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(*N*-Butyl-*N*-phenyldithiocarbamato- κ S)-triphenyltin(IV)

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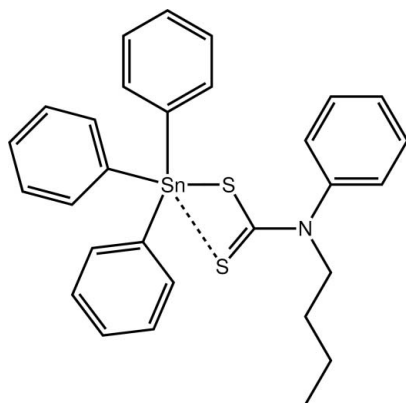
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 Key indicators: single-crystal X-ray study; $T = 150$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.024; wR factor = 0.060; data-to-parameter ratio = 20.4.

The title compound, $[\text{Sn}(\text{C}_6\text{H}_5)_3(\text{C}_{11}\text{H}_{14}\text{NS}_2)]$, features a tetrahedrally coordinated Sn atom, as the dithiocarbamate ligand coordinates in a monodentate fashion. Due to the proximity of the non-coordinating thione S atom, distortions from ideal tetrahedral geometry about the metal atom are evident with the widest C—Sn—S angle being $117.26(5)^\circ$. In the crystal, molecules are linked by C—H \cdots S interactions, which generate helical supramolecular chains along the b axis.

Related literature

For a review on the applications and structural chemistry of tin dithiocarbamates, see: Tiekink (2008). For a recently reported related structure, see: Awang *et al.* (2010).


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Experimental

Crystal data

 $[\text{Sn}(\text{C}_6\text{H}_5)_3(\text{C}_{11}\text{H}_{14}\text{NS}_2)]$
 $M_r = 574.34$

 Monoclinic, $P2_1/n$
 $a = 10.0488(1)$ Å

 $b = 18.0008(2)$ Å

 $c = 15.2054(2)$ Å

 $\beta = 102.442(1)^\circ$
 $V = 2685.85(5)$ Å³
 $Z = 4$

 Mo $K\alpha$ radiation

 $\mu = 1.12$ mm⁻¹
 $T = 150$ K

 $0.24 \times 0.22 \times 0.10$ mm

Data collection

Oxford Diffraction Xcaliber Eos

Gemini diffractometer

Absorption correction: multi-scan

 (*CrysAlis PRO*; Oxford

Diffraction, 2010)

 $T_{\min} = 0.781$, $T_{\max} = 0.894$

34109 measured reflections

6099 independent reflections

 5277 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.044$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.024$
 $wR(F^2) = 0.060$
 $S = 1.02$

6099 reflections

299 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.49$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.27$ e Å⁻³
Table 1

Selected geometric parameters (Å, °).

| | | | |
|------------|-------------|-----------|-------------|
| Sn—S1 | 2.4772 (5) | Sn—C24 | 2.1521 (18) |
| Sn—S2 | 3.1048 (5) | S1—C1 | 1.758 (2) |
| Sn—C12 | 2.1286 (18) | S2—C1 | 1.675 (2) |
| Sn—C18 | 2.1380 (19) | | |
| C12—Sn—C18 | 113.76 (7) | C12—Sn—S1 | 117.26 (5) |
| C12—Sn—C24 | 107.51 (7) | C18—Sn—S1 | 115.54 (5) |
| C18—Sn—C24 | 107.45 (7) | C24—Sn—S1 | 92.18 (5) |

Table 2

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|----------------------------------|-------|-------------|-------------|---------------|
| C28—H28 \cdots S2 ⁱ | 0.95 | 2.83 | 3.612 (2) | 140 |

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5836).

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supporting information

Acta Cryst. (2011). E67, m555–m556 [doi:10.1107/S1600536811012426]

(*N*-Butyl-*N*-phenyldithiocarbamate- κ S)triphenyltin(IV)

Nurul Farahana Kamaludin, Ibrahim Baba, Normah Awang, Mohamed Ibrahim Mohamed Tahir and Edward R. T. Tiekink

S1. Comment

Their potential as anti-cancer agents, anti-microbials and insecticides, and as convenient synthetic precursors for tin sulfide nanoparticles, attract continued attention to organotin dithiocarbamates (Tiekink, 2008). As part of on-going of structural studies of triphenyltin(IV) dithiocarbamates (Awang *et al.*, 2010), the analysis of the title compound, (I), was undertaken.

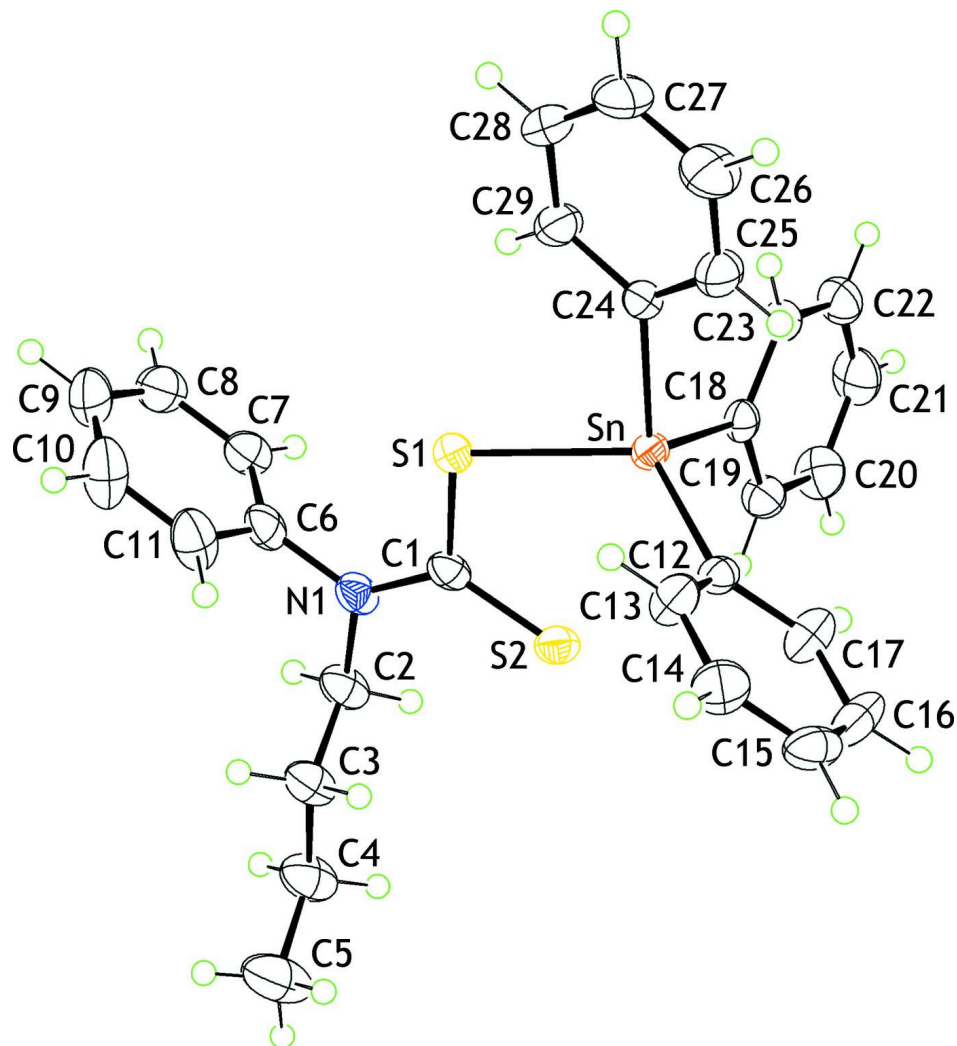
The molecular structure, Fig. 1, features Sn coordinated by the dithiocarbamate ligand and three *ipso*-C atoms of three benzene rings. The dithiocarbamate ligand coordinates essentially in a monodentate fashion, an assignment supported by the large disparity in the C—S bond distances, Table 1. The coordination geometry is based on a tetrahedron with the range of tetrahedral angles being 92.18 (5) to 117.26 (5) °. The wider angles are ascribed to the influence of the proximate S2 atom. The crystal packing of (I) features helical supramolecular chains along the *b* axis that is sustained by C—H···S interactions, Fig. 2 and Table 2.

S2. Experimental

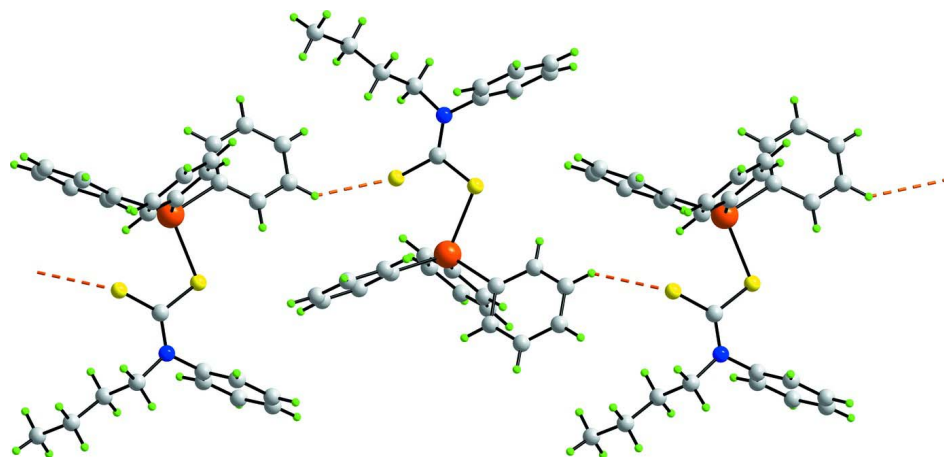
The title compound was prepared using an *in situ* method by the addition of carbon disulfide (0.01 mol) to an ethanolic solution of *N*-butylphenylamine (0.01 mol). The mixture was stirred for 1 h at 277 K. The solution was then added dropwise to a solution of triphenyltin(IV) chloride (0.01 mol) in ethanol (20 ml). The mixture was stirred for 1 h. The white precipitate that formed was filtered, washed with cold ethanol and dried in a desiccator. Crystallization was carried out by using an ethanol:chloroform (1:1 *v/v*) mixture to yield colourless prisms of (I). Yield: 34%. *M*.pt. 374–375 K. Elemental analysis. Found (calculated) for C₂₉H₂₉NS₂Sn: C, 60.54 (60.64); H 5.08 (5.09); N 2.34 (2.44); S 11.31 (11.17); Sn 20.19 (20.66) %. UV (CHCl₃) λ_{max} 252 nm ($L(\pi) \rightarrow L(\pi^*)$). IR (KBr): $\nu(\text{C—H})$ 2960 m; $\nu(\text{C}\equiv\text{N})$ 1477 m; $\nu(\text{N—C})$ 1139 s; $\nu(\text{C}\equiv\text{S})$ 997 s; $\nu(\text{C—S})$ 356 s cm⁻¹.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 to 0.99 Å) and were included in the refinement in the riding model approximation, with $U_{\text{iso}}(\text{H})$ set to 1.2 to 1.5 $U_{\text{equiv}}(\text{C})$.

**Figure 1**

The molecular structure of (I) showing the displacement ellipsoids at the 50% probability level.

**Figure 2**

A view of the helical supramolecular chain in (I) mediated by C—H...S interactions (orange dashed lines) along the *b* axis in (I).

(*N*-Butyl-*N*-phenyldithiocarbamate- κ S)triphenyltin(IV)

Crystal data

[Sn(C₆H₅)₃(C₁₁H₁₄NS₂)]

$M_r = 574.34$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 10.0488$ (1) Å

$b = 18.0008$ (2) Å

$c = 15.2054$ (2) Å

$\beta = 102.442$ (1)°

$V = 2685.85$ (5) Å³

$Z = 4$

$F(000) = 1168$

$D_x = 1.420$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 18395 reflections

$\theta = 2\text{--}29^\circ$

$\mu = 1.12$ mm⁻¹

$T = 150$ K

Prism, colourless

$0.24 \times 0.22 \times 0.10$ mm

Data collection

Oxford Diffraction Xcaliber Eos Gemini diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 16.1952 pixels mm⁻¹

ω scans

Absorption correction: multi-scan

(*CrysAlis PRO*; Oxford Diffraction, 2010)

$T_{\min} = 0.781$, $T_{\max} = 0.894$

34109 measured reflections

6099 independent reflections

5277 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.044$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 2.2^\circ$

$h = -13 \rightarrow 13$

$k = -23 \rightarrow 23$

$l = -19 \rightarrow 19$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.024$

$wR(F^2) = 0.060$

$S = 1.02$

6099 reflections

299 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-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0284P)^2 + 0.6995P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.003$

$\Delta\rho_{\max} = 0.49$ e Å⁻³

$\Delta\rho_{\min} = -0.27$ e Å⁻³

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|---------------|--------------|--------------|----------------------------------|
| Sn | 0.636843 (12) | 0.514323 (7) | 0.706567 (8) | 0.02366 (5) |
| S1 | 0.74819 (5) | 0.56428 (3) | 0.85614 (3) | 0.03110 (11) |
| S2 | 0.60687 (5) | 0.42144 (3) | 0.87326 (3) | 0.03087 (11) |
| N1 | 0.72072 (18) | 0.50776 (9) | 1.01112 (11) | 0.0316 (4) |
| C1 | 0.6917 (2) | 0.49591 (10) | 0.92221 (13) | 0.0280 (4) |
| C2 | 0.6806 (2) | 0.45399 (12) | 1.07424 (13) | 0.0366 (5) |
| H2A | 0.5941 | 0.4299 | 1.0445 | 0.044* |
| H2B | 0.6642 | 0.4811 | 1.1276 | 0.044* |
| C3 | 0.7875 (2) | 0.39454 (12) | 1.10512 (14) | 0.0392 (5) |
| H3A | 0.8713 | 0.4180 | 1.1404 | 0.047* |
| H3B | 0.8106 | 0.3705 | 1.0518 | 0.047* |
| C4 | 0.7378 (3) | 0.33576 (13) | 1.16269 (15) | 0.0471 (6) |
| H4A | 0.6524 | 0.3135 | 1.1280 | 0.057* |
| H4B | 0.7172 | 0.3597 | 1.2168 | 0.057* |
| C5 | 0.8423 (3) | 0.27455 (16) | 1.19190 (19) | 0.0671 (8) |
| H5A | 0.8668 | 0.2525 | 1.1386 | 0.101* |
| H5B | 0.8035 | 0.2362 | 1.2247 | 0.101* |
| H5C | 0.9239 | 0.2955 | 1.2312 | 0.101* |
| C6 | 0.7940 (2) | 0.57343 (12) | 1.05062 (13) | 0.0338 (5) |
| C7 | 0.7210 (2) | 0.63472 (12) | 1.06800 (14) | 0.0365 (5) |
| H7 | 0.6242 | 0.6337 | 1.0544 | 0.044* |
| C8 | 0.7902 (3) | 0.69796 (13) | 1.10562 (15) | 0.0442 (5) |
| H8 | 0.7407 | 0.7403 | 1.1178 | 0.053* |
| C9 | 0.9303 (3) | 0.69916 (15) | 1.12510 (15) | 0.0518 (6) |
| H9 | 0.9775 | 0.7427 | 1.1498 | 0.062* |
| C10 | 1.0025 (3) | 0.63747 (16) | 1.10886 (17) | 0.0578 (7) |
| H10 | 1.0993 | 0.6384 | 1.1228 | 0.069* |
| C11 | 0.9344 (2) | 0.57402 (15) | 1.07221 (15) | 0.0485 (6) |
| H11 | 0.9842 | 0.5312 | 1.0620 | 0.058* |
| C12 | 0.71232 (19) | 0.41209 (10) | 0.66655 (12) | 0.0258 (4) |
| C13 | 0.8499 (2) | 0.40110 (12) | 0.67362 (15) | 0.0377 (5) |
| H13 | 0.9118 | 0.4400 | 0.6962 | 0.045* |
| C14 | 0.8999 (2) | 0.33402 (12) | 0.64823 (16) | 0.0442 (5) |
| H14 | 0.9952 | 0.3274 | 0.6540 | 0.053* |
| C15 | 0.8124 (3) | 0.27783 (12) | 0.61507 (15) | 0.0421 (5) |

| | | | | |
|-----|--------------|--------------|--------------|------------|
| H15 | 0.8465 | 0.2319 | 0.5986 | 0.050* |
| C16 | 0.6745 (3) | 0.28803 (12) | 0.60564 (17) | 0.0498 (6) |
| H16 | 0.6132 | 0.2494 | 0.5811 | 0.060* |
| C17 | 0.6240 (2) | 0.35448 (12) | 0.63171 (15) | 0.0404 (5) |
| H17 | 0.5285 | 0.3607 | 0.6257 | 0.048* |
| C18 | 0.41962 (19) | 0.52313 (10) | 0.67250 (13) | 0.0263 (4) |
| C19 | 0.3332 (2) | 0.47347 (11) | 0.70304 (14) | 0.0329 (4) |
| H19 | 0.3709 | 0.4336 | 0.7413 | 0.039* |
| C20 | 0.1932 (2) | 0.48155 (13) | 0.67828 (17) | 0.0439 (6) |
| H20 | 0.1357 | 0.4477 | 0.7004 | 0.053* |
| C21 | 0.1365 (2) | 0.53874 (15) | 0.62151 (17) | 0.0489 (6) |
| H21 | 0.0403 | 0.5446 | 0.6052 | 0.059* |
| C22 | 0.2205 (2) | 0.58712 (13) | 0.58878 (15) | 0.0426 (5) |
| H22 | 0.1819 | 0.6256 | 0.5485 | 0.051* |
| C23 | 0.3614 (2) | 0.57999 (11) | 0.61427 (13) | 0.0328 (4) |
| H23 | 0.4184 | 0.6140 | 0.5919 | 0.039* |
| C24 | 0.71761 (18) | 0.60219 (10) | 0.63749 (12) | 0.0260 (4) |
| C25 | 0.7478 (2) | 0.59142 (12) | 0.55345 (14) | 0.0388 (5) |
| H25 | 0.7282 | 0.5450 | 0.5238 | 0.047* |
| C26 | 0.8063 (3) | 0.64789 (14) | 0.51222 (16) | 0.0510 (6) |
| H26 | 0.8271 | 0.6395 | 0.4550 | 0.061* |
| C27 | 0.8344 (2) | 0.71606 (13) | 0.55379 (16) | 0.0472 (6) |
| H27 | 0.8737 | 0.7546 | 0.5252 | 0.057* |
| C28 | 0.8049 (3) | 0.72759 (12) | 0.63682 (16) | 0.0455 (6) |
| H28 | 0.8242 | 0.7743 | 0.6659 | 0.055* |
| C29 | 0.7472 (2) | 0.67142 (11) | 0.67806 (14) | 0.0383 (5) |
| H29 | 0.7272 | 0.6802 | 0.7355 | 0.046* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| Sn | 0.02646 (8) | 0.02098 (8) | 0.02380 (8) | −0.00103 (5) | 0.00594 (5) | −0.00096 (5) |
| S1 | 0.0410 (3) | 0.0271 (2) | 0.0234 (2) | −0.0021 (2) | 0.0029 (2) | 0.00049 (19) |
| S2 | 0.0389 (3) | 0.0250 (2) | 0.0299 (2) | 0.0037 (2) | 0.0100 (2) | 0.00173 (19) |
| N1 | 0.0396 (10) | 0.0330 (9) | 0.0223 (8) | 0.0080 (7) | 0.0072 (7) | 0.0010 (7) |
| C1 | 0.0301 (10) | 0.0281 (10) | 0.0259 (10) | 0.0106 (8) | 0.0061 (8) | 0.0028 (8) |
| C2 | 0.0456 (12) | 0.0418 (12) | 0.0253 (10) | 0.0110 (10) | 0.0138 (9) | 0.0053 (9) |
| C3 | 0.0446 (13) | 0.0421 (12) | 0.0316 (11) | 0.0116 (10) | 0.0101 (10) | 0.0074 (9) |
| C4 | 0.0654 (16) | 0.0486 (14) | 0.0314 (11) | 0.0150 (12) | 0.0196 (11) | 0.0083 (10) |
| C5 | 0.087 (2) | 0.0596 (17) | 0.0554 (17) | 0.0233 (16) | 0.0181 (15) | 0.0239 (14) |
| C6 | 0.0410 (12) | 0.0404 (12) | 0.0194 (9) | 0.0069 (9) | 0.0051 (8) | 0.0001 (8) |
| C7 | 0.0408 (12) | 0.0376 (12) | 0.0317 (11) | 0.0069 (9) | 0.0091 (9) | 0.0032 (9) |
| C8 | 0.0604 (15) | 0.0376 (12) | 0.0352 (12) | 0.0068 (11) | 0.0111 (11) | −0.0012 (10) |
| C9 | 0.0596 (16) | 0.0566 (15) | 0.0342 (12) | −0.0082 (13) | −0.0009 (11) | −0.0076 (11) |
| C10 | 0.0419 (14) | 0.078 (2) | 0.0483 (15) | 0.0000 (13) | −0.0023 (12) | −0.0180 (14) |
| C11 | 0.0415 (13) | 0.0615 (16) | 0.0389 (13) | 0.0146 (11) | 0.0005 (10) | −0.0115 (11) |
| C12 | 0.0340 (10) | 0.0218 (9) | 0.0230 (9) | −0.0014 (8) | 0.0090 (8) | 0.0004 (7) |
| C13 | 0.0342 (11) | 0.0316 (11) | 0.0468 (13) | −0.0021 (9) | 0.0076 (10) | −0.0081 (9) |

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C14 | 0.0435 (13) | 0.0396 (12) | 0.0501 (14) | 0.0115 (10) | 0.0111 (11) | -0.0039 (11) |
| C15 | 0.0688 (16) | 0.0272 (11) | 0.0359 (12) | 0.0091 (11) | 0.0238 (11) | 0.0014 (9) |
| C16 | 0.0684 (17) | 0.0299 (12) | 0.0554 (15) | -0.0169 (11) | 0.0226 (13) | -0.0156 (11) |
| C17 | 0.0415 (12) | 0.0348 (12) | 0.0482 (13) | -0.0096 (9) | 0.0171 (10) | -0.0120 (10) |
| C18 | 0.0270 (9) | 0.0280 (10) | 0.0234 (9) | 0.0008 (7) | 0.0046 (8) | -0.0057 (7) |
| C19 | 0.0310 (10) | 0.0334 (11) | 0.0344 (11) | -0.0019 (8) | 0.0073 (9) | 0.0015 (9) |
| C20 | 0.0322 (11) | 0.0515 (14) | 0.0491 (14) | -0.0063 (10) | 0.0111 (10) | -0.0004 (11) |
| C21 | 0.0295 (11) | 0.0597 (15) | 0.0526 (15) | 0.0049 (11) | -0.0017 (11) | -0.0041 (12) |
| C22 | 0.0413 (12) | 0.0402 (12) | 0.0402 (12) | 0.0093 (10) | -0.0045 (10) | -0.0001 (10) |
| C23 | 0.0393 (11) | 0.0291 (10) | 0.0276 (10) | -0.0006 (9) | 0.0023 (9) | -0.0013 (8) |
| C24 | 0.0265 (9) | 0.0249 (9) | 0.0253 (9) | -0.0006 (7) | 0.0025 (8) | 0.0026 (7) |
| C25 | 0.0540 (14) | 0.0325 (11) | 0.0312 (11) | -0.0070 (10) | 0.0122 (10) | -0.0023 (9) |
| C26 | 0.0723 (17) | 0.0504 (15) | 0.0358 (12) | -0.0063 (13) | 0.0237 (12) | 0.0062 (11) |
| C27 | 0.0547 (14) | 0.0398 (13) | 0.0481 (14) | -0.0105 (11) | 0.0131 (12) | 0.0156 (11) |
| C28 | 0.0639 (15) | 0.0261 (11) | 0.0432 (13) | -0.0108 (10) | 0.0046 (12) | 0.0037 (9) |
| C29 | 0.0588 (14) | 0.0265 (10) | 0.0308 (11) | -0.0036 (10) | 0.0122 (10) | -0.0013 (8) |

Geometric parameters (Å, °)

| | | | |
|--------|-------------|---------|-----------|
| Sn—S1 | 2.4772 (5) | C12—C13 | 1.377 (3) |
| Sn—S2 | 3.1048 (5) | C12—C17 | 1.393 (3) |
| Sn—C12 | 2.1286 (18) | C13—C14 | 1.394 (3) |
| Sn—C18 | 2.1380 (19) | C13—H13 | 0.9500 |
| Sn—C24 | 2.1521 (18) | C14—C15 | 1.364 (3) |
| S1—C1 | 1.758 (2) | C14—H14 | 0.9500 |
| S2—C1 | 1.675 (2) | C15—C16 | 1.374 (3) |
| N1—C1 | 1.337 (2) | C15—H15 | 0.9500 |
| N1—C6 | 1.453 (3) | C16—C17 | 1.390 (3) |
| N1—C2 | 1.479 (3) | C16—H16 | 0.9500 |
| C2—C3 | 1.517 (3) | C17—H17 | 0.9500 |
| C2—H2A | 0.9900 | C18—C19 | 1.394 (3) |
| C2—H2B | 0.9900 | C18—C23 | 1.396 (3) |
| C3—C4 | 1.524 (3) | C19—C20 | 1.384 (3) |
| C3—H3A | 0.9900 | C19—H19 | 0.9500 |
| C3—H3B | 0.9900 | C20—C21 | 1.385 (3) |
| C4—C5 | 1.521 (3) | C20—H20 | 0.9500 |
| C4—H4A | 0.9900 | C21—C22 | 1.378 (3) |
| C4—H4B | 0.9900 | C21—H21 | 0.9500 |
| C5—H5A | 0.9800 | C22—C23 | 1.391 (3) |
| C5—H5B | 0.9800 | C22—H22 | 0.9500 |
| C5—H5C | 0.9800 | C23—H23 | 0.9500 |
| C6—C11 | 1.378 (3) | C24—C25 | 1.389 (3) |
| C6—C7 | 1.382 (3) | C24—C29 | 1.394 (3) |
| C7—C8 | 1.391 (3) | C25—C26 | 1.390 (3) |
| C7—H7 | 0.9500 | C25—H25 | 0.9500 |
| C8—C9 | 1.375 (3) | C26—C27 | 1.381 (3) |
| C8—H8 | 0.9500 | C26—H26 | 0.9500 |
| C9—C10 | 1.377 (4) | C27—C28 | 1.373 (3) |

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|------------|-------------|-------------|-------------|
| C9—H9 | 0.9500 | C27—H27 | 0.9500 |
| C10—C11 | 1.385 (4) | C28—C29 | 1.382 (3) |
| C10—H10 | 0.9500 | C28—H28 | 0.9500 |
| C11—H11 | 0.9500 | C29—H29 | 0.9500 |
| C12—Sn—C18 | 113.76 (7) | C13—C12—C17 | 118.00 (18) |
| C12—Sn—C24 | 107.51 (7) | C13—C12—Sn | 121.01 (14) |
| C18—Sn—C24 | 107.45 (7) | C17—C12—Sn | 120.99 (15) |
| C12—Sn—S1 | 117.26 (5) | C12—C13—C14 | 121.2 (2) |
| C18—Sn—S1 | 115.54 (5) | C12—C13—H13 | 119.4 |
| C24—Sn—S1 | 92.18 (5) | C14—C13—H13 | 119.4 |
| C1—S1—Sn | 97.64 (7) | C15—C14—C13 | 120.1 (2) |
| C1—N1—C6 | 121.91 (17) | C15—C14—H14 | 119.9 |
| C1—N1—C2 | 121.41 (18) | C13—C14—H14 | 119.9 |
| C6—N1—C2 | 116.68 (16) | C16—C15—C14 | 119.7 (2) |
| N1—C1—S2 | 123.79 (16) | C16—C15—H15 | 120.2 |
| N1—C1—S1 | 116.04 (15) | C14—C15—H15 | 120.2 |
| S2—C1—S1 | 120.16 (12) | C15—C16—C17 | 120.5 (2) |
| N1—C2—C3 | 112.88 (17) | C15—C16—H16 | 119.8 |
| N1—C2—H2A | 109.0 | C17—C16—H16 | 119.8 |
| C3—C2—H2A | 109.0 | C16—C17—C12 | 120.5 (2) |
| N1—C2—H2B | 109.0 | C16—C17—H17 | 119.8 |
| C3—C2—H2B | 109.0 | C12—C17—H17 | 119.8 |
| H2A—C2—H2B | 107.8 | C19—C18—C23 | 118.40 (18) |
| C2—C3—C4 | 111.70 (18) | C19—C18—Sn | 123.25 (14) |
| C2—C3—H3A | 109.3 | C23—C18—Sn | 118.31 (14) |
| C4—C3—H3A | 109.3 | C20—C19—C18 | 120.8 (2) |
| C2—C3—H3B | 109.3 | C20—C19—H19 | 119.6 |
| C4—C3—H3B | 109.3 | C18—C19—H19 | 119.6 |
| H3A—C3—H3B | 107.9 | C19—C20—C21 | 120.4 (2) |
| C3—C4—C5 | 112.3 (2) | C19—C20—H20 | 119.8 |
| C3—C4—H4A | 109.1 | C21—C20—H20 | 119.8 |
| C5—C4—H4A | 109.1 | C22—C21—C20 | 119.5 (2) |
| C3—C4—H4B | 109.1 | C22—C21—H21 | 120.2 |
| C5—C4—H4B | 109.1 | C20—C21—H21 | 120.2 |
| H4A—C4—H4B | 107.9 | C21—C22—C23 | 120.5 (2) |
| C4—C5—H5A | 109.5 | C21—C22—H22 | 119.8 |
| C4—C5—H5B | 109.5 | C23—C22—H22 | 119.8 |
| H5A—C5—H5B | 109.5 | C22—C23—C18 | 120.4 (2) |
| C4—C5—H5C | 109.5 | C22—C23—H23 | 119.8 |
| H5A—C5—H5C | 109.5 | C18—C23—H23 | 119.8 |
| H5B—C5—H5C | 109.5 | C25—C24—C29 | 117.65 (18) |
| C11—C6—C7 | 120.5 (2) | C25—C24—Sn | 121.76 (14) |
| C11—C6—N1 | 120.44 (19) | C29—C24—Sn | 120.53 (14) |
| C7—C6—N1 | 119.07 (19) | C24—C25—C26 | 120.7 (2) |
| C6—C7—C8 | 119.5 (2) | C24—C25—H25 | 119.7 |
| C6—C7—H7 | 120.2 | C26—C25—H25 | 119.7 |
| C8—C7—H7 | 120.2 | C27—C26—C25 | 120.5 (2) |

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|-----------------|--------------|-----------------|--------------|
| C9—C8—C7 | 120.0 (2) | C27—C26—H26 | 119.7 |
| C9—C8—H8 | 120.0 | C25—C26—H26 | 119.7 |
| C7—C8—H8 | 120.0 | C28—C27—C26 | 119.5 (2) |
| C8—C9—C10 | 120.2 (2) | C28—C27—H27 | 120.3 |
| C8—C9—H9 | 119.9 | C26—C27—H27 | 120.3 |
| C10—C9—H9 | 119.9 | C29—C28—C27 | 120.1 (2) |
| C9—C10—C11 | 120.2 (2) | C29—C28—H28 | 120.0 |
| C9—C10—H10 | 119.9 | C27—C28—H28 | 120.0 |
| C11—C10—H10 | 119.9 | C28—C29—C24 | 121.6 (2) |
| C6—C11—C10 | 119.6 (2) | C28—C29—H29 | 119.2 |
| C6—C11—H11 | 120.2 | C24—C29—H29 | 119.2 |
| C10—C11—H11 | 120.2 | | |
| C12—Sn—S1—C1 | -68.43 (8) | C13—C14—C15—C16 | 0.9 (4) |
| C18—Sn—S1—C1 | 70.03 (8) | C14—C15—C16—C17 | -1.6 (4) |
| C24—Sn—S1—C1 | -179.43 (8) | C15—C16—C17—C12 | 1.0 (4) |
| C6—N1—C1—S2 | -179.67 (14) | C13—C12—C17—C16 | 0.4 (3) |
| C2—N1—C1—S2 | 0.9 (3) | Sn—C12—C17—C16 | 179.86 (17) |
| C6—N1—C1—S1 | 0.3 (2) | C12—Sn—C18—C19 | 58.98 (18) |
| C2—N1—C1—S1 | -179.14 (14) | C24—Sn—C18—C19 | 177.86 (16) |
| Sn—S1—C1—N1 | -173.43 (14) | S1—Sn—C18—C19 | -80.93 (16) |
| Sn—S1—C1—S2 | 6.51 (12) | C12—Sn—C18—C23 | -118.75 (14) |
| C1—N1—C2—C3 | 88.8 (2) | C24—Sn—C18—C23 | 0.13 (16) |
| C6—N1—C2—C3 | -90.7 (2) | S1—Sn—C18—C23 | 101.34 (14) |
| N1—C2—C3—C4 | -174.46 (18) | C23—C18—C19—C20 | -1.8 (3) |
| C2—C3—C4—C5 | 178.3 (2) | Sn—C18—C19—C20 | -179.52 (16) |
| C1—N1—C6—C11 | -87.1 (2) | C18—C19—C20—C21 | 0.9 (4) |
| C2—N1—C6—C11 | 92.3 (2) | C19—C20—C21—C22 | 0.8 (4) |
| C1—N1—C6—C7 | 94.2 (2) | C20—C21—C22—C23 | -1.7 (4) |
| C2—N1—C6—C7 | -86.3 (2) | C21—C22—C23—C18 | 0.8 (3) |
| C11—C6—C7—C8 | 1.5 (3) | C19—C18—C23—C22 | 0.9 (3) |
| N1—C6—C7—C8 | -179.84 (18) | Sn—C18—C23—C22 | 178.78 (15) |
| C6—C7—C8—C9 | 0.1 (3) | C12—Sn—C24—C25 | 29.77 (18) |
| C7—C8—C9—C10 | -1.1 (4) | C18—Sn—C24—C25 | -93.05 (17) |
| C8—C9—C10—C11 | 0.5 (4) | S1—Sn—C24—C25 | 149.29 (16) |
| C7—C6—C11—C10 | -2.1 (3) | C12—Sn—C24—C29 | -147.32 (16) |
| N1—C6—C11—C10 | 179.2 (2) | C18—Sn—C24—C29 | 89.86 (17) |
| C9—C10—C11—C6 | 1.1 (4) | S1—Sn—C24—C29 | -27.81 (16) |
| C18—Sn—C12—C13 | 172.10 (15) | C29—C24—C25—C26 | 0.5 (3) |
| C24—Sn—C12—C13 | 53.25 (18) | Sn—C24—C25—C26 | -176.71 (18) |
| S1—Sn—C12—C13 | -48.72 (17) | C24—C25—C26—C27 | -0.6 (4) |
| C18—Sn—C12—C17 | -7.36 (19) | C25—C26—C27—C28 | 0.5 (4) |
| C24—Sn—C12—C17 | -126.21 (16) | C26—C27—C28—C29 | -0.2 (4) |
| S1—Sn—C12—C17 | 131.82 (15) | C27—C28—C29—C24 | 0.1 (4) |
| C17—C12—C13—C14 | -1.1 (3) | C25—C24—C29—C28 | -0.2 (3) |
| Sn—C12—C13—C14 | 179.44 (17) | Sn—C24—C29—C28 | 177.00 (17) |
| C12—C13—C14—C15 | 0.5 (4) | | |

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> |
|---------------------------|-------------|---------------|-----------------------|-------------------------|
| C28—H28···S2 ⁱ | 0.95 | 2.83 | 3.612 (2) | 140 |

Symmetry code: (i) $-x+3/2, y+1/2, -z+3/2$.