

## *Supporting Information*

### **A Highly Hydroxylated 6-Tin Oxide Cluster Serves as An Efficient E-beam and EUV-Photoresists to Reach High-resolution Patterns**

Cheng-Dun Li,<sup>a</sup> Chun-Fu Chou,<sup>a</sup> Yu-Fang Tseng,<sup>a</sup> Burn-Jeng Lin,<sup>b,c\*</sup> Tsai-Sheng Gau,<sup>b,c</sup> Po-Hsiung Chen,<sup>b,c</sup> Po-Wen Chiu<sup>b,c</sup> Sun-Zen Chen,<sup>d</sup> Shin-Lin Tsai<sup>e</sup>, Wen-Bin Jian,<sup>e</sup> and Jui-Hsiung Liu<sup>a,c\*</sup>

Department of Chemistry,<sup>a</sup> TSMC-NTHU Joint Research Center,<sup>b</sup> College of Semiconductor Research<sup>c</sup>, Center for Nanotechnology, Materials Science and Microsystem,<sup>d</sup> National Tsing Hua University, Hsinchu, 300044, Taiwan

Department of Electrophysics,<sup>e</sup> National Yang Ming Chao Tung University. Hsinchu, 300013, Taiwan

#### Content:

1. Representative Synthetic procedures -----	s1
2. Powder X-ray diffraction pattern for cluster (2) -----	s2
3. ESI(+)-MS of photoresist 2 -----	s2
4. SEM images for cluster (1) EUV lithography patterns -----	s3
5. SEM images for e-beam lithography patterns -----	s4
6. SEM images for cluster (2) EUV lithography patterns -----	s5
7. Spectral data of key compounds -----	s7
8. X-ray crystallographic data of cluster (1) -----	s7
9. <sup>1</sup> H, <sup>13</sup> C and <sup>119</sup> Sn NMR of cluster (1) -----	s20
10. <sup>1</sup> H, <sup>13</sup> C, and <sup>119</sup> Sn NMR of cluster (2) -----	s23

## 1. Representative synthetic procedures

Unless otherwise noted, all reactions were carried out under nitrogen atmosphere in oven-dried glassware using standard syringe, cannula and septa apparatus. Dichloromethane and toluene were dried over  $\text{CaH}_2$  and distilled. Reagents were purchased from commercial sources and used without purification, unless otherwise stated.  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra were recorded on a Bruker 400 MHz and Bruker 500 MHz spectrometers using chloroform-d ( $\text{CDCl}_3$ ) as the internal standard. The ESI-Mass were performed using JEOL JMS-700. The EA analysis was performed by elemental vario EL cube. The TGA were performed using Mettler-Toledo 2-HT. FTIR Spectroscopy of powder samples was in a Bruker Vertex 80v spectrometer. The AFM measurements were using SEIKO SPA-300HV. Electron-beam lithography was done by utilizing Elionix ELS-7800 with an accelerating voltage of 80 kV and a beam current of 200 pA. The EUV-IL system at the Swiss Light Sources (SLS), Paul Scherrer Institute, utilizes 13.5 nm EUV light. HRXPS measurements were performed in a ULVAC-PHI Quantera II, with a monochromatic Al  $K\alpha$  source (energy of 1486.7 eV).

## 2. Powder X-ray diffraction pattern

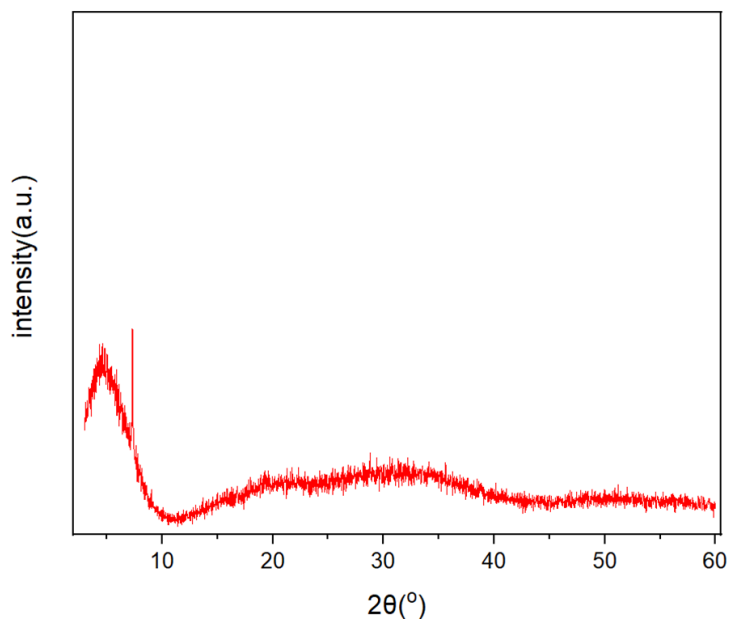


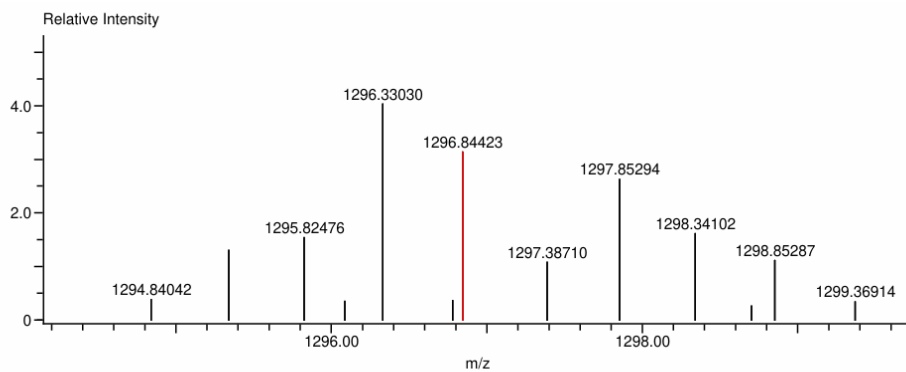
Figure s1A. Powder X-ray diffraction : photoresist 2

## 3. ESI-LC-MS spectrum

Ionization Mode:ESI+  
History:Average(MS[1] 0.95..1.09)

Created:2025/1/6  
Created by:AccuTOF

Charge number:1 Tolerance:500.00[ppm], 500.00 .. 500.... Unsaturation Number:-500.5 .. 500.0 (...)  
Element:<sup>12</sup>C:24 .. 24, <sup>1</sup>H:64 .. 65, <sup>23</sup>Na:0 .. 1, <sup>16</sup>O:14 .. 14, <sup>120</sup>Sn:6 .. 6



Mass	Intensity	Calc. Mass	Mass Difference [mDa]	Mass Difference [ppm]	Possible Formula
1296.84423	313.73	1296.85062	-6.39	-4.92	<sup>12</sup> C <sub>24</sub> <sup>1</sup> H <sub>65</sub> <sup>16</sup> O <sub>14</sub> <sup>120</sup> Sn <sub>6</sub>

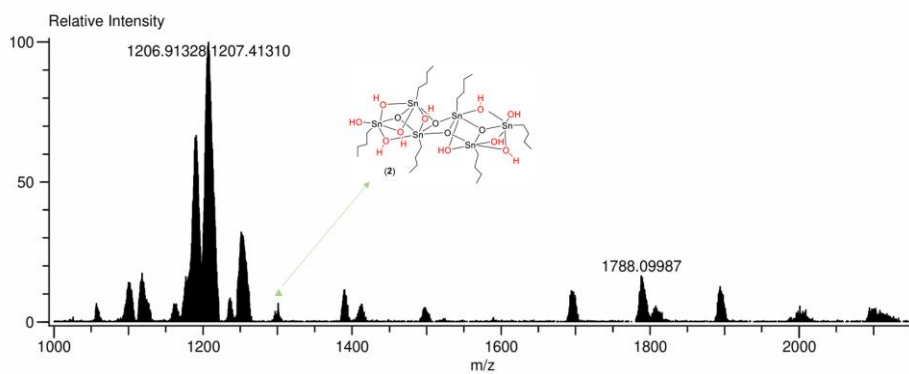


Figure s1B. ESI(+)-MS of photoresist 2

4. SEM images for cluster 1 EUV lithography patterns

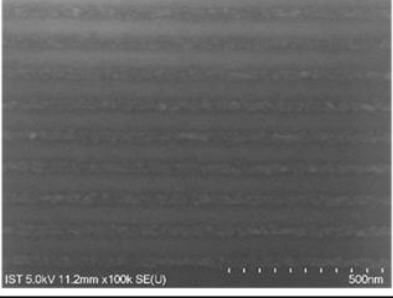
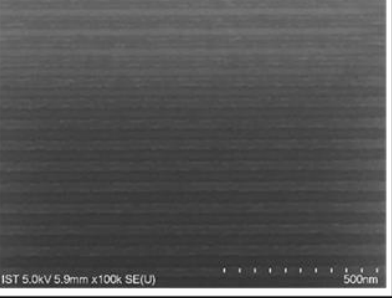
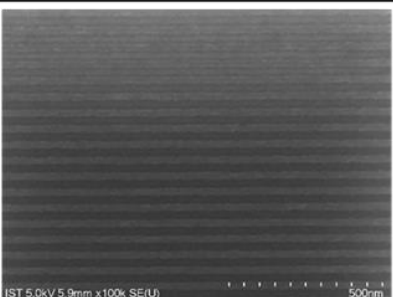
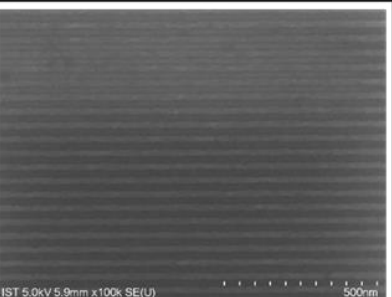
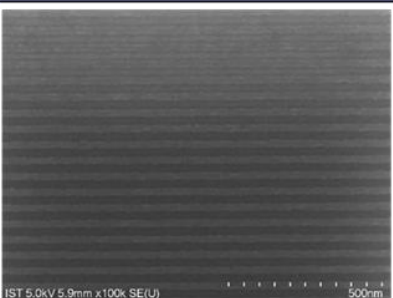
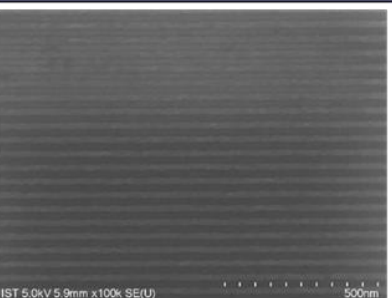
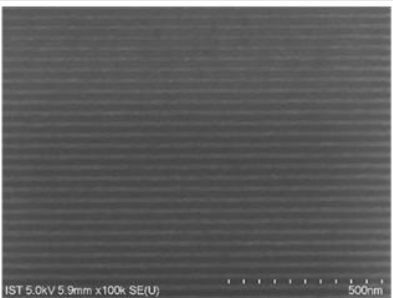
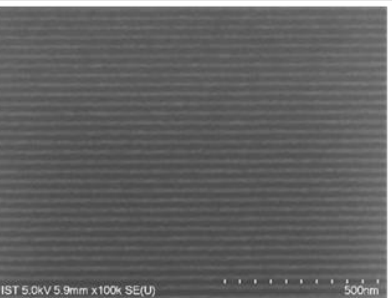
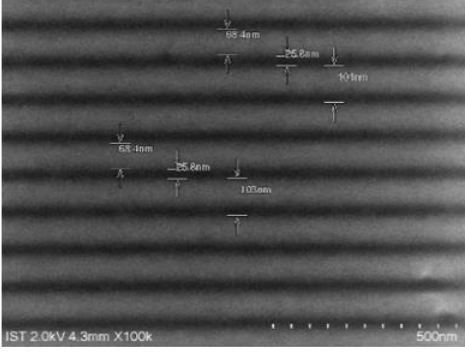
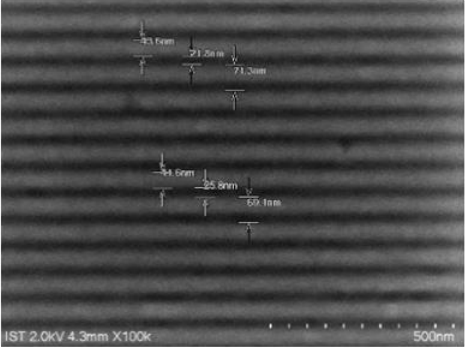
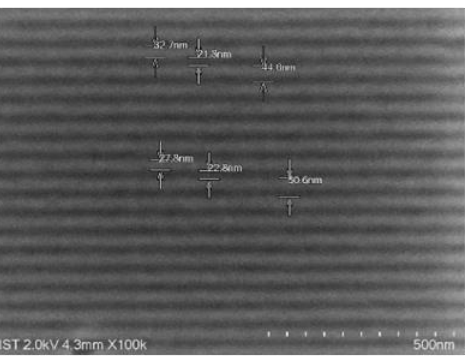
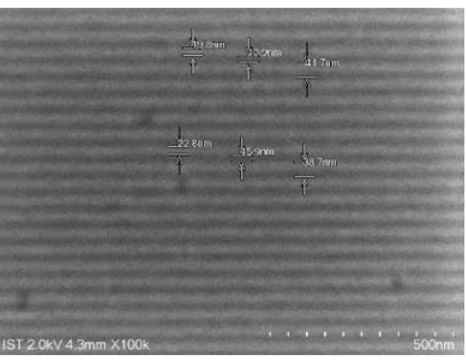
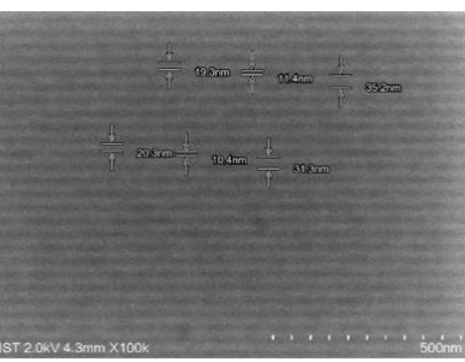
Dose HP	Dose = 200 mJ/cm <sup>2</sup> , L/S = 0.85 HP = 50 nm, CD = 47 nm	Dose = 200 mJ/cm <sup>2</sup> , L/S = 1.09 HP = 34 nm, CD = 35 nm	Dose HP
Design HP = 50 nm			Design HP = 35 nm
	Dose = 200 mJ/cm <sup>2</sup> , L/S = 1.04 HP = 25 nm, CD = 25 nm	Dose = 200 mJ/cm <sup>2</sup> , L/S = 0.94 HP = 22 nm, CD = 21 nm	
Design HP = 25 nm			Design HP = 22 nm
Dose HP	Dose = 200 mJ/cm <sup>2</sup> , L/S = 1.04 HP = 25 nm, CD = 25 nm	Dose = 200 mJ/cm <sup>2</sup> , L/S = 0.94 HP = 22 nm, CD = 21 nm	Dose HP
Design HP = 25 nm			Design HP = 22 nm
	Dose = 200 mJ/cm <sup>2</sup> , L/S = 0.99 HP = 18 nm, CD = 18 nm	Dose = 200 mJ/cm <sup>2</sup> , L/S = 0.94 HP = 16 nm, CD = 16 nm	
Design HP = 18 nm			Design HP = 16 nm

Figure s2. SEM images of EUV lithography patterns on photoresist 1 HP= 50-16 nm at different dose. Process parameter: 1.2wt%, THK= 18.2 nm, Developer: Acetone 60 s, PAB=60 °C for 60s, PEB=



wt%, THK= 27.8 nm, PAB=90 °C for 60s, PEB=110 °C for 60s Development: Acetone, 10s. (Dose = 1440, 1760 and  $\mu\text{C}/\text{cm}^2$ ).

6. SEM image of cluster 2 EUV lithography patterns

Dose HP	Dose = 73 mJ/cm <sup>2</sup> , HP = 50 nm	Dose = 66 mJ/cm <sup>2</sup> , HP = 35 nm	Dose HP
Design HP = 50 nm			Design HP = 35 nm
	Dose = 60 mJ/cm <sup>2</sup> , HP = 25 nm	Dose = 68 mJ/cm <sup>2</sup> , HP = 19 nm	
Design HP = 25 nm			Design HP = 20 nm
	Dose = 56 mJ/cm <sup>2</sup> , HP = 16 nm		
Design HP = 16 nm			

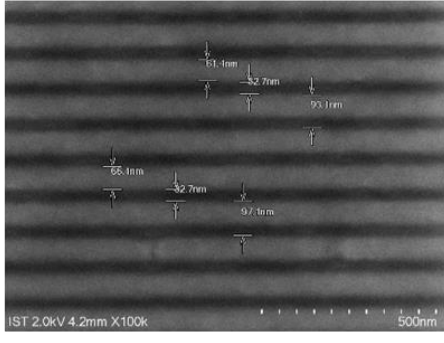
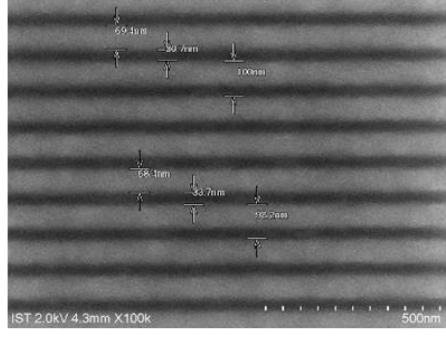
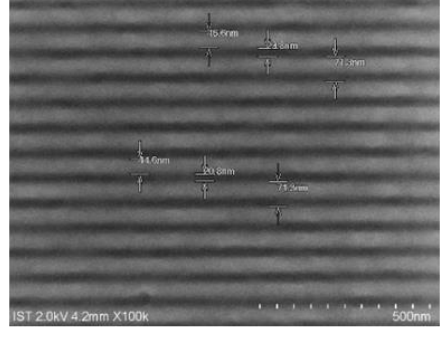
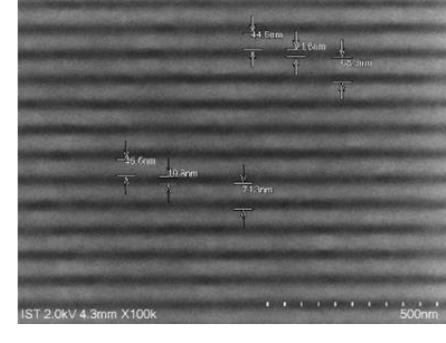
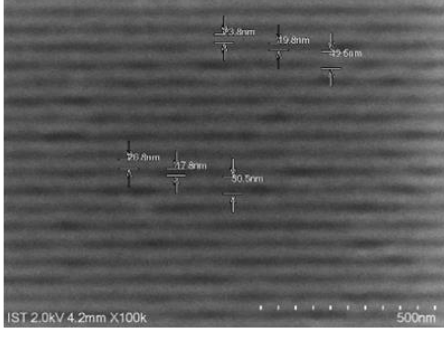
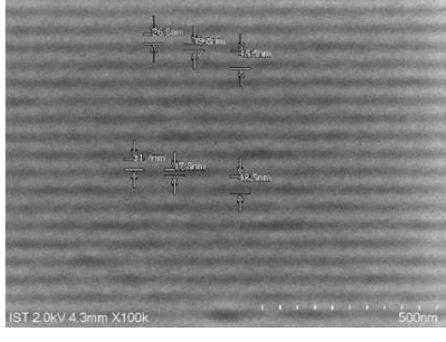
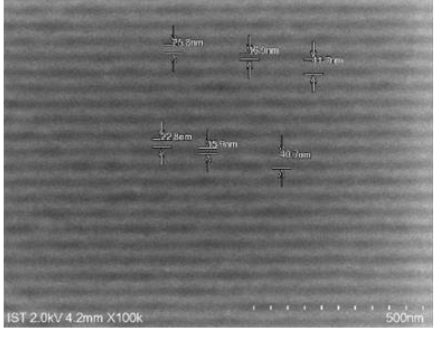
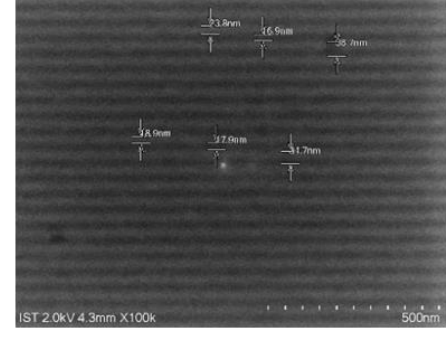
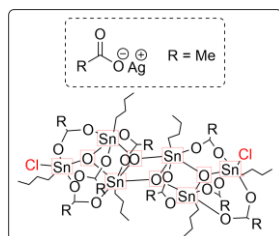
Dose HP	Dose = 66 mJ/cm <sup>2</sup> , HP = 50 nm	Dose = 70 mJ/cm <sup>2</sup> , HP = 50 nm
Design HP = 50 nm		
	Dose = 60 mJ/cm <sup>2</sup> , HP = 35 nm	Dose = 63 mJ/cm <sup>2</sup> , HP = 35 nm
Design HP = 35 nm		
	Dose = 55 mJ/cm <sup>2</sup> , HP = 25 nm	Dose = 58 mJ/cm <sup>2</sup> , HP = 24 nm
Design HP = 25 nm		
	Dose = 62 mJ/cm <sup>2</sup> , HP = 20 nm	Dose = 65 mJ/cm <sup>2</sup> , HP = 19 nm
Design HP = 20 nm		

Figure S4. SEM images of EUV lithography patterns on photoresist 2 HP= 50, 35, 25, 20, 16 nm at different dose. Process parameter: 1.75 wt%, THK= 27.8 nm, Developer: Acetone:Hexane=6:1 , 10s , PEB= 110°C, 90 s.(dose = 55-73 mJ/cm<sup>2</sup>).

## 7. Spectral data of key compounds.



Cluster 1 was purified on recrystallization using DCM/hexane in low temperature. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 2.07 (s, 24H), 1.70-1.60 (m, 12H), 1.36-1.22 (m, 24H), 0.89(t, J=7.3, 18H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 182.9, 180.4, 179.6, 179.4, 27.6, 27.3, 27.0, 26.7, 26.5, 26.3, 26.1, 26.0, 24.2, 14.0, 13.8, 13.7, 13.6, 13.5, 13.5, 13.5; <sup>119</sup>Sn NMR (186.362 MHz, CDCl<sub>3</sub>): δ -521.27, -525.42, -557.05. HRMS (ESI<sup>+</sup>) m/z calculated for Sn<sub>6</sub>O<sub>20</sub>C<sub>40</sub>H<sub>78</sub>Cl<sub>2</sub>Na<sub>2</sub> [1/2M+Na]<sub>x2</sub>: 1713.8390, found: 1713.8438.

## 8. X-ray crystallographic structures and data.

### 1.1 X-ray structure of (1)

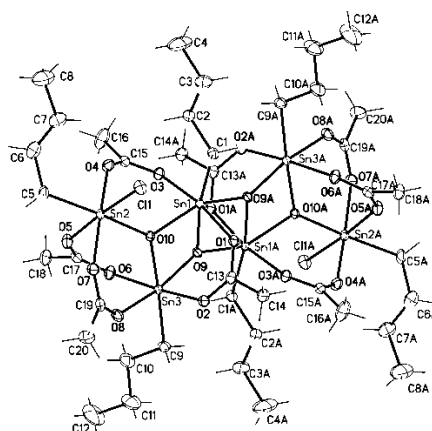
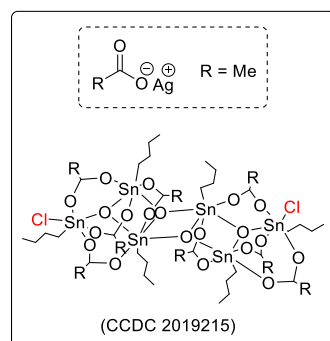


Table 1. Crystal data and structure refinement for 19080/LI\_UM.

Identification code	190807LT_0m	
Empirical formula	C <sub>20</sub> H <sub>39</sub> Cl O <sub>10</sub> Sn <sub>3</sub>	
Formula weight	831.03	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.5238(3) Å	α = 86.917(2)°.
	b = 12.4341(5) Å	β = 80.685(2)°.



	$c = 14.2811(6) \text{ \AA}$	$\gamma = 81.456(2)^\circ$ .
Volume	$1476.37(10) \text{ \AA}^3$	
Z	2	
Density (calculated)	$1.869 \text{ Mg/m}^3$	
Absorption coefficient	$2.653 \text{ mm}^{-1}$	
F(000)	812	
Crystal size	$0.10 \times 0.03 \times 0.03 \text{ mm}^3$	
Theta range for data collection	$1.657 \text{ to } 26.407^\circ$ .	
Index ranges	$-10 \leq h \leq 10, -15 \leq k \leq 15, -17 \leq l \leq 17$	
Reflections collected	19788	
Independent reflections	6033 [R(int) = 0.0266]	
Completeness to $\theta = 25.242^\circ$	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7454 and 0.6523	
Refinement method	Full-matrix least-squares on $F^2$	
Data / restraints / parameters	6033 / 0 / 314	
Goodness-of-fit on $F^2$	1.126	
Final R indices [ $I > 2\sigma(I)$ ]	R1 = 0.0210, wR2 = 0.0575	
R indices (all data)	R1 = 0.0240, wR2 = 0.0593	
Extinction coefficient	n/a	
Largest diff. peak and hole	$1.445 \text{ and } -0.582 \text{ e.\AA}^{-3}$	

Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 190807LT\_0M.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	U(eq)
Sn(1)	6396(1)	3815(1)	6663(1)	13(1)
Sn(2)	5278(1)	6309(1)	7987(1)	11(1)
Sn(3)	6091(1)	4138(1)	9241(1)	10(1)
Cl(1)	8994(1)	2935(1)	7004(1)	24(1)
O(1)	4055(2)	4714(2)	6411(1)	19(1)
O(2)	3152(2)	5934(2)	7539(1)	17(1)
O(3)	6207(2)	4707(2)	7809(1)	12(1)
O(4)	4706(2)	5642(2)	9318(1)	12(1)
O(5)	3990(2)	3440(2)	9053(1)	15(1)
O(6)	4888(3)	2801(2)	7592(1)	19(1)
O(7)	6317(2)	6603(2)	6528(1)	18(1)

O(8)	7534(3)	5057(2)	5832(1)	20(1)
O(9)	7563(2)	6521(2)	8342(1)	16(1)
O(10)	8100(2)	5014(2)	9251(1)	15(1)
C(1)	2965(3)	5362(2)	6874(2)	16(1)
C(2)	3850(3)	2935(2)	8336(2)	17(1)
C(3)	1301(4)	5463(3)	6619(2)	24(1)
C(4)	7263(4)	6083(2)	5882(2)	16(1)
C(5)	8135(4)	6724(3)	5099(2)	28(1)
C(6)	8380(3)	5929(2)	8895(2)	14(1)
C(7)	9808(3)	6358(3)	9140(2)	19(1)
C(8)	4394(4)	8001(2)	8077(2)	20(1)
C(9)	3031(4)	8376(3)	7503(3)	32(1)
C(10)	2462(5)	9588(3)	7531(3)	42(1)
C(11)	1105(6)	9930(4)	6948(4)	66(2)
C(12)	6357(4)	2942(3)	5427(2)	22(1)
C(13)	5958(5)	1801(3)	5538(3)	40(1)
C(14)	7108(6)	963(3)	5956(3)	46(1)
C(15)	6860(7)	-194(3)	5903(4)	67(2)
C(16)	2343(4)	2446(4)	8362(3)	41(1)
C(17)	7638(3)	2642(2)	9382(2)	15(1)
C(18)	7052(4)	1593(2)	9193(2)	18(1)
C(19)	8240(4)	595(3)	9383(3)	30(1)
C(20)	7671(6)	-459(3)	9192(4)	57(1)

Table 3. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for 190807LT\_0M.

Sn(1)-O(3)	1.9980(19)
Sn(1)-C(12)	2.129(3)
Sn(1)-O(8)	2.147(2)
Sn(1)-O(6)	2.179(2)
Sn(1)-O(1)	2.2101(19)
Sn(1)-Cl(1)	2.4317(8)
Sn(2)-O(3)	2.0454(19)
Sn(2)-O(4)	2.0464(18)
Sn(2)-C(8)	2.129(3)
Sn(2)-O(2)	2.138(2)
Sn(2)-O(9)	2.146(2)

Sn(2)-O(7)	2.1632(19)
Sn(2)-Sn(3)	3.2096(3)
Sn(3)-O(4)	2.0568(19)
Sn(3)-O(4)#1	2.0798(18)
Sn(3)-O(3)	2.1187(18)
Sn(3)-C(17)	2.135(3)
Sn(3)-O(5)	2.162(2)
Sn(3)-O(10)	2.165(2)
Sn(3)-Sn(3)#1	3.2815(4)
O(1)-C(1)	1.260(3)
O(2)-C(1)	1.261(4)
O(4)-Sn(3)#1	2.0798(18)
O(5)-C(2)	1.260(3)
O(6)-C(2)	1.270(4)
O(7)-C(4)	1.260(3)
O(8)-C(4)	1.266(4)
O(9)-C(6)	1.270(3)
O(10)-C(6)	1.260(3)
C(1)-C(3)	1.506(4)
C(2)-C(16)	1.495(4)
C(3)-H(1)	0.9800
C(3)-H(2)	0.9800
C(3)-H(3)	0.9800
C(4)-C(5)	1.500(4)
C(5)-H(5)	0.9800
C(5)-H(6)	0.9800
C(5)-H(4)	0.9800
C(6)-C(7)	1.496(4)
C(7)-H(8)	0.9800
C(7)-H(7)	0.9800
C(7)-H(9)	0.9800
C(8)-C(9)	1.531(5)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(10)	1.514(5)
C(9)-H(10)	0.9900
C(9)-H(16)	0.9900
C(10)-C(11)	1.530(6)

C(10)-H(15)	0.9900
C(10)-H(11)	0.9900
C(11)-H(12)	0.9800
C(11)-H(13)	0.9800
C(11)-H(14)	0.9800
C(12)-C(13)	1.501(5)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.491(5)
C(13)-H(17)	0.9900
C(13)-H(23)	0.9900
C(14)-C(15)	1.492(6)
C(14)-H(18)	0.9900
C(14)-H(19)	0.9900
C(15)-H(21)	0.9800
C(15)-H(20)	0.9800
C(15)-H(22)	0.9800
C(16)-H(24)	0.9800
C(16)-H(26)	0.9800
C(16)-H(25)	0.9800
C(17)-C(18)	1.516(4)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-C(19)	1.522(4)
C(18)-H(33)	0.9900
C(18)-H(27)	0.9900
C(19)-C(20)	1.515(5)
C(19)-H(31)	0.9900
C(19)-H(32)	0.9900
C(20)-H(28)	0.9800
C(20)-H(30)	0.9800
C(20)-H(29)	0.9800
O(3)-Sn(1)-C(12)	174.19(10)
O(3)-Sn(1)-O(8)	88.80(8)
C(12)-Sn(1)-O(8)	91.58(10)
O(3)-Sn(1)-O(6)	84.85(8)
C(12)-Sn(1)-O(6)	93.88(11)
O(8)-Sn(1)-O(6)	169.35(8)

O(3)-Sn(1)-O(1)	87.76(7)
C(12)-Sn(1)-O(1)	86.45(10)
O(8)-Sn(1)-O(1)	88.23(8)
O(6)-Sn(1)-O(1)	83.00(8)
O(3)-Sn(1)-Cl(1)	88.52(6)
C(12)-Sn(1)-Cl(1)	97.28(9)
O(8)-Sn(1)-Cl(1)	90.08(6)
O(6)-Sn(1)-Cl(1)	98.28(6)
O(1)-Sn(1)-Cl(1)	175.95(6)
O(3)-Sn(2)-O(4)	77.56(7)
O(3)-Sn(2)-C(8)	176.04(10)
O(4)-Sn(2)-C(8)	106.34(10)
O(3)-Sn(2)-O(2)	87.30(8)
O(4)-Sn(2)-O(2)	92.81(8)
C(8)-Sn(2)-O(2)	93.10(10)
O(3)-Sn(2)-O(9)	86.46(8)
O(4)-Sn(2)-O(9)	88.69(7)
C(8)-Sn(2)-O(9)	92.92(10)
O(2)-Sn(2)-O(9)	173.12(8)
O(3)-Sn(2)-O(7)	87.43(7)
O(4)-Sn(2)-O(7)	164.45(8)
C(8)-Sn(2)-O(7)	88.63(10)
O(2)-Sn(2)-O(7)	90.52(8)
O(9)-Sn(2)-O(7)	86.29(8)
O(3)-Sn(2)-Sn(3)	40.42(5)
O(4)-Sn(2)-Sn(3)	38.65(5)
C(8)-Sn(2)-Sn(3)	143.22(8)
O(2)-Sn(2)-Sn(3)	98.48(5)
O(9)-Sn(2)-Sn(3)	78.56(5)
O(7)-Sn(2)-Sn(3)	125.80(5)
O(4)-Sn(3)-O(4)#1	75.01(8)
O(4)-Sn(3)-O(3)	75.71(7)
O(4)#1-Sn(3)-O(3)	150.72(7)
O(4)-Sn(3)-C(17)	170.30(9)
O(4)#1-Sn(3)-C(17)	96.89(9)
O(3)-Sn(3)-C(17)	112.18(9)
O(4)-Sn(3)-O(5)	88.68(8)
O(4)#1-Sn(3)-O(5)	92.89(7)

O(3)-Sn(3)-O(5)	87.12(7)
C(17)-Sn(3)-O(5)	97.16(10)
O(4)-Sn(3)-O(10)	85.63(7)
O(4)#1-Sn(3)-O(10)	92.36(7)
O(3)-Sn(3)-O(10)	84.72(7)
C(17)-Sn(3)-O(10)	89.45(9)
O(5)-Sn(3)-O(10)	171.00(7)
O(4)-Sn(3)-Sn(2)	38.42(5)
O(4)#1-Sn(3)-Sn(2)	112.35(5)
O(3)-Sn(3)-Sn(2)	38.75(5)
C(17)-Sn(3)-Sn(2)	147.43(8)
O(5)-Sn(3)-Sn(2)	95.44(5)
O(10)-Sn(3)-Sn(2)	75.80(5)
O(4)-Sn(3)-Sn(3)#1	37.75(5)
O(4)#1-Sn(3)-Sn(3)#1	37.26(5)
O(3)-Sn(3)-Sn(3)#1	113.46(5)
C(17)-Sn(3)-Sn(3)#1	133.93(8)
O(5)-Sn(3)-Sn(3)#1	91.01(5)
O(10)-Sn(3)-Sn(3)#1	88.76(5)
Sn(2)-Sn(3)-Sn(3)#1	75.520(8)
C(1)-O(1)-Sn(1)	135.59(18)
C(1)-O(2)-Sn(2)	131.19(18)
Sn(1)-O(3)-Sn(2)	128.58(9)
Sn(1)-O(3)-Sn(3)	127.19(9)
Sn(2)-O(3)-Sn(3)	100.83(8)
Sn(2)-O(4)-Sn(3)	102.93(8)
Sn(2)-O(4)-Sn(3)#1	148.92(10)
Sn(3)-O(4)-Sn(3)#1	104.99(8)
C(2)-O(5)-Sn(3)	125.33(18)
C(2)-O(6)-Sn(1)	136.26(19)
C(4)-O(7)-Sn(2)	137.48(19)
C(4)-O(8)-Sn(1)	130.71(19)
C(6)-O(9)-Sn(2)	127.89(18)
C(6)-O(10)-Sn(3)	131.27(18)
O(1)-C(1)-O(2)	125.2(3)
O(1)-C(1)-C(3)	117.8(3)
O(2)-C(1)-C(3)	117.1(3)
O(5)-C(2)-O(6)	125.4(3)

O(5)-C(2)-C(16)	117.6(3)
O(6)-C(2)-C(16)	117.0(3)
C(1)-C(3)-H(1)	109.5
C(1)-C(3)-H(2)	109.5
H(1)-C(3)-H(2)	109.5
C(1)-C(3)-H(3)	109.5
H(1)-C(3)-H(3)	109.5
H(2)-C(3)-H(3)	109.5
O(7)-C(4)-O(8)	125.4(3)
O(7)-C(4)-C(5)	117.8(3)
O(8)-C(4)-C(5)	116.8(3)
C(4)-C(5)-H(5)	109.5
C(4)-C(5)-H(6)	109.5
H(5)-C(5)-H(6)	109.5
C(4)-C(5)-H(4)	109.5
H(5)-C(5)-H(4)	109.5
H(6)-C(5)-H(4)	109.5
O(10)-C(6)-O(9)	126.0(3)
O(10)-C(6)-C(7)	117.3(2)
O(9)-C(6)-C(7)	116.8(3)
C(6)-C(7)-H(8)	109.5
C(6)-C(7)-H(7)	109.5
H(8)-C(7)-H(7)	109.5
C(6)-C(7)-H(9)	109.5
H(8)-C(7)-H(9)	109.5
H(7)-C(7)-H(9)	109.5
C(9)-C(8)-Sn(2)	113.9(2)
C(9)-C(8)-H(8A)	108.8
Sn(2)-C(8)-H(8A)	108.8
C(9)-C(8)-H(8B)	108.8
Sn(2)-C(8)-H(8B)	108.8
H(8A)-C(8)-H(8B)	107.7
C(10)-C(9)-C(8)	113.7(3)
C(10)-C(9)-H(10)	108.8
C(8)-C(9)-H(10)	108.8
C(10)-C(9)-H(16)	108.8
C(8)-C(9)-H(16)	108.8
H(10)-C(9)-H(16)	107.7

C(9)-C(10)-C(11)	112.1(4)
C(9)-C(10)-H(15)	109.2
C(11)-C(10)-H(15)	109.2
C(9)-C(10)-H(11)	109.2
C(11)-C(10)-H(11)	109.2
H(15)-C(10)-H(11)	107.9
C(10)-C(11)-H(12)	109.5
C(10)-C(11)-H(13)	109.5
H(12)-C(11)-H(13)	109.5
C(10)-C(11)-H(14)	109.5
H(12)-C(11)-H(14)	109.5
H(13)-C(11)-H(14)	109.5
C(13)-C(12)-Sn(1)	119.1(2)
C(13)-C(12)-H(12A)	107.5
Sn(1)-C(12)-H(12A)	107.5
C(13)-C(12)-H(12B)	107.5
Sn(1)-C(12)-H(12B)	107.5
H(12A)-C(12)-H(12B)	107.0
C(14)-C(13)-C(12)	117.2(3)
C(14)-C(13)-H(17)	108.0
C(12)-C(13)-H(17)	108.0
C(14)-C(13)-H(23)	108.0
C(12)-C(13)-H(23)	108.0
H(17)-C(13)-H(23)	107.2
C(13)-C(14)-C(15)	116.6(4)
C(13)-C(14)-H(18)	108.1
C(15)-C(14)-H(18)	108.1
C(13)-C(14)-H(19)	108.1
C(15)-C(14)-H(19)	108.1
H(18)-C(14)-H(19)	107.3
C(14)-C(15)-H(21)	109.5
C(14)-C(15)-H(20)	109.5
H(21)-C(15)-H(20)	109.5
C(14)-C(15)-H(22)	109.5
H(21)-C(15)-H(22)	109.5
H(20)-C(15)-H(22)	109.5
C(2)-C(16)-H(24)	109.5
C(2)-C(16)-H(26)	109.5



H(24)-C(16)-H(26)	109.5
C(2)-C(16)-H(25)	109.5
H(24)-C(16)-H(25)	109.5
H(26)-C(16)-H(25)	109.5
C(18)-C(17)-Sn(3)	118.30(19)
C(18)-C(17)-H(17A)	107.7
Sn(3)-C(17)-H(17A)	107.7
C(18)-C(17)-H(17B)	107.7
Sn(3)-C(17)-H(17B)	107.7
H(17A)-C(17)-H(17B)	107.1
C(17)-C(18)-C(19)	112.1(3)
C(17)-C(18)-H(33)	109.2
C(19)-C(18)-H(33)	109.2
C(17)-C(18)-H(27)	109.2
C(19)-C(18)-H(27)	109.2
H(33)-C(18)-H(27)	107.9
C(20)-C(19)-C(18)	112.6(3)
C(20)-C(19)-H(31)	109.1
C(18)-C(19)-H(31)	109.1
C(20)-C(19)-H(32)	109.1
C(18)-C(19)-H(32)	109.1
H(31)-C(19)-H(32)	107.8
C(19)-C(20)-H(28)	109.5
C(19)-C(20)-H(30)	109.5
H(28)-C(20)-H(30)	109.5
C(19)-C(20)-H(29)	109.5
H(28)-C(20)-H(29)	109.5
H(30)-C(20)-H(29)	109.5

---

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+2

Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 190807LT\_0M. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

---

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
Sn(1)	14(1)	14(1)	9(1)	-2(1)	-2(1)	-1(1)

---

Sn(2)	12(1)	12(1)	9(1)	0(1)	-2(1)	-1(1)
Sn(3)	10(1)	12(1)	9(1)	-1(1)	-2(1)	-1(1)
Cl(1)	20(1)	29(1)	21(1)	-2(1)	-3(1)	2(1)
O(1)	19(1)	22(1)	17(1)	-7(1)	-7(1)	4(1)
O(2)	13(1)	22(1)	16(1)	-5(1)	-5(1)	0(1)
O(3)	14(1)	13(1)	9(1)	-1(1)	-3(1)	-1(1)
O(4)	15(1)	12(1)	8(1)	-1(1)	-2(1)	0(1)
O(5)	14(1)	16(1)	15(1)	-3(1)	-1(1)	-4(1)
O(6)	24(1)	18(1)	16(1)	-3(1)	-1(1)	-6(1)
O(7)	22(1)	20(1)	11(1)	-1(1)	0(1)	0(1)
O(8)	23(1)	22(1)	14(1)	-2(1)	0(1)	-3(1)
O(9)	17(1)	17(1)	16(1)	2(1)	-6(1)	-3(1)
O(10)	14(1)	15(1)	16(1)	0(1)	-3(1)	-2(1)
C(1)	16(2)	20(2)	12(1)	4(1)	-3(1)	-3(1)
C(2)	17(2)	17(2)	18(2)	1(1)	-5(1)	-5(1)
C(3)	17(2)	30(2)	22(2)	-7(1)	-6(1)	2(1)
C(4)	18(2)	19(2)	13(1)	2(1)	-5(1)	-3(1)
C(5)	33(2)	24(2)	23(2)	0(1)	8(1)	-5(2)
C(6)	13(1)	17(2)	11(1)	-4(1)	1(1)	-1(1)
C(7)	15(2)	22(2)	20(2)	1(1)	-4(1)	-6(1)
C(8)	24(2)	15(2)	17(2)	-2(1)	-1(1)	0(1)
C(9)	31(2)	22(2)	43(2)	2(2)	-11(2)	6(2)
C(10)	47(2)	29(2)	43(2)	6(2)	-4(2)	10(2)
C(11)	66(3)	54(3)	71(3)	5(2)	-22(3)	32(3)
C(12)	31(2)	20(2)	16(2)	-6(1)	-7(1)	0(1)
C(13)	58(3)	37(2)	28(2)	-9(2)	-10(2)	-11(2)
C(14)	70(3)	26(2)	44(2)	-8(2)	-19(2)	0(2)
C(15)	110(5)	26(2)	65(3)	1(2)	-12(3)	-10(3)
C(16)	30(2)	61(3)	36(2)	-19(2)	2(2)	-26(2)
C(17)	14(1)	15(2)	14(1)	0(1)	-3(1)	-1(1)
C(18)	19(2)	17(2)	19(2)	-2(1)	-5(1)	0(1)
C(19)	31(2)	18(2)	38(2)	-1(1)	-6(2)	4(1)
C(20)	60(3)	16(2)	94(4)	-6(2)	-12(3)	0(2)

---

Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^{-3}$ ) for 190807LT\_0M.

---

	x	y	z	U(eq)
H(1)	1372	5453	5928	35
H(2)	677	6150	6852	35
H(3)	772	4853	6912	35
H(5)	7574	6783	4547	42
H(6)	9234	6355	4921	42
H(4)	8166	7454	5316	42
H(8)	9872	7081	8841	28
H(7)	10786	5865	8908	28
H(9)	9700	6408	9830	28
H(8A)	4007	8172	8751	23
H(8B)	5292	8419	7849	23
H(10)	3401	8173	6834	39
H(16)	2112	7985	7752	39
H(15)	3376	9983	7280	50
H(11)	2083	9795	8198	50
H(12)	1506	9793	6277	100
H(13)	716	10708	7025	100
H(14)	223	9510	7169	100
H(12A)	5574	3374	5062	27
H(12B)	7427	2916	5030	27
H(17)	4892	1820	5939	48
H(23)	5854	1560	4904	48
H(18)	7056	1126	6633	55
H(19)	8206	1038	5633	55
H(21)	5824	-304	6278	101
H(20)	7724	-672	6156	101
H(22)	6869	-365	5240	101
H(24)	2370	2097	7759	61
H(26)	1414	3018	8461	61
H(25)	2256	1902	8884	61
H(17A)	8657	2687	8947	18
H(17B)	7894	2586	10037	18
H(33)	6878	1604	8524	22
H(27)	6009	1544	9603	22
H(31)	9284	647	8976	36

H(32)	8410	584	10053	36
H(28)	7560	-472	8521	86
H(30)	6630	-511	9587	86
H(29)	8456	-1075	9346	86

---

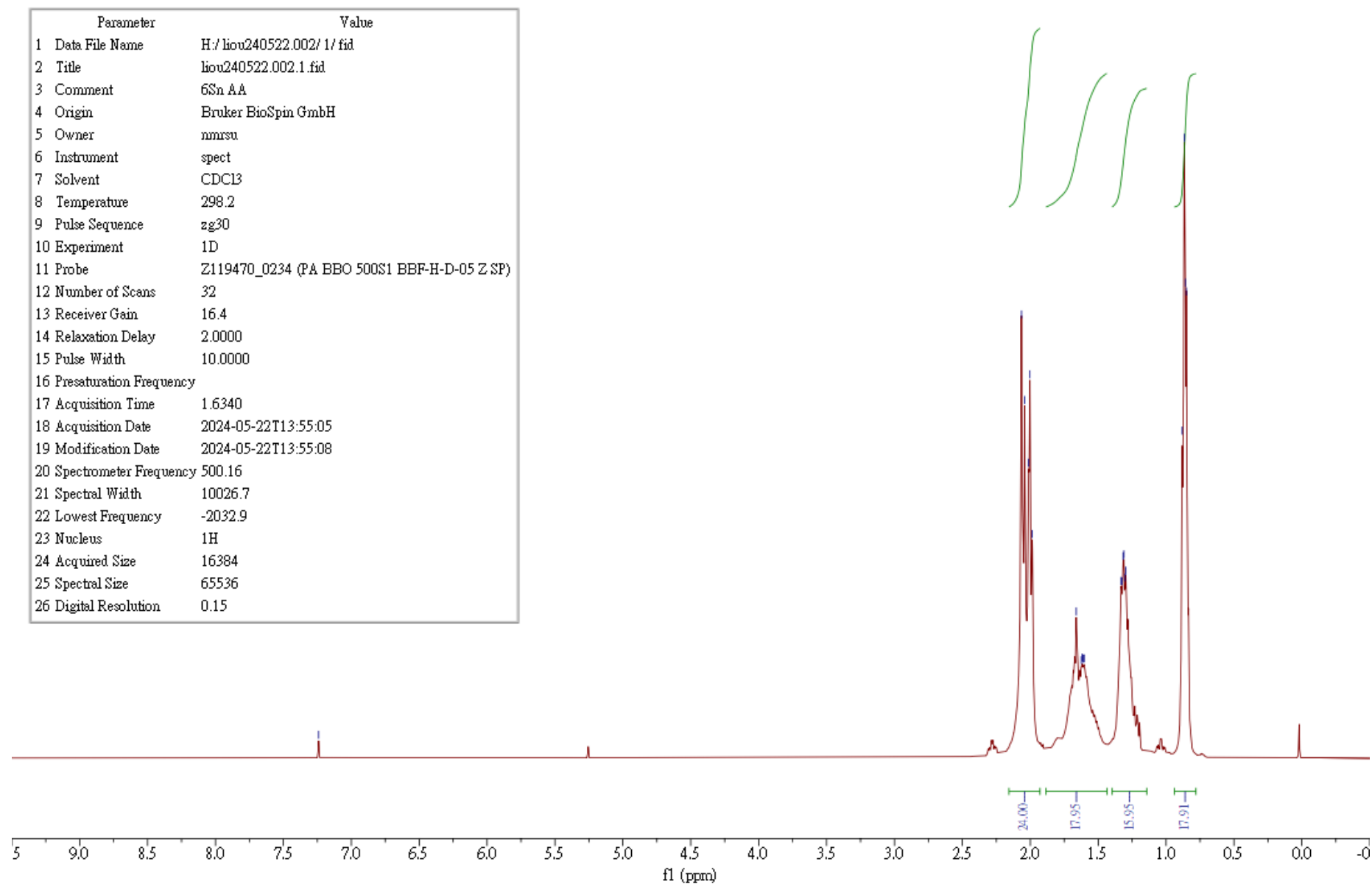


Figure S5. <sup>1</sup>H NMR of cluster 1

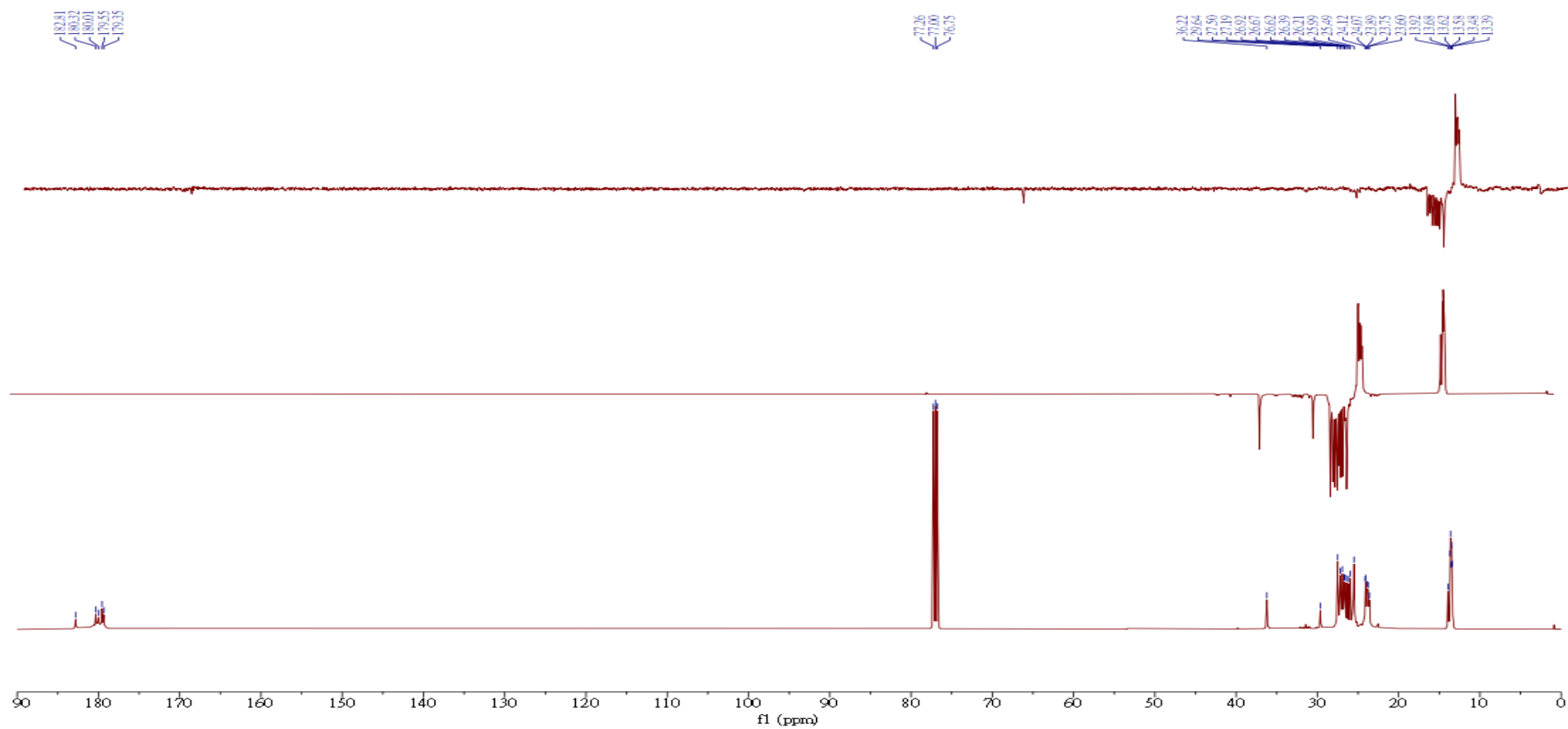


Figure S6. <sup>13</sup>C NMR of cluster 1

-484.85  
-521.07  
-525.33  
-556.89

Parameter	Value
1 Data File Name	H:/liou240522.002/ 5/ fid
2 Title	liou240522.002.5.fid
3 Comment	6Sn AA
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Instrument	spect
7 Solvent	CDCl3
8 Temperature	298.9
9 Pulse Sequence	zgpg
10 Experiment	1D
11 Probe	Z119470_0234 (PA BBO 500S1 BBF-H-D-05 Z SP)
12 Number of Scans	2048
13 Receiver Gain	191.0
14 Relaxation Delay	2.0000
15 Pulse Width	15.0000
16 Presaturation Frequency	
17 Acquisition Time	0.0437
18 Acquisition Date	2024-05-23T06:57:37
19 Modification Date	2024-05-23T06:57:38
20 Spectrometer Frequency	186.51
21 Spectral Width	750000.0
22 Lowest Frequency	-374978.9
23 Nucleus	$^{119}\text{Sn}$
24 Acquired Size	32768
25 Spectral Size	65536
26 Digital Resolution	11.44

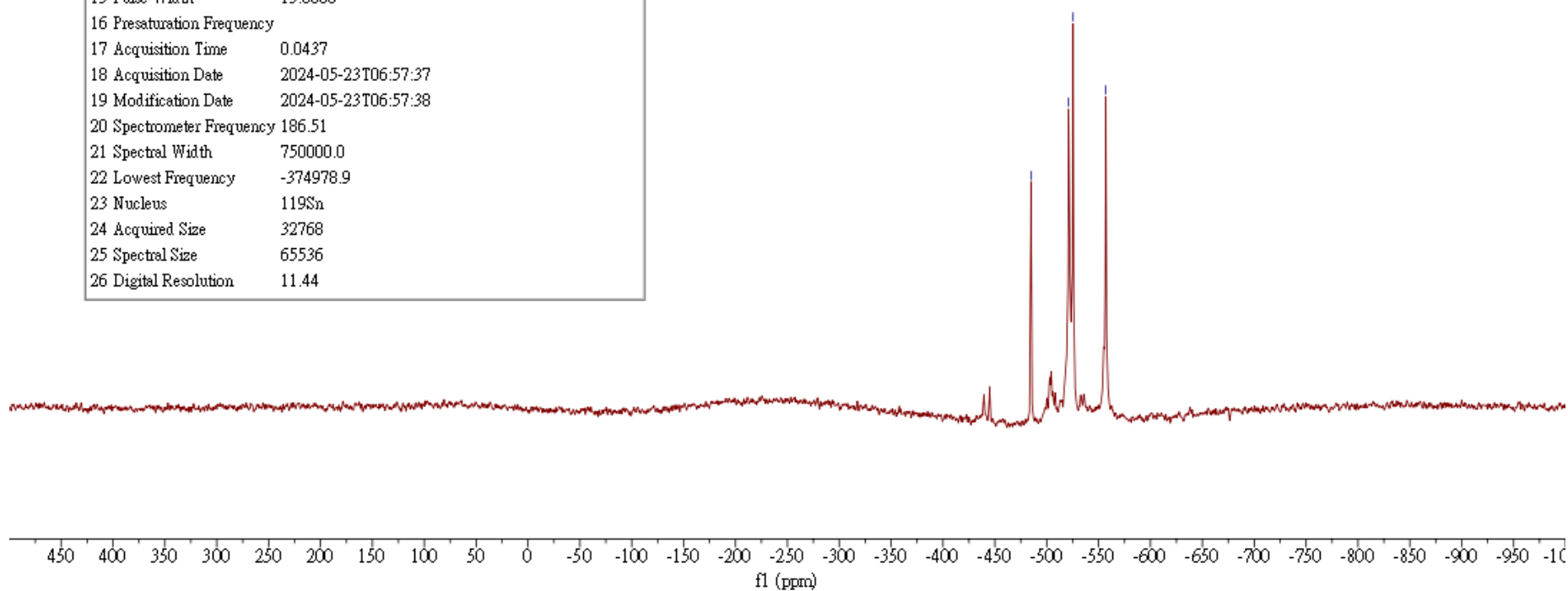


Figure S7.  $^{119}\text{Sn}$  NMR of cluster 1

sample 3.1.fid

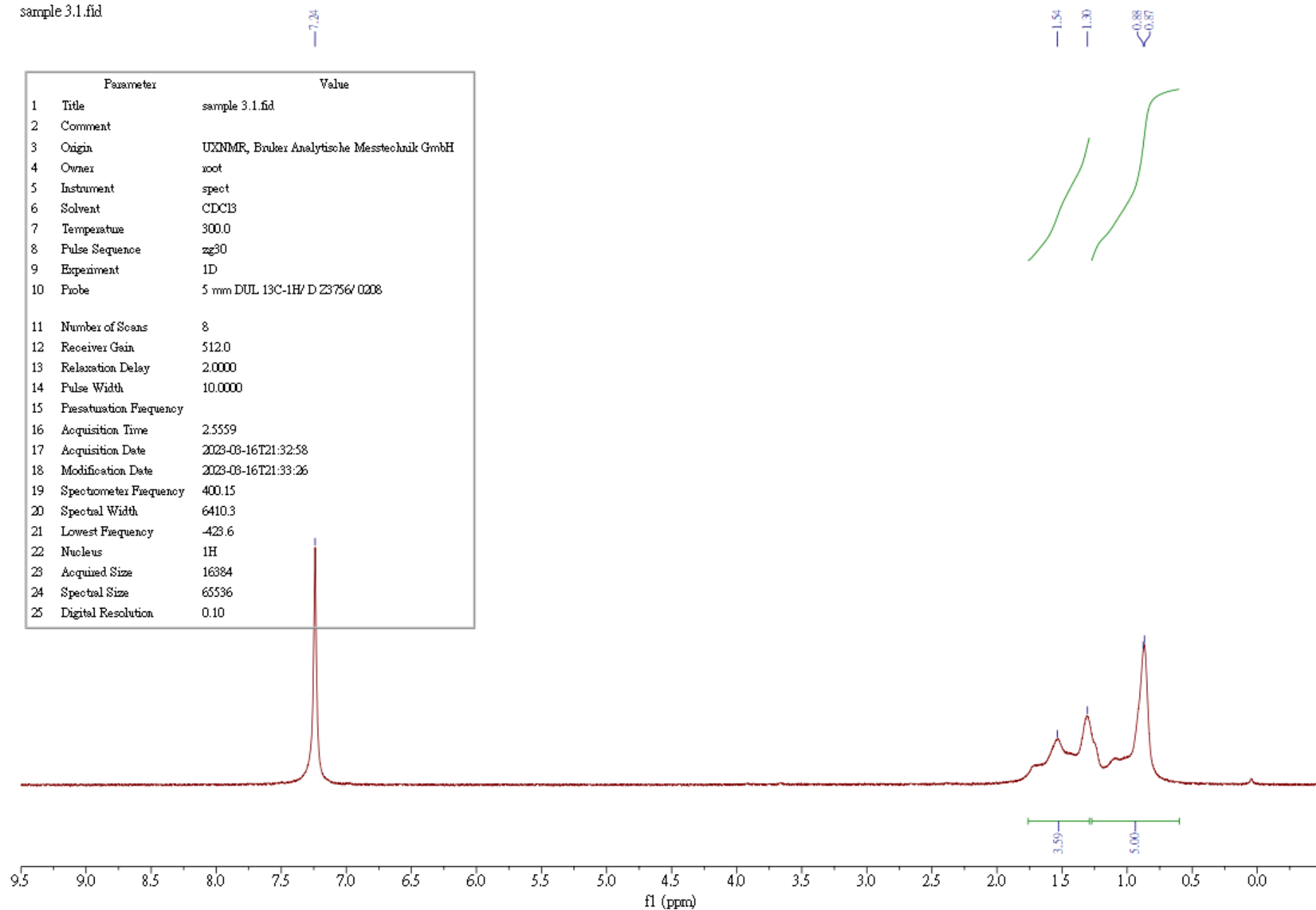


Figure S8. <sup>1</sup>H NMR of cluster 2



liou240522.001.4.fid  
6Sn OH

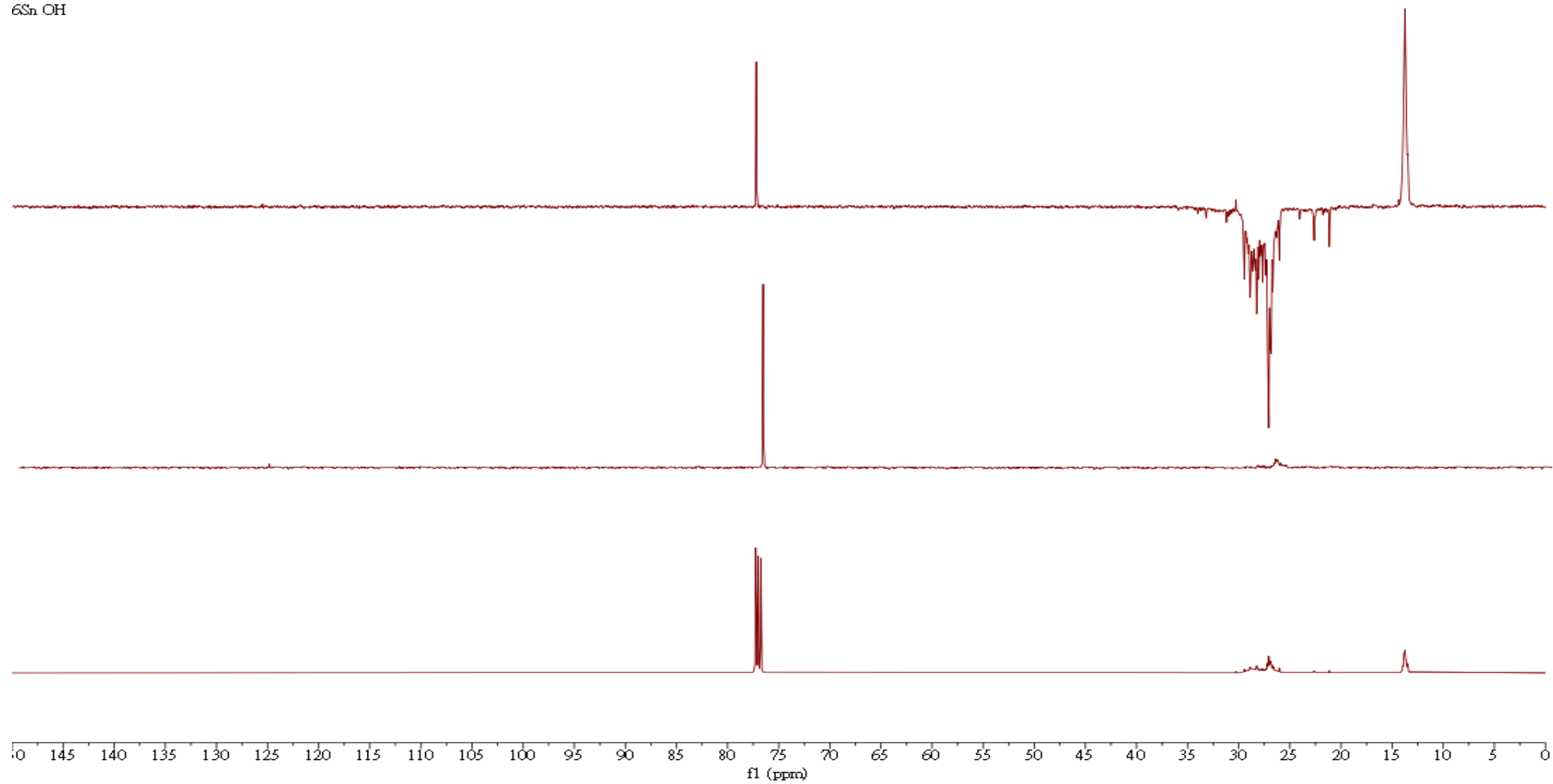


Figure S9.  $^{13}\text{C}$  NMR of cluster 2

451.10  
465.08  
469.89  
485.57

Parameter	Value
1 Title	liou230921.001.2.fid
2 Comment	Jeff-06
3 Origin	Bruker BioSpin GmbH
4 Owner	nmrsu
5 Instrument	spect
6 Solvent	CDCl3
7 Temperature	233.1
8 Pulse Sequence	zgpg
9 Experiment	1D
10 Probe	Z119470_0234 (PA BBO 500S1 BBF-H-D-05 Z SP)
11 Number of Scans	4096
12 Receiver Gain	191.0
13 Relaxation Delay	2.0000
14 Pulse Width	15.0000
15 Presaturation Frequency	
16 Acquisition Time	0.0437
17 Acquisition Date	2023-09-21 T11:38:49
18 Modification Date	2023-09-21 T11:38:50
19 Spectrometer Frequency	186.51
20 Spectral Width	750000.0
21 Lowest Frequency	-374978.8
22 Nucleus	119Sn
23 Acquired Size	32768
24 Spectral Size	65536
25 Digital Resolution	11.44

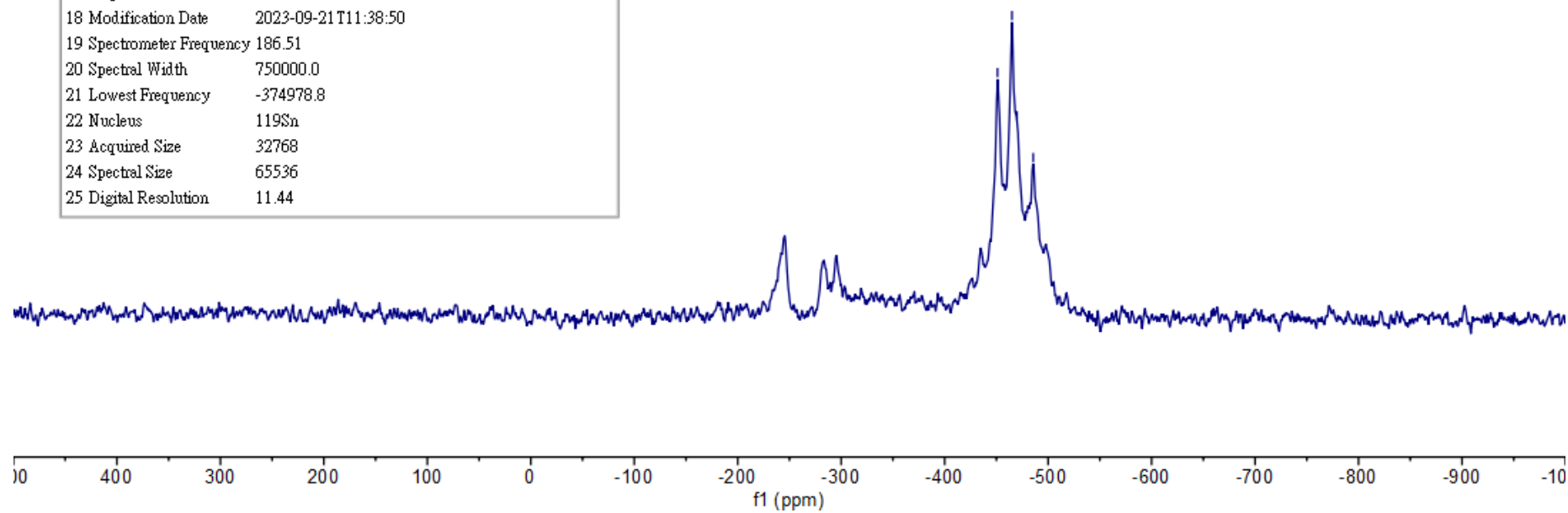


Figure S10. <sup>119</sup>Sn NMR of cluster 2