N2—Mo—S1	90.86 (8)	C15—C16—C17	120.0 (3)
O4—Mo—S1	90.67 (6)	C16—C17—C18	120.9 (3)
O2—Mo—S1	78.12 (6)	C17—C18—C13	119.7 (3)
S2—Mo—S1	164.14 (3)	C17—C18—C19	116.8 (3)
C13—S1—Mo	102.18 (10)	C13—C18—C19	123.5 (3)
C20—S2—Mo	114.22 (10)	O1—C19—O2	122.2 (3)
C19—O2—Mo	134.8 (2)	O1—C19—C18	116.7 (3)
C26—O4—Mo	141.8 (2)	O2—C19—C18	121.1 (3)
N2—N1—C7	119.1 (2)	C25—C20—C21	118.1 (3)
N2—N1—C1	118.5 (2)	C25—C20—S2	128.5 (2)
C7—N1—C1	122.2 (2)	C21—C20—S2	113.5 (2)
N1—N2—Mo	176.1 (2)	C22—C21—C20	121.6 (3)
C2—C1—C6	120.7 (3)	C23—C22—C21	120.4 (3)
C2—C1—N1	119.5 (3)	C22—C23—C24	119.2 (3)
C6—C1—N1	119.8 (3)	C23—C24—C25	122.0 (3)
C1—C2—C3	118.9 (4)	C20—C25—C24	118.7 (3)
C4—C3—C2	120.0 (4)	C20—C25—C26	125.8 (2)
C5—C4—C3	120.8 (4)	C24—C25—C26	115.5 (3)
C4—C5—C6	119.4 (4)	O3—C26—O4	120.4 (3)
C5—C6—C1	120.1 (4)	O3—C26—C25	117.0 (2)
C12—C7—C8	120.1 (3)	O4—C26—C25	122.6 (3)
C12—C7—N1	120.4 (3)		

The structure was solved through a combination of direct methods and difference Fourier synthesis. Refinement was on F^2 using the whole data set. H atoms were included at their expected positions, with fixed thermal parameters, and allowed to ride on their host atoms. The two disordered NHEt3 groups were subject to a mild similarity restraint in homologous bond distances.

Data collection: *P3/P4-PC* (Siemens, 1991). Cell refinement: *P3/P4-PC*. Data reduction: *XDISK* in *SHELXTL/PC* (Sheldrick, 1991). Program(s) used to solve structure: *XS* in *SHELXTL/PC*. Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *XP* in *SHELXTL/PC*. Software used to prepare material for publication: *CIFTAB*.

Lists of structure factors, anisotropic displacement parameters, least-squares-planes data, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: CR1181). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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(N,N-Dimethylthiocarbamoylthioacetato)-triphenyltin

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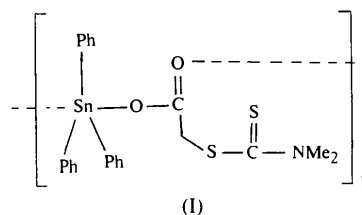*Department of Chemistry, University of Malaya, 59100 Kuala Lumpur, Malaysia*

Abstract

Carboxylate bridges link the two independent molecules in the asymmetric unit of the title compound, $[Sn(C_5H_8NO_2S_2)(C_6H_5)_3]$, into a helical chain parallel to **b** {*i.e. catena*-poly[triphenyltin-μ-(N,N-dimethylthiocarbamoylthioacetato)-O:O']}. Both five-coordinate Sn atoms show *trans*-C_3SnO_2 trigonal bipyramidal coordination geometry.

Comment

The bond lengths around the Sn atoms in this fungicidal compound, (I) (Kumar Das, Kuthubutheen, Ng & Ng, 1987), compare well with those found in other carboxylate-bridged triorganotin carboxylates (Ng, Chen

(I)

& Kumar Das, 1988). The repeat distance of the chain (4.33 Å) is much shorter than that found for $(C_4H_9)_3SnO_2CCH_2SC(S)N(CH_3)(C_6H_5)$ (5.12 Å; Ng, Chen, Kumar Das, Yap & Butcher, 1992), and is in agreement with the flexible chain structure previously inferred from variable-temperature Mössbauer spectroscopy ($a = -0.0152\,\mathrm{K}^{-1}$) (Ng & Kumar Das,
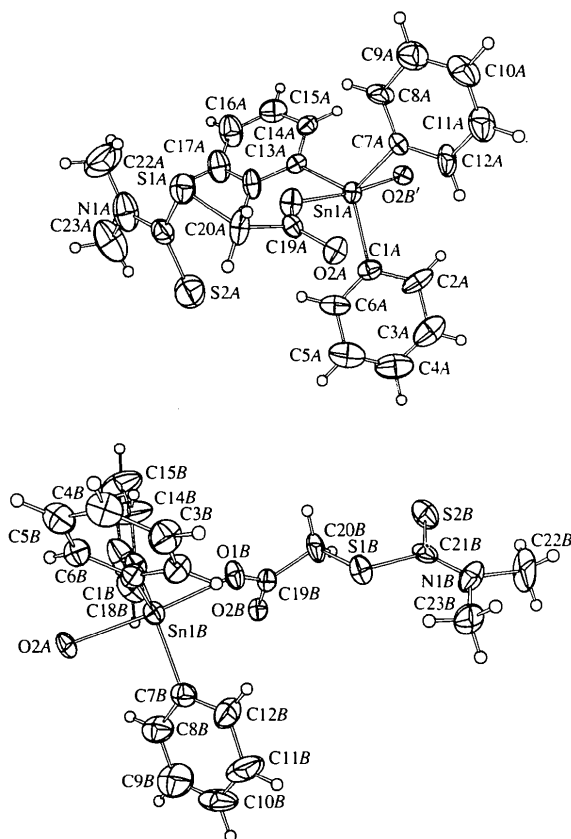
Fig. 1. Atomic labelling for the two independent molecules of the title compound. Displacement ellipsoids are plotted at the 30% probability level.
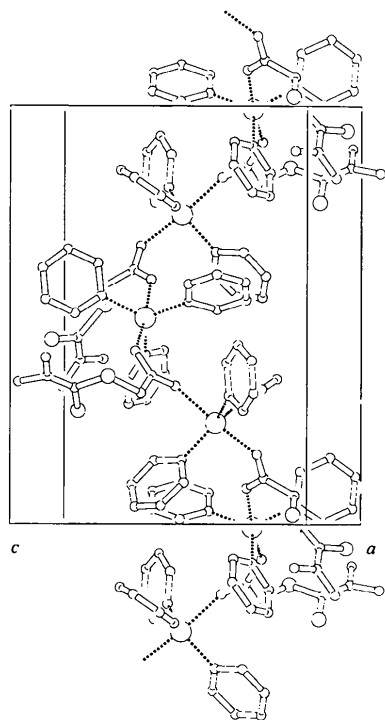

Fig. 2. View of the polymeric chain.

1991). The slope exceeds that ($a = -0.0143\,\mathrm{K}^{-1}$) for (C6H5)3SnO2CCH3 (Ng, Chin, Chen, Kumar Das & Butcher, 1989), which is more rigid and has a repeat distance of 5.07 Å (Molloy, Purcell, Quill & Nowell, 1984). Tiekink (1991) has reviewed the structures of organotin carboxylates.

Experimental

The compound was synthesized by condensing triphenyltin hydroxide with N,N-dimethylthiocarbamoylthioacetic acid in either ethanol or toluene (Ng & Kumar Das, 1991). Transparent crystals were grown from an ethanol solution of the compound.

Crystal data

[Sn(C5H8NO2S2)(C6H5)3]	Mo $K\alpha$ radiation
$M_r = 528.26$	$\lambda = 0.71073$ Å
Monoclinic	Cell parameters from 25
$P2_1/c$	reflections
$a = 12.391\,(5)$ Å	$\theta = 8-10°$
$b = 17.316\,(4)$ Å	$\mu = 1.285$ mm^{-1}
$c = 21.908\,(7)$ Å	$T = 300$ K
$\beta = 95.92\,(2)°$	Irregular
$V = 4676\,(3)$ Å^3	$0.29 \times 0.25 \times 0.22$ mm
$Z = 8$	Colorless
$D_x = 1.501$ Mg m^{-3}	

Data collection

Enraf–Nonius CAD-4 diffractometer	3270 observed reflections [$I > 3\sigma(I)$]
ω scans	$R_{int} = 0.027$
Absorption correction:	$\theta_{max} = 22.5°$
ψ scan (North, Phillips & Mathews, 1968)	$h = 0 \rightarrow 13$
	$k = 0 \rightarrow 8$
$T_{min} = 0.873$, $T_{max} = 0.999$	$l = -23 \rightarrow 23$
6687 measured reflections	3 standard reflections frequency: 60 min
6420 independent reflections	intensity decay: none

Refinement

Refinement on F	$w = 1/[\sigma^2(F) + 0.0004|F|^2 + 1]$
$R = 0.050$	
$wR = 0.055$	$(\Delta/\sigma)_{max} = 0.03$
$S = 0.446$	$\Delta\rho_{max} = 0.83\,(9)$ e Å^{-3}
3270 reflections	$\Delta\rho_{min} = -0.17\,(9)$ e Å^{-3}
547 parameters	Extinction correction: none
H-atom parameters not refined	Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

B_{iso} for S1Bb to C23Bb, $B_{eq} = (4/3)\Sigma_i\Sigma_j\beta_{ij}a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$ for all others.

	x	y	z	B_{iso}/B_{eq}
Sn1A	0.32276 (7)	0.49233 (5)	0.27287 (4)	3.52 (2)
S1A	0.2323 (3)	0.3531 (3)	0.4646 (2)	5.7 (1)
S2A	0.1131 (5)	0.2708 (4)	0.3580 (2)	9.2 (2)

O1A	0.3042 (6)	0.4139 (5)	0.3500 (4)	4.6 (2)
O2A	0.4373 (6)	0.3304 (5)	0.3390 (4)	4.3 (2)
N1A	0.024 (1)	0.3527 (9)	0.4388 (7)	8.3 (4)
C1A	0.311 (1)	0.4049 (8)	0.2045 (6)	4.3 (3)
C2A	0.364 (1)	0.4149 (9)	0.1530 (6)	6.0 (4)
C3A	0.358 (1)	0.360 (1)	0.1078 (7)	8.0 (5)
C4A	0.297 (2)	0.296 (1)	0.1138 (8)	9.4 (5)
C5A	0.248 (2)	0.287 (1)	0.1642 (9)	9.3 (6)
C6A	0.254 (1)	0.3407 (9)	0.2094 (7)	6.7 (4)
C7A	0.4765 (9)	0.5308 (7)	0.3103 (5)	3.2 (3)
C8A	0.485 (1)	0.5745 (9)	0.3616 (7)	5.7 (4)
C9A	0.586 (1)	0.598 (1)	0.3879 (8)	7.6 (5)
C10A	0.676 (1)	0.579 (1)	0.3647 (7)	7.8 (5)
C11A	0.670 (1)	0.535 (1)	0.3139 (7)	7.3 (5)
C12A	0.569 (1)	0.512 (1)	0.2866 (6)	5.9 (4)
C13A	0.1791 (9)	0.5454 (7)	0.2968 (5)	3.6 (3)
C14A	0.167 (1)	0.6252 (8)	0.2949 (6)	4.7 (3)
C15A	0.069 (1)	0.6585 (9)	0.3081 (8)	6.7 (4)
C16A	−0.013 (1)	0.614 (1)	0.3240 (9)	9.5 (5)
C17A	−0.003 (1)	0.537 (1)	0.3277 (9)	7.9 (5)
C18A	0.094 (1)	0.5036 (9)	0.3146 (7)	5.9 (4)
C19A	0.3617 (8)	0.3552 (7)	0.3668 (5)	3.0 (3)
C20A	0.336 (1)	0.3136 (8)	0.4234 (6)	4.6 (3)
C21A	0.113 (1)	0.3256 (8)	0.4198 (7)	5.1 (4)
C22A	0.028 (2)	0.398 (2)	0.493 (1)	14.6 (9)
C23A	−0.080 (1)	0.340 (1)	0.410 (1)	12.6 (8)
Sn1B	0.57656 (7)	0.24164 (6)	0.35759 (4)	3.69 (2)
S1B†	0.8499 (4)	0.0225 (3)	0.4299 (2)	4.7 (1)
S2B†	1.0168 (5)	−0.0591 (4)	0.3641 (3)	6.7 (2)
O1B	0.7191 (7)	0.1663 (5)	0.3769 (4)	4.4 (2)
O2B	0.6711 (6)	0.0859 (5)	0.3016 (4)	3.7 (2)
N1B†	0.939 (1)	−0.1086 (9)	0.4659 (8)	5.3 (4)
C1B	0.636 (1)	0.3071 (7)	0.4363 (6)	3.9 (3)
C2B	0.692 (1)	0.2712 (8)	0.4864 (6)	4.8 (3)
C3B	0.736 (1)	0.3130 (9)	0.5368 (7)	6.3 (4)
C4B	0.729 (1)	0.390 (1)	0.5372 (6)	6.4 (4)
C5B	0.675 (1)	0.4283 (9)	0.4883 (7)	5.9 (4)
C6B	0.628 (1)	0.3851 (8)	0.4377 (6)	4.5 (3)
C7B	0.464 (1)	0.1526 (8)	0.3687 (6)	4.8 (3)
C8B	0.365 (1)	0.151 (1)	0.3309 (8)	7.5 (5)
C9B	0.291 (2)	0.094 (1)	0.339 (1)	11.0 (7)
C10B	0.310 (1)	0.0412 (9)	0.3823 (9)	10.2 (5)
C11B	0.404 (2)	0.044 (1)	0.4206 (9)	10.2 (6)
C12B	0.480 (1)	0.099 (1)	0.4129 (9)	8.0 (5)
C13B	0.628 (1)	0.2799 (8)	0.2734 (5)	4.1 (3)
C14B	0.717 (1)	0.322 (1)	0.2717 (8)	9.9 (5)
C15B	0.757 (2)	0.347 (1)	0.2193 (9)	12.9 (6)
C16B	0.703 (2)	0.330 (1)	0.1659 (8)	9.3 (5)
C17B	0.613 (1)	0.287 (1)	0.1641 (7)	9.5 (6)
C18B	0.574 (1)	0.262 (1)	0.2182 (7)	7.7 (5)
C19B	0.7374 (9)	0.1091 (7)	0.3452 (6)	3.8 (3)
C20B	0.842 (1)	0.0681 (8)	0.3603 (6)	5.3 (4)
C21B†	0.940 (1)	−0.055 (1)	0.421 (1)	4.3 (5)
C22B†	1.000 (3)	−0.172 (1)	0.467 (2)	11 (1)
C23B†	0.871 (2)	−0.106 (1)	0.514 (1)	6.3 (6)
S1Bb‡	0.9442 (9)	0.1041 (7)	0.4060 (5)	4.9 (2)
S2Bb‡	0.805 (1)	0.0505 (9)	0.5009 (7)	7.1 (3)
N1Bb‡	0.980 (3)	0.124 (2)	0.527 (2)	7 (1)
C21Bb‡	0.914 (3)	0.094 (2)	0.484 (2)	3.6 (8)
C22Bb‡	0.985 (5)	0.121 (3)	0.592 (3)	9 (2)
C23Bb‡	1.096 (4)	0.159 (3)	0.497 (2)	8 (1)

† Site occupancy = 0.67.
‡ Site occupancy = 0.33.

Table 2. Selected geometric parameters (Å, °)

Sn1A—O1A	2.199 (9)	Sn1B—O1B	2.201 (9)
Sn1A—O2B'	2.307 (9)	Sn1B—O2A	2.315 (8)
Sn1A—C1A	2.13 (1)	Sn1B—C1B	2.13 (1)
Sn1A—C7A	2.10 (1)	Sn1B—C7B	2.11 (2)
Sn1A—C13A	2.12 (1)	Sn1B—C13B	2.12 (1)
O1A—Sn1A—C1A	95.5 (5)	O2A—Sn1B—O1B	174.8 (3)
O1A—Sn1A—C7A	93.4 (4)	O2A—Sn1B—C1B	88.7 (4)
O1A—Sn1A—C13A	85.4 (4)	O2A—Sn1B—C7B	91.0 (5)
O1A—Sn1A—O2B'	172.5 (3)	O2A—Sn1B—C13B	85.8 (4)

O2B'—Sn1A—C1A	90.4 (4)	O1B—Sn1B—C1B	87.5 (4)
O2B'—Sn1A—C7A	87.6 (4)	O1B—Sn1B—C7B	94.0 (5)
O2B'—Sn1A—C13A	87.7 (4)	O1B—Sn1B—C13B	92.5 (4)
C1A—Sn1A—C7A	119.7 (5)	C1B—Sn1B—C7B	118.2 (5)
C1A—Sn1A—C13A	119.0 (5)	C1B—Sn1B—C13B	115.3 (5)
C7A—Sn1A—C13A	121.1 (5)	C7B—Sn1B—C13B	126.3 (6)
Sn1A—O1A—C19A	127.9 (8)	Sn1B—O1B—C19B	123.6 (8)
Sn1A—O2B'—C19B'	133.9 (9)	Sn1B—O2A—C19A	136.7 (8)

Symmetry code: (i) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$.

The Sn atoms were found by direct methods and the other non-H atoms were located from difference Fourier maps. The thiocarbamoylthio group of molecule B was disordered over two positions, the occupancies of which were set at 0.67 and 0.33. The atoms of the thiocarbamoylthio group with the site occupancy factor of 0.33 were refined isotropically; other non-H atoms were refined anisotropically. H atoms were placed at calculated positions (C—H = 0.95 Å) and included in the structure-factor calculations.

Data collection and cell refinement: CAD-4 diffractometer software (Enraf–Nonius, 1988). Data reduction: *MolEN* (Fair, 1990). Structure refinement: *MolEN*. Molecular graphics: *ORTEP*II (Johnson, 1976); *PLUTON* (Spek, 1994). Preparation of material for publication: *MolEN*.

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