

catena-Poly[[trimethyltin(IV)]- μ -4-methyl-4*H*-1,2,4-triazole-3-thiolato- κ^2 S:N¹]

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Key indicators

Single-crystal X-ray study
 $T = 100$ K
 Mean $\sigma(N-C) = 0.004$ Å
 R factor = 0.017
 wR factor = 0.041
 Data-to-parameter ratio = 19.7

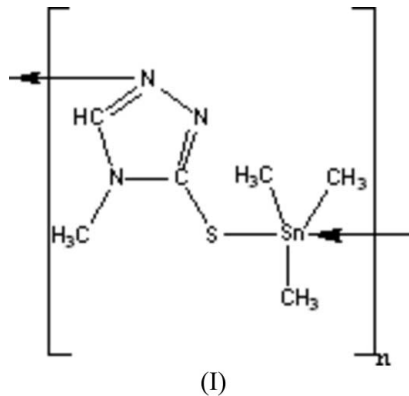
For details of how these key indicators were
 automatically derived from the article, see
<http://journals.iucr.org/e>.

The crystal structure of the title compound, $[\text{Sn}(\text{CH}_3)_3(\text{C}_3\text{H}_4\text{N}_3\text{S})]_n$, consists of a linear chain in which adjacent trimethyltin groups are bridged by the 4-methyl-4*H*-1,2,4-triazole-3-thiolate anion through its N and S atoms.

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Comment

The synthesis and structural chemistry of organotin compounds is still a fertile area of research because of their extensive biological applications. However, there is relatively little information available on organotin compounds as anti-cancer agents *in vivo*. Diorganotins represent the largest group of tin compounds to have been extensively examined for cytotoxicity *in vitro*; they have been found to be less toxic than platinum complexes (Narayan, 1983). We report here the structure of the title compound, (I), in a continuation of our work on the synthesis and structural characterization of organotin complexes of sulfur donor ligands (Shahzadi, Ali, Bhatti *et al.*, 2006, Shahzadi, Ali & Fettouhi, 2006).



In the crystal structure of (I) (Fig. 1), the Sn atom is bonded to three methyl groups in equatorial positions. The axial positions are occupied by N and S atoms of a 4-methyl-4*H*-1,2,4-triazole-3-thiolate anion, with an almost linear S—Sn—N angle; the Sn atom has a distorted trigonal-bipyramidal coordination geometry. The Sn—S bond length is 2.7116 (7) Å, which is shorter than the Sn—S bond distance reported earlier (Shahzadi, Ali, Bhatti *et al.*, 2006, Shahzadi, Ali & Fettouhi, 2006).

Experimental

3-Mercapto-4-methyl-4*H*-1,2,4-triazole (0.15 g, 1 mmol) and triethylamine (0.1 g, 1 mmol) were suspended in dry toluene (150 ml) in a two-necked round-bottomed flask equipped with a water condenser. The mixture was stirred for 25 min at room temperature

and then trimethyltin chloride (0.2 g, 1 mmol) was added. The reaction mixture was refluxed for 4–5 h. After cooling at room temperature, triethylammonium chloride formed, was filtered off and the solvent was removed on a rotary evaporator under reduced pressure. The solid product was recrystallized from chloroform to obtain crystals suitable for X-ray analysis (yield 80%; m.p. 433 K).

Crystal data

[Sn(CH ₃) ₃ (C ₃ H ₄ N ₃ S)]	Z = 4
<i>M_r</i> = 277.94	<i>D_x</i> = 1.822 Mg m ⁻³
Orthorhombic, <i>Pna</i> 2 ₁	Mo <i>K</i> α radiation
<i>a</i> = 13.7254 (11) Å	<i>μ</i> = 2.68 mm ⁻¹
<i>b</i> = 11.0183 (9) Å	<i>T</i> = 100 (2) K
<i>c</i> = 6.6998 (5) Å	Plate, colourless
<i>V</i> = 1013.21 (14) Å ³	0.40 × 0.30 × 0.05 mm

Data collection

Bruker APEX CCD diffractometer	7581 measured reflections
<i>φ</i> and <i>ω</i> scans	2051 independent reflections
Absorption correction: multi-scan	2032 reflections with <i>I</i> > 2σ(<i>I</i>)
(<i>SADABS</i> ; Bruker, 2001)	<i>R</i> _{int} = 0.025
<i>T</i> _{min} = 0.414, <i>T</i> _{max} = 0.878	<i>θ</i> _{max} = 26.3°

Refinement

Refinement on <i>F</i> ²	$w = 1/[\sigma^2(F_o^2) + (0.0189P)^2 + 0.5609P]$
$R[F^2 > 2\sigma(F^2)] = 0.017$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.042$	(Δ/σ) _{max} = 0.003
<i>S</i> = 1.07	$\Delta\rho_{\text{max}} = 0.65 \text{ e } \text{Å}^{-3}$
2051 reflections	$\Delta\rho_{\text{min}} = -0.25 \text{ e } \text{Å}^{-3}$
104 parameters	Absolute structure: Flack (1983),
H-atom parameters constrained	928 Friedel pairs
	Flack parameter: 0.06 (2)

H atoms were included in calculated positions using the riding method, with C–H = 0.95–0.98 Å and *U*_{iso}(H) = 1.2*U*_{eq}(C) or 1.5*U*_{eq}(methyl C).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINTE* (Bruker, 2002); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics:

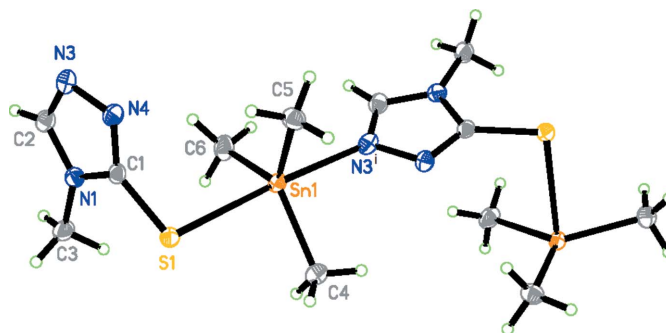


Figure 1

The structure of (I), with displacement ellipsoids drawn at the 50% probability level. [Symmetry code: (i) $-x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$]

SHELXTL (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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