Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Chloro[5,6-diphenyl-1,2,4-triazine-3(2*H*)-thionato]dimethyltin(IV)

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.004 Å
R factor = 0.028
wR factor = 0.071
Data-to-parameter ratio = 15.7

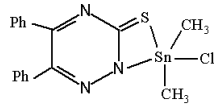
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 20 June 2003
Accepted 11 July 2003
Online 8 August 2003

The reaction between dichlorodimethyltin(IV) and 5-methoxy-5,6-diphenyl-4,5-dihydro-2*H*-1,2,4-triazine-3-thione yields the title complex, $[SnClMe_2(C_{15}H_{10}N_3S)]$. The coordination sphere of the Sn atom is formed by the S, amine N and Cl atoms and two methyl groups, giving a pentacoordinate geometry. The distances Sn—N = 2.525 (2) Å, Sn—S = 2.4671 (7) Å, Sn—C = 2.109 (3) and 2.111 (4) Å, and Sn—Cl = 2.4220 (7) Å are in the ranges expected for this type of complex. The coordination mode of the triazinethione ligand results in a four-membered chelate ring.

Comment

In the title molecule, (I), the geometry is intermediate between a square-base pyramid and a trigonal bipyramid (t = 0.41; Addison et al., 1984). The thione bond distance of 1.738 (3) Å is longer than in the uncoordinated precursor molecule [1.628 (2) Å; Arquero *et al.*, 1998] and is intermediate between the theoretical C—S single- and double-bond lengths (Sutton, 1965); this is also the case for the N—N bonds. The X-ray analysis confirms the structure proposed from spectroscopy measurements.



(I)

Experimental

The complex was synthesized as described by López-Torres *et al.* (2003). Recrystallization from chloroform afforded yellow crystals suitable for X-ray analysis.

Crystal data

$[SnCl(CH_3)_2(C_{15}H_{10}N_3S)]$
M_r = 448.53
Triclinic, $P\overline{1}$
a = 7.5737 (1) Å
b = 10.6393 (1) Å
c = 12.4602 (1) Å
α = 79.524 (1)°
β = 74.738 (1)°
γ = 73.828 (1)°
V = 923.890 (17) Å^3
Z = 2
D_x = 1.612 Mg m^{-3}
Cu $K\alpha$ radiation
μ = 13.39 mm^{-1}
T = 296 (2) K
Prism, yellow
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997–2001)
T_{min} = 0.062, T_{max} = 0.069
10 236 measured reflections
3309 independent reflections
3256 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 70.4°
$h = -9 \rightarrow 9$
$k = -12 \rightarrow 12$
$l = -15 \rightarrow 15$

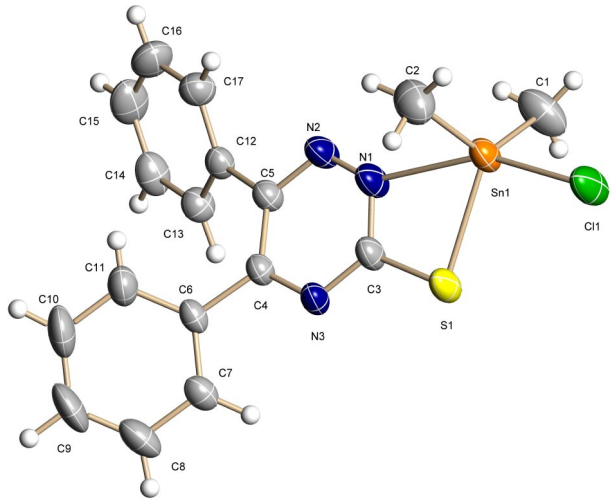


Figure 1
A view of (I), with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0419P)^2 + 0.3651P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.028$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.071$	$\Delta\rho_{max} = 0.91$ e Å^{-3}
$S = 1.04$	$\Delta\rho_{min} = -0.73$ e Å^{-3}
3309 reflections	Extinction correction: *SHELXL*97
211 parameters	Extinction coefficient: 0.0023 (2)
H-atom parameters constrained	

H atoms were placed in idealized positions, with C—H distances of 0.93 Å (0.96 Å for methyl), and were included in the refinement in the riding-model approximation, with U_{iso} values equal to $1.2U_{eq}$ ($1.5U_{eq}$ for methyl) of the carrier atom.

Data collection: *SMART* (Bruker, 1997–2001); cell refinement: *SMART*; data reduction: *SAINT-Plus-NT* (Bruker, 1997–2001); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

The authors thank DGICYT for financial support (project No. BQU2001-0151) and the Servicio Interdepartamental de Investigación (SIdI) of the Universidad Autónoma de Madrid for providing the instrumentation facilities.

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