

## Supporting Information for the Communication Entitled “Synthesis and Structure of Pentaorganostannate Having Five Carbon Substituents”

Masaichi Saito,<sup>\*,†</sup> Sanae Imaizumi,<sup>†</sup> Tomoyuki Tajima,<sup>†</sup> Kazuya Ishimura<sup>§</sup> and Shigeru Nagase<sup>§</sup>

<sup>†</sup>*Department of Chemistry, Graduate School of Science and Engineering, Saitama University*

<sup>§</sup>*Department of Theoretical Molecular Science, Institute for Molecular Science, Myodaiji, Okazaki, Aichi, 444-8585 Japan*

*E-mail: masaichi@chem.saitama-u.ac.jp*

### Experimental

**Reaction of spirostannabifluorene **3** with methyllithium.** A THF (1 mL) solution of spirostannabifluorene **3** (52 mg, 0.12 mmol) was treated with methyllithium (0.13 mL; 0.98 N in diethyl ether, 0.13 mmol) at  $-78$  °C. When a dichloromethane (0.5 mL) solution of tetrabutylammonium bromide (55 mg, 0.17 mmol) was added to the resulting solution at the same temperature, precipitates were formed. After being warmed to room temperature, precipitates were filtered off and washed with methanol to give 9-(2-biphenyl)-9-methyl-9-stannafluorene (**5**) (48 mg, 88%). **5**: mp 132-132 °C (dichloromethane+methanol). <sup>1</sup>H NMR(400 MHz, CDCl<sub>3</sub>) δ 0.11 (s,  $J(\text{Sn-H}) = 61, 63$  Hz, 3H), 7.26-7.33 (m, 3H), 7.37-7.46 (m, 6H), 7.49-7.62 (m, 6H), 7.93-7.98 (m, 2H); <sup>13</sup>C NMR(101 MHz, CDCl<sub>3</sub>) δ  $-8.03$  (q,  $J(\text{Sn-C}) = 381, 400$  Hz), 122.63 (d,  $J(\text{Sn-C}) = 40$  Hz), 126.94 (d,  $J(\text{Sn-C}) = 51$  Hz), 127.59 (d,  $J(\text{Sn-C}) = 43$  Hz), 127.62 (d), 128.59 (d), 128.71 (d), 128.83 (d), 129.10 (d,  $J(\text{Sn-C}) = 11$  Hz), 129.28 (d,  $J(\text{Sn-C}) = 9$  Hz), 136.14 (d,  $J(\text{Sn-C}) = 42$  Hz), 137.19 (d,  $J(\text{Sn-C}) = 40$  Hz), 140.48 (s), 140.50 (s), 145.,75 (s), 148.21 (s,  $J(\text{Sn-C}) = 67$  Hz), 149.84 (s); <sup>119</sup>Sn NMR(149 MHz, CDCl<sub>3</sub>) δ  $-105.93$ . Anal. Calcd for C<sub>25</sub>H<sub>20</sub>Sn: C, 68.37; H, 4.59. Found: C, 68.10; H, 4.43.

### Full authors list of ref. 20.

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Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

#### **X-ray Crystallographic Analysis of Lithium Pentamethylstannate 4.**

**Table 1.** Crystal data and structure refinement for lithium pentamethylstannate 4.

Empirical formula	$C_{37} H_{33} Li O_6 Sn$	
Formula weight	699.26	
Temperature	93(2) K	
Wavelength	0.71069 Å	
Crystal system	monoclinic	
Space group	$C2/c$	
Unit cell dimensions	$a = 11.5850(10)$ Å	$\alpha = 90^\circ$ .
	$b = 20.8836(17)$ Å	$\beta = 102.415(2)^\circ$ .
	$c = 15.2368(12)$ Å	$\gamma = 90^\circ$ .
Volume	$3600.1(5)$ Å <sup>3</sup>	
Z	4	
Density (calculated)	1.290 Mg/m <sup>3</sup>	
Absorption coefficient	0.750 mm <sup>-1</sup>	
F(000)	1424	
Crystal size	0.50 x 0.20 x 0.20 mm <sup>3</sup>	
Theta range for data collection	2.05 to 25.10°.	
Index ranges	-9<=h<=13, -24<=k<=23, -18<=l<=18	
Reflections collected	10560	
Independent reflections	3206 [R(int) = 0.0310]	

Completeness to $\theta = 25.10^\circ$	99.9%
Max. and min. transmission	0.8644 and 0.7054
Refinement method	Full-matrix least-squares on $F^2$
Data / restraints / parameters	3206 / 1 / 251
Goodness-of-fit on $F^2$	1.115
Final R indices [ $I > 2\sigma(I)$ ]	$R_1 = 0.0670$ , $wR_2 = 0.1390$
R indices (all data)	$R_1 = 0.0789$ , $wR_2 = 0.1472$
Largest diff. peak and hole	1.773 and -2.226 e. $\text{\AA}^{-3}$

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

	x	y	z	U(eq)
Sn(1)	0	1184(1)	2500	57(1)
C(1)	0	138(5)	2500	92(4)
C(2)	644(5)	1294(3)	1204(4)	55(2)
C(3)	179(5)	1058(4)	352(5)	70(2)
C(4)	706(6)	1164(4)	-367(5)	70(2)
C(5)	1748(6)	1516(3)	-243(5)	62(2)
C(6)	2243(5)	1747(3)	602(4)	54(2)
C(7)	1709(4)	1636(2)	1327(4)	43(1)
C(8)	1678(4)	1697(3)	2953(4)	46(1)
C(9)	2240(4)	1859(2)	2254(4)	42(1)
C(10)	3270(6)	2218(3)	2462(5)	67(2)
C(11)	3739(6)	2411(3)	3335(5)	75(2)
C(12)	3210(5)	2245(3)	4015(5)	54(2)
C(13)	2177(5)	1892(3)	3820(4)	48(1)
Li(1)	0	4439(5)	2500	43(3)
C(14)	1200(8)	5395(5)	1310(6)	100(3)
O(1)	123(6)	5098(3)	1431(6)	54(2)
C(15)	-950(8)	5451(4)	1217(7)	56(3)
C(16)	-2025(6)	4945(4)	1047(5)	78(2)
O(2)	-1765(6)	4581(3)	1884(5)	45(2)
C(17)	-2619(6)	4091(4)	1863(6)	71(2)
C(18)	-219(8)	3572(6)	4125(9)	156(6)
O(3)	-344(8)	3646(4)	3291(7)	48(2)
C(19)	133(7)	3073(4)	3005(6)	52(3)
C(20)	92(19)	5835(11)	2141(12)	180(30)

O(4)	655(16)	5228(6)	1911(11)	59(4)
O(5)	-1646(12)	4343(7)	1508(10)	47(3)
C(22)	-1947(16)	3550(9)	2530(11)	57(5)
O(6)	-885(13)	3770(8)	3131(10)	43(3)

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**Table 3.** Bond lengths [Å] and angles [°] for lithium pentamethylstannane **4**.

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Sn(1)-C(1)	2.186(11)
Sn(1)-C(8)	2.196(5)
Sn(1)-C(8)#1	2.196(5)
Sn(1)-C(2)#1	2.268(7)
Sn(1)-C(2)	2.268(7)
C(1)-H(1)	0.9800
C(1)-H(2)	0.9800
C(1)-H(3)	0.9800
C(2)-C(3)	1.385(9)
C(2)-C(7)	1.402(8)
C(3)-C(4)	1.381(10)
C(3)-H(4)	0.9500
C(4)-C(5)	1.391(9)
C(4)-H(5)	0.9500
C(5)-C(6)	1.379(9)
C(5)-H(6)	0.9500
C(6)-C(7)	1.397(8)
C(6)-H(7)	0.9500
C(7)-C(9)	1.489(8)
C(8)-C(13)	1.384(8)
C(8)-C(9)	1.404(8)
C(9)-C(10)	1.387(8)
C(10)-C(11)	1.384(10)
C(10)-H(8)	0.9500
C(11)-C(12)	1.358(10)
C(11)-H(9)	0.9500
C(12)-C(13)	1.382(8)
C(12)-H(10)	0.9500
C(13)-H(11)	0.9500
Li(1)-O(2)#1	2.079(6)
Li(1)-O(2)	2.079(6)

Li(1)-O(6)	2.085(17)
Li(1)-O(6)#1	2.085(17)
Li(1)-O(4)	2.096(16)
Li(1)-O(4)#1	2.096(16)
Li(1)-O(3)	2.135(12)
Li(1)-O(3)#1	2.135(12)
Li(1)-O(1)#1	2.160(10)
Li(1)-O(1)	2.160(10)
Li(1)-O(5)#1	2.173(13)
Li(1)-O(5)	2.173(13)
C(14)-O(4)	1.267(16)
C(14)-O(1)	1.440(10)
O(1)-C(15)	1.421(11)
C(15)-C(16)	1.611(12)
C(15)-H(18)	0.9900
C(15)-H(19)	0.9900
C(16)-O(2)	1.460(10)
C(16)-O(5)	1.461(15)
O(2)-C(17)	1.419(9)
C(17)-O(5)	1.449(16)
C(17)-C(22)	1.60(2)
C(18)-O(3)	1.256(14)
C(18)-O(6)	1.598(18)
C(18)-H(12)	0.9800
C(18)-H(13)	0.9800
C(18)-H(14)	0.9800
C(18)-H(15)	0.9800
C(18)-H(16)	0.9800
C(18)-H(17)	0.9800
O(3)-C(19)	1.425(12)
C(19)-C(19)#1	1.503(19)
C(19)-H(24)	0.9900
C(19)-H(25)	0.9900

C(20)-C(20)#1	1.16(4)
C(20)-O(4)	1.50(2)
C(20)-H(22)	0.9900
C(20)-H(23)	0.9900
C(22)-O(6)	1.44(2)
C(22)-H(20)	0.9900
C(22)-H(21)	0.9900
C(1)-Sn(1)-C(8)	119.15(13)
C(1)-Sn(1)-C(8)#1	119.15(13)
C(8)-Sn(1)-C(8)#1	121.7(3)
C(1)-Sn(1)-C(2)#1	95.79(16)
C(8)-Sn(1)-C(2)#1	96.4(2)
C(8)#1-Sn(1)-C(2)#1	77.8(2)
C(1)-Sn(1)-C(2)	95.79(16)
C(8)-Sn(1)-C(2)	77.8(2)
C(8)#1-Sn(1)-C(2)	96.4(2)
C(2)#1-Sn(1)-C(2)	168.4(3)
Sn(1)-C(1)-H(1)	109.5
Sn(1)-C(1)-H(2)	109.5
H(1)-C(1)-H(2)	109.5
Sn(1)-C(1)-H(3)	109.5
H(1)-C(1)-H(3)	109.5
H(2)-C(1)-H(3)	109.5
C(3)-C(2)-C(7)	117.4(6)
C(3)-C(2)-Sn(1)	130.2(5)
C(7)-C(2)-Sn(1)	112.3(4)
C(4)-C(3)-C(2)	122.5(6)
C(4)-C(3)-H(4)	118.8
C(2)-C(3)-H(4)	118.8
C(3)-C(4)-C(5)	119.8(6)
C(3)-C(4)-H(5)	120.1
C(5)-C(4)-H(5)	120.1



C(6)-C(5)-C(4)	119.1(7)
C(6)-C(5)-H(6)	120.5
C(4)-C(5)-H(6)	120.5
C(5)-C(6)-C(7)	120.9(6)
C(5)-C(6)-H(7)	119.5
C(7)-C(6)-H(7)	119.5
C(6)-C(7)-C(2)	120.4(6)
C(6)-C(7)-C(9)	122.3(5)
C(2)-C(7)-C(9)	117.3(5)
C(13)-C(8)-C(9)	119.1(5)
C(13)-C(8)-Sn(1)	127.1(5)
C(9)-C(8)-Sn(1)	113.8(4)
C(10)-C(9)-C(8)	118.3(6)
C(10)-C(9)-C(7)	123.1(6)
C(8)-C(9)-C(7)	118.6(5)
C(11)-C(10)-C(9)	121.1(7)
C(11)-C(10)-H(8)	119.4
C(9)-C(10)-H(8)	119.4
C(12)-C(11)-C(10)	120.7(6)
C(12)-C(11)-H(9)	119.6
C(10)-C(11)-H(9)	119.6
C(11)-C(12)-C(13)	118.9(6)
C(11)-C(12)-H(10)	120.5
C(13)-C(12)-H(10)	120.5
C(12)-C(13)-C(8)	121.8(6)
C(12)-C(13)-H(11)	119.1
C(8)-C(13)-H(11)	119.1
O(2)#1-Li(1)-O(2)	163.6(7)
O(2)#1-Li(1)-O(6)	114.9(5)
O(2)-Li(1)-O(6)	76.7(5)
O(2)#1-Li(1)-O(6)#1	76.7(5)
O(2)-Li(1)-O(6)#1	114.9(5)
O(6)-Li(1)-O(6)#1	95.9(10)

O(2)#1-Li(1)-O(4)	70.7(5)
O(2)-Li(1)-O(4)	96.1(6)
O(6)-Li(1)-O(4)	169.5(7)
O(6)#1-Li(1)-O(4)	94.0(6)
O(2)#1-Li(1)-O(4)#1	96.1(6)
O(2)-Li(1)-O(4)#1	70.7(5)
O(6)-Li(1)-O(4)#1	94.0(6)
O(6)#1-Li(1)-O(4)#1	169.5(7)
O(4)-Li(1)-O(4)#1	76.2(9)
O(2)#1-Li(1)-O(3)	98.1(4)
O(2)-Li(1)-O(3)	94.6(4)
O(6)-Li(1)-O(3)	18.3(3)
O(6)#1-Li(1)-O(3)	84.9(6)
O(4)-Li(1)-O(3)	168.6(5)
O(4)#1-Li(1)-O(3)	103.9(5)
O(2)#1-Li(1)-O(3)#1	94.6(4)
O(2)-Li(1)-O(3)#1	98.1(4)
O(6)-Li(1)-O(3)#1	84.9(6)
O(6)#1-Li(1)-O(3)#1	18.3(3)
O(4)-Li(1)-O(3)#1	103.9(5)
O(4)#1-Li(1)-O(3)#1	168.6(5)
O(3)-Li(1)-O(3)#1	78.3(6)
O(2)#1-Li(1)-O(1)#1	77.7(3)
O(2)-Li(1)-O(1)#1	91.8(4)
O(6)-Li(1)-O(1)#1	87.7(5)
O(6)#1-Li(1)-O(1)#1	153.3(4)
O(4)-Li(1)-O(1)#1	84.8(6)
O(4)#1-Li(1)-O(1)#1	24.1(4)
O(3)-Li(1)-O(1)#1	91.0(3)
O(3)#1-Li(1)-O(1)#1	166.0(5)
O(2)#1-Li(1)-O(1)	91.8(4)
O(2)-Li(1)-O(1)	77.7(3)
O(6)-Li(1)-O(1)	153.3(4)

O(6)#1-Li(1)-O(1)	87.7(5)
O(4)-Li(1)-O(1)	24.1(4)
O(4)#1-Li(1)-O(1)	84.8(6)
O(3)-Li(1)-O(1)	166.0(5)
O(3)#1-Li(1)-O(1)	91.0(3)
O(1)#1-Li(1)-O(1)	100.8(6)
O(2)#1-Li(1)-O(5)#1	21.3(3)
O(2)-Li(1)-O(5)#1	163.3(4)
O(6)-Li(1)-O(5)#1	93.6(6)
O(6)#1-Li(1)-O(5)#1	79.3(6)
O(4)-Li(1)-O(5)#1	91.5(6)
O(4)#1-Li(1)-O(5)#1	96.9(7)
O(3)-Li(1)-O(5)#1	77.2(5)
O(3)#1-Li(1)-O(5)#1	94.5(5)
O(1)#1-Li(1)-O(5)#1	74.0(4)
O(1)-Li(1)-O(5)#1	113.1(5)
O(2)#1-Li(1)-O(5)	163.3(4)
O(2)-Li(1)-O(5)	21.3(3)
O(6)-Li(1)-O(5)	79.3(6)
O(6)#1-Li(1)-O(5)	93.6(6)
O(4)-Li(1)-O(5)	96.9(7)
O(4)#1-Li(1)-O(5)	91.5(6)
O(3)-Li(1)-O(5)	94.5(5)
O(3)#1-Li(1)-O(5)	77.2(5)
O(1)#1-Li(1)-O(5)	113.1(5)
O(1)-Li(1)-O(5)	74.0(4)
O(5)#1-Li(1)-O(5)	169.4(10)
O(4)-C(14)-O(1)	37.8(7)
C(15)-O(1)-C(14)	119.1(7)
C(15)-O(1)-Li(1)	107.9(6)
C(14)-O(1)-Li(1)	124.8(6)
O(1)-C(15)-C(16)	107.8(7)
O(1)-C(15)-H(18)	110.2

C(16)-C(15)-H(18)	110.2
O(1)-C(15)-H(19)	110.2
C(16)-C(15)-H(19)	110.2
H(18)-C(15)-H(19)	108.5
O(2)-C(16)-O(5)	31.5(5)
O(2)-C(16)-C(15)	101.1(6)
O(5)-C(16)-C(15)	110.2(7)
C(17)-O(2)-C(16)	110.1(6)
C(17)-O(2)-Li(1)	121.4(6)
C(16)-O(2)-Li(1)	117.8(5)
O(2)-C(17)-O(5)	32.1(5)
O(2)-C(17)-C(22)	104.6(7)
O(5)-C(17)-C(22)	100.5(9)
O(3)-C(18)-O(6)	23.6(6)
O(3)-C(18)-H(12)	97.9
O(6)-C(18)-H(12)	109.5
O(3)-C(18)-H(13)	95.5
O(6)-C(18)-H(13)	109.5
H(12)-C(18)-H(13)	109.5
O(3)-C(18)-H(14)	133.0
O(6)-C(18)-H(14)	109.5
H(12)-C(18)-H(14)	109.5
H(13)-C(18)-H(14)	109.5
O(3)-C(18)-H(15)	109.5
O(6)-C(18)-H(15)	91.6
H(12)-C(18)-H(15)	76.8
H(13)-C(18)-H(15)	153.4
H(14)-C(18)-H(15)	46.1
O(3)-C(18)-H(16)	109.5
O(6)-C(18)-H(16)	131.8
H(12)-C(18)-H(16)	41.6
H(13)-C(18)-H(16)	68.7
H(14)-C(18)-H(16)	116.4

H(15)-C(18)-H(16)	109.5
O(3)-C(18)-H(17)	109.5
O(6)-C(18)-H(17)	102.8
H(12)-C(18)-H(17)	147.0
H(13)-C(18)-H(17)	51.2
H(14)-C(18)-H(17)	64.3
H(15)-C(18)-H(17)	109.5
H(16)-C(18)-H(17)	109.5
C(18)-O(3)-C(19)	103.8(9)
C(18)-O(3)-Li(1)	132.1(8)
C(19)-O(3)-Li(1)	110.3(7)
O(3)-C(19)-C(19)#1	107.8(6)
O(3)-C(19)-H(24)	110.1
C(19)#1-C(19)-H(24)	110.1
O(3)-C(19)-H(25)	110.1
C(19)#1-C(19)-H(25)	110.1
H(24)-C(19)-H(25)	108.5
C(20)#1-C(20)-O(4)	113.5(13)
C(20)#1-C(20)-H(22)	108.9
O(4)-C(20)-H(22)	108.9
C(20)#1-C(20)-H(23)	108.9
O(4)-C(20)-H(23)	108.9
H(22)-C(20)-H(23)	107.7
C(14)-O(4)-C(20)	104.2(12)
C(14)-O(4)-Li(1)	143.9(11)
C(20)-O(4)-Li(1)	110.4(13)
C(17)-O(5)-C(16)	108.3(10)
C(17)-O(5)-Li(1)	114.2(9)
C(16)-O(5)-Li(1)	112.5(8)
O(6)-C(22)-C(17)	114.2(13)
O(6)-C(22)-H(20)	108.7
C(17)-C(22)-H(20)	108.7
O(6)-C(22)-H(21)	108.7

C(17)-C(22)-H(21)	108.7
H(20)-C(22)-H(21)	107.6
C(22)-O(6)-C(18)	133.7(14)
C(22)-O(6)-Li(1)	110.9(11)
C(18)-O(6)-Li(1)	115.1(9)

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Symmetry transformations used to generate equivalent atoms:

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

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

	U11	U22	U33	U23	U13	U12
Sn(1)	22(1)	67(1)	77(1)	0	0(1)	0
C(1)	66(7)	63(7)	156(12)	0	44(8)	0
C(2)	27(3)	61(4)	71(4)	-4(3)	-2(3)	4(3)
C(3)	31(3)	94(5)	78(5)	-10(4)	-5(3)	-8(3)
C(4)	45(4)	92(5)	63(4)	-11(4)	-13(3)	3(4)
C(5)	53(4)	68(4)	58(4)	11(3)	-3(3)	7(3)
C(6)	43(3)	44(3)	66(4)	11(3)	-4(3)	1(3)
C(7)	30(3)	30(3)	66(4)	5(2)	-1(2)	9(2)
C(8)	24(2)	39(3)	68(4)	0(3)	-4(2)	10(2)
C(9)	31(3)	22(2)	68(4)	-1(2)	3(2)	4(2)
C(10)	64(4)	54(4)	85(5)	-18(4)	19(4)	-25(3)
C(11)	61(4)	67(4)	95(6)	-32(4)	14(4)	-33(4)
C(12)	44(3)	40(3)	74(4)	-19(3)	0(3)	5(3)
C(13)	31(3)	43(3)	67(4)	-4(3)	3(3)	13(2)
Li(1)	27(6)	27(6)	69(9)	0	-4(6)	0
C(14)	79(6)	129(8)	86(6)	40(6)	3(5)	-47(5)
O(1)	49(4)	33(3)	73(5)	4(3)	-4(4)	-1(3)
C(15)	57(6)	49(5)	56(6)	10(4)	1(4)	19(4)
C(16)	55(4)	83(5)	90(5)	35(4)	3(4)	27(4)
O(2)	32(3)	38(4)	57(5)	-5(3)	-10(3)	2(3)
C(17)	40(3)	69(4)	102(6)	-7(4)	9(4)	-14(3)
C(18)	76(6)	215(13)	195(12)	156(11)	65(7)	47(7)
O(3)	37(5)	32(4)	71(6)	6(3)	2(4)	-1(4)
C(19)	31(4)	23(4)	96(7)	7(4)	-2(5)	-3(3)
C(20)	270(40)	48(13)	140(30)	-7(14)	-160(40)	0(20)
O(4)	87(12)	28(6)	60(9)	7(6)	10(9)	-3(7)
O(5)	44(7)	39(8)	50(9)	-9(6)	-9(6)	-6(6)

C(22)	64(11)	70(12)	42(9)	-22(9)	23(8)	-45(10)
O(6)	33(8)	44(8)	48(8)	0(6)	-3(7)	-6(7)

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**Table 5.** Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for lithium pentamethylstannate **4**.

	x	y	z	U(eq)
H(1)	-808	-19	2280	138
H(2)	302	-19	3113	138
H(3)	506	-19	2107	138
H(4)	-529	814	258	84
H(5)	357	998	-943	84
H(6)	2114	1596	-734	74
H(7)	2958	1985	693	64
H(8)	3661	2334	1997	81
H(9)	4439	2662	3459	90
H(10)	3544	2369	4616	65
H(11)	1799	1780	4293	57
H(18)	-974	5712	672	67
H(19)	-1011	5741	1719	67
H(12)	482	3842	4316	234
H(13)	21	3122	4129	234
H(14)	-752	3631	4538	234
H(15)	-528	3949	4382	234
H(16)	622	3520	4399	234
H(17)	-653	3190	4243	234
H(24)	-229	2694	3229	63
H(25)	998	3057	3243	63
H(22)	617	6200	2085	220
H(23)	-662	5900	1701	220
H(20)	-2495	3382	2892	68
H(21)	-1742	3191	2168	68

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**Table 6.** Torsion angles [°] for lithium pentamethylstannane **4**.

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C(1)-Sn(1)-C(2)-C(3)	56.3(6)
C(8)-Sn(1)-C(2)-C(3)	175.0(6)
C(8)#1-Sn(1)-C(2)-C(3)	-63.9(6)
C(2)#1-Sn(1)-C(2)-C(3)	-123.7(6)
C(1)-Sn(1)-C(2)-C(7)	-120.8(4)
C(8)-Sn(1)-C(2)-C(7)	-2.1(4)
C(8)#1-Sn(1)-C(2)-C(7)	119.0(4)
C(2)#1-Sn(1)-C(2)-C(7)	59.2(4)
C(7)-C(2)-C(3)-C(4)	-1.9(10)
Sn(1)-C(2)-C(3)-C(4)	-178.9(5)
C(2)-C(3)-C(4)-C(5)	0.5(11)
C(3)-C(4)-C(5)-C(6)	0.6(10)
C(4)-C(5)-C(6)-C(7)	-0.4(9)
C(5)-C(6)-C(7)-C(2)	-1.0(8)
C(5)-C(6)-C(7)-C(9)	177.9(5)
C(3)-C(2)-C(7)-C(6)	2.1(8)
Sn(1)-C(2)-C(7)-C(6)	179.6(4)
C(3)-C(2)-C(7)-C(9)	-176.8(5)
Sn(1)-C(2)-C(7)-C(9)	0.7(6)
C(1)-Sn(1)-C(8)-C(13)	-90.1(5)
C(8)#1-Sn(1)-C(8)-C(13)	89.9(5)
C(2)#1-Sn(1)-C(8)-C(13)	10.3(5)
C(2)-Sn(1)-C(8)-C(13)	-180.0(5)
C(1)-Sn(1)-C(8)-C(9)	93.2(4)
C(8)#1-Sn(1)-C(8)-C(9)	-86.8(4)
C(2)#1-Sn(1)-C(8)-C(9)	-166.4(4)
C(2)-Sn(1)-C(8)-C(9)	3.3(4)
C(13)-C(8)-C(9)-C(10)	-0.9(8)
Sn(1)-C(8)-C(9)-C(10)	176.1(4)
C(13)-C(8)-C(9)-C(7)	178.8(4)
Sn(1)-C(8)-C(9)-C(7)	-4.2(6)

C(6)-C(7)-C(9)-C(10)	3.2(8)
C(2)-C(7)-C(9)-C(10)	-177.9(6)
C(6)-C(7)-C(9)-C(8)	-176.5(5)
C(2)-C(7)-C(9)-C(8)	2.3(7)
C(8)-C(9)-C(10)-C(11)	0.3(10)
C(7)-C(9)-C(10)-C(11)	-179.4(6)
C(9)-C(10)-C(11)-C(12)	1.0(12)
C(10)-C(11)-C(12)-C(13)	-1.5(11)
C(11)-C(12)-C(13)-C(8)	0.9(9)
C(9)-C(8)-C(13)-C(12)	0.3(8)
Sn(1)-C(8)-C(13)-C(12)	-176.2(4)
O(4)-C(14)-O(1)-C(15)	105.8(15)
O(4)-C(14)-O(1)-Li(1)	-38.7(12)
O(2)#1-Li(1)-O(1)-C(15)	-141.7(7)
O(2)-Li(1)-O(1)-C(15)	25.6(6)
O(6)-Li(1)-O(1)-C(15)	42.9(18)
O(6)#1-Li(1)-O(1)-C(15)	141.6(7)
O(4)-Li(1)-O(1)-C(15)	-113.2(15)
O(4)#1-Li(1)-O(1)-C(15)	-45.8(6)
O(3)-Li(1)-O(1)-C(15)	83.4(18)
O(3)#1-Li(1)-O(1)-C(15)	123.6(6)
O(1)#1-Li(1)-O(1)-C(15)	-63.9(6)
O(5)#1-Li(1)-O(1)-C(15)	-141.0(7)
O(5)-Li(1)-O(1)-C(15)	47.3(7)
O(2)#1-Li(1)-O(1)-C(14)	6.1(9)
O(2)-Li(1)-O(1)-C(14)	173.3(9)
O(6)-Li(1)-O(1)-C(14)	-169.3(14)
O(6)#1-Li(1)-O(1)-C(14)	-70.6(10)
O(4)-Li(1)-O(1)-C(14)	34.5(12)
O(4)#1-Li(1)-O(1)-C(14)	102.0(11)
O(3)-Li(1)-O(1)-C(14)	-128.9(15)
O(3)#1-Li(1)-O(1)-C(14)	-88.6(9)
O(1)#1-Li(1)-O(1)-C(14)	83.9(8)

O(5)#1-Li(1)-O(1)-C(14)	6.7(11)
O(5)-Li(1)-O(1)-C(14)	-165.0(10)
C(14)-O(1)-C(15)-C(16)	158.6(8)
Li(1)-O(1)-C(15)-C(16)	-51.5(8)
O(1)-C(15)-C(16)-O(2)	55.0(9)
O(1)-C(15)-C(16)-O(5)	23.6(12)
O(5)-C(16)-O(2)-C(17)	-68.3(13)
C(15)-C(16)-O(2)-C(17)	-178.9(7)
O(5)-C(16)-O(2)-Li(1)	76.7(13)
C(15)-C(16)-O(2)-Li(1)	-33.9(8)
O(2)#1-Li(1)-O(2)-C(17)	-160.3(7)
O(6)-Li(1)-O(2)-C(17)	-23.5(8)
O(6)#1-Li(1)-O(2)-C(17)	67.0(10)
O(4)-Li(1)-O(2)-C(17)	164.3(8)
O(4)#1-Li(1)-O(2)-C(17)	-122.6(8)
O(3)-Li(1)-O(2)-C(17)	-19.6(8)
O(3)#1-Li(1)-O(2)-C(17)	59.3(8)
O(1)#1-Li(1)-O(2)-C(17)	-110.7(8)
O(1)-Li(1)-O(2)-C(17)	148.6(8)
O(5)#1-Li(1)-O(2)-C(17)	-79(3)
O(5)-Li(1)-O(2)-C(17)	71.0(13)
O(2)#1-Li(1)-O(2)-C(16)	58.8(6)
O(6)-Li(1)-O(2)-C(16)	-164.4(8)
O(6)#1-Li(1)-O(2)-C(16)	-74.0(9)
O(4)-Li(1)-O(2)-C(16)	23.3(8)
O(4)#1-Li(1)-O(2)-C(16)	96.4(8)
O(3)-Li(1)-O(2)-C(16)	-160.5(6)
O(3)#1-Li(1)-O(2)-C(16)	-81.6(8)
O(1)#1-Li(1)-O(2)-C(16)	108.3(7)
O(1)-Li(1)-O(2)-C(16)	7.6(7)
O(5)#1-Li(1)-O(2)-C(16)	140(2)
O(5)-Li(1)-O(2)-C(16)	-70.0(14)
C(16)-O(2)-C(17)-O(5)	67.2(13)

Li(1)-O(2)-C(17)-O(5)	-76.4(12)
C(16)-O(2)-C(17)-C(22)	153.7(9)
Li(1)-O(2)-C(17)-C(22)	10.1(11)
O(6)-C(18)-O(3)-C(19)	-137(2)
O(6)-C(18)-O(3)-Li(1)	88(2)
O(2)#1-Li(1)-O(3)-C(18)	54.9(10)
O(2)-Li(1)-O(3)-C(18)	-114.6(10)
O(6)-Li(1)-O(3)-C(18)	-102(2)
O(6)#1-Li(1)-O(3)-C(18)	130.8(12)
O(4)-Li(1)-O(3)-C(18)	46(3)
O(4)#1-Li(1)-O(3)-C(18)	-43.4(12)
O(3)#1-Li(1)-O(3)-C(18)	148.0(12)
O(1)#1-Li(1)-O(3)-C(18)	-22.8(10)
O(1)-Li(1)-O(3)-C(18)	-170.7(13)
O(5)#1-Li(1)-O(3)-C(18)	50.6(10)
O(5)-Li(1)-O(3)-C(18)	-136.0(11)
O(2)#1-Li(1)-O(3)-C(19)	-77.6(7)
O(2)-Li(1)-O(3)-C(19)	112.8(6)
O(6)-Li(1)-O(3)-C(19)	125(2)
O(6)#1-Li(1)-O(3)-C(19)	-1.8(6)
O(4)-Li(1)-O(3)-C(19)	-87(3)
O(4)#1-Li(1)-O(3)-C(19)	-176.0(7)
O(3)#1-Li(1)-O(3)-C(19)	15.5(4)
O(1)#1-Li(1)-O(3)-C(19)	-155.3(6)
O(1)-Li(1)-O(3)-C(19)	56.7(18)
O(5)#1-Li(1)-O(3)-C(19)	-82.0(7)
O(5)-Li(1)-O(3)-C(19)	91.4(7)
C(18)-O(3)-C(19)-C(19)#1	172.0(9)
Li(1)-O(3)-C(19)-C(19)#1	-42.2(9)
O(1)-C(14)-O(4)-C(20)	-99.3(17)
O(1)-C(14)-O(4)-Li(1)	63.9(19)
C(20)#1-C(20)-O(4)-C(14)	-155(3)
C(20)#1-C(20)-O(4)-Li(1)	35(3)

O(2)#1-Li(1)-O(4)-C(14)	86(2)
O(2)-Li(1)-O(4)-C(14)	-104(2)
O(6)-Li(1)-O(4)-C(14)	-150(3)
O(6)#1-Li(1)-O(4)-C(14)	11(2)
O(4)#1-Li(1)-O(4)-C(14)	-173(3)
O(3)-Li(1)-O(4)-C(14)	96(4)
O(3)#1-Li(1)-O(4)-C(14)	-4(2)
O(1)#1-Li(1)-O(4)-C(14)	165(2)
O(1)-Li(1)-O(4)-C(14)	-64(2)
O(5)#1-Li(1)-O(4)-C(14)	91(2)
O(5)-Li(1)-O(4)-C(14)	-83(2)
O(2)#1-Li(1)-O(4)-C(20)	-111.5(13)
O(2)-Li(1)-O(4)-C(20)	58.5(13)
O(6)-Li(1)-O(4)-C(20)	12(4)
O(6)#1-Li(1)-O(4)-C(20)	174.1(13)
O(4)#1-Li(1)-O(4)-C(20)	-9.9(9)
O(3)-Li(1)-O(4)-C(20)	-102(3)
O(3)#1-Li(1)-O(4)-C(20)	158.4(12)
O(1)#1-Li(1)-O(4)-C(20)	-32.7(12)
O(1)-Li(1)-O(4)-C(20)	98.8(19)
O(5)#1-Li(1)-O(4)-C(20)	-106.6(13)
O(5)-Li(1)-O(4)-C(20)	80.0(13)
O(2)-C(17)-O(5)-C(16)	-65.7(13)
C(22)-C(17)-O(5)-C(16)	-166.6(10)
O(2)-C(17)-O(5)-Li(1)	60.6(11)
C(22)-C(17)-O(5)-Li(1)	-40.3(11)
O(2)-C(16)-O(5)-C(17)	64.2(13)
C(15)-C(16)-O(5)-C(17)	142.4(9)
O(2)-C(16)-O(5)-Li(1)	-63.0(10)
C(15)-C(16)-O(5)-Li(1)	15.1(12)
O(2)#1-Li(1)-O(5)-C(17)	170(2)
O(2)-Li(1)-O(5)-C(17)	-60.1(13)
O(6)-Li(1)-O(5)-C(17)	20.8(10)

O(6)#1-Li(1)-O(5)-C(17)	116.2(11)
O(4)-Li(1)-O(5)-C(17)	-149.3(10)
O(4)#1-Li(1)-O(5)-C(17)	-73.0(10)
O(3)-Li(1)-O(5)-C(17)	31.0(10)
O(3)#1-Li(1)-O(5)-C(17)	108.0(10)
O(1)#1-Li(1)-O(5)-C(17)	-62.0(11)
O(1)-Li(1)-O(5)-C(17)	-157.2(11)
O(5)#1-Li(1)-O(5)-C(17)	69.0(9)
O(2)#1-Li(1)-O(5)-C(16)	-66(3)
O(2)-Li(1)-O(5)-C(16)	63.9(12)
O(6)-Li(1)-O(5)-C(16)	144.9(12)
O(6)#1-Li(1)-O(5)-C(16)	-119.7(10)
O(4)-Li(1)-O(5)-C(16)	-25.2(11)
O(4)#1-Li(1)-O(5)-C(16)	51.1(11)
O(3)-Li(1)-O(5)-C(16)	155.1(10)
O(3)#1-Li(1)-O(5)-C(16)	-127.9(10)
O(1)#1-Li(1)-O(5)-C(16)	62.1(11)
O(1)-Li(1)-O(5)-C(16)	-33.1(9)
O(5)#1-Li(1)-O(5)-C(16)	-166.9(10)
O(2)-C(17)-C(22)-O(6)	17.2(16)
O(5)-C(17)-C(22)-O(6)	49.8(16)
C(17)-C(22)-O(6)-C(18)	149.6(15)
C(17)-C(22)-O(6)-Li(1)	-35.9(17)
O(3)-C(18)-O(6)-C(22)	117(3)
O(3)-C(18)-O(6)-Li(1)	-56.9(18)
O(2)#1-Li(1)-O(6)-C(22)	-161.6(12)
O(2)-Li(1)-O(6)-C(22)	30.8(12)
O(6)#1-Li(1)-O(6)-C(22)	-83.4(13)
O(4)-Li(1)-O(6)-C(22)	78(4)
O(4)#1-Li(1)-O(6)-C(22)	99.8(13)
O(3)-Li(1)-O(6)-C(22)	-137(3)
O(3)#1-Li(1)-O(6)-C(22)	-68.8(12)
O(1)#1-Li(1)-O(6)-C(22)	123.1(13)



O(1)-Li(1)-O(6)-C(22)	13(2)
O(5)#1-Li(1)-O(6)-C(22)	-163.0(13)
O(5)-Li(1)-O(6)-C(22)	9.1(13)
O(2)#1-Li(1)-O(6)-C(18)	14.1(13)
O(2)-Li(1)-O(6)-C(18)	-153.6(12)
O(6)#1-Li(1)-O(6)-C(18)	92.2(12)
O(4)-Li(1)-O(6)-C(18)	-106(3)
O(4)#1-Li(1)-O(6)-C(18)	-84.5(13)
O(3)-Li(1)-O(6)-C(18)	39.0(14)
O(3)#1-Li(1)-O(6)-C(18)	106.8(12)
O(1)#1-Li(1)-O(6)-C(18)	-61.2(11)
O(1)-Li(1)-O(6)-C(18)	-171.0(11)
O(5)#1-Li(1)-O(6)-C(18)	12.6(12)
O(5)-Li(1)-O(6)-C(18)	-175.3(13)

---

Symmetry transformations used to generate equivalent atoms:

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

#### CIF file for Lithium Pentamethylstannate 4.

data\_pentamethylstannate

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_publ_contact_author_address
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Shimo-okubo, Sakura-ku, Saitama-city, Saitama, 338-8570 Japan
;
_publ_contact_author_email 'masaichi@chem.saitama-u.ac.jp'
_publ_contact_author_fax '+81-48-858-9029'
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 '-x, -y, -z'  
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 \_cell\_measurement\_temperature 93(2)

_cell_measurement_reflns_used	3907
_cell_measurement_theta_min	2.24
_cell_measurement_theta_max	26.88
_exptl_crystal_description	?
_exptl_crystal_colour	?
_exptl_crystal_size_max	0.50
_exptl_crystal_size_mid	0.20
_exptl_crystal_size_min	0.20
_exptl_crystal_density_meas	?
_exptl_crystal_density_diffn	1.290
_exptl_crystal_density_method	'not measured'
_exptl_crystal_F_000	1424
_exptl_absorpt_coefficient_mu	0.750
_exptl_absorpt_correction_type	empirical
_exptl_absorpt_correction_T_min	0.835
_exptl_absorpt_correction_T_max	0.861
_exptl_absorpt_process_details	
;	
SADABS; Sheldrick 1996	
;	
_exptl_special_details	
;	
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;	
_diffn_ambient_temperature	93(2)
_diffn_radiation_wavelength	0.71069
_diffn_radiation_type	MoK $\alpha$
_diffn_radiation_source	'fine-focus sealed tube'
_diffn_radiation_monochromator	graphite
_diffn_measurement_device_type	'CCD area detector'
_diffn_measurement_method	'phi and omega scans'

_diffraction_detector_area_resol_mean	?
_diffraction_reflections_number	10560
_diffraction_reflections_av_R_equivalents	0.0310
_diffraction_reflections_av_sigmaI/netI	0.0349
_diffraction_reflections_limit_h_min	-9
_diffraction_reflections_limit_h_max	13
_diffraction_reflections_limit_k_min	-24
_diffraction_reflections_limit_k_max	23
_diffraction_reflections_limit_l_min	-18
_diffraction_reflections_limit_l_max	18
_diffraction_reflections_theta_min	2.05
_diffraction_reflections_theta_max	25.10
_reflections_number_total	3208
_reflections_number_gt	2760
_reflections_threshold_expression	>2sigma(I)
_computing_data_collection	'Bruker SMART'
_computing_cell_refinement	'Bruker SMART'
_computing_data_reduction	'Bruker SAINT'
_computing_structure_solution	'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement	'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics	'Bruker SHELXTL'
_computing_publication_material	'Bruker SHELXTL'

\_refinement\_special\_details

;

Refinement of  $F^2$  against ALL reflections. The weighted R-factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional R-factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > 2\sigma(F^2)$  is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and R-factors based on ALL data will be even larger.

;

\_refine\_ls\_structure\_factor\_coef Fsqd  
\_refine\_ls\_matrix\_type full  
\_refine\_ls\_weighting\_scheme calc  
\_refine\_ls\_weighting\_details  
'calc w=1/[ $\sum s^2(F_o^2)^2 + (0.0218P)^2 + 35.5358P$ ] where  $P=(F_o^2+2F_c^2)/3$ '  
\_atom\_sites\_solution\_primary direct  
\_atom\_sites\_solution\_secondary difmap  
\_atom\_sites\_solution\_hydrogens geom  
\_refine\_ls\_hydrogen\_treatment constr  
\_refine\_ls\_extinction\_method none  
\_refine\_ls\_extinction\_coef ?  
\_refine\_ls\_number\_reflns 3208  
\_refine\_ls\_number\_parameters 251  
\_refine\_ls\_number\_restraints 1  
\_refine\_ls\_R\_factor\_all 0.0789  
\_refine\_ls\_R\_factor\_gt 0.0670  
\_refine\_ls\_wR\_factor\_ref 0.1472  
\_refine\_ls\_wR\_factor\_gt 0.1390  
\_refine\_ls\_goodness\_of\_fit\_ref 1.115  
\_refine\_ls\_restrained\_S\_all 1.115  
\_refine\_ls\_shift/su\_max 0.000  
\_refine\_ls\_shift/su\_mean 0.000

loop\_

\_atom\_site\_label  
\_atom\_site\_type\_symbol  
\_atom\_site\_fract\_x  
\_atom\_site\_fract\_y  
\_atom\_site\_fract\_z  
\_atom\_site\_U\_iso\_or\_equiv  
\_atom\_site\_adp\_type

\_atom\_site\_occupancy  
 \_atom\_site\_symmetry\_multiplicity  
 \_atom\_site\_calc\_flag  
 \_atom\_site\_refinement\_flags  
 \_atom\_site\_disorder\_assembly  
 \_atom\_site\_disorder\_group  
 Sn1 Sn 0.0000 0.11844(3) 0.2500 0.0570(2) Uani 1 2 d S . .  
 C1 C 0.0000 0.0138(5) 0.2500 0.092(4) Uani 1 2 d S . .  
 H1 H -0.0808 -0.0019 0.2280 0.138 Uiso 0.50 1 calc PR . .  
 H2 H 0.0302 -0.0019 0.3113 0.138 Uiso 0.50 1 calc PR . .  
 H3 H 0.0506 -0.0019 0.2107 0.138 Uiso 0.50 1 calc PR . .  
 C2 C 0.0644(5) 0.1294(3) 0.1204(4) 0.0549(16) Uani 1 1 d . . .  
 C3 C 0.0179(5) 0.1058(4) 0.0352(5) 0.070(2) Uani 1 1 d . . .  
 H4 H -0.0529 0.0814 0.0258 0.084 Uiso 1 1 calc R . .  
 C4 C 0.0706(6) 0.1164(4) -0.0367(5) 0.0702(19) Uani 1 1 d . . .  
 H5 H 0.0357 0.0998 -0.0943 0.084 Uiso 1 1 calc R . .  
 C5 C 0.1748(6) 0.1516(3) -0.0243(5) 0.0619(17) Uani 1 1 d . . .  
 H6 H 0.2114 0.1596 -0.0734 0.074 Uiso 1 1 calc R . .  
 C6 C 0.2243(5) 0.1747(3) 0.0602(4) 0.0535(15) Uani 1 1 d . . .  
 H7 H 0.2958 0.1985 0.0693 0.064 Uiso 1 1 calc R . .  
 C7 C 0.1709(4) 0.1636(2) 0.1327(4) 0.0434(13) Uani 1 1 d . . .  
 C8 C 0.1678(4) 0.1697(3) 0.2953(4) 0.0455(14) Uani 1 1 d . . .  
 C9 C 0.2240(4) 0.1859(2) 0.2254(4) 0.0417(13) Uani 1 1 d . . .  
 C10 C 0.3270(6) 0.2218(3) 0.2462(5) 0.0672(19) Uani 1 1 d . . .  
 H8 H 0.3661 0.2334 0.1997 0.081 Uiso 1 1 calc R . .  
 C11 C 0.3739(6) 0.2411(3) 0.3335(5) 0.075(2) Uani 1 1 d . . .  
 H9 H 0.4439 0.2662 0.3459 0.090 Uiso 1 1 calc R . .  
 C12 C 0.3210(5) 0.2245(3) 0.4015(5) 0.0544(16) Uani 1 1 d . . .  
 H10 H 0.3544 0.2369 0.4616 0.065 Uiso 1 1 calc R . .  
 C13 C 0.2177(5) 0.1892(3) 0.3820(4) 0.0477(14) Uani 1 1 d . . .  
 H11 H 0.1799 0.1780 0.4293 0.057 Uiso 1 1 calc R . .  
 Li1 Li 0.0000 0.4439(5) 0.2500 0.043(3) Uani 1 2 d S . .  
 C14 C 0.1200(8) 0.5395(5) 0.1310(6) 0.100(3) Uani 1 1 d D . .

O1 O 0.0123(6) 0.5098(3) 0.1431(6) 0.0542(19) Uani 0.657(9) 1 d P A 2  
C15 C -0.0950(8) 0.5451(4) 0.1217(7) 0.056(3) Uani 0.657(9) 1 d P A 2  
H18 H -0.0974 0.5712 0.0672 0.067 Uiso 0.657(9) 1 calc PR A 2  
H19 H -0.1011 0.5741 0.1719 0.067 Uiso 0.657(9) 1 calc PR A 2  
C16 C -0.2025(6) 0.4945(4) 0.1047(5) 0.078(2) Uani 1 1 d . . .  
O2 O -0.1765(6) 0.4581(3) 0.1884(5) 0.0452(18) Uani 0.657(9) 1 d P A 2  
C17 C -0.2619(6) 0.4091(4) 0.1863(6) 0.071(2) Uani 1 1 d . . .  
C18 C -0.0219(8) 0.3572(6) 0.4125(9) 0.156(6) Uani 1 1 d . . .  
H12 H 0.0482 0.3842 0.4316 0.234 Uiso 0.343(9) 1 calc PR A 1  
H13 H 0.0021 0.3122 0.4129 0.234 Uiso 0.343(9) 1 calc PR A 1  
H14 H -0.0752 0.3631 0.4538 0.234 Uiso 0.343(9) 1 calc PR A 1  
H15 H -0.0528 0.3949 0.4382 0.234 Uiso 0.657(9) 1 calc PR A 2  
H16 H 0.0622 0.3520 0.4399 0.234 Uiso 0.657(9) 1 calc PR A 2  
H17 H -0.0653 0.3190 0.4243 0.234 Uiso 0.657(9) 1 calc PR A 2  
O3 O -0.0344(8) 0.3646(4) 0.3291(7) 0.048(2) Uani 0.657(9) 1 d P A 2  
C19 C 0.0133(7) 0.3073(4) 0.3005(6) 0.052(3) Uani 0.657(9) 1 d P . 2  
H24 H -0.0229 0.2694 0.3229 0.063 Uiso 0.657(9) 1 calc PR A 2  
H25 H 0.0998 0.3057 0.3243 0.063 Uiso 0.657(9) 1 calc PR A 2  
C20 C 0.0092(19) 0.5835(11) 0.2141(12) 0.18(3) Uani 0.343(9) 1 d PD . 1  
H22 H 0.0617 0.6200 0.2085 0.220 Uiso 0.343(9) 1 calc PR A 1  
H23 H -0.0662 0.5900 0.1701 0.220 Uiso 0.343(9) 1 calc PR A 1  
O4 O 0.0655(16) 0.5228(6) 0.1911(11) 0.059(4) Uani 0.343(9) 1 d P A 1  
O5 O -0.1646(12) 0.4343(7) 0.1508(10) 0.047(3) Uani 0.343(9) 1 d P A 1  
C22 C -0.1947(16) 0.3550(9) 0.2530(11) 0.057(5) Uani 0.343(9) 1 d P A 1  
H20 H -0.2495 0.3382 0.2892 0.068 Uiso 0.343(9) 1 calc PR A 1  
H21 H -0.1742 0.3191 0.2168 0.068 Uiso 0.343(9) 1 calc PR A 1  
O6 O -0.0885(13) 0.3770(8) 0.3131(10) 0.043(3) Uani 0.343(9) 1 d P A 1

loop\_

\_atom\_site\_aniso\_label

\_atom\_site\_aniso\_U\_11

\_atom\_site\_aniso\_U\_22

\_atom\_site\_aniso\_U\_33



\_atom\_site\_aniso\_U\_23

\_atom\_site\_aniso\_U\_13

\_atom\_site\_aniso\_U\_12

Sn1 0.0224(3) 0.0669(4) 0.0767(5) 0.000 -0.0002(3) 0.000  
C1 0.066(7) 0.063(7) 0.156(12) 0.000 0.044(8) 0.000  
C2 0.027(3) 0.061(4) 0.071(4) -0.004(3) -0.002(3) 0.004(3)  
C3 0.031(3) 0.094(5) 0.078(5) -0.010(4) -0.005(3) -0.008(3)  
C4 0.045(4) 0.092(5) 0.063(4) -0.011(4) -0.013(3) 0.003(4)  
C5 0.053(4) 0.068(4) 0.058(4) 0.011(3) -0.003(3) 0.007(3)  
C6 0.043(3) 0.044(3) 0.066(4) 0.011(3) -0.004(3) 0.001(3)  
C7 0.030(3) 0.030(3) 0.066(4) 0.005(2) -0.001(2) 0.009(2)  
C8 0.024(2) 0.039(3) 0.068(4) 0.000(3) -0.004(2) 0.010(2)  
C9 0.031(3) 0.022(2) 0.068(4) -0.001(2) 0.003(2) 0.004(2)  
C10 0.064(4) 0.054(4) 0.085(5) -0.018(4) 0.019(4) -0.025(3)  
C11 0.061(4) 0.067(4) 0.095(6) -0.032(4) 0.014(4) -0.033(4)  
C12 0.044(3) 0.040(3) 0.074(4) -0.019(3) 0.000(3) 0.005(3)  
C13 0.031(3) 0.043(3) 0.067(4) -0.004(3) 0.003(3) 0.013(2)  
Li1 0.027(6) 0.027(6) 0.069(9) 0.000 -0.004(6) 0.000  
C14 0.079(6) 0.129(8) 0.086(6) 0.040(6) 0.003(5) -0.047(5)  
O1 0.049(4) 0.033(3) 0.073(5) 0.004(3) -0.004(4) -0.001(3)  
C15 0.057(6) 0.049(5) 0.056(6) 0.010(4) 0.001(4) 0.019(4)  
C16 0.055(4) 0.083(5) 0.090(5) 0.035(4) 0.003(4) 0.027(4)  
O2 0.032(3) 0.038(4) 0.057(5) -0.005(3) -0.010(3) 0.002(3)  
C17 0.040(3) 0.069(4) 0.102(6) -0.007(4) 0.009(4) -0.014(3)  
C18 0.076(6) 0.215(13) 0.195(12) 0.156(11) 0.065(7) 0.047(7)  
O3 0.037(5) 0.032(4) 0.071(6) 0.006(3) 0.002(4) -0.001(4)  
C19 0.031(4) 0.023(4) 0.096(7) 0.007(4) -0.002(5) -0.003(3)  
C20 0.27(4) 0.048(13) 0.14(3) -0.007(14) -0.16(4) 0.00(2)  
O4 0.087(12) 0.028(6) 0.060(9) 0.007(6) 0.010(9) -0.003(7)  
O5 0.044(7) 0.039(8) 0.050(9) -0.009(6) -0.009(6) -0.006(6)  
C22 0.064(11) 0.070(12) 0.042(9) -0.022(9) 0.023(8) -0.045(10)  
O6 0.033(8) 0.044(8) 0.048(8) 0.000(6) -0.003(7) -0.006(7)

\_geom\_special\_details

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All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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loop\_

\_geom\_bond\_atom\_site\_label\_1

\_geom\_bond\_atom\_site\_label\_2

\_geom\_bond\_distance

\_geom\_bond\_site\_symmetry\_2

\_geom\_bond\_publ\_flag

Sn1 C1 2.186(11) . ?

Sn1 C8 2.196(5) . ?

Sn1 C8 2.196(5) 2 ?

Sn1 C2 2.268(7) 2 ?

Sn1 C2 2.268(7) . ?

C1 H1 0.9800 . ?

C1 H2 0.9800 . ?

C1 H3 0.9800 . ?

C2 C3 1.385(9) . ?

C2 C7 1.402(8) . ?

C3 C4 1.381(10) . ?

C3 H4 0.9500 . ?

C4 C5 1.391(9) . ?

C4 H5 0.9500 . ?

C5 C6 1.379(9) . ?

C5 H6 0.9500 . ?

C6 C7 1.397(8) . ?

C6 H7 0.9500 . ?  
C7 C9 1.489(8) . ?  
C8 C13 1.384(8) . ?  
C8 C9 1.404(8) . ?  
C9 C10 1.387(8) . ?  
C10 C11 1.384(10) . ?  
C10 H8 0.9500 . ?  
C11 C12 1.358(10) . ?  
C11 H9 0.9500 . ?  
C12 C13 1.382(8) . ?  
C12 H10 0.9500 . ?  
C13 H11 0.9500 . ?  
Li1 O2 2.079(6) 2 ?  
Li1 O2 2.079(6) . ?  
Li1 O6 2.085(17) . ?  
Li1 O6 2.085(17) 2 ?  
Li1 O4 2.096(16) . ?  
Li1 O4 2.096(16) 2 ?  
Li1 O3 2.135(12) . ?  
Li1 O3 2.135(12) 2 ?  
Li1 O1 2.160(10) 2 ?  
Li1 O1 2.160(10) . ?  
Li1 O5 2.173(13) 2 ?  
Li1 O5 2.173(13) . ?  
C14 O4 1.267(16) . ?  
C14 O1 1.440(10) . ?  
O1 C15 1.421(11) . ?  
C15 C16 1.611(12) . ?  
C15 H18 0.9900 . ?  
C15 H19 0.9900 . ?  
C16 O2 1.460(10) . ?  
C16 O5 1.461(15) . ?  
O2 C17 1.419(9) . ?

C17 O5 1.449(16) . ?  
C17 C22 1.60(2) . ?  
C18 O3 1.256(14) . ?  
C18 O6 1.598(18) . ?  
C18 H12 0.9800 . ?  
C18 H13 0.9800 . ?  
C18 H14 0.9800 . ?  
C18 H15 0.9800 . ?  
C18 H16 0.9800 . ?  
C18 H17 0.9800 . ?  
O3 C19 1.425(12) . ?  
C19 C19 1.503(19) 2 ?  
C19 H24 0.9900 . ?  
C19 H25 0.9900 . ?  
C20 C20 1.16(4) 2 ?  
C20 O4 1.50(2) . ?  
C20 H22 0.9900 . ?  
C20 H23 0.9900 . ?  
C22 O6 1.44(2) . ?  
C22 H20 0.9900 . ?  
C22 H21 0.9900 . ?

loop\_

  \_geom\_angle\_atom\_site\_label\_1  
  \_geom\_angle\_atom\_site\_label\_2  
  \_geom\_angle\_atom\_site\_label\_3  
  \_geom\_angle  
  \_geom\_angle\_site\_symmetry\_1  
  \_geom\_angle\_site\_symmetry\_3  
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C1 Sn1 C8 119.15(13) . . ?  
C1 Sn1 C8 119.15(13) . 2 ?  
C8 Sn1 C8 121.7(3) . 2 ?

C1 Sn1 C2 95.79(16) . 2 ?  
C8 Sn1 C2 96.4(2) . 2 ?  
C8 Sn1 C2 77.8(2) 2 2 ?  
C1 Sn1 C2 95.79(16) . . ?  
C8 Sn1 C2 77.8(2) . . ?  
C8 Sn1 C2 96.4(2) 2 . ?  
C2 Sn1 C2 168.4(3) 2 . ?  
Sn1 C1 H1 109.5 . . ?  
Sn1 C1 H2 109.5 . . ?  
H1 C1 H2 109.5 . . ?  
Sn1 C1 H3 109.5 . . ?  
H1 C1 H3 109.5 . . ?  
H2 C1 H3 109.5 . . ?  
C3 C2 C7 117.4(6) . . ?  
C3 C2 Sn1 130.2(5) . . ?  
C7 C2 Sn1 112.3(4) . . ?  
C4 C3 C2 122.5(6) . . ?  
C4 C3 H4 118.8 . . ?  
C2 C3 H4 118.8 . . ?  
C3 C4 C5 119.8(6) . . ?  
C3 C4 H5 120.1 . . ?  
C5 C4 H5 120.1 . . ?  
C6 C5 C4 119.1(7) . . ?  
C6 C5 H6 120.5 . . ?  
C4 C5 H6 120.5 . . ?  
C5 C6 C7 120.9(6) . . ?  
C5 C6 H7 119.5 . . ?  
C7 C6 H7 119.5 . . ?  
C6 C7 C2 120.4(6) . . ?  
C6 C7 C9 122.3(5) . . ?  
C2 C7 C9 117.3(5) . . ?  
C13 C8 C9 119.1(5) . . ?  
C13 C8 Sn1 127.1(5) . . ?

C9 C8 Sn1 113.8(4) . . ?  
C10 C9 C8 118.3(6) . . ?  
C10 C9 C7 123.1(6) . . ?  
C8 C9 C7 118.6(5) . . ?  
C11 C10 C9 121.1(7) . . ?  
C11 C10 H8 119.4 . . ?  
C9 C10 H8 119.4 . . ?  
C12 C11 C10 120.7(6) . . ?  
C12 C11 H9 119.6 . . ?  
C10 C11 H9 119.6 . . ?  
C11 C12 C13 118.9(6) . . ?  
C11 C12 H10 120.5 . . ?  
C13 C12 H10 120.5 . . ?  
C12 C13 C8 121.8(6) . . ?  
C12 C13 H11 119.1 . . ?  
C8 C13 H11 119.1 . . ?  
O2 Li1 O2 163.6(7) 2 . ?  
O2 Li1 O6 114.9(5) 2 . ?  
O2 Li1 O6 76.7(5) . . ?  
O2 Li1 O6 76.7(5) 2 2 ?  
O2 Li1 O6 114.9(5) . 2 ?  
O6 Li1 O6 95.9(10) . 2 ?  
O2 Li1 O4 70.7(5) 2 . ?  
O2 Li1 O4 96.1(6) . . ?  
O6 Li1 O4 169.5(7) . . ?  
O6 Li1 O4 94.0(6) 2 . ?  
O2 Li1 O4 96.1(6) 2 2 ?  
O2 Li1 O4 70.7(5) . 2 ?  
O6 Li1 O4 94.0(6) . 2 ?  
O6 Li1 O4 169.5(7) 2 2 ?  
O4 Li1 O4 76.2(9) . 2 ?  
O2 Li1 O3 98.1(4) 2 . ?  
O2 Li1 O3 94.6(4) . . ?

O6 Li1 O3 18.3(3) . . ?  
O6 Li1 O3 84.9(6) 2 . ?  
O4 Li1 O3 168.6(5) . . ?  
O4 Li1 O3 103.9(5) 2 . ?  
O2 Li1 O3 94.6(4) 2 2 ?  
O2 Li1 O3 98.1(4) . 2 ?  
O6 Li1 O3 84.9(6) . 2 ?  
O6 Li1 O3 18.3(3) 2 2 ?  
O4 Li1 O3 103.9(5) . 2 ?  
O4 Li1 O3 168.6(5) 2 2 ?  
O3 Li1 O3 78.3(6) . 2 ?  
O2 Li1 O1 77.7(3) 2 2 ?  
O2 Li1 O1 91.8(4) . 2 ?  
O6 Li1 O1 87.7(5) . 2 ?  
O6 Li1 O1 153.3(4) 2 2 ?  
O4 Li1 O1 84.8(6) . 2 ?  
O4 Li1 O1 24.1(4) 2 2 ?  
O3 Li1 O1 91.0(3) . 2 ?  
O3 Li1 O1 166.0(5) 2 2 ?  
O2 Li1 O1 91.8(4) 2 . ?  
O2 Li1 O1 77.7(3) . . ?  
O6 Li1 O1 153.3(4) . . ?  
O6 Li1 O1 87.7(5) 2 . ?  
O4 Li1 O1 24.1(4) . . ?  
O4 Li1 O1 84.8(6) 2 . ?  
O3 Li1 O1 166.0(5) . . ?  
O3 Li1 O1 91.0(3) 2 . ?  
O1 Li1 O1 100.8(6) 2 . ?  
O2 Li1 O5 21.3(3) 2 2 ?  
O2 Li1 O5 163.3(4) . 2 ?  
O6 Li1 O5 93.6(6) . 2 ?  
O6 Li1 O5 79.3(6) 2 2 ?  
O4 Li1 O5 91.5(6) . 2 ?

O4 Li1 O5 96.9(7) 2 2 ?  
O3 Li1 O5 77.2(5) . 2 ?  
O3 Li1 O5 94.5(5) 2 2 ?  
O1 Li1 O5 74.0(4) 2 2 ?  
O1 Li1 O5 113.1(5) . 2 ?  
O2 Li1 O5 163.3(4) 2 . ?  
O2 Li1 O5 21.3(3) . . ?  
O6 Li1 O5 79.3(6) . . ?  
O6 Li1 O5 93.6(6) 2 . ?  
O4 Li1 O5 96.9(7) . . ?  
O4 Li1 O5 91.5(6) 2 . ?  
O3 Li1 O5 94.5(5) . . ?  
O3 Li1 O5 77.2(5) 2 . ?  
O1 Li1 O5 113.1(5) 2 . ?  
O1 Li1 O5 74.0(4) . . ?  
O5 Li1 O5 169.4(10) 2 . ?  
O4 C14 O1 37.8(7) . . ?  
C15 O1 C14 119.1(7) . . ?  
C15 O1 Li1 107.9(6) . . ?  
C14 O1 Li1 124.8(6) . . ?  
O1 C15 C16 107.8(7) . . ?  
O1 C15 H18 110.2 . . ?  
C16 C15 H18 110.2 . . ?  
O1 C15 H19 110.2 . . ?  
C16 C15 H19 110.2 . . ?  
H18 C15 H19 108.5 . . ?  
O2 C16 O5 31.5(5) . . ?  
O2 C16 C15 101.1(6) . . ?  
O5 C16 C15 110.2(7) . . ?  
C17 O2 C16 110.1(6) . . ?  
C17 O2 Li1 121.4(6) . . ?  
C16 O2 Li1 117.8(5) . . ?  
O2 C17 O5 32.1(5) . . ?



O2 C17 C22 104.6(7) . . ?  
O5 C17 C22 100.5(9) . . ?  
O3 C18 O6 23.6(6) . . ?  
O3 C18 H12 97.9 . . ?  
O6 C18 H12 109.5 . . ?  
O3 C18 H13 95.5 . . ?  
O6 C18 H13 109.5 . . ?  
H12 C18 H13 109.5 . . ?  
O3 C18 H14 133.0 . . ?  
O6 C18 H14 109.5 . . ?  
H12 C18 H14 109.5 . . ?  
H13 C18 H14 109.5 . . ?  
O3 C18 H15 109.5 . . ?  
O6 C18 H15 91.6 . . ?  
H12 C18 H15 76.8 . . ?  
H13 C18 H15 153.4 . . ?  
H14 C18 H15 46.1 . . ?  
O3 C18 H16 109.5 . . ?  
O6 C18 H16 131.8 . . ?  
H12 C18 H16 41.6 . . ?  
H13 C18 H16 68.7 . . ?  
H14 C18 H16 116.4 . . ?  
H15 C18 H16 109.5 . . ?  
O3 C18 H17 109.5 . . ?  
O6 C18 H17 102.8 . . ?  
H12 C18 H17 147.0 . . ?  
H13 C18 H17 51.2 . . ?  
H14 C18 H17 64.3 . . ?  
H15 C18 H17 109.5 . . ?  
H16 C18 H17 109.5 . . ?  
C18 O3 C19 103.8(9) . . ?  
C18 O3 Li1 132.1(8) . . ?  
C19 O3 Li1 110.3(7) . . ?

O3 C19 C19 107.8(6) . 2 ?  
O3 C19 H24 110.1 . . ?  
C19 C19 H24 110.1 2 . ?  
O3 C19 H25 110.1 . . ?  
C19 C19 H25 110.1 2 . ?  
H24 C19 H25 108.5 . . ?  
C20 C20 O4 113.5(13) 2 . ?  
C20 C20 H22 108.9 2 . ?  
O4 C20 H22 108.9 . . ?  
C20 C20 H23 108.9 2 . ?  
O4 C20 H23 108.9 . . ?  
H22 C20 H23 107.7 . . ?  
C14 O4 C20 104.2(12) . . ?  
C14 O4 Li1 143.9(11) . . ?  
C20 O4 Li1 110.4(13) . . ?  
C17 O5 C16 108.3(10) . . ?  
C17 O5 Li1 114.2(9) . . ?  
C16 O5 Li1 112.5(8) . . ?  
O6 C22 C17 114.2(13) . . ?  
O6 C22 H20 108.7 . . ?  
C17 C22 H20 108.7 . . ?  
O6 C22 H21 108.7 . . ?  
C17 C22 H21 108.7 . . ?  
H20 C22 H21 107.6 . . ?  
C22 O6 C18 133.7(14) . . ?  
C22 O6 Li1 110.9(11) . . ?  
C18 O6 Li1 115.1(9) . . ?

loop\_

\_geom\_torsion\_atom\_site\_label\_1  
\_geom\_torsion\_atom\_site\_label\_2  
\_geom\_torsion\_atom\_site\_label\_3  
\_geom\_torsion\_atom\_site\_label\_4

\_geom\_torsion  
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 \_geom\_torsion\_site\_symmetry\_2  
 \_geom\_torsion\_site\_symmetry\_3  
 \_geom\_torsion\_site\_symmetry\_4  
 \_geom\_torsion\_publ\_flag  
 C1 Sn1 C2 C3 56.3(6) . . . . ?  
 C8 Sn1 C2 C3 175.0(6) . . . . ?  
 C8 Sn1 C2 C3 -63.9(6) 2 . . . ?  
 C2 Sn1 C2 C3 -123.7(6) 2 . . . ?  
 C1 Sn1 C2 C7 -120.8(4) . . . . ?  
 C8 Sn1 C2 C7 -2.1(4) . . . . ?  
 C8 Sn1 C2 C7 119.0(4) 2 . . . ?  
 C2 Sn1 C2 C7 59.2(4) 2 . . . ?  
 C7 C2 C3 C4 -1.9(10) . . . . ?  
 Sn1 C2 C3 C4 -178.9(5) . . . . ?  
 C2 C3 C4 C5 0.5(11) . . . . ?  
 C3 C4 C5 C6 0.6(10) . . . . ?  
 C4 C5 C6 C7 -0.4(9) . . . . ?  
 C5 C6 C7 C2 -1.0(8) . . . . ?  
 C5 C6 C7 C9 177.9(5) . . . . ?  
 C3 C2 C7 C6 2.1(8) . . . . ?  
 Sn1 C2 C7 C6 179.6(4) . . . . ?  
 C3 C2 C7 C9 -176.8(5) . . . . ?  
 Sn1 C2 C7 C9 0.7(6) . . . . ?  
 C1 Sn1 C8 C13 -90.1(5) . . . . ?  
 C8 Sn1 C8 C13 89.9(5) 2 . . . ?  
 C2 Sn1 C8 C13 10.3(5) 2 . . . ?  
 C2 Sn1 C8 C13 -180.0(5) . . . . ?  
 C1 Sn1 C8 C9 93.2(4) . . . . ?  
 C8 Sn1 C8 C9 -86.8(4) 2 . . . ?  
 C2 Sn1 C8 C9 -166.4(4) 2 . . . ?  
 C2 Sn1 C8 C9 3.3(4) . . . . ?

C13 C8 C9 C10 -0.9(8) . . . . ?  
Sn1 C8 C9 C10 176.1(4) . . . . ?  
C13 C8 C9 C7 178.8(4) . . . . ?  
Sn1 C8 C9 C7 -4.2(6) . . . . ?  
C6 C7 C9 C10 3.2(8) . . . . ?  
C2 C7 C9 C10 -177.9(6) . . . . ?  
C6 C7 C9 C8 -176.5(5) . . . . ?  
C2 C7 C9 C8 2.3(7) . . . . ?  
C8 C9 C10 C11 0.3(10) . . . . ?  
C7 C9 C10 C11 -179.4(6) . . . . ?  
C9 C10 C11 C12 1.0(12) . . . . ?  
C10 C11 C12 C13 -1.5(11) . . . . ?  
C11 C12 C13 C8 0.9(9) . . . . ?  
C9 C8 C13 C12 0.3(8) . . . . ?  
Sn1 C8 C13 C12 -176.2(4) . . . . ?  
O4 C14 O1 C15 105.8(15) . . . . ?  
O4 C14 O1 Li1 -38.7(12) . . . . ?  
O2 Li1 O1 C15 -141.7(7) 2 . . . . ?  
O2 Li1 O1 C15 25.6(6) . . . . ?  
O6 Li1 O1 C15 42.9(18) . . . . ?  
O6 Li1 O1 C15 141.6(7) 2 . . . . ?  
O4 Li1 O1 C15 -113.2(15) . . . . ?  
O4 Li1 O1 C15 -45.8(6) 2 . . . . ?  
O3 Li1 O1 C15 83.4(18) . . . . ?  
O3 Li1 O1 C15 123.6(6) 2 . . . . ?  
O1 Li1 O1 C15 -63.9(6) 2 . . . . ?  
O5 Li1 O1 C15 -141.0(7) 2 . . . . ?  
O5 Li1 O1 C15 47.3(7) . . . . ?  
O2 Li1 O1 C14 6.1(9) 2 . . . . ?  
O2 Li1 O1 C14 173.3(9) . . . . ?  
O6 Li1 O1 C14 -169.3(14) . . . . ?  
O6 Li1 O1 C14 -70.6(10) 2 . . . . ?  
O4 Li1 O1 C14 34.5(12) . . . . ?

O4 Li1 O1 C14 102.0(11) 2 . . . ?  
O3 Li1 O1 C14 -128.9(15) . . . . ?  
O3 Li1 O1 C14 -88.6(9) 2 . . . ?  
O1 Li1 O1 C14 83.9(8) 2 . . . ?  
O5 Li1 O1 C14 6.7(11) 2 . . . ?  
O5 Li1 O1 C14 -165.0(10) . . . . ?  
C14 O1 C15 C16 158.6(8) . . . . ?  
Li1 O1 C15 C16 -51.5(8) . . . . ?  
O1 C15 C16 O2 55.0(9) . . . . ?  
O1 C15 C16 O5 23.6(12) . . . . ?  
O5 C16 O2 C17 -68.3(13) . . . . ?  
C15 C16 O2 C17 -178.9(7) . . . . ?  
O5 C16 O2 Li1 76.7(13) . . . . ?  
C15 C16 O2 Li1 -33.9(8) . . . . ?  
O2 Li1 O2 C17 -160.3(7) 2 . . . ?  
O6 Li1 O2 C17 -23.5(8) . . . . ?  
O6 Li1 O2 C17 67.0(10) 2 . . . ?  
O4 Li1 O2 C17 164.3(8) . . . . ?  
O4 Li1 O2 C17 -122.6(8) 2 . . . ?  
O3 Li1 O2 C17 -19.6(8) . . . . ?  
O3 Li1 O2 C17 59.3(8) 2 . . . ?  
O1 Li1 O2 C17 -110.7(8) 2 . . . ?  
O1 Li1 O2 C17 148.6(8) . . . . ?  
O5 Li1 O2 C17 -79(3) 2 . . . ?  
O5 Li1 O2 C17 71.0(13) . . . . ?  
O2 Li1 O2 C16 58.8(6) 2 . . . ?  
O6 Li1 O2 C16 -164.4(8) . . . . ?  
O6 Li1 O2 C16 -74.0(9) 2 . . . ?  
O4 Li1 O2 C16 23.3(8) . . . . ?  
O4 Li1 O2 C16 96.4(8) 2 . . . ?  
O3 Li1 O2 C16 -160.5(6) . . . . ?  
O3 Li1 O2 C16 -81.6(8) 2 . . . ?  
O1 Li1 O2 C16 108.3(7) 2 . . . ?

O1 Li1 O2 C16 7.6(7) . . . . ?  
O5 Li1 O2 C16 140(2) 2 . . . ?  
O5 Li1 O2 C16 -70.0(14) . . . . ?  
C16 O2 C17 O5 67.2(13) . . . . ?  
Li1 O2 C17 O5 -76.4(12) . . . . ?  
C16 O2 C17 C22 153.7(9) . . . . ?  
Li1 O2 C17 C22 10.1(11) . . . . ?  
O6 C18 O3 C19 -137(2) . . . . ?  
O6 C18 O3 Li1 88(2) . . . . ?  
O2 Li1 O3 C18 54.9(10) 2 . . . ?  
O2 Li1 O3 C18 -114.6(10) . . . . ?  
O6 Li1 O3 C18 -102(2) . . . . ?  
O6 Li1 O3 C18 130.8(12) 2 . . . ?  
O4 Li1 O3 C18 46(3) . . . . ?  
O4 Li1 O3 C18 -43.4(12) 2 . . . ?  
O3 Li1 O3 C18 148.0(12) 2 . . . ?  
O1 Li1 O3 C18 -22.8(10) 2 . . . ?  
O1 Li1 O3 C18 -170.7(13) . . . . ?  
O5 Li1 O3 C18 50.6(10) 2 . . . ?  
O5 Li1 O3 C18 -136.0(11) . . . . ?  
O2 Li1 O3 C19 -77.6(7) 2 . . . ?  
O2 Li1 O3 C19 112.8(6) . . . . ?  
O6 Li1 O3 C19 125(2) . . . . ?  
O6 Li1 O3 C19 -1.8(6) 2 . . . ?  
O4 Li1 O3 C19 -87(3) . . . . ?  
O4 Li1 O3 C19 -176.0(7) 2 . . . ?  
O3 Li1 O3 C19 15.5(4) 2 . . . ?  
O1 Li1 O3 C19 -155.3(6) 2 . . . ?  
O1 Li1 O3 C19 56.7(18) . . . . ?  
O5 Li1 O3 C19 -82.0(7) 2 . . . ?  
O5 Li1 O3 C19 91.4(7) . . . . ?  
C18 O3 C19 C19 172.0(9) . . . 2 ?  
Li1 O3 C19 C19 -42.2(9) . . . 2 ?

O1 C14 O4 C20 -99.3(17) . . . . ?  
O1 C14 O4 Li1 63.9(19) . . . . ?  
C20 C20 O4 C14 -155(3) 2 . . . . ?  
C20 C20 O4 Li1 35(3) 2 . . . . ?  
O2 Li1 O4 C14 86(2) 2 . . . . ?  
O2 Li1 O4 C14 -104(2) . . . . ?  
O6 Li1 O4 C14 -150(3) . . . . ?  
O6 Li1 O4 C14 11(2) 2 . . . . ?  
O4 Li1 O4 C14 -173(3) 2 . . . . ?  
O3 Li1 O4 C14 96(4) . . . . ?  
O3 Li1 O4 C14 -4(2) 2 . . . . ?  
O1 Li1 O4 C14 165(2) 2 . . . . ?  
O1 Li1 O4 C14 -64(2) . . . . ?  
O5 Li1 O4 C14 91(2) 2 . . . . ?  
O5 Li1 O4 C14 -83(2) . . . . ?  
O2 Li1 O4 C20 -111.5(13) 2 . . . . ?  
O2 Li1 O4 C20 58.5(13) . . . . ?  
O6 Li1 O4 C20 12(4) . . . . ?  
O6 Li1 O4 C20 174.1(13) 2 . . . . ?  
O4 Li1 O4 C20 -9.9(9) 2 . . . . ?  
O3 Li1 O4 C20 -102(3) . . . . ?  
O3 Li1 O4 C20 158.4(12) 2 . . . . ?  
O1 Li1 O4 C20 -32.7(12) 2 . . . . ?  
O1 Li1 O4 C20 98.8(19) . . . . ?  
O5 Li1 O4 C20 -106.6(13) 2 . . . . ?  
O5 Li1 O4 C20 80.0(13) . . . . ?  
O2 C17 O5 C16 -65.7(13) . . . . ?  
C22 C17 O5 C16 -166.6(10) . . . . ?  
O2 C17 O5 Li1 60.6(11) . . . . ?  
C22 C17 O5 Li1 -40.3(11) . . . . ?  
O2 C16 O5 C17 64.2(13) . . . . ?  
C15 C16 O5 C17 142.4(9) . . . . ?  
O2 C16 O5 Li1 -63.0(10) . . . . ?

C15 C16 O5 Li1 15.1(12) . . . . ?  
O2 Li1 O5 C17 170(2) 2 . . . ?  
O2 Li1 O5 C17 -60.1(13) . . . . ?  
O6 Li1 O5 C17 20.8(10) . . . . ?  
O6 Li1 O5 C17 116.2(11) 2 . . . ?  
O4 Li1 O5 C17 -149.3(10) . . . . ?  
O4 Li1 O5 C17 -73.0(10) 2 . . . ?  
O3 Li1 O5 C17 31.0(10) . . . . ?  
O3 Li1 O5 C17 108.0(10) 2 . . . ?  
O1 Li1 O5 C17 -62.0(11) 2 . . . ?  
O1 Li1 O5 C17 -157.2(11) . . . . ?  
O5 Li1 O5 C17 69.0(9) 2 . . . ?  
O2 Li1 O5 C16 -66(3) 2 . . . ?  
O2 Li1 O5 C16 63.9(12) . . . . ?  
O6 Li1 O5 C16 144.9(12) . . . . ?  
O6 Li1 O5 C16 -119.7(10) 2 . . . ?  
O4 Li1 O5 C16 -25.2(11) . . . . ?  
O4 Li1 O5 C16 51.1(11) 2 . . . ?  
O3 Li1 O5 C16 155.1(10) . . . . ?  
O3 Li1 O5 C16 -127.9(10) 2 . . . ?  
O1 Li1 O5 C16 62.1(11) 2 . . . ?  
O1 Li1 O5 C16 -33.1(9) . . . . ?  
O5 Li1 O5 C16 -166.9(10) 2 . . . ?  
O2 C17 C22 O6 17.2(16) . . . . ?  
O5 C17 C22 O6 49.8(16) . . . . ?  
C17 C22 O6 C18 149.6(15) . . . . ?  
C17 C22 O6 Li1 -35.9(17) . . . . ?  
O3 C18 O6 C22 117(3) . . . . ?  
O3 C18 O6 Li1 -56.9(18) . . . . ?  
O2 Li1 O6 C22 -161.6(12) 2 . . . ?  
O2 Li1 O6 C22 30.8(12) . . . . ?  
O6 Li1 O6 C22 -83.4(13) 2 . . . ?  
O4 Li1 O6 C22 78(4) . . . . ?



O4 Li1 O6 C22 99.8(13) 2 . . . ?  
 O3 Li1 O6 C22 -137(3) . . . . ?  
 O3 Li1 O6 C22 -68.8(12) 2 . . . ?  
 O1 Li1 O6 C22 123.1(13) 2 . . . ?  
 O1 Li1 O6 C22 13(2) . . . . ?  
 O5 Li1 O6 C22 -163.0(13) 2 . . . ?  
 O5 Li1 O6 C22 9.1(13) . . . . ?  
 O2 Li1 O6 C18 14.1(13) 2 . . . ?  
 O2 Li1 O6 C18 -153.6(12) . . . . ?  
 O6 Li1 O6 C18 92.2(12) 2 . . . ?  
 O4 Li1 O6 C18 -106(3) . . . . ?  
 O4 Li1 O6 C18 -84.5(13) 2 . . . ?  
 O3 Li1 O6 C18 39.0(14) . . . . ?  
 O3 Li1 O6 C18 106.8(12) 2 . . . ?  
 O1 Li1 O6 C18 -61.2(11) 2 . . . ?  
 O1 Li1 O6 C18 -171.0(11) . . . . ?  
 O5 Li1 O6 C18 12.6(12) 2 . . . ?  
 O5 Li1 O6 C18 -175.3(13) . . . . ?

_diffn_measured_fraction_theta_max	0.999
_diffn_reflns_theta_full	25.10
_diffn_measured_fraction_theta_full	0.999
_refine_diff_density_max	1.773
_refine_diff_density_min	-2.226
_refine_diff_density_rms	0.101

## Theoretical Calculations

**Table 7.** Optimized Structure of Pentamethylstannate Anion **4** (B3LYP/LANL2DZP for Sn, 6-31G(d) for C and H).

Sn	-0.000678	-0.002423	0.665877
C	0.615916	2.779951	-0.864960
C	1.425834	3.691830	-1.551151
C	2.766430	3.376107	-1.777807
C	3.285827	2.163242	-1.323122
C	2.543221	-2.168394	0.972644
C	3.886085	-2.547022	0.852728
C	4.789510	-1.673275	0.244665
C	4.346170	-0.440394	-0.236159
C	1.118293	1.563475	-0.391402
C	2.064013	-0.943646	0.489189
C	2.478335	1.245948	-0.626898
C	2.993800	-0.069731	-0.124894
C	0.041526	-0.025075	2.853983
H	-0.433779	3.018469	-0.703079
H	1.015264	4.634588	-1.910062
H	3.410786	4.070187	-2.315538
H	4.329570	1.936830	-1.527651
H	1.853331	-2.858364	1.462404
H	4.226662	-3.510136	1.232404
H	5.839505	-1.945786	0.148551
H	5.072720	0.229263	-0.691822
H	0.882337	0.576744	3.218820
H	0.190392	-1.049285	3.215939
H	-0.887733	0.368996	3.277675

C	-0.628137	-2.779922	-0.868397
C	-1.442003	-3.687971	-1.555030
C	-2.781986	-3.367684	-1.778813
C	-3.297021	-2.154187	-1.320744
C	-2.538605	2.166826	0.990979
C	-3.880075	2.550821	0.871986
C	-4.786136	1.683546	0.258689
C	-4.346963	0.451365	-0.227772
C	-1.126347	-1.563209	-0.391196
C	-2.063689	0.942476	0.502043
C	-2.485681	-1.241073	-0.623613
C	-2.996247	0.074792	-0.116746
H	0.421294	-3.021493	-0.709351
H	-1.034895	-4.631192	-1.916648
H	-3.429339	-4.058737	-2.316827
H	-4.340508	-1.924424	-1.522790
H	-4.217352	3.513360	1.255998
H	-5.834940	1.960584	0.162601
H	-5.075490	-0.213085	-0.687836
H	-1.846356	2.851863	1.484146

**Table 8.** Optimized Structure of Pentamethylstannate Anion **6** (B3LYP/LANL2DZP for Sn, 6-31G(d) for C and H).

Sn	0.603039	-1.467121	-0.007264
C	-2.335316	-2.907166	0.028659
C	-3.735114	-2.938970	0.031650
C	-4.442257	-1.735733	0.006170
C	-3.754810	-0.521043	-0.021642

C	0.592512	1.864211	-0.089688
C	-0.012799	3.125434	-0.113451
C	-1.407185	3.216913	-0.107359
C	-2.178977	2.055111	-0.078131
C	-1.625844	-1.702338	0.000852
C	-0.157759	0.682861	-0.059900
C	-2.348952	-0.488006	-0.024275
C	-1.564818	0.789432	-0.054430
C	2.237331	-1.132080	-2.837478
C	3.402058	-0.879990	-3.569246
C	4.584680	-0.584950	-2.888959
C	4.595095	-0.544073	-1.495205
C	2.186368	-0.996002	2.830210
C	3.336022	-0.700571	3.569478
C	4.529371	-0.432266	2.896977
C	4.565615	-0.461795	1.503363
C	2.220559	-1.098757	-1.438907
C	2.195452	-1.032833	1.431619
C	3.427894	-0.797326	-0.749550
C	3.414004	-0.759898	0.750140
C	0.931660	-3.689201	0.038661
H	-1.786505	-3.847095	0.048666
H	-4.268336	-3.888772	0.053529
H	-5.531410	-1.738751	0.007604
H	-4.330921	0.401223	-0.042048
H	1.681195	1.805132	-0.094930
H	0.594068	4.030361	-0.136593
H	-1.895040	4.190551	-0.125376
H	-3.262965	2.151289	-0.073464

H	1.319915	-1.357815	-3.380622
H	3.387837	-0.912035	-4.657802
H	5.501537	-0.385224	-3.441161
H	5.531410	-0.311134	-0.994021
H	1.260268	-1.199623	3.367211
H	3.301689	-0.677903	4.657802
H	5.434516	-0.198562	3.455130
H	5.509289	-0.246409	1.008205
H	0.509567	-4.190551	-0.843543
H	0.493815	-4.160502	0.929580
H	2.010705	-3.884523	0.051236