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Structures of 4-tolyl 2-(triphenylstannyl)ethyl sulphone and 4-tolyl 4-(triphenylstannyl)butyl sulphone

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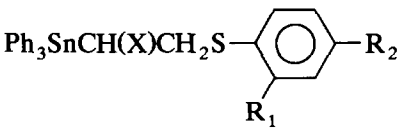
Abstract

The crystal structures of $Ph_3SnCH_2CH_2SO_2C_6H_4Me$-4 (**4**) and $Ph_3SnCH_2CH_2CH_2CH_2SO_2C_6H_4Me$-4 (**5**) have been determined. Both molecules contain tetrahedral tin atoms; the C–Sn–C angles in **4** range from 106.4(4) to 112.7(4)° and from 105.4(4) to 113.1(4)° in the two crystallographically independent molecules, while those in **5** lie between 107.2(2) and 113.6(2)°. The $Sn-C_{aryl}$ bond lengths in **4** and **5** fall in the range from 2.132(10) to 2.154(10) Å; the $Sn-C_{alkyl}$ bond lengths are also normal, being 2.158(10) and 2.165(10) Å in **4** and 2.147(5) Å in **5**. The environments about the sulphur atoms in **4** and **5** are similar and are essentially tetrahedral. A molecular mechanics plot showing the variation in potential energy of **4** with the Sn–C–C–S torsion angle is presented.

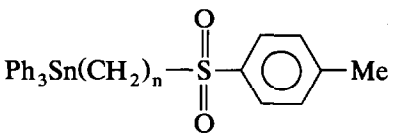
Key words: Tin; Crystal structure; X-ray diffraction; Organotin

1. Introduction

The crystal structures of β-sulphidoalkylstannanes, $Ph_3SnCHClCH_2SC_6H_3NO_2$-2-Me-4 (**1**) [1], $Ph_3SnCH(SCN)CH_2SC_6H_4NO_2$-2 (**2**) [1] and $Ph_3SnCH_2CH_2SC_6H_4Me$-4 (**3**) [2] have been determined previously. As expected, in all these compounds the solid state conformations about the central C–C bonds are staggered, but in **1** and **2** the Sn–C–C–S dihedral angles are about 60°, in contrast with the Sn–C–C–S dihedral angle in **3** of nearly 180°.



where X = Cl, $R_1 = NO_2$, R_2 = Me (**1**), X = SCN, $R_1 = NO_2$, R_2 = H (**2**) and X = R_1 = H, R_2 = Me.



where $n = 2$ (**4**) or $n = 4$ (**5**).

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The synthesis, NMR spectra and some reactions of the sulphone analogue of (3), viz $Ph_3SnCH_2CH_2SO_2C_6H_4Me$-4 (4), were reported previously [3]. In order to establish the solid state conformation of **4**, the crystal structure of **4** has been determined. A molecular mechanics study of **4** using the program HYPERCHEM [4] has also been performed. The crystal structure of $Ph_3SnCH_2CH_2CH_2CH_2SO_2C_6H_4Me$-4 (**5**) has also been determined.

2. Experimental details

Compound **4** was prepared from Ph_3SnH and $CH_2{=}CHSO_2C_6H_4Me$-4. Compound **5** was obtained by oxidation of $Ph_3SnCH_2CH_2CH_2CH_2SC_6H_4Me$-4 with 3-chloroperbenzoic acid in CH_2Cl_2 solution by previously reported procedures [3]. Both compounds were recrystallized from ethanol.

$Ph_3SnCH_2CH_2SO_2C_6H_4Me$-4: melting point (m.p.), 121–122°C, literature [3] m.p. 120–121°C. Anal. Found: C, 60.6; H, 4.8; S, 6.0. $C_{27}H_{26}O_2SSn$ Calc.: C, 60.8; H, 4.9; S, 6.0%.

$Ph_3SnCH_2CH_2CH_2CH_2SO_2C_6H_4Me$-4: m.p., 87–89°C; literature [3] m.p., 88.5–89.50°C. Anal. Found: C,

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62.1; H, 5.3; S, 5.6. $C_{29}H_{30}O_2SSn$ calc.: C, 62.0; H, 5.4; S, 5.7%.

The X-ray data were collected on a Delft Instruments Fast diffractometer and corrected for Lorentz and polarization effects but not for absorption. Details of the crystal data and the structure refinements using SHELXL-93 [5] are shown in Table 1. For **4**, only Sn and S were refined with anisotropic temperature factors whereas for **5** all non-hydrogen atoms were refined with anisotropic temperature factors. Hydrogen atoms were included at calculated positions in riding mode.

TABLE 1. Crystal data and structure refinement

	4	**5**
Empirical formula	$C_{27}H_{26}O_2SSn$	$C_{29}H_{30}O_2SSn$
Formula weight	533.23	561.28
Temperature (K)	150 (2)	150 (2)
Wavelength (Å)	0.71069	0.71069
Crystal system	Triclinic	Monoclinic
Space group	$P\bar{1}$	$P2_1/a$
Unit-cell dimensions		
a (Å)	9.913(2)	16.486(2)
b (Å)	10.931(2)	7.360(2)
c (Å)	22.452(9)	22.653(3)
α (°)	98.521(6)	90
β (°)	94.187(14)	108.346(13)
γ (°)	91.66(2)	90
Volume (Å^3)	2397.6(11)	2608.7(7)
Z	4	4
Density (calculated) (Mg m^{-3})	1.477	1.429
Absorption coefficient (mm^{-1})	1.173	1.082
$F(000)$	1080	1144
Crystal size (mm)	0.50×0.08×0.05	0.40×0.40×0.20
θ range for data collection (°)	1.97–25.51	1.89–25.06
Index ranges	$-8 \leq h \leq 10$	$-17 \leq h \leq 13$
	$-12 \leq k \leq 11$	$-8 \leq k \leq 5$
	$-12 \leq l \leq 25$	$-24 \leq l \leq 24$
Number of reflections collected	7868	7754
Number of independent reflections	6731	3778
Number of reflections ($I > 2\sigma(I)$)	1631	2951
Refinement method	Full matrix least squares on F^2	
Number of parameters	273	301
Goodness of fit on F^2	0.378	0.464
Final R indices R_1 ($I > 2\sigma(I)$)	0.0380	0.0252
R indices wR_2 (all data)	0.1904	0.0939
Residual diffraction maximum (electrons Å^{-3})	0.479	0.594
Residual diffraction minimum (electrons Å^{-3})	−0.428	−0.469

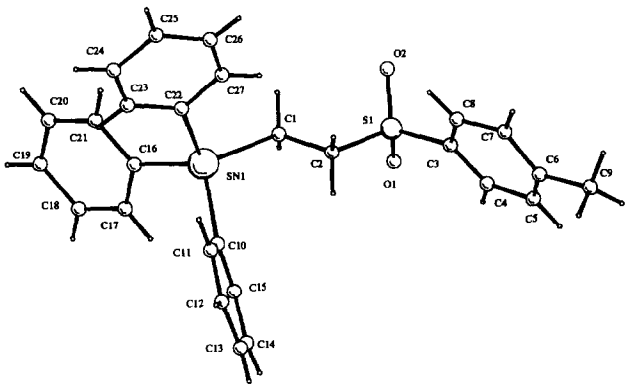

Fig. 1. The atomic arrangement in $Ph_3SnCH_2CH_2SO_2C_6H_4Me$-4 (**4**).

Molecular plots were obtained with the program SNOOPI [6].

3. Results and discussion

Atomic coordinates, bond lengths and valency angles for $Ph_3SnCH_2CH_2SO_2C_6H_4Me$-4 (**4**) are listed in

TABLE 2. Atomic coordinates and equivalent isotropic displacement parameters for **4**, where U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor

Atom	x (×10^{-4})	y (×10^{-4})	z (×10^{-4})	U_{eq} (×10^{-3} Å^2)
Sn(1)	1971(1)	4367(1)	1898(1)	33(1)
S(1)	5038(3)	6082(2)	3538(1)	37(1)
O(1)	5563(7)	4946(7)	3703(4)	44(2)
O(2)	5850(8)	6840(7)	3219(4)	48(2)
C(1)	3771(10)	5003(9)	2472(5)	33(2)
C(2)	3494(10)	5660(10)	3086(5)	36(2)
C(3)	4563(11)	7016(11)	4201(6)	42(3)
C(4)	4697(12)	6595(12)	4740(6)	54(3)
C(5)	4275(13)	7309(13)	5258(7)	66(4)
C(6)	3732(14)	8379(14)	5228(7)	66(4)
C(7)	3655(16)	8891(18)	4694(9)	91(5)
C(8)	4010(15)	8147(14)	4165(8)	77(4)
C(9)	3304(16)	9222(16)	5785(8)	89(5)
C(10)	387(10)	3877(9)	2426(5)	33(2)
C(11)	−810(12)	4499(12)	2410(6)	56(3)
C(12)	−1864(12)	4236(11)	2767(6)	46(3)
C(13)	−1721(13)	3370(12)	3148(6)	54(3)
C(14)	−570(12)	2742(12)	3164(6)	55(3)
C(15)	481(12)	2973(11)	2794(6)	45(3)
C(16)	2433(9)	2870(9)	1215(5)	29(2)
C(17)	2462(10)	1654(9)	1317(5)	35(2)
C(18)	2701(11)	717(11)	862(6)	47(3)
C(19)	2883(11)	995(11)	288(6)	47(3)
C(20)	2875(10)	2190(10)	178(5)	37(3)
C(21)	2634(11)	3126(11)	636(5)	42(3)
C(22)	1252(10)	5854(9)	1452(5)	31(2)
C(23)	428(10)	5648(10)	921(5)	37(3)

TABLE 2 (continued)

Atom	x ($\times 10^{-4}$)	y ($\times 10^{-4}$)	z ($\times 10^{-4}$)	U_{eq} ($\times 10^{-3}$ Å^2)
C(24)	−43(11)	6608(11)	642(6)	48(3)
C(25)	311(12)	7855(11)	892(6)	50(3)
C(26)	1108(11)	8055(10)	1427(5)	41(3)
C(27)	1589(10)	7085(9)	1694(5)	34(2)
Sn(1')	7001(1)	9550(1)	1976(1)	32(1)
S(1')	9937(3)	8445(2)	3548(1)	36(1)
O(1')	10448(7)	9677(7)	3802(4)	45(2)
O(2')	10827(7)	7633(7)	3203(4)	44(2)
C(1')	8768(10)	9268(9)	2559(5)	34(2)
C(2')	8449(10)	8602(9)	3068(5)	34(2)
C(3')	9393(10)	7699(10)	4137(5)	38(3)
C(4')	9246(12)	6403(11)	4066(6)	52(3)
C(5')	8757(11)	5856(12)	4525(6)	49(3)
C(6')	8460(12)	6530(11)	5061(6)	47(3)
C(7')	8643(12)	7802(12)	5131(6)	53(3)
C(8')	9081(11)	8387(11)	4679(5)	43(3)
C(9')	7999(14)	5873(13)	5560(7)	67(4)
C(10')	6310(10)	7766(9)	1500(5)	32(2)
C(11')	5060(10)	7600(10)	1164(5)	38(3)
C(12')	4594(11)	6471(10)	848(5)	37(3)
C(13')	5415(11)	5460(11)	866(6)	45(3)
C(14')	6664(11)	5608(11)	1176(6)	46(3)
C(15')	7123(12)	6752(11)	1500(6)	46(3)
C(16')	5334(10)	10235(9)	2466(5)	34(2)
C(17')	4337(10)	9400(9)	2591(5)	33(2)
C(18')	3280(11)	9777(10)	2927(5)	42(3)
C(19')	3227(12)	10970(11)	3174(6)	49(3)
C(20')	4157(12)	11869(11)	3060(6)	49(3)
C(21')	5233(10)	11482(10)	2694(5)	36(3)
C(22')	7464(9)	10810(9)	1373(5)	27(2)
C(23')	8764(10)	11027(10)	1203(5)	37(3)
C(24')	8959(11)	11804(10)	773(5)	39(3)
C(25')	7882(11)	12357(10)	502(6)	43(3)
C(26')	6612(11)	12148(10)	671(6)	42(3)
C(27')	6367(10)	11399(9)	1101(5)	33(2)

Tables 2 and 3; those for $Ph_3SnCH_2CH_2CH_2CH_2SO_2C_6H_4Me$-4 (**5**) are in Tables 4 and 5. The atomic arrangements for **4** and **5** are shown in Figs. 1 and 2. [1]

The geometries about tin in the two independent molecules of **4** are essentially tetrahedral, with C–Sn–C valency angles ranging from 106.4(4) to 112.7(4)° in one molecule and 105.4(4) to 113.1(4)° in the second. Compound **4** in the solid state takes up staggered conformations about the central C(1)–C(2) bonds, with Sn–C–C–S dihedral angles of 177.1(5) and −178.0(4)°. Thus there are no indications of even weak Sn–$S(O)_2$ interactions in the solid state. Molecular mechanics calculations were performed to examine the variation in molecular potential energy with the Sn–C–C–S torsion

[1] Lists of thermal parameters and H atom coordinates have been deposited with the Cambridge Crystallographic Data Centre. Lists of torsion angles and structure factor lists may be obtained from P.J.C.

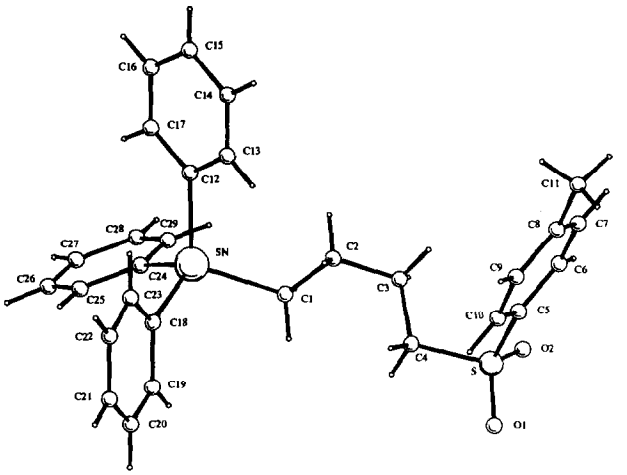

Fig. 2. The atomic arrangement in $Ph_3SnCH_2CH_2CH_2CH_2SO_2C_6H_4Me$-4 (**5**).

angle in **4**. The minimum energy value was associated with a torsion angle of −179.8° (Fig. 3), a value very close to those observed experimentally for the two crystallographically independent molecules.

Compound **5** also contains a tetrahedral tin atom with C–Sn–C valency angles ranging from 107.2(2) to 113.6(2)°.

The $Sn-C_{aryl}$ bond lengths in both **4** and **5** fall in the narrow range of 2.132(10)–2.154(10) Å; the $Sn-C_{alkyl}$ bond lengths are also unexceptional, being 2.158(10) and 2.165(10) Å in **4** and 2.147(5) Å in **5**.

The environments about the sulphur atoms in **4** and **5** are similar; the S–O bond lengths are between 1.439(8) and 1.451(8) Å. The $S-C_{aryl}$ bond lengths (1.762(12)–1.777(12) Å) and $S-C_{alkyl}$ bond lengths (1.775(4)–1.789(11) Å) are essentially the same and are comparable with those published for structures of alkyl aryl sulphones, including the tin-substituted derivative [6] $(4\text{-}MeSO_2C_6H_4)_4Sn$ (S–O, 1.415(10)–1.438(7) Å; $S-C_{alkyl}$, 1.773(4) and 1.774(4) Å; $S-C_{aryl}$ 1.781(16)–1.789(11) Å).

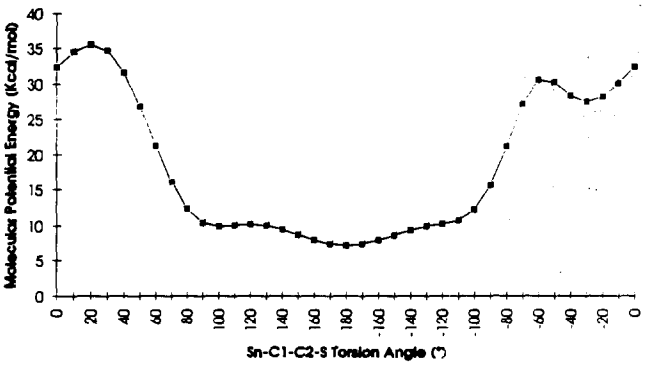

Fig. 3. Torsional potential energy diagram for **4**.

TABLE 3. Bond lengths (Å) and angles (°) for **4**

Bond angles			
Sn(1)–C(10)	2.137(10)	Sn(1')–C(22')	2.132(10)
Sn(1)–C(22)	2.145(11)	Sn(1')–C(16')	2.143(10)
Sn(1)–C(16)	2.154(10)	Sn(1')–C(10')	2.148(10)
Sn(1)–C(1)	2.158(10)	Sn(1')–C(1')	2.165(10)
S(1)–O(2)	1.439(8)	S(1')–O(1')	1.444(8)
S(1)–O(1)	1.446(8)	S(1')–O(2')	1.451(8)
S(1)–C(3)	1.777(12)	S(1')–C(3')	1.762(12)
S(1)–C(2)	1.783(10)	S(1')–C(2')	1.789(11)
C(1)–C(2)	1.505(14)	C(1')–C(2')	1.49(2)
C(3)–C(4)	1.36(2)	C(3')–C(8')	1.39(2)
C(3)–C(8)	1.38(2)	C(3')–C(4')	1.40(2)
C(4)–C(5)	1.40(2)	C(4')–C(5')	1.38(2)
C(5)–C(6)	1.31(2)	C(5')–C(6')	1.37(2)
C(6)–C(7)	1.40(2)	C(6')–C(7')	1.38(2)
C(6)–C(9)	1.53(2)	C(6')–C(9')	1.51(2)
C(7)–C(8)	1.41(2)	C(7')–C(8')	1.37(2)
C(10)–C(15)	1.38(2)	C(10')–C(15')	1.39(2)
C(10)–C(11)	1.39(2)	C(10')–C(11')	1.395(14)
C(11)–C(12)	1.41(2)	C(11')–C(12')	1.379(14)
C(12)–C(13)	1.37(2)	C(12')–C(13')	1.39(2)
C(13)–C(14)	1.35(2)	C(13')–C(14')	1.37(2)
C(14)–C(15)	1.42(2)	C(14')–C(15')	1.40(2)
C(16)–C(17)	1.383(14)	C(16')–C(21')	1.393(14)
C(16)–C(21)	1.40(2)	C(16')–C(17')	1.398(14)
C(17)–C(18)	1.37(2)	C(17')–C(18')	1.372(14)
C(18)–C(19)	1.39(2)	C(18')–C(19')	1.34(2)
C(19)–C(20)	1.37(2)	C(19')–C(20')	1.39(2)
C(20)–C(21)	1.38(2)	C(20')–C(21')	1.43(2)
C(22)–C(23)	1.38(2)	C(22')–C(23')	1.394(14)
C(22)–C(27)	1.396(13)	C(22')–C(27')	1.425(14)
C(23)–C(24)	1.38(2)	C(23')–C(24')	1.40(2)
C(24)–C(25)	1.42(2)	C(24')–C(25')	1.39(2)
C(25)–C(26)	1.37(2)	C(25')–C(26')	1.36(2)
C(26)–C(27)	1.37(2)	C(26')–C(27')	1.39(2)
Bond angles			
C(10)–Sn(1)–C(22)	106.4(4)	C(26)–C(27)–C(22)	122.0(11)
C(10)–Sn(1)–C(16)	112.7(4)	C(22')–Sn(1')–C(16')	108.3(4)
C(22)–Sn(1)–C(16)	107.9(4)	C(22')–Sn(1')–C(10')	111.8(4)
C(10)–Sn(1)–C(1)	110.5(4)	C(16')–Sn(1')–C(10')	105.4(4)
C(22)–Sn(1)–C(1)	109.1(4)	C(22')–Sn(1')–C(1')	111.0(4)
C(16)–Sn(1)–C(1)	110.0(4)	C(16')–Sn(1')–C(1')	113.1(4)
O(2)–S(1)–O(1)	119.7(5)	C(10')–Sn(1')–C(1')	107.2(4)
O(2)–S(1)–C(3)	108.2(5)	O(1')–S(1')–O(2')	118.2(4)
O(1)–S(1)–C(3)	108.6(5)	O(1')–S(1')–C(3')	108.4(5)
O(2)–S(1)–C(2)	107.7(5)	O(2')–S(1')–C(3')	108.3(5)
O(1)–S(1)–C(2)	106.4(5)	O(1')–S(1')–C(2')	107.5(5)
C(3)–S(1)–C(2)	105.3(5)	O(2')–S(1')–C(2')	107.9(5)
C(2)–C(1)–Sn(1)	114.0(7)	C(3')–S(1')–C(2')	105.9(5)
C(1)–C(2)–S(1)	110.7(7)	C(2')–C(1')–Sn(1')	113.3(7)
C(4)–C(3)–C(8)	119.8(14)	C(1')–C(2')–S(1')	111.2(7)
C(4)–C(3)–S(1)	120.0(10)	C(8')–C(3')–C(4')	118.8(11)
C(8)–C(3)–S(1)	120.1(11)	C(8')–C(3')–S(1')	120.5(9)
C(3)–C(4)–C(5)	120.0(14)	C(4')–C(3')–S(1')	120.7(9)
C(6)–C(5)–C(4)	121(2)	C(5')–C(4')–C(3')	119.0(12)
C(5)–C(6)–C(7)	122(2)	C(6')–C(5')–C(4')	122.3(12)
C(5)–C(6)–C(9)	123(2)	C(5')–C(6')–C(7')	118.0(13)
C(7)–C(6)–C(9)	115(2)	C(5')–C(6')–C(9')	119.8(12)
C(6)–C(7)–C(8)	118(2)	C(7')–C(6')–C(9')	122.1(12)
C(3)–C(8)–C(7)	120(2)	C(8')–C(7')–C(6')	121.6(12)

TABLE 3 (continued)

C(15)–C(10)–C(11)	116.9(11)	C(7′)–C(8′)–C(3′)	120.2(11)
C(15)–C(10)–Sn(1)	123.9(8)	C(15′)–C(10′)–C(11′)	118.1(10)
C(11)–C(10)–Sn(1)	119.2(9)	C(15′)–C(10′)–Sn(1′)	120.6(8)
C(10)–C(11)–C(12)	121.1(13)	C(11′)–C(10′)–Sn(1′)	121.2(7)
C(13)–C(12)–C(11)	120.8(12)	C(12′)–C(11′)–C(10′)	122.7(10)
C(14)–C(13)–C(12)	119.0(13)	C(11′)–C(12′)–C(13′)	118.1(11)
C(13)–C(14)–C(15)	120.7(13)	C(14′)–C(13′)–C(12′)	120.3(11)
C(10)–C(15)–C(14)	121.4(11)	C(13′)–C(14′)–C(15′)	121.2(11)
C(17)–C(16)–C(21)	118.5(10)	C(10′)–C(15′)–C(14′)	119.6(11)
C(17)–C(16)–Sn(1)	122.6(8)	C(21′)–C(16′)–C(17′)	118.0(9)
C(21)–C(16)–Sn(1)	118.8(7)	C(21′)–C(16′)–Sn(1′)	122.6(7)
C(18)–C(17)–C(16)	120.9(11)	C(17′)–C(16′)–Sn(1′)	119.4(7)
C(17)–C(18)–C(19)	119.4(11)	C(18′)–C(17′)–C(16′)	122.0(10)
C(20)–C(19)–C(18)	120.8(12)	C(19′)–C(18′)–C(17′)	119.8(11)
C(19)–C(20)–C(21)	119.6(12)	C(18′)–C(19′)–C(20′)	121.9(12)
C(20)–C(21)–C(16)	120.8(11)	C(19′)–C(20′)–C(21′)	118.1(11)
C(23)–C(22)–C(27)	117.0(10)	C(16′)–C(21′)–C(20′)	120.0(10)
C(23)–C(22)–Sn(1)	122.1(7)	C(23′)–C(22′)–C(27′)	118.4(10)
C(27)–C(22)–Sn(1)	120.9(8)	C(23′)–C(22′)–Sn(1′)	123.6(8)
C(24)–C(23)–C(22)	121.8(10)	C(27′)–C(22′)–Sn(1′)	117.8(7)
C(23)–C(24)–C(25)	120.7(12)	C(22′)–C(23′)–C(24′)	119.7(11)
C(26)–C(25)–C(24)	117.2(12)	C(25′)–C(24′)–C(23′)	121.5(10)
C(27)–C(26)–C(25)	121.3(11)	C(26′)–C(25′)–C(24′)	118.7(12)
		C(25′)–C(26′)–C(27′)	122.0(12)
		C(26′)–C(27′)–C(22′)	119.7(10)

TABLE 4. Atomic coordinates and equivalent isotropic displacement parameters for **5**, where U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor

Atom	x ($\times 10^{-4}$)	y ($\times 10^{-4}$)	z ($\times 10^{-4}$)	U_{eq} ($\times 10^{-3}$ Å^2)
Sn	2062(1)	829(1)	1825(1)	22(1)
S	1935(1)	7413(1)	3932(1)	22(1)
O(1)	1758(2)	9181(4)	3646(2)	31(1)
O(2)	1376(2)	6721(4)	4260(1)	29(1)
C(1)	1677(3)	2450(6)	2478(2)	27(1)
C(2)	2388(3)	2758(6)	3088(2)	26(1)
C(3)	2126(3)	3912(5)	3560(2)	24(1)
C(4)	1946(3)	5858(5)	3336(2)	23(1)
C(5)	2991(3)	7367(5)	4444(2)	22(1)
C(6)	3178(3)	6592(6)	5024(2)	24(1)
C(7)	4010(3)	6526(6)	5409(2)	29(1)
C(8)	4673(3)	7216(5)	5214(2)	23(1)
C(9)	4472(3)	7975(5)	4626(2)	27(1)
C(10)	3643(3)	8073(5)	4242(2)	24(1)
C(11)	5581(3)	7107(6)	5636(2)	35(1)
C(12)	3144(3)	−833(6)	2292(2)	25(1)
C(13)	3873(3)	−69(7)	2714(2)	29(1)
C(14)	4564(3)	−1161(7)	3030(2)	34(1)
C(15)	4543(3)	−2997(7)	2918(2)	38(1)
C(16)	3835(3)	−3767(7)	2487(2)	39(1)
C(17)	3141(3)	−2699(6)	2177(2)	30(1)
C(18)	2447(3)	2601(5)	1213(2)	21(1)
C(19)	1905(3)	3982(6)	885(2)	28(1)
C(20)	2170(3)	5176(7)	518(2)	36(1)
C(21)	2981(4)	5070(7)	481(2)	39(1)
C(22)	3539(3)	3754(7)	804(2)	40(1)
C(23)	3266(3)	2513(6)	1164(2)	30(1)
C(24)	1037(3)	−949(5)	1356(2)	22(1)
C(25)	772(3)	−1260(6)	722(2)	28(1)
C(26)	117(3)	−2476(6)	449(2)	34(1)
C(27)	−275(3)	−3406(7)	807(2)	37(1)
C(28)	−30(3)	−3097(6)	1439(2)	40(1)
C(29)	619(3)	−1881(6)	1708(2)	31(1)

TABLE 5. Bond lengths (Å) and angles (°) for **5**

Bond lengths			
Sn–C(24)	2.138(4)	C(12)–C(13)	1.396(6)
Sn–C(18)	2.140(4)	C(12)–C(17)	1.398(6)
Sn–C(1)	2.145(4)	C(13)–C(14)	1.394(6)
Sn–C(12)	2.147(5)	C(14)–C(15)	1.374(6)
S–O(1)	1.442(3)	C(15)–C(16)	1.384(7)
S–O(2)	1.446(3)	C(16)–C(17)	1.384(6)
S–C(5)	1.763(4)	C(18)–C(23)	1.390(6)
S–C(4)	1.775(4)	C(18)–C(19)	1.402(6)
C(1)–C(2)	1.521(6)	C(19)–C(20)	1.373(6)
C(2)–C(3)	1.531(5)	C(20)–C(21)	1.368(7)
C(3)–C(4)	1.517(5)	C(21)–C(22)	1.378(7)
C(5)–C(6)	1.375(6)	C(22)–C(23)	1.391(6)
C(5)–C(10)	1.395(6)	C(24)–C(25)	1.381(6)
C(6)–C(7)	1.376(6)	C(24)–C(29)	1.388(6)
C(7)–C(8)	1.397(6)	C(25)–C(26)	1.389(6)
C(8)–C(9)	1.386(6)	C(26)–C(27)	1.369(7)
C(8)–C(11)	1.503(6)	C(27)–C(28)	1.379(7)
C(9)–C(10)	1.371(6)	C(28)–C(29)	1.380(6)
Bond angles			
C(24)–Sn–C(18)	113.6(2)	C(9)–C(10)–C(5)	119.4(4)
C(24)–Sn–C(1)	108.9(2)	C(13)–C(12)–C(17)	118.4(4)
C(18)–Sn–C(1)	108.7(2)	C(13)–C(12)–Sn	120.7(3)
C(24)–Sn–C(12)	107.5(2)	C(17)–C(12)–Sn	121.0(3)
C(18)–Sn–C(12)	107.2(2)	C(14)–C(13)–C(12)	120.5(4)
C(1)–Sn–C(12)	110.9(2)	C(15)–C(14)–C(13)	120.2(5)
O(1)–S–O(2)	118.5(2)	C(14)–C(15)–C(16)	120.0(5)
O(1)–S–C(5)	109.3(2)	C(17)–C(16)–C(15)	120.3(5)
O(2)–S–C(5)	108.2(2)	C(16)–C(17)–C(12)	120.7(5)
O(1)–S–C(4)	106.8(2)	C(23)–C(18)–C(19)	117.7(4)
O(2)–S–C(4)	108.9(2)	C(23)–C(18)–Sn	121.1(3)
C(5)–S–C(4)	104.1(2)	C(19)–C(18)–Sn	121.0(3)
C(2)–C(1)–Sn	113.4(3)	C(20)–C(19)–C(18)	120.9(4)
C(1)–C(2)–C(3)	114.2(4)	C(21)–C(20)–C(19)	120.3(5)
C(4)–C(3)–C(2)	111.0(3)	C(20)–C(21)–C(22)	120.6(4)
C(3)–C(4)–S	113.6(3)	C(21)–C(22)–C(23)	119.2(5)
C(6)–C(5)–C(10)	120.3(4)	C(18)–C(23)–C(22)	121.2(4)
C(6)–C(5)–S	120.9(3)	C(25)–C(24)–C(29)	117.6(4)
C(10)–C(5)–S	118.8(3)	C(25)–C(24)–Sn	124.1(3)
C(5)–C(6)–C(7)	119.9(4)	C(29)–C(24)–Sn	118.3(3)
C(6)–C(7)–C(8)	120.7(4)	C(24)–C(25)–C(26)	121.1(4)
C(9)–C(8)–C(7)	118.4(4)	C(27)–C(26)–C(25)	120.3(4)
C(9)–C(8)–C(11)	121.5(4)	C(26)–C(27)–C(28)	119.6(4)
C(7)–C(8)–C(11)	120.1(4)	C(27)–C(28)–C(29)	119.9(4)
C(10)–C(9)–C(8)	121.3(4)	C(28)–C(29)–C(24)	121.5(4)

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