	42
O(10)	12067(1)	4135(1)	4231(1)	1	46(1)
H(50A)	12460(14)	3696(17)	4336(16)	1	69

H(50B)	11777(15)	4239(19)	3716(10)	1	69
O(11A)	12433(2)	876(2)	-40(2)	0.697(4)	36(1)
H(60A)	12540(20)	318(15)	190(20)	0.697(4)	54
H(60B)	12210(20)	1270(20)	160(20)	0.697(4)	54
O(11B)	12442(3)	1579(3)	-208(3)	0.303(4)	36(2)
H(60C)	12750(50)	1980(40)	-330(50)	0.303(4)	53
H(60D)	12250(50)	1860(40)	100(40)	0.303(4)	53

---

\* $U_{eq}$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

Table S10. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for  $\text{C}_{12}\text{H}_{26}\text{N}_4\text{O}_{11}\text{Sn}$  (**3**) at 150(2) K with estimated standard deviations in parentheses.

Label	$U_{11}$	$U_{22}$	$U_{33}$	$U_{12}$	$U_{13}$	$U_{23}$
Sn(1)	26(1)	17(1)	25(1)	2(1)	11(1)	0(1)
O(1)	28(1)	19(1)	39(1)	1(1)	14(1)	5(1)
O(2)	34(1)	25(1)	26(1)	3(1)	8(1)	5(1)
O(3)	29(1)	40(1)	44(1)	3(1)	21(1)	10(1)
O(4)	34(1)	18(1)	22(1)	-1(1)	5(1)	-2(1)
O(5)	25(1)	33(1)	24(1)	-3(1)	6(1)	-3(1)
O(6)	46(1)	17(1)	37(1)	0(1)	4(1)	-3(1)
O(7)	33(1)	36(1)	25(1)	0(1)	6(1)	5(1)
O(8)	46(1)	26(1)	38(1)	-2(1)	1(1)	1(1)
O(9)	50(1)	20(1)	80(1)	-5(1)	44(1)	-1(1)
N(1)	23(1)	31(1)	22(1)	0(1)	8(1)	1(1)
N(2)	29(1)	17(1)	28(1)	-1(1)	9(1)	-3(1)
N(3)	34(1)	17(1)	44(1)	-2(1)	23(1)	-1(1)
C(1)	21(1)	25(1)	22(1)	2(1)	7(1)	6(1)
C(2)	70(2)	38(1)	131(2)	-6(1)	76(2)	5(2)
C(3)	24(1)	21(1)	23(1)	2(1)	9(1)	0(1)
C(4)	35(1)	36(1)	38(1)	3(1)	15(1)	11(1)
C(5)	37(1)	30(1)	27(1)	-4(1)	0(1)	-5(1)
C(6)	22(1)	21(1)	22(1)	2(1)	8(1)	0(1)
C(7)	21(1)	22(1)	23(1)	0(1)	9(1)	-3(1)
C(8)	25(1)	28(1)	26(1)	2(1)	8(1)	-4(1)
C(9)	42(1)	34(1)	28(1)	-8(1)	4(1)	-6(1)
C(10)	39(1)	25(1)	47(1)	6(1)	25(1)	-1(1)
C(11)	24(1)	30(1)	24(1)	-2(1)	9(1)	-3(1)

C(12)	56(2)	21(1)	54(2)	6(1)	5(1)	6(1)
N(4)	29(1)	27(1)	23(1)	4(1)	7(1)	0(1)
O(10)	62(1)	36(1)	32(1)	6(1)	15(1)	3(1)
O(11A)	36(1)	43(2)	34(1)	2(1)	20(1)	4(1)
O(11B)	44(2)	25(2)	50(3)	0(2)	33(2)	2(2)

---

The anisotropic displacement factor exponent takes the form:  $-2\pi^2[h^2a^{*2}U_{11} + \dots + 2hka^*b^*U_{12}]$ .

Table S11. Bond lengths [ $\text{\AA}$ ] for  $\text{C}_{12}\text{H}_{26}\text{N}_4\text{O}_{11}\text{Sn}$  (**3**) at 150(2) K with estimated standard deviations in parentheses.

Label	Distances
Sn(1)-O(5)	2.1782(12)
Sn(1)-O(1)	2.1792(12)
Sn(1)-O(4)	2.1988(12)
O(1)-C(1)	1.2895(18)
O(2)-C(6)	1.2337(17)
O(3)-C(1)	1.2237(18)
O(4)-C(6)	1.2842(17)
O(5)-C(8)	1.2873(18)
O(6)-N(2)	1.3976(16)
O(6)-C(12)	1.430(2)
O(7)-N(1)	1.3973(16)
O(7)-C(4)	1.440(2)
O(8)-C(8)	1.230(2)
O(9)-N(3)	1.3843(16)
O(9)-C(2)	1.439(2)
N(1)-C(11)	1.278(2)
N(2)-C(7)	1.2749(19)
N(3)-C(3)	1.2744(18)
C(1)-C(3)	1.5101(19)
C(3)-C(10)	1.4905(19)
C(5)-C(7)	1.488(2)
C(6)-C(7)	1.5103(19)
C(8)-C(11)	1.509(2)
C(9)-C(11)	1.494(2)

Table S12. Bond angles [°] for C<sub>12</sub>H<sub>26</sub>N<sub>4</sub>O<sub>11</sub>Sn (**3**) at 150(2) K with estimated standard deviations in parentheses.

Label	Angles
O(5)-Sn(1)-O(1)	82.45(4)
O(5)-Sn(1)-O(4)	77.36(4)
O(1)-Sn(1)-O(4)	81.55(4)
C(1)-O(1)-Sn(1)	133.15(9)
C(6)-O(4)-Sn(1)	113.13(8)
C(8)-O(5)-Sn(1)	112.68(10)
N(2)-O(6)-C(12)	108.18(13)
N(1)-O(7)-C(4)	108.27(12)
N(3)-O(9)-C(2)	108.95(13)
C(11)-N(1)-O(7)	112.07(12)
C(7)-N(2)-O(6)	111.72(12)
C(3)-N(3)-O(9)	113.36(12)
O(3)-C(1)-O(1)	123.29(14)
O(3)-C(1)-C(3)	118.27(13)
O(1)-C(1)-C(3)	118.45(12)
N(3)-C(3)-C(10)	126.26(13)
N(3)-C(3)-C(1)	113.58(12)
C(10)-C(3)-C(1)	120.15(13)
O(2)-C(6)-O(4)	124.11(13)
O(2)-C(6)-C(7)	119.07(13)
O(4)-C(6)-C(7)	116.82(12)
N(2)-C(7)-C(5)	126.00(13)
N(2)-C(7)-C(6)	114.71(12)
C(5)-C(7)-C(6)	119.29(12)
O(8)-C(8)-O(5)	123.64(15)
O(8)-C(8)-C(11)	119.33(14)
O(5)-C(8)-C(11)	117.02(13)
N(1)-C(11)-C(9)	125.84(14)
N(1)-C(11)-C(8)	114.57(13)
C(9)-C(11)-C(8)	119.51(14)

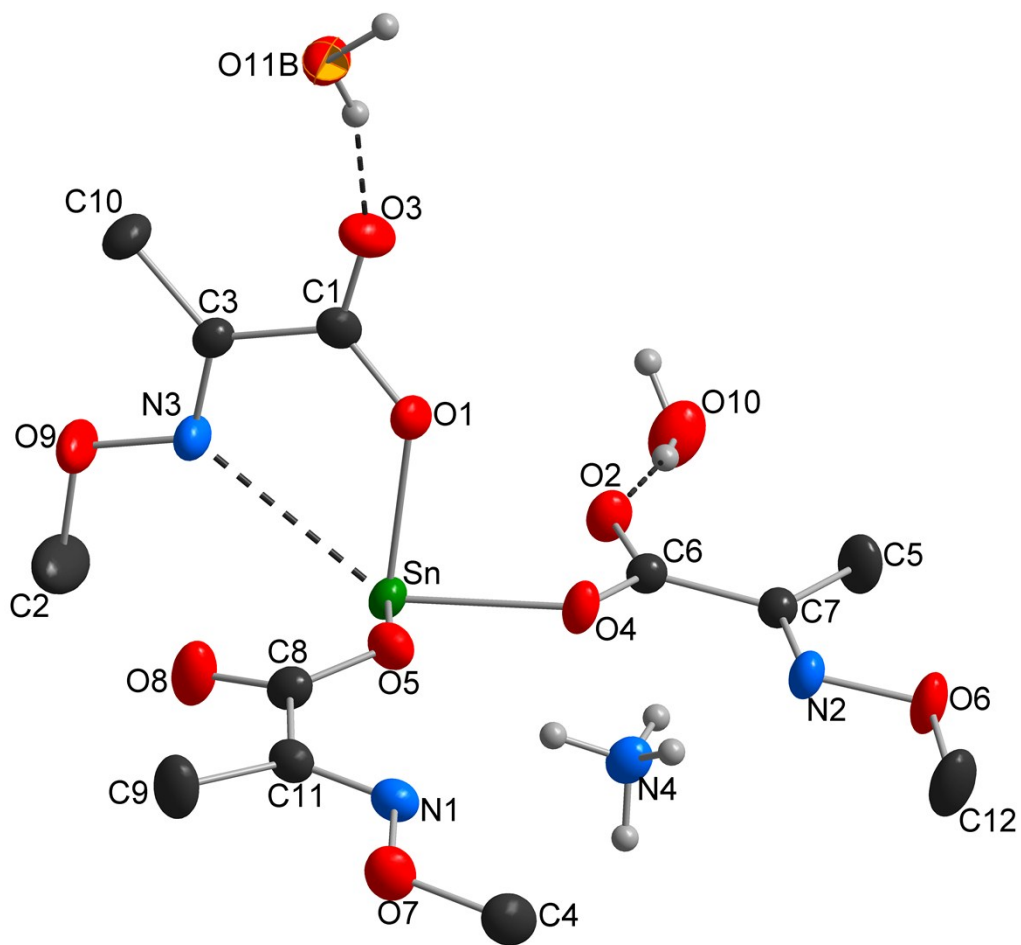


Fig. S2 Solid state structure of **3** with thermal ellipsoids are drawn at the 50 % probability level showing water molecule in the structure and its hydrogen bonding.



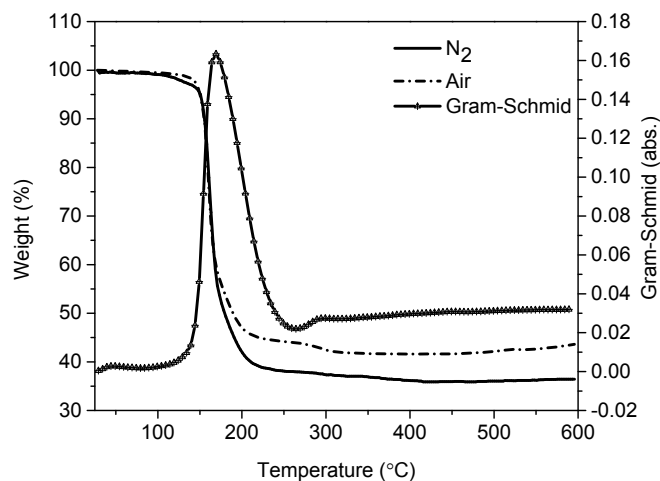
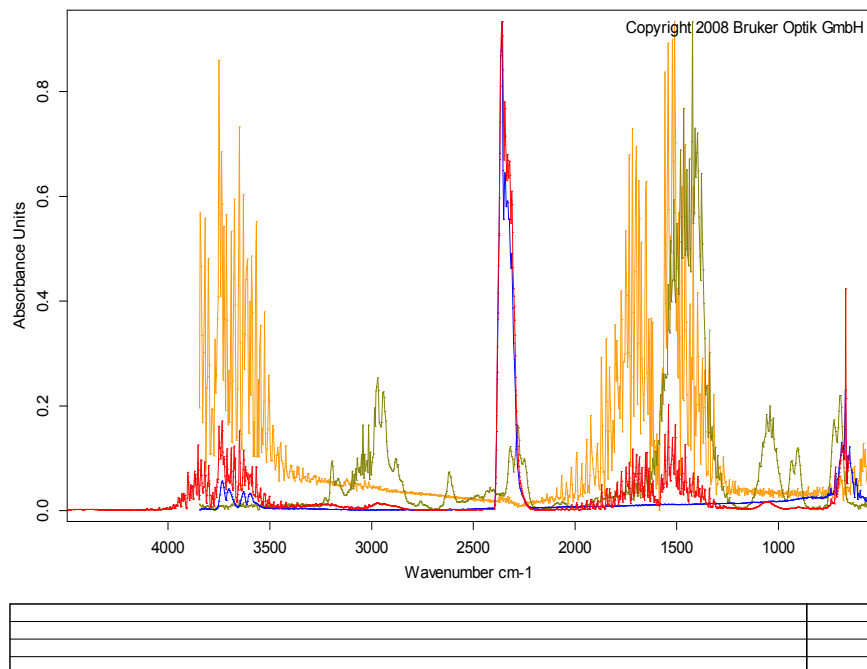


Fig. S3 TG and Gram-Schmid (TG-IR) plot for decomposition of **1**. Measurement were performed by heating the sample at 5 °C/min. in N<sub>2</sub> flow of 20 mL/min.



Page 1/1

Fig. S4 TG-IR spectra of *bis*[2-(hydroxyimino)propionato] tin (II) complex **1** measured by heating at 5 °C/min. in N<sub>2</sub> flow of 20 mL/min. The red line is the gas phase IR spectrum of the product released at T = 161 °C. The spectra for CO<sub>2</sub>, CH<sub>3</sub>CH and H<sub>2</sub>O are the best match shown by the database.

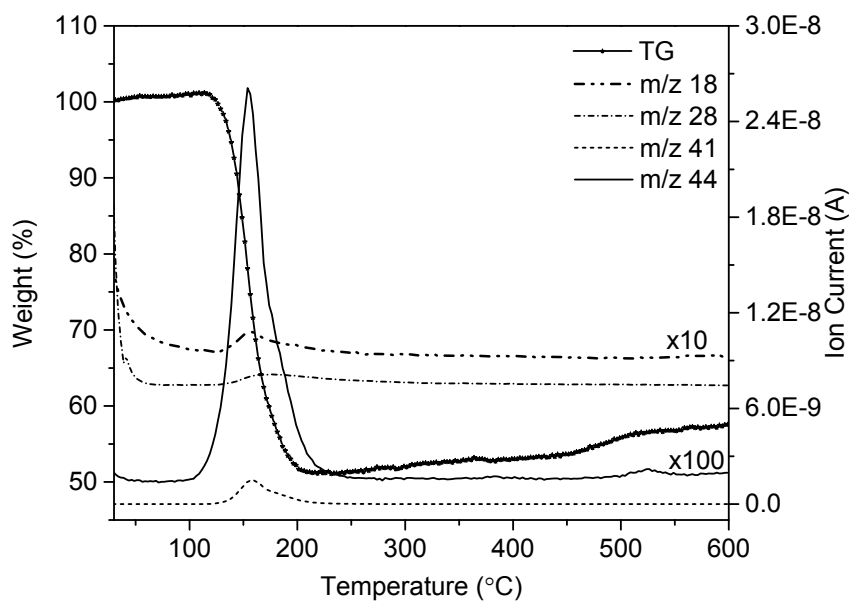


Fig. S5 TG-MS of *bis*[2-(hydroxyimino)propionato] tin (II) **1** measured by heating at 5 °C/min. in helium flow of 20 mL/min. TG-MS of *bis*[2-(hydroxyimino)3-phenyl-propionato] tin (II) **2** show similar ion current profile for m/z 18, 28, 41 and 44 as that of **1**.

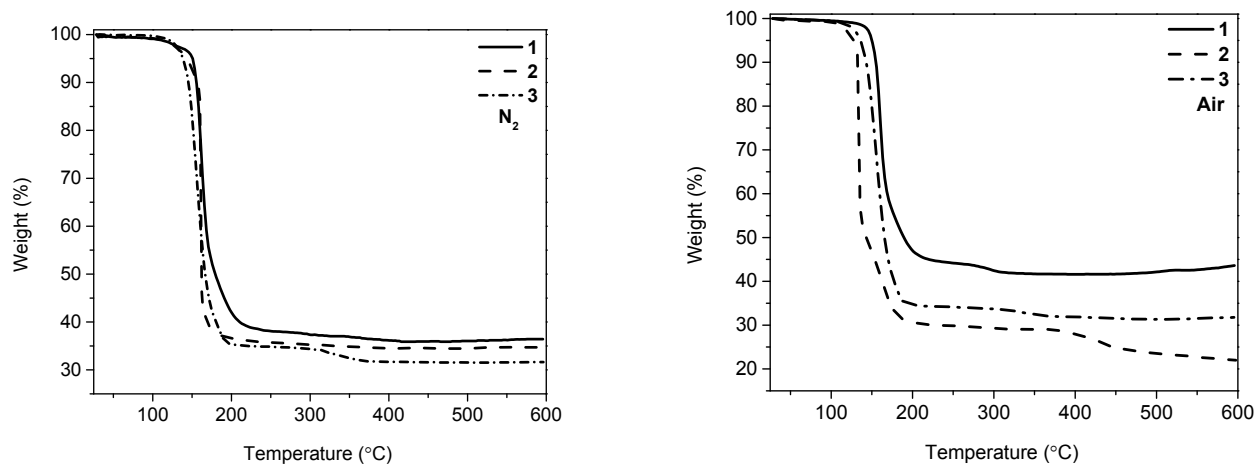


Fig. S6 Thermogravimetric plot for **1**, **2**, and **3** in nitrogen(left) and air atmosphere (right).

Table S13: C, H, N analysis of the residue obtained after heating **1** at different temperatures.

T °C	C %	H %	N %
140	1.61	0.32	0.24
160	1.70	0.39	0.19
180	1.63	0.36	0.15
200	0.86	0.19	0

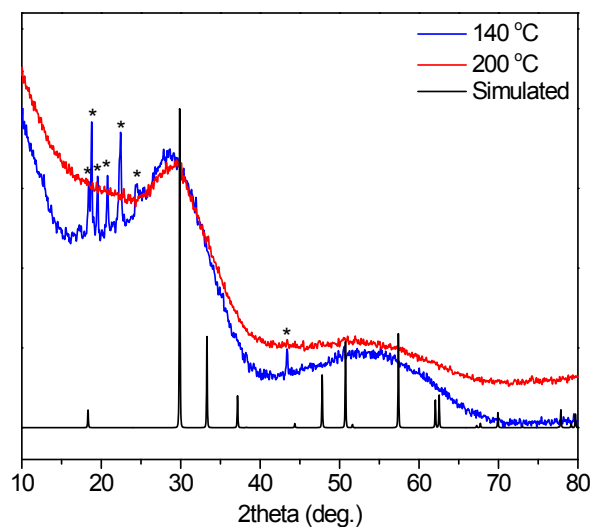


Fig. S7 XRD of amorphous SnO formed by the decomposition of Synthesis of *bis*[2-(hydroxyimino)3-phenylpropionato] tin (II) **2** at 140 and 200 °C.\* indicate unidentified decomposition product.

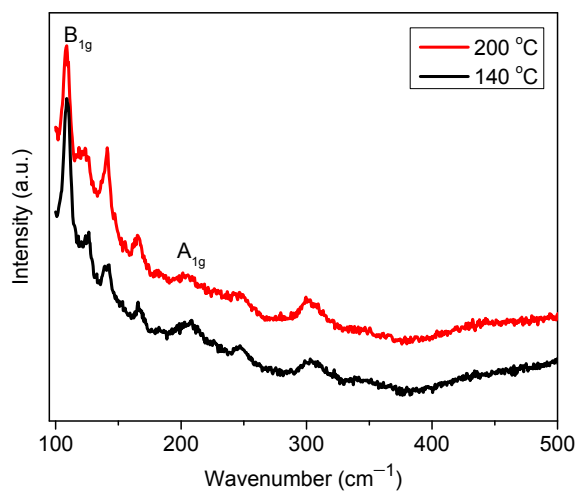


Fig. S8 Raman spectra of SnO powder formed by the decomposition of *bis*(2-(hydroxyimino)propionato) tin (II) **1** at 140 and 200 °C.

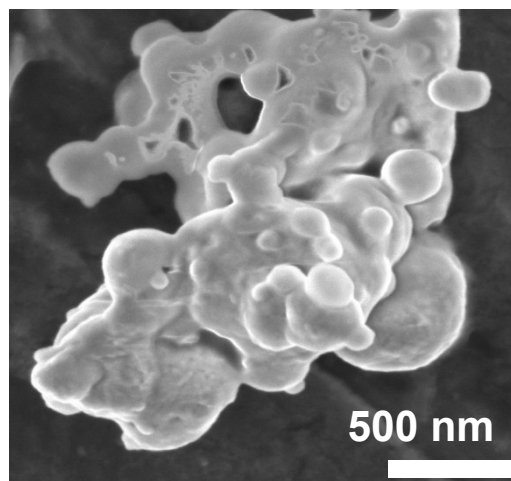


Fig. S9 SEM of SnO from **1** at 140 °C. The SnO particles are lumped together, with fewer non-agglomerated particles.

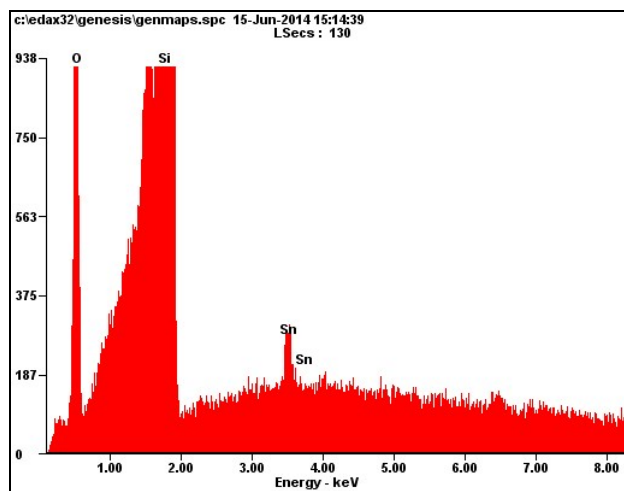


Fig. S10 EDX of the SnO film after one layer of spin coating. The Sn signal indicates the presence of Sn on the surface of the substrate.

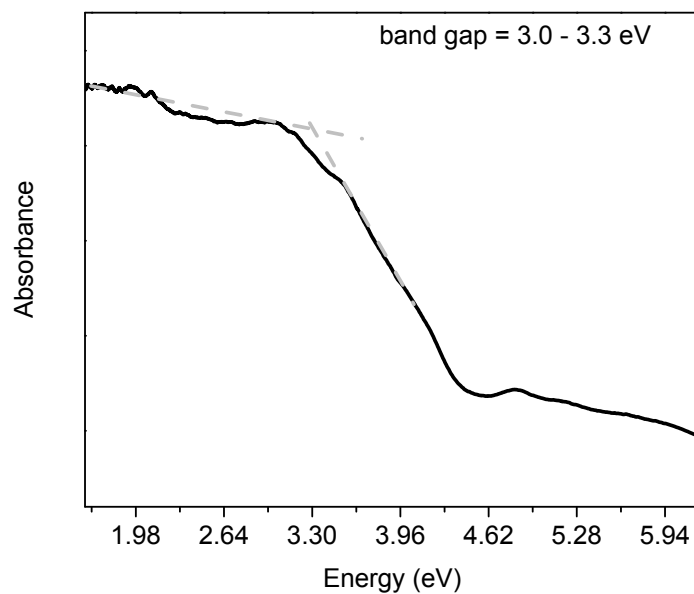


Fig. S11 UV-Vis spectra of SnO thin film on Si formed by spin coating of complex **1**, heating it to 180 °C for 15 minutes.

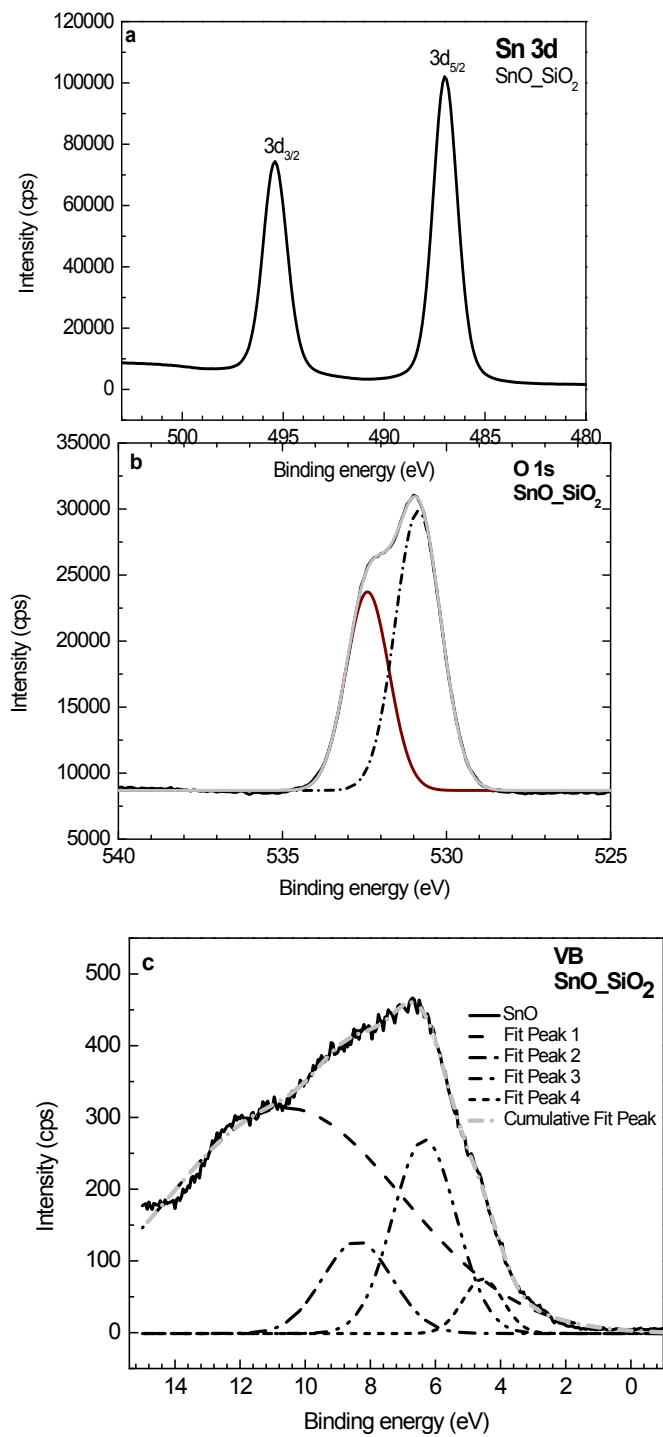


Fig. S12 XPS spectrum of a) 3d and b) O1s c) valence band of SnO thin film after 10 x spin coating/200 °C/15 minute heating cycle for 10 layers SnO from 1.

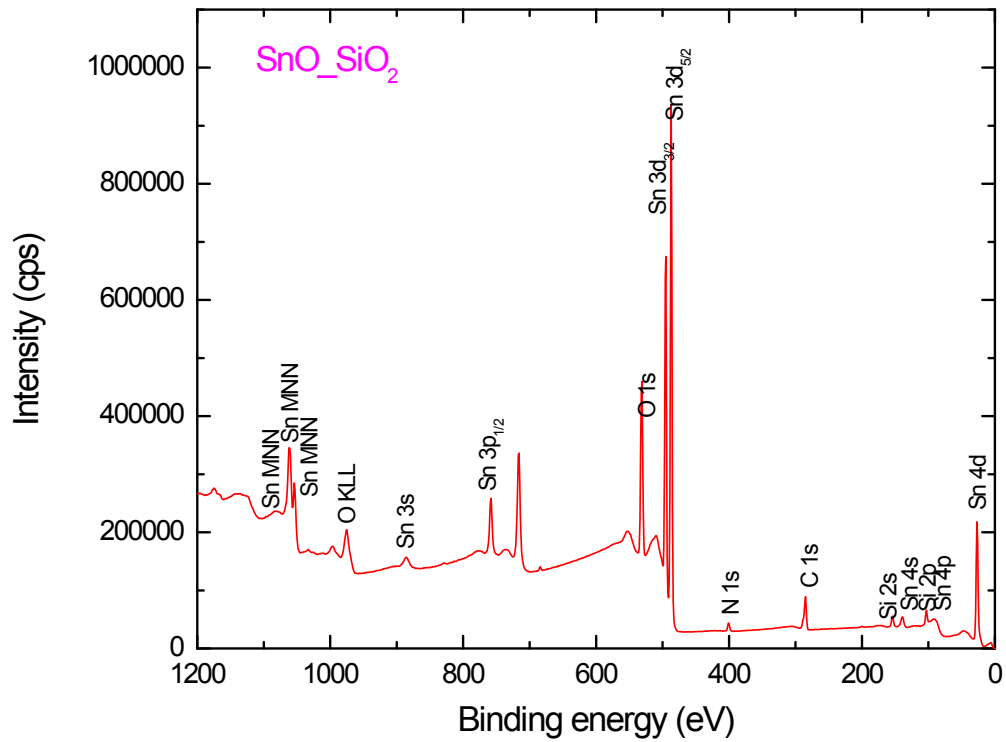


Fig. S13 XPS survey spectrum of 10 layers SnO from **1**.

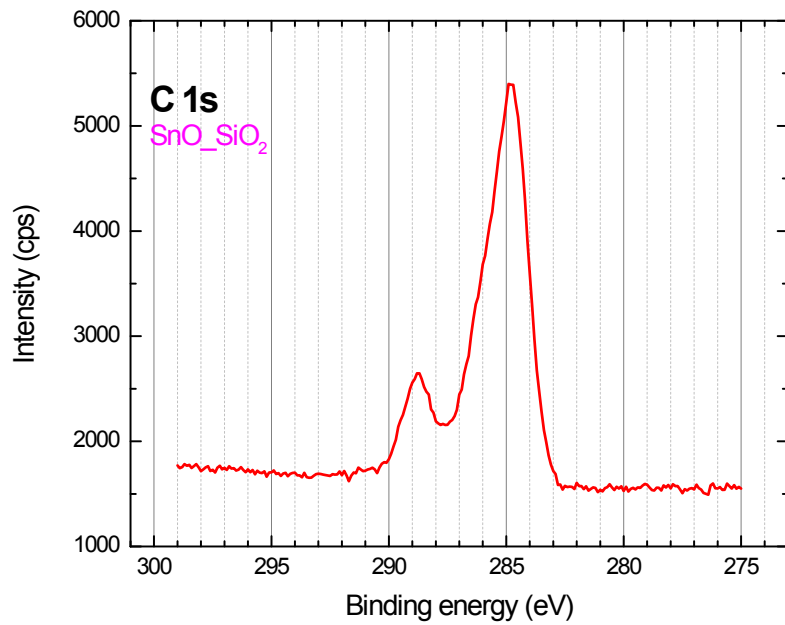


Fig. S14 C 1s XPS spectrum of 10 layer SnO from **1**.



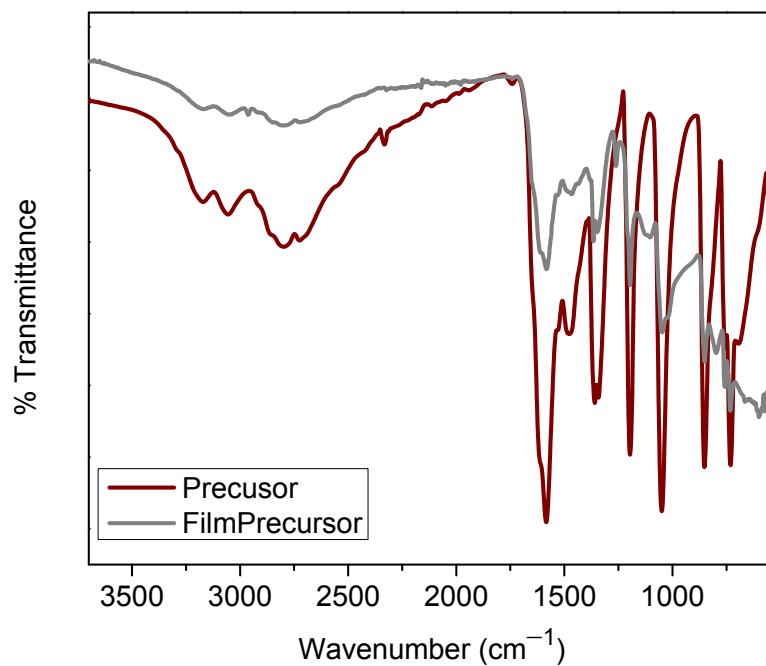


Fig. S15 IR spectra of **1** and film of **1** on Si substrate after drop casting from DMF solution measured by ATR set up.

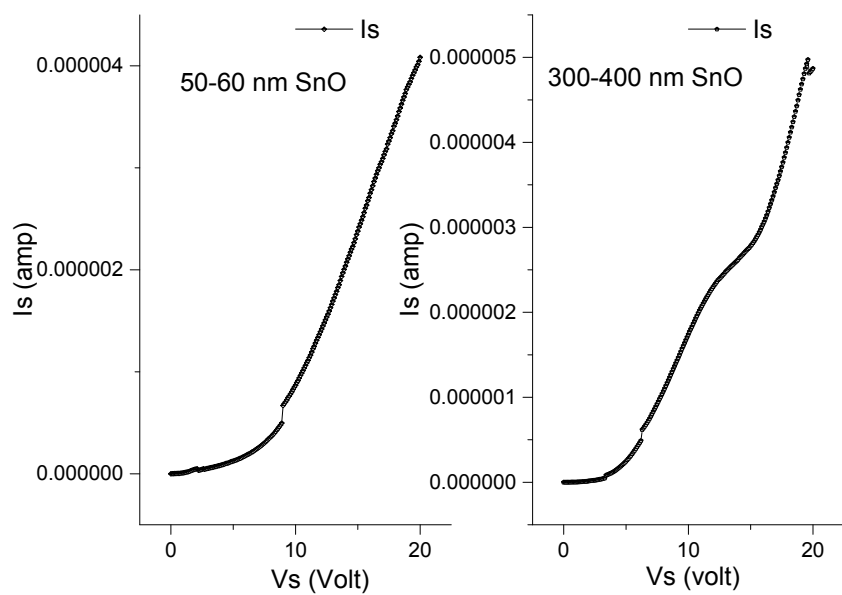


Fig. S16 I-V characteristics of two different thicknesses of SnO on interdigital substrate..

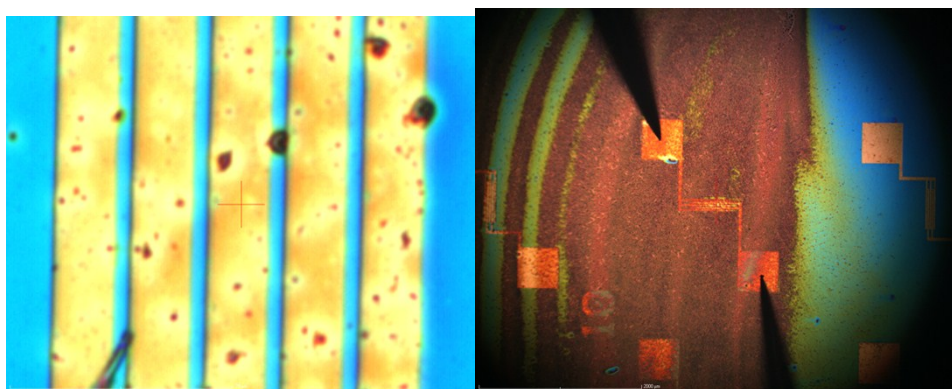


Fig. S17 Optical microscope images of films from which the I-V measurements were carried out. Left (30-50nm) right (300 – 400nm).

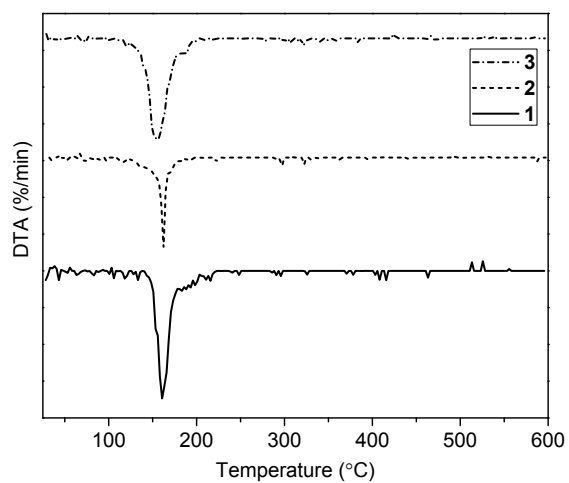


Fig. S18 DTA plot for **1**, **2**, and **3** in nitrogen and air atmosphere. The peak data are taken for reporting the melting/decomposition of **1**, **2**, and **3**.