Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

Aziz-ur-Rehman,[a] Saqib Ali,[a]* Saira Shahzadi[a] and Madeleine Helliwell[b]

[a]Department of Chemistry, Quaid-i-Azam University, Islamabad 45320, Pakistan, and [b]School of Chemistry, The University of Manchester, Manchester M13 9PL, England

Correspondence e-mail: drsa54@yahoo.com

Key indicators

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

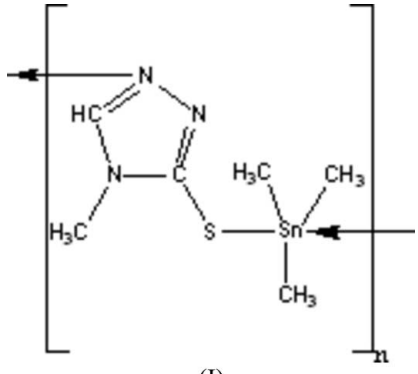
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 8 August 2006
Accepted 22 August 2006

The crystal structure of the title compound, $[Sn(CH_3)_3(C_3H_4N_3S)]_n$, 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.

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).



(I)

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

$[Sn(CH_3)_3(C_3H_4N_3S)]$	$Z = 4$
$M_r = 277.94$	$D_x = 1.822$ Mg m^{-3}
Orthorhombic, $Pna2_1$	Mo $K\alpha$ radiation
$a = 13.7254$ (11) Å	$\mu = 2.68$ mm^{-1}
$b = 11.0183$ (9) Å	$T = 100$ (2) K
$c = 6.6998$ (5) Å	Plate, colourless
$V = 1013.21$ (14) Å^3	0.40 × 0.30 × 0.05 mm

Data collection

Bruker APEX CCD diffractometer	7581 measured reflections
φ and ω scans	2051 independent reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)	2032 reflections with $I > 2\sigma(I)$
$T_{min} = 0.414$, $T_{max} = 0.878$	$R_{int} = 0.025$
	$\theta_{max} = 26.3°$

Refinement

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

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

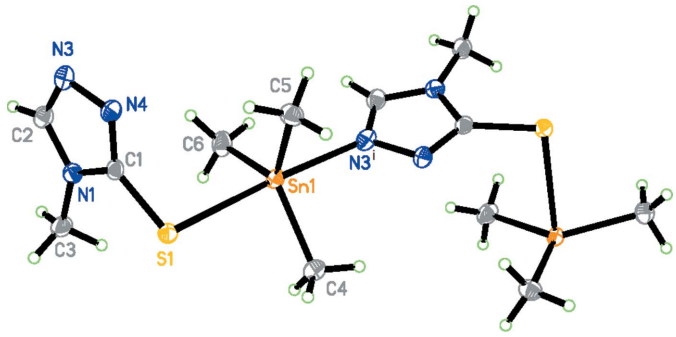


Figure 1
The structure of (I), with displacement ellipsoids drawn at the 50% probability level. [Symmetry code: (i) $-x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$.]

AR is grateful to HEC (Higher Education Commision, Islamabad, Pakistan) for financial support under the PhD Fellowship Scheme Batch-II (PIN code: 042–111621-PS2–179).

References

Bruker (2001). *SMART* (Version 5.625), *SADABS* (Version 2.03a) and *SHELXTL* (Version 6.12). Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2002). *SAINT*. Version 6.36a. Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Narayan, V. L. (1983). *Organotin Compounds as Antitumour Agents.* In *Structure–Activity Relationship of Antitumour Agents*, edited by D. N. Reinhoudt, T. A. Connors, H. M. Pinedo & K. W. Van De Poll, pp. 77-106. The Hague: Martinus Nijhoff.
Shahzadi, S., Ali, S., Bhatti, M. H., Fettouhi, M. & Athar, M. (2006). *J. Organomet. Chem.* **691**, 1797–1802.
Shahzadi, S., Ali, S. & Fettouhi, M. (2006). *Acta Cryst.* E**62**, m1178–m1180.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.