4,5-Diphenyl-2-(trimethylstannylsulfanyl)-1,3-oxazole

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The mononuclear title complex, $[Sn(CH_3)_3(C_{15}H_{10}NOS)]$, features a distorted C_3S tetrahedral geometry for Sn with some of the distortion ascribed to an intramolecular $Sn\cdots N$ interaction. Intermolecular $Sn\cdots S$ interactions lead to the formation of a helical chain.

Comment

In recent years, organotin complexes have attracted increasing attention owing to their wide industrial applications and biological activities (Duboy & Roy, 2003). In order to explore the relationships between these applications and their structures, a large number of organotin compounds have been prepared and studied (Gielen, 2002). In this connection, we report the structure of the title compound, (I). As shown in Fig. 1, the Sn atom in (I) is four-coordinated so that the C_3S donor set defines a distorted tetrahedral geometry. Some of the distortion is ascribed to an intramolecular $Sn\cdots N1$ interaction of 3.147 (3) Å. If this interaction was considered significant, the geometry would be best considered as distorted trigonal bipyramidal, the axial N1—Sn1—C18 angle being 157.06 (13)°. The Sn—C and Sn—S bond lengths (Table 1) are in good agreement with those found in (1-phenyl-1*H*-tetrazole-5-thiolato)trimethyltin (Cea-Olivares *et al.*, 1994); the $Sn\cdots N$ interaction in this structure, of 3.285 (12) Å, is also comparable to that found in (I). There is an intermolecular $Sn\cdots S^i$ contact of 3.6857 (12) Å, such that molecules are associated into a helical chain along the *b* axis, as shown in Fig. 2 [symmetry code: (i) $\frac{3}{2} - x$, $-\frac{1}{2} + y$, $\frac{1}{2} - z$].

(I)
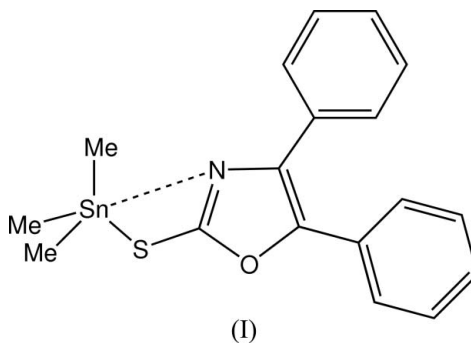
Experimental

All reagents and solvents were used as obtained and the reaction was carried out under a nitrogen atmosphere. 4,5-Diphenyl-4-oxazoline-2-thione (0.253 g, 1 mmol) was added to sodium ethoxide (0.068 g, 1 mmol) in benzene (20 ml). After stirring for 10 min, trimethyltin chloride (0.199 g, 1 mmol) was added and the reaction was continued
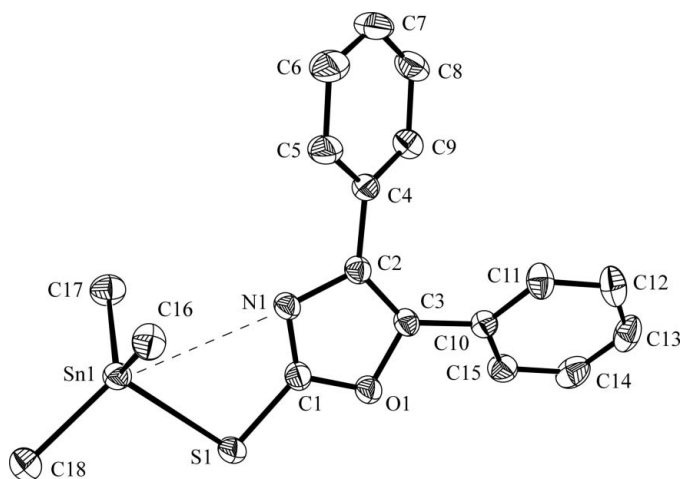
Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted for clarity. The dashed line indicates the intramolecular Sn···N1 interaction.

for 12 h at 313 K. After cooling to room temperature, the solution was filtered. The filtrate was gradually removed by evaporation under vacuum until a solid product was obtained. This solid was recrystallized from dichloromethane and colorless crystals suitable for X-ray diffraction were obtained. Yield 0.384 g, 85%. M.p. 424 K. Analysis found: C 51.93, H 4.61, N 3.36%; $C_{18}H_{19}NOSSn$ requires: C 51.96, H 4.60, N 3.37%.

Crystal data

$[Sn(CH_3)_3(C_{15}H_{10}NOS)]$	$D_x = 1.516$ Mg m^{-3}
$M_r = 416.09$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 5503
$a = 9.267$ (3) Å	reflections
$b = 9.824$ (3) Å	$\theta = 2.3$–27.9°
$c = 20.477$ (6) Å	$\mu = 1.52$ mm^{-1}
$\beta = 102.144$ (4)°	$T = 298$ (2) K
$V = 1822.5$ (9) Å^3	Block, colorless
$Z = 4$	$0.49 \times 0.42 \times 0.35$ mm

Data collection

Siemens SMART CCD area detector diffractometer	3201 independent reflections
	2687 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.031$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 25.0°$
	$h = -11 \rightarrow 8$
$T_{min} = 0.498$, $T_{max} = 0.588$	$k = -11 \rightarrow 10$
9231 measured reflections	$l = -12 \rightarrow 24$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0669P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.032$	$+ 0.3413P]$
$wR(F^2) = 0.097$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.001$
3201 reflections	$\Delta\rho_{max} = 0.41$ e Å^{-3}
199 parameters	$\Delta\rho_{min} = -0.95$ e Å^{-3}
H-atom parameters constrained	
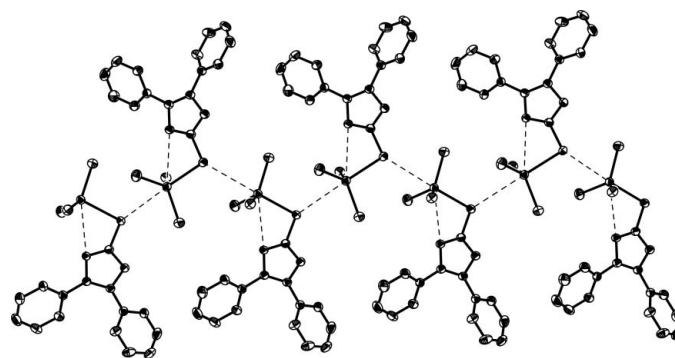
Figure 2
A supramolecular one-dimensional chain in (I), mediated by Sn···S interactions. H atoms have been omitted.

Table 1
Selected geometric parameters (Å, °).

Sn1—S1	2.4932 (11)	Sn1—C17	2.124 (4)
Sn1—N1	3.147 (3)	Sn1—C18	2.129 (4)
Sn1—C16	2.120 (4)	Sn1—S1^i	3.6857 (12)
S1—Sn1—N1	56.53 (5)	N1—Sn1—C18	157.06 (13)
S1—Sn1—C16	102.38 (12)	C16—Sn1—C17	118.54 (17)
S1—Sn1—C17	104.54 (13)	C16—Sn1—C18	115.46 (17)
S1—Sn1—C18	100.53 (13)	C17—Sn1—C18	112.30 (18)
N1—Sn1—C16	73.56 (13)	S1—Sn1—S1^i	168.995 (18)
N1—Sn1—C17	77.35 (14)		

Symmetry code: (i) $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$.

The H atoms were included in the riding-model approximation, with C—H(aromatic) = 0.93 Å and C—H(methyl) = 0.96 Å, and with $U_{iso}(H) = 1.2U_{eq}$(C aromatic) and $U_{iso}(H) = 1.5U_{eq}$(C methyl).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

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