

μ_2 -Oxalato-bis[triphenyl(thiourea- κ S)-tin(IV)]

 Yaya Sow,^{a*} Libasse Diop,^a Kieran C. Molloy^b and Gabrielle Kociok-Kohn^b

^aLaboratoire de Chimie Minérale et Analytique (LACHIMIA), Département de Chimie, Faculté des Sciences et Techniques, Université Cheikh, Anta Diop Dakar Senegal, and ^bDepartment of Chemistry, University of Bath, Bath BA2 7AY, England
Correspondence e-mail: yayasow81@yahoo.fr

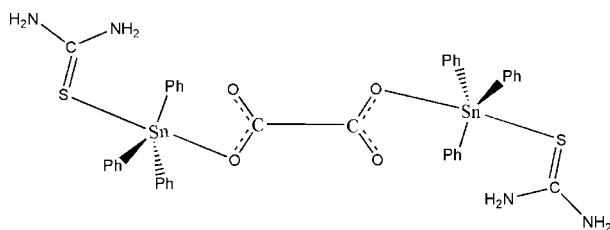
Received 15 July 2012; accepted 26 September 2012

Key indicators: single-crystal X-ray study; $T = 150$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.030; wR factor = 0.066; data-to-parameter ratio = 17.8.

The asymmetric unit of the binuclear title compound, $[\text{Sn}_2(\text{C}_2\text{O}_4)(\text{C}_6\text{H}_5)_6(\text{CH}_4\text{N}_2\text{S})_2]$, consists of one half of the organotin(IV) molecule. The remainder is generated by a twofold rotation axis passing through the mid-point of the oxalate C—C bond. The Sn^{IV} atom exhibits a distorted trigonal-bipyramidal coordination environment with the phenyl groups in equatorial positions and the thiourea and the monodentately bridging oxalate anion in axial positions. The molecules are linked through $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds involving the amino group of the thiourea ligand and the uncoordinating oxalate O atoms, forming layers parallel to (001). Weak $\text{C}-\text{H}\cdots\text{O}$ interactions are also present.

Related literature

For background to organotin(IV) chemistry, see: Evans & Karpel (1985); Gielen *et al.* (1995). For triphenyltin(IV)-containing compounds and their biological activity, see: Kamruddin *et al.* (1996). For related compounds, see: Diallo *et al.* (2009); Diasse-Sarr *et al.* (1997); Diop *et al.* (1997, 1999, 2003); Tiekink (1992).



Experimental

Crystal data

$[\text{Sn}_2(\text{C}_2\text{O}_4)(\text{C}_6\text{H}_5)_6(\text{CH}_4\text{N}_2\text{S})_2]$
 $M_r = 940.24$
 Monoclinic, $C2/c$
 $a = 12.9161$ (2) Å
 $b = 13.9870$ (2) Å

$c = 21.8215$ (3) Å
 $\beta = 99.238$ (1)°
 $V = 3891.09$ (10) Å³
 $Z = 4$
 Mo $K\alpha$ radiation

$\mu = 1.44$ mm⁻¹
 $T = 150$ K

$0.30 \times 0.30 \times 0.20$ mm

Data collection

Nonius KappaCCD diffractometer
 Absorption correction: multi-scan
 (*SORTAV*; Blessing, 1995)
 $T_{\text{min}} = 0.659$, $T_{\text{max}} = 0.747$

31403 measured reflections
 4472 independent reflections
 3665 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.057$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.066$
 $S = 1.09$
 4472 reflections
 251 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 1.34$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.11$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1A}\cdots\text{O2}^{\text{i}}$	0.81 (4)	2.06 (4)	2.824 (3)	157 (4)
$\text{N2}-\text{H2A}\cdots\text{O2}^{\text{ii}}$	0.86 (4)	2.14 (4)	2.970 (3)	164 (3)
$\text{C6}-\text{H6}\cdots\text{O1}$	0.95	2.44	2.957 (3)	114
$\text{C18}-\text{H18}\cdots\text{O2}$	0.95	2.39	3.234 (3)	147

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

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2662).

References

- Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
- Blessing, R. H. (1995). *Acta Cryst.* **A51**, 33–38.
- Diallo, W., Okio, K. Y. A., Diop, C. A. K., Diop, L., Diop, L. A. & Russo, U. (2009). *Main Group Met. Chem.* **32**, 93–100.
- Diasse-Sarr, A., Diop, L., Mahon, M. & Molloy, K. C. (1997). *Main Group Met. Chem.* **20**, 223–229.
- Diop, C. A. K., Diop, L. & Russo, U. (1999). *Main Group Met. Chem.* **22**, 217–220.
- Diop, C. A. K., Lahlou, M., Diop, L., Mahieu, B. & Russo, U. (1997). *Main Group Met. Chem.* **20**, 681–686.
- Diop, L., Mahieu, B., Mahon, M. F., Molloy, K. C. & Okio, K. Y. A. (2003). *Appl. Organomet. Chem.* **17**, 881–882.
- Evans, C. J. & Karpel, S. (1985). *Organotin Compounds in Modern Technology*, *J. Organomet. Chem. Library*, Vol. 16. Amsterdam: Elsevier.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
- Gielen, M., Bouhdid, A., Kayser, S., Biesemans, M., De Vos, D., Mahieu, B. & Willem, R. (1995). *Appl. Organomet. Chem.* **9**, 251–257.
- Kamruddin, S. K., Chattopadhyaya, T. K., Roy, A. & Tiekink, E. R. T. (1996). *Appl. Organomet. Chem.* **10**, 513–521.
- Nonius (1999). *COLLECT*. Nonius BV, Delft, The Netherlands.
- Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C.W.Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Tiekink, E. R. T. (1992). *Main Group Met. Chem.* **15**, 161–186.

supporting information

Acta Cryst. (2012). E68, m1337 [doi:10.1107/S1600536812040706]

 μ_2 -Oxalato-bis[triphenyl(thiourea- κ S)tin(IV)]**Yaya Sow, Libasse Diop, Kieran C. Molloy and Gabrielle Kociok-Kohn****S1. Comment**

Interest in organotin (IV) chemistry remains high because of several applications found in molecules belonging to this family (Evans & Karpel, 1985; Gielen *et al.*, 1995), specifically triphenyltin(IV)-residue containing compounds for which biological activity has been reported (Kamruddin *et al.*, 1996). Our specific interest lies also in the coordinating behavior of oxy-anions to these organometallic centers; we have previously published several crystal structures dealing with such systems (Diallo *et al.*, 2009; Diasse-Sarr *et al.*, 1997; Diop *et al.*, 1997). Moreover, we have reported spectroscopic data (Diop *et al.*, 1999) and the crystal structure of $[\text{Sn}_2(\text{C}_2\text{O}_4)(\text{C}_6\text{H}_5)_6]$ which exhibits tetrahedrally coordinate tin atoms (Diop *et al.*, 2003). Here we report a study of the interactions between this species and thiourea, which has yielded the title compound, $[\text{Sn}_2(\text{C}_2\text{O}_4)(\text{C}_6\text{H}_5)_6(\text{CH}_4\text{N}_2\text{S})_2]$.

The molecule of the title compound has site symmetry 2 with the twofold rotation axis passing through the mid-point of the central oxalate C—C bond. The Sn(IV) atom is five-coordinate by one oxygen atom of the oxalate anion, a sulfur atom of the thiourea ligand [Sn—O 2.2471 (17), Sn—S 2.6945 (7) Å] which are in apical positions and to three phenyl groups [Sn—C 2.146 (2), 2.139 (2), 2.139 (2) Å] occupying the equatorial positions of the trigonal bipyramid (Fig. 1). The Sn—S bond length is longer than the Sn—S bond length [2.573 (1) Å] found, for example, in $\{(\text{C}_4\text{H}_9)_2\text{Sn}[\text{S}_2\text{CN}(\text{CH}_3)_2]_2\}$ which contains a trigonal bipyramidally coordinate tin(IV) atom (Tiekink, 1992). The angle S—Sn—O [175.97 (5)°] deviates slightly from linearity. The sum of the C—Sn—C angles (359.96°) indicates a nearly perfectly planar $\text{Sn}(\text{C}_6\text{H}_5)_3$ residue consistent with the near linearity of the axial substituents. The Sn—O bond length is remarkably long when compared with the Sn—O distance [2.111 (1) Å] in the tetrahedrally coordinate tin(IV) atom in $[\text{Sn}_2(\text{C}_2\text{O}_4)(\text{C}_6\text{H}_5)_6]$ (Diop *et al.*, 2003). The addition of $\text{SC}(\text{NH}_2)_2$ apparently has caused a change in the coordination from tetrahedral to trigonal-bipyramidal along with a Sn—O bond length increase. The two C—O bond length of the oxalate anion are slightly different because the O atom of the C19—O1 bond [1.269 (3) Å] is also involved in bonding to the Sn(IV) atom, whereas the O atom of the C19—O2 bond [1.243 (3) Å] is involved in hydrogen bonding with the amino group. These interactions lead to the formation of layers parallel to (001) (Figs. 2,3). Weak C—H \cdots O hydrogen bonding is also observed.

S2. Experimental

All chemicals were purchased from Aldrich or Merck and used without any further purification. $[\text{Sn}_2(\text{C}_2\text{O}_4)(\text{C}_6\text{H}_5)_6]$ has been obtained on allowing $\text{Sn}(\text{C}_6\text{H}_5)_3\text{OH}$ to react with oxalic acid in a 2:1 ratio in ethanol. A white powder is collected after slow evaporation. When $[\text{Sn}_2(\text{C}_2\text{O}_4)(\text{C}_6\text{H}_5)_6]$ is mixed with $\text{SC}(\text{NH}_2)_2$ in a 1:2 ratio, both as ethanolic solutions, a colorless solution is obtained which gives crystals of $[\text{Sn}_2(\text{C}_2\text{O}_4)(\text{C}_6\text{H}_5)_6(\text{CH}_4\text{N}_2\text{S})_2]$ suitable for X-ray work, after a slow solvent evaporation.

S3. Refinement

The maximum remaining electron density is 0.79 Å from C3 while the minimum density is in the immediate vicinity of tin. Hydrogen atoms bonded to the N atom have been located in difference Fourier maps and have been freely refined. The other hydrogen atoms have been placed onto calculated position and refined using a riding model, with C—H distances of 0.95 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

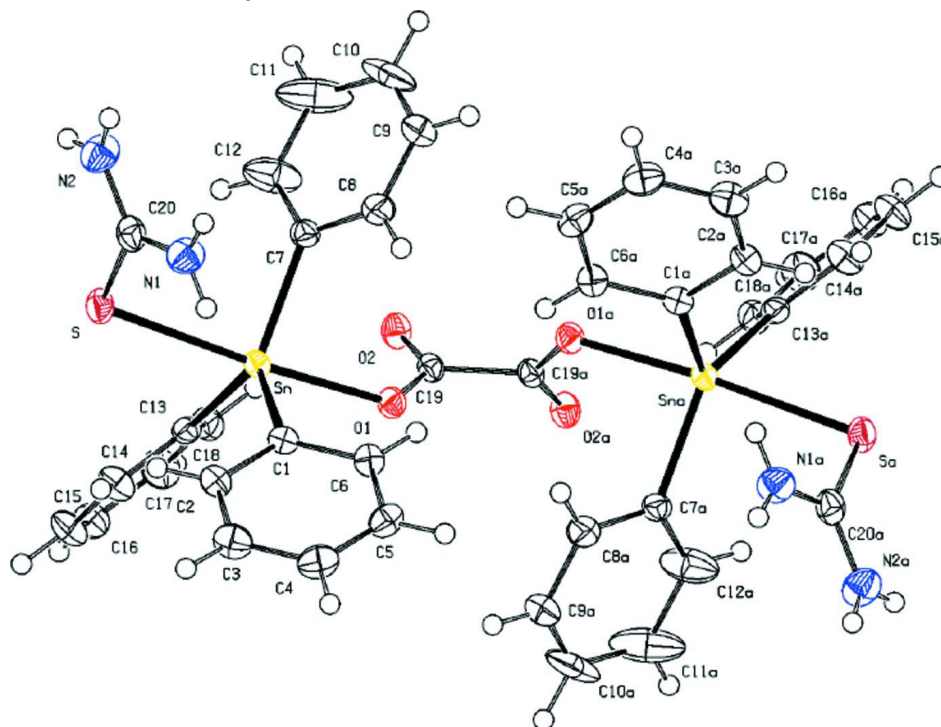
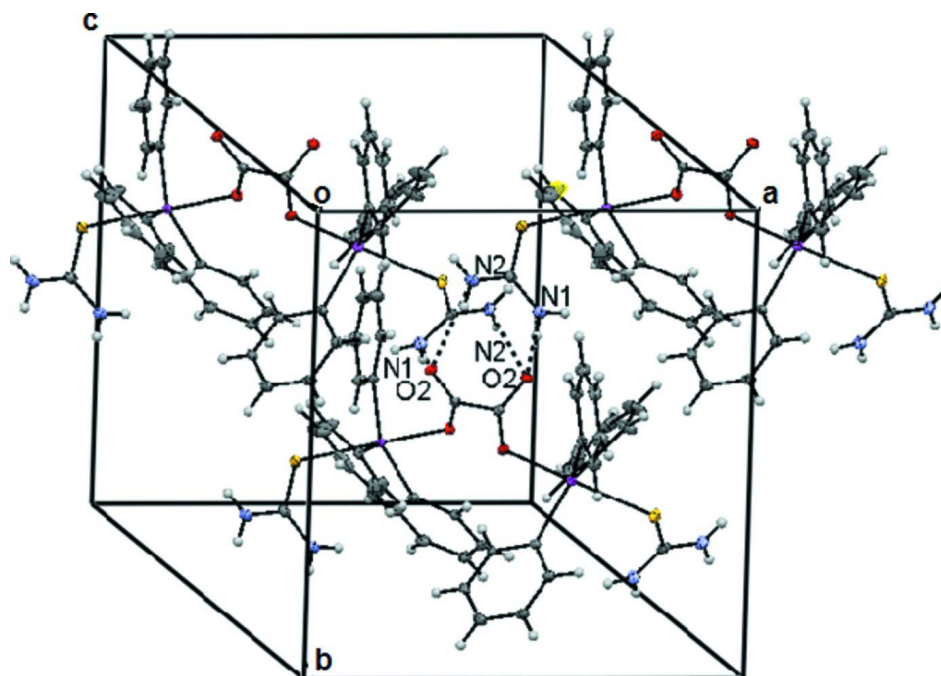
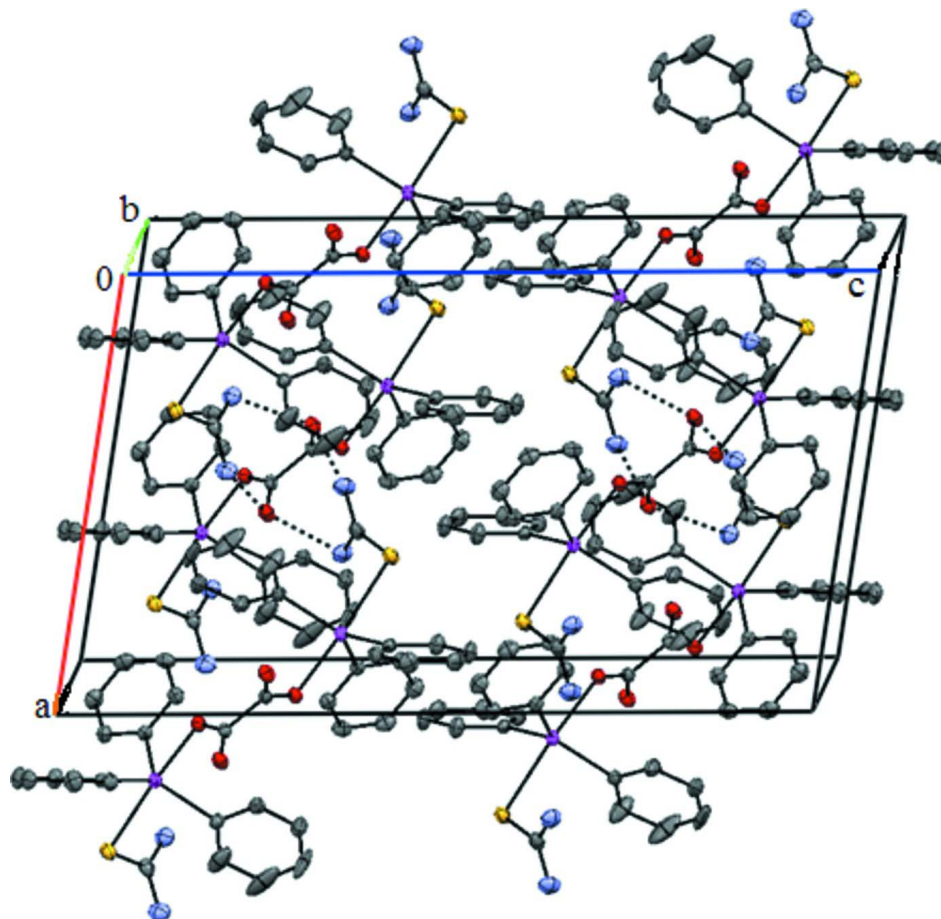


Figure 1

The molecule of the title complex showing the numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code a) $-x, y, -z + 1/2$.]

**Figure 2**

View of the N—H···O hydrogen bonding system (dashed lines) assured by pairs of oxygen atoms of the oxalate and H atoms of thiourea.

**Figure 3**

The packing of the structure showing N—H···O hydrogen bonding interactions as dashed lines

μ_2 -Oxalato-bis[triphenyl(thiourea- κ S)tin(IV)]

Crystal data

[Sn₂(C₂O₄)(C₆H₅)₆(CH₄N₂S)₂]

$M_r = 940.24$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 12.9161\ (2)\ \text{\AA}$

$b = 13.9870\ (2)\ \text{\AA}$

$c = 21.8215\ (3)\ \text{\AA}$

$\beta = 99.238\ (1)^\circ$

$V = 3891.09\ (10)\ \text{\AA}^3$

$Z = 4$

$F(000) = 1880$

$D_x = 1.605\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 26977 reflections

$\theta = 2.9\text{--}27.5^\circ$

$\mu = 1.44\ \text{mm}^{-1}$

$T = 150\ \text{K}$

Block, colourless

$0.30 \times 0.30 \times 0.20\ \text{mm}$

Data collection

Nonius KappaCCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

400 1.5 degree images with φ and ω scans

Absorption correction: multi-scan
(*SORTAV*; Blessing, 1995)

$T_{\min} = 0.659$, $T_{\max} = 0.747$

31403 measured reflections

4472 independent reflections

3665 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.057$
 $\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 3.8^\circ$
 $h = -16 \rightarrow 16$

$k = -18 \rightarrow 18$
 $l = -28 \rightarrow 28$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.066$
 $S = 1.09$
 4472 reflections
 251 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H atoms treated by a mixture of independent
 and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0248P)^2 + 7.4801P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 1.34 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -1.11 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Sn	0.165377 (13)	0.128741 (12)	0.141781 (7)	0.01783 (7)
S	0.33347 (5)	0.18709 (5)	0.09290 (3)	0.02648 (16)
O1	0.03210 (13)	0.08111 (13)	0.18919 (8)	0.0223 (4)
O2	0.09855 (14)	-0.05868 (13)	0.22806 (8)	0.0247 (4)
N1	0.3214 (2)	0.34372 (19)	0.16116 (13)	0.0319 (6)
H1A	0.340 (3)	0.385 (3)	0.1866 (18)	0.050 (12)*
H1B	0.256 (3)	0.351 (2)	0.1449 (16)	0.040 (10)*
N2	0.4815 (2)	0.2725 (2)	0.17068 (13)	0.0342 (6)
H2A	0.509 (3)	0.319 (3)	0.1931 (16)	0.044 (10)*
H2B	0.519 (3)	0.228 (3)	0.1620 (17)	0.050 (12)*
C1	0.07308 (19)	0.25438 (17)	0.11628 (11)	0.0190 (5)
C2	0.0815 (2)	0.30357 (19)	0.06162 (12)	0.0245 (6)
H2	0.1363	0.2876	0.0392	0.029*
C3	0.0110 (2)	0.3755 (2)	0.03950 (14)	0.0308 (6)
H3	0.0181	0.4082	0.0023	0.037*
C4	-0.0697 (2)	0.3998 (2)	0.07159 (14)	0.0317 (7)
H4	-0.1187	0.4480	0.0560	0.038*
C5	-0.0780 (2)	0.35315 (19)	0.12646 (13)	0.0266 (6)
H5	-0.1323	0.3702	0.1491	0.032*
C6	-0.0075 (2)	0.28136 (19)	0.14865 (12)	0.0229 (6)
H6	-0.0140	0.2500	0.1865	0.027*

C7	0.2578 (2)	0.11799 (18)	0.23207 (12)	0.0215 (5)
C8	0.2292 (2)	0.1691 (3)	0.28081 (13)	0.0410 (8)
H8	0.1752	0.2157	0.2724	0.049*
C9	0.2764 (3)	0.1547 (4)	0.34114 (15)	0.0574 (11)
H9	0.2549	0.1913	0.3735	0.069*
C10	0.3516 (3)	0.0900 (3)	0.35449 (15)	0.0576 (12)
H10	0.3830	0.0797	0.3964	0.069*
C11	0.3848 (4)	0.0368 (3)	0.3069 (2)	0.0700 (14)
H11	0.4388	-0.0095	0.3162	0.084*
C12	0.3373 (3)	0.0529 (2)	0.24521 (16)	0.0515 (10)
H12	0.3605	0.0184	0.2125	0.062*
C13	0.15172 (19)	0.01853 (18)	0.07300 (11)	0.0202 (5)
C14	0.1501 (2)	0.0447 (2)	0.01093 (12)	0.0298 (6)
H14	0.1558	0.1102	0.0004	0.036*
C15	0.1403 (2)	-0.0245 (2)	-0.03532 (13)	0.0360 (7)
H15	0.1396	-0.0062	-0.0773	0.043*
C16	0.1317 (2)	-0.1194 (2)	-0.02054 (14)	0.0333 (7)
H16	0.1249	-0.1665	-0.0523	0.040*
C17	0.1328 (2)	-0.1461 (2)	0.04042 (14)	0.0343 (7)
H17	0.1266	-0.2117	0.0506	0.041*
C18	0.1429 (2)	-0.0774 (2)	0.08685 (12)	0.0270 (6)
H18	0.1438	-0.0964	0.1287	0.032*
C19	0.03827 (19)	0.01088 (18)	0.22640 (11)	0.0190 (5)
C20	0.3813 (2)	0.2744 (2)	0.14526 (12)	0.0260 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn	0.02036 (10)	0.01769 (10)	0.01559 (9)	0.00087 (7)	0.00337 (6)	-0.00049 (7)
S	0.0272 (3)	0.0299 (4)	0.0242 (3)	-0.0054 (3)	0.0098 (3)	-0.0070 (3)
O1	0.0227 (9)	0.0238 (10)	0.0211 (9)	0.0002 (8)	0.0056 (7)	0.0060 (8)
O2	0.0294 (10)	0.0208 (10)	0.0254 (10)	0.0042 (8)	0.0093 (8)	0.0000 (8)
N1	0.0311 (15)	0.0292 (14)	0.0346 (14)	-0.0033 (12)	0.0029 (11)	-0.0081 (12)
N2	0.0297 (14)	0.0301 (15)	0.0427 (16)	-0.0074 (13)	0.0057 (12)	-0.0087 (13)
C1	0.0217 (13)	0.0153 (12)	0.0193 (12)	-0.0001 (10)	0.0011 (10)	0.0000 (10)
C2	0.0277 (14)	0.0250 (14)	0.0208 (13)	0.0001 (11)	0.0039 (11)	0.0013 (11)
C3	0.0364 (16)	0.0237 (15)	0.0309 (15)	0.0021 (13)	0.0015 (12)	0.0069 (12)
C4	0.0295 (15)	0.0247 (15)	0.0389 (17)	0.0063 (12)	-0.0006 (12)	0.0012 (13)
C5	0.0222 (14)	0.0216 (14)	0.0358 (15)	0.0014 (11)	0.0046 (11)	-0.0065 (12)
C6	0.0255 (14)	0.0197 (13)	0.0240 (13)	-0.0012 (11)	0.0054 (10)	-0.0013 (11)
C7	0.0205 (12)	0.0232 (14)	0.0201 (12)	-0.0027 (11)	0.0015 (10)	0.0026 (11)
C8	0.0254 (15)	0.072 (2)	0.0251 (15)	0.0055 (16)	0.0021 (12)	-0.0117 (15)
C9	0.0331 (18)	0.117 (4)	0.0207 (16)	-0.010 (2)	0.0009 (13)	-0.0065 (19)
C10	0.069 (3)	0.075 (3)	0.0207 (16)	-0.046 (2)	-0.0189 (16)	0.0201 (17)
C11	0.077 (3)	0.037 (2)	0.077 (3)	0.012 (2)	-0.045 (2)	0.006 (2)
C12	0.062 (2)	0.039 (2)	0.044 (2)	0.0230 (18)	-0.0196 (17)	-0.0121 (16)
C13	0.0170 (12)	0.0228 (14)	0.0202 (12)	0.0005 (10)	0.0017 (10)	-0.0059 (10)
C14	0.0387 (17)	0.0275 (15)	0.0224 (14)	0.0005 (13)	0.0024 (12)	-0.0017 (11)

C15	0.0424 (18)	0.046 (2)	0.0187 (14)	-0.0021 (15)	0.0026 (12)	-0.0073 (13)
C16	0.0330 (16)	0.0374 (18)	0.0292 (15)	-0.0032 (14)	0.0036 (12)	-0.0176 (13)
C17	0.0414 (17)	0.0265 (16)	0.0350 (16)	-0.0030 (13)	0.0064 (13)	-0.0084 (13)
C18	0.0292 (14)	0.0288 (15)	0.0234 (14)	-0.0015 (12)	0.0051 (11)	-0.0032 (12)
C19	0.0217 (13)	0.0192 (13)	0.0164 (12)	-0.0032 (11)	0.0042 (10)	-0.0016 (10)
C20	0.0303 (15)	0.0252 (14)	0.0241 (14)	-0.0062 (12)	0.0095 (11)	0.0012 (11)

Geometric parameters (Å, °)

Sn—C7	2.139 (2)	C6—H6	0.9500
Sn—C13	2.139 (2)	C7—C12	1.368 (4)
Sn—C1	2.146 (2)	C7—C8	1.381 (4)
Sn—O1	2.2471 (17)	C8—C9	1.374 (4)
Sn—S	2.6945 (7)	C8—H8	0.9500
S—C20	1.718 (3)	C9—C10	1.325 (6)
O1—C19	1.269 (3)	C9—H9	0.9500
O2—C19	1.243 (3)	C10—C11	1.398 (6)
N1—C20	1.321 (4)	C10—H10	0.9500
N1—H1A	0.81 (4)	C11—C12	1.406 (5)
N1—H1B	0.86 (4)	C11—H11	0.9500
N2—C20	1.324 (4)	C12—H12	0.9500
N2—H2A	0.85 (4)	C13—C18	1.384 (4)
N2—H2B	0.82 (4)	C13—C14	1.400 (4)
C1—C2	1.396 (3)	C14—C15	1.389 (4)
C1—C6	1.400 (4)	C14—H14	0.9500
C2—C3	1.391 (4)	C15—C16	1.375 (4)
C2—H2	0.9500	C15—H15	0.9500
C3—C4	1.388 (4)	C16—C17	1.380 (4)
C3—H3	0.9500	C16—H16	0.9500
C4—C5	1.383 (4)	C17—C18	1.388 (4)
C4—H4	0.9500	C17—H17	0.9500
C5—C6	1.390 (4)	C18—H18	0.9500
C5—H5	0.9500	C19—C19 ⁱ	1.538 (5)
C7—Sn—C13	124.52 (10)	C9—C8—C7	122.0 (3)
C7—Sn—C1	120.08 (9)	C9—C8—H8	119.0
C13—Sn—C1	115.36 (9)	C7—C8—H8	119.0
C7—Sn—O1	84.87 (8)	C10—C9—C8	120.5 (4)
C13—Sn—O1	97.26 (8)	C10—C9—H9	119.7
C1—Sn—O1	85.84 (8)	C8—C9—H9	119.7
C7—Sn—S	91.14 (7)	C9—C10—C11	120.1 (3)
C13—Sn—S	85.49 (7)	C9—C10—H10	120.0
C1—Sn—S	95.66 (7)	C11—C10—H10	120.0
O1—Sn—S	175.97 (5)	C10—C11—C12	119.2 (3)
C20—S—Sn	100.29 (9)	C10—C11—H11	120.4
C19—O1—Sn	123.37 (16)	C12—C11—H11	120.4
C20—N1—H1A	126 (3)	C7—C12—C11	120.3 (3)
C20—N1—H1B	123 (2)	C7—C12—H12	119.8

H1A—N1—H1B	111 (3)	C11—C12—H12	119.8
C20—N2—H2A	121 (2)	C18—C13—C14	118.4 (2)
C20—N2—H2B	119 (3)	C18—C13—Sn	123.08 (19)
H2A—N2—H2B	120 (3)	C14—C13—Sn	118.5 (2)
C2—C1—C6	117.7 (2)	C15—C14—C13	120.4 (3)
C2—C1—Sn	120.59 (19)	C15—C14—H14	119.8
C6—C1—Sn	121.12 (18)	C13—C14—H14	119.8
C3—C2—C1	121.1 (3)	C16—C15—C14	120.2 (3)
C3—C2—H2	119.4	C16—C15—H15	119.9
C1—C2—H2	119.4	C14—C15—H15	119.9
C4—C3—C2	120.3 (3)	C15—C16—C17	120.0 (3)
C4—C3—H3	119.8	C15—C16—H16	120.0
C2—C3—H3	119.8	C17—C16—H16	120.0
C5—C4—C3	119.4 (3)	C16—C17—C18	120.1 (3)
C5—C4—H4	120.3	C16—C17—H17	120.0
C3—C4—H4	120.3	C18—C17—H17	120.0
C4—C5—C6	120.3 (3)	C13—C18—C17	120.9 (3)
C4—C5—H5	119.9	C13—C18—H18	119.5
C6—C5—H5	119.9	C17—C18—H18	119.5
C5—C6—C1	121.2 (3)	O2—C19—O1	126.8 (2)
C5—C6—H6	119.4	O2—C19—C19 ⁱ	116.57 (17)
C1—C6—H6	119.4	O1—C19—C19 ⁱ	116.58 (18)
C12—C7—C8	117.9 (3)	N1—C20—N2	118.6 (3)
C12—C7—Sn	121.9 (2)	N1—C20—S	122.2 (2)
C8—C7—Sn	119.6 (2)	N2—C20—S	119.2 (2)

Symmetry code: (i) $-x, y, -z+1/2$.

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H1A...O2 ⁱⁱ	0.81 (4)	2.06 (4)	2.824 (3)	157 (4)
N2—H2A...O2 ⁱⁱⁱ	0.86 (4)	2.14 (4)	2.970 (3)	164 (3)
C6—H6...O1	0.95	2.44	2.957 (3)	114
C18—H18...O2	0.95	2.39	3.234 (3)	147

Symmetry codes: (ii) $-x+1/2, y+1/2, -z+1/2$; (iii) $x+1/2, y+1/2, z$.