

[2-Oxido-1-naphthaldehyde (2-hydroxybenzoyl)hydrazonato]diphenyltin(IV)

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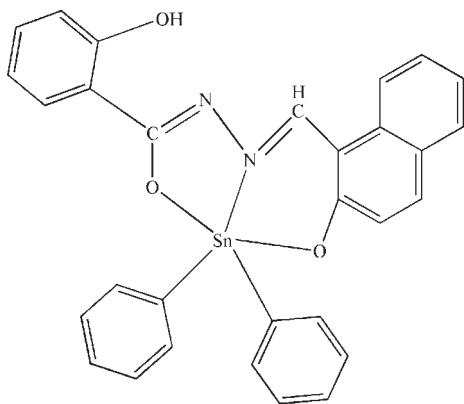
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 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.033; wR factor = 0.073; data-to-parameter ratio = 13.6.

In the title compound, $[\text{Sn}(\text{C}_6\text{H}_5)_2(\text{C}_{18}\text{H}_{12}\text{N}_2\text{O}_3)]$, the Sn^{IV} atom has a distorted trigonal-bipyramidal geometry. The Schiff base molecule is coordinated to the Sn^{IV} atom in a tridentate fashion *via* the azomethine N atom, the hydroxy O atom and the carbonyl O atom. The complex involves an intramolecular $\text{O}-\text{H}\cdots\text{N}$ hydrogen bond.

Related literature

For related structures, see: Chen *et al.* (2006); Yearwood *et al.* (2002). For covalent radii, see: Sanderson (1967).



Experimental

Crystal data

 $[\text{Sn}(\text{C}_6\text{H}_5)_2(\text{C}_{18}\text{H}_{12}\text{N}_2\text{O}_3)]$
 $M_r = 577.19$

 Monoclinic, $P2_1/c$
 $a = 9.418$ (1) Å

 $b = 11.0861$ (12) Å

 $c = 25.668$ (2) Å

 $\beta = 109.547$ (2)°

 $V = 2525.5$ (4) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 1.05$ mm⁻¹
 $T = 293$ K
 $0.43 \times 0.29 \times 0.20$ mm

Data collection

 Siemens SMART 1000 CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.662$, $T_{\text{max}} = 0.818$

 12414 measured reflections
 4435 independent reflections
 3263 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.031$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.073$
 $S = 1.03$
 4435 reflections

 325 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.43$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.33$ e Å⁻³

Table 1
Selected bond lengths (Å).

| | | | |
|--------|-----------|---------|-----------|
| Sn1—O1 | 2.121 (2) | Sn1—C19 | 2.106 (4) |
| Sn1—O3 | 2.061 (2) | Sn1—C25 | 2.113 (4) |
| Sn1—N2 | 2.154 (3) | | |

Table 2
Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|--------------------------------------|--------------|--------------------|-------------|----------------------|
| $\text{O2}-\text{H2}\cdots\text{N1}$ | 0.82 | 1.89 | 2.611 (5) | 146 |

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2239).

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supplementary materials

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[2-Oxido-1-naphthaldehyde (2-hydroxybenzoyl)hydrazonato]diphenyltin(IV)

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Comment

The molecular structure of the title compound is shown in Fig. 1. The Sn^{IV} atom is five-coordinated by two O atoms, two C atoms and one N atom. The distortion around the Sn^{IV} atom is a result of the constraints imposed by the Sn1–N2–N1–C1–O1 and Sn1–N2–C8–C9–C10–O3 rings. The dihedral angles between the two benzene rings (C19 to C24 and C25 to C30) and the O3–Sn1–N2 plane are 61.5 (1) and 67.2 (1)°, respectively. The Sn1–N2 distance is 2.154 (3) Å, close to the sum of the covalent radii (2.15 Å; Sanderson, 1967), indicating a strong Sn–N interaction. The O atoms coordinate to the Sn atom with one shorter and one longer Sn–O bond. Very similar structural parameters were observed in the compound studied by Yearwood *et al.* (2002). The angles at Sn1 confirm that the complex has a distorted trigonal-bipyramidal geometry.

Experimental

2-Hydroxybenzhydrazide (5 mol) was added to 30 ml ethanol. The mixture was stirred for 0.5 h and then 2-hydroxy-1-naphthaldehyde (5 mol) was added, generating a yellow sediment immediately. The product was recrystallized from ethanol and DMF mixed solvent to get yellow crystals of 2-hydroxy-1-naphthaldehyde 2-benzoylhydrazone (*L*). The preparation of the title compound was carried out under nitrogen atmosphere. *L* (4 mmol) was added to a mixture of ethanol and benzene (v/v 1:3, 30 ml) with sodium ethoxide (4 mmol). The mixture was stirred for 0.5 h and then dichlorodiphenyltin (4 mmol) was added. The mixture was stirred for 12 h under reflux. After cooling to room temperature, the mixture was filtered and evaporated to dryness. The resulting solid was then recrystallized from dichloromethane-hexane (v/v 1:1). Analysis, calculated for C₃₀H₂₂N₂O₃Sn: C 62.42, H 3.84, N 4.85, O 8.32%; found: C 62.30, H 3.75, N 4.92, O 8.28%.

Refinement

H atoms were positioned geometrically and refined as riding atoms, with C–H = 0.93 and O–H = 0.82 Å and with $U_{\text{iso}}(\text{H}) = 1.2(1.5 \text{ for hydroxyl})U_{\text{eq}}(\text{C}, \text{O})$.

Figures

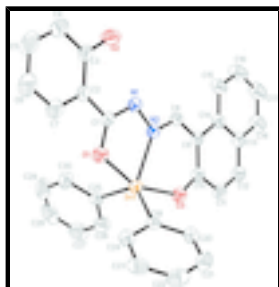


Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids. H atoms have been omitted for clarity.

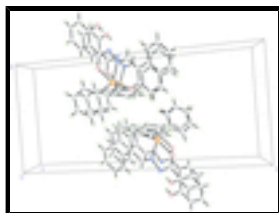


Fig. 2. The crystal packing of the title compound.

[2-Oxido-1-naphthaldehyde (2-hydroxybenzoyl)hydrazonato]diphenyltin(IV)

Crystal data

[Sn(C₆H₅)₂(C₁₈H₁₂N₂O₃)]

$M_r = 577.19$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 9.418 (1) \text{ \AA}$

$b = 11.0861 (12) \text{ \AA}$

$c = 25.668 (2) \text{ \AA}$

$\beta = 109.547 (2)^\circ$

$V = 2525.5 (4) \text{ \AA}^3$

$Z = 4$

$F_{000} = 1160$

$D_x = 1.518 \text{ Mg m}^{-3}$

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

Cell parameters from 4435 reflections

$\theta = 2.5\text{--}24.5^\circ$

$\mu = 1.05 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Block, colorless

$0.43 \times 0.29 \times 0.20 \text{ mm}$

Data collection

Siemens SMART 1000 CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293 \text{ K}$

ϕ and ω scans

Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)

$T_{\min} = 0.662$, $T_{\max} = 0.818$

12414 measured reflections

4435 independent reflections

3263 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.031$

$\theta_{\max} = 25.0^\circ$

$\theta_{\min} = 1.7^\circ$

$h = -11 \rightarrow 11$

$k = -11 \rightarrow 13$

$l = -30 \rightarrow 30$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.033$

$wR(F^2) = 0.073$

$S = 1.03$

4435 reflections

325 parameters

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0238P)^2 + 1.7663P]$$

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

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

$\Delta\rho_{\max} = 0.43 \text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -0.33 \text{ e \AA}^{-3}$

Primary atom site location: structure-invariant direct methods Extinction correction: none

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

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|-------------|---------------|----------------------------------|
| Sn1 | 0.89811 (3) | 0.74107 (2) | 0.920886 (10) | 0.04851 (10) |
| N1 | 0.8396 (4) | 0.4718 (2) | 0.91811 (11) | 0.0465 (8) |
| N2 | 0.8343 (3) | 0.5736 (2) | 0.94938 (11) | 0.0434 (7) |
| O1 | 0.9135 (3) | 0.6067 (2) | 0.86422 (10) | 0.0647 (8) |
| O2 | 0.7809 (4) | 0.2520 (2) | 0.88057 (12) | 0.0834 (10) |
| H2 | 0.7848 | 0.3089 | 0.9015 | 0.125* |
| O3 | 0.8815 (3) | 0.8048 (2) | 0.99407 (10) | 0.0589 (7) |
| C1 | 0.8817 (4) | 0.4984 (3) | 0.87560 (14) | 0.0459 (9) |
| C2 | 0.8935 (4) | 0.4009 (3) | 0.83892 (14) | 0.0493 (9) |
| C3 | 0.8422 (5) | 0.2849 (3) | 0.84222 (15) | 0.0576 (11) |
| C4 | 0.8529 (6) | 0.1978 (4) | 0.80504 (18) | 0.0794 (14) |
| H4 | 0.8193 | 0.1198 | 0.8075 | 0.095* |
| C5 | 0.9126 (7) | 0.2261 (5) | 0.7647 (2) | 0.0918 (17) |
| H5 | 0.9166 | 0.1676 | 0.7392 | 0.110* |
| C6 | 0.9665 (7) | 0.3391 (5) | 0.7614 (2) | 0.1001 (19) |
| H6 | 1.0100 | 0.3573 | 0.7347 | 0.120* |
| C7 | 0.9554 (6) | 0.4251 (4) | 0.79798 (17) | 0.0753 (14) |
| H7 | 0.9905 | 0.5025 | 0.7954 | 0.090* |
| C8 | 0.7840 (4) | 0.5562 (3) | 0.99031 (14) | 0.0449 (9) |
| H8 | 0.7550 | 0.4779 | 0.9950 | 0.054* |
| C9 | 0.7683 (4) | 0.6439 (3) | 1.02883 (13) | 0.0428 (9) |
| C10 | 0.8202 (4) | 0.7625 (3) | 1.02946 (14) | 0.0482 (9) |
| C11 | 0.8110 (5) | 0.8440 (3) | 1.07056 (15) | 0.0557 (10) |
| H11 | 0.8460 | 0.9225 | 1.0708 | 0.067* |
| C12 | 0.7523 (5) | 0.8097 (4) | 1.10938 (16) | 0.0609 (11) |
| H12 | 0.7496 | 0.8648 | 1.1364 | 0.073* |
| C13 | 0.6946 (5) | 0.6924 (4) | 1.11023 (16) | 0.0561 (11) |
| C14 | 0.7010 (4) | 0.6071 (3) | 1.07003 (15) | 0.0507 (10) |
| C15 | 0.6398 (5) | 0.4933 (4) | 1.07211 (17) | 0.0640 (12) |
| H15 | 0.6401 | 0.4363 | 1.0455 | 0.077* |
| C16 | 0.5797 (6) | 0.4627 (4) | 1.1119 (2) | 0.0826 (15) |
| H16 | 0.5410 | 0.3856 | 1.1122 | 0.099* |
| C17 | 0.5756 (6) | 0.5453 (5) | 1.1519 (2) | 0.0878 (16) |
| H17 | 0.5346 | 0.5242 | 1.1790 | 0.105* |
| C18 | 0.6327 (6) | 0.6582 (4) | 1.15106 (18) | 0.0751 (14) |
| H18 | 0.6308 | 0.7137 | 1.1780 | 0.090* |
| C19 | 1.1244 (4) | 0.7942 (3) | 0.93967 (14) | 0.0444 (9) |
| C20 | 1.2167 (5) | 0.8207 (3) | 0.99286 (15) | 0.0572 (11) |
| H20 | 1.1779 | 0.8179 | 1.0217 | 0.069* |
| C21 | 1.3657 (5) | 0.8514 (4) | 1.0035 (2) | 0.0748 (13) |
| H21 | 1.4275 | 0.8661 | 1.0396 | 0.090* |
| C22 | 1.4234 (6) | 0.8602 (4) | 0.9612 (2) | 0.0763 (13) |
| H22 | 1.5236 | 0.8821 | 0.9686 | 0.092* |

supplementary materials

| | | | | |
|-----|------------|------------|--------------|-------------|
| C23 | 1.3339 (6) | 0.8371 (4) | 0.9084 (2) | 0.0707 (13) |
| H23 | 1.3723 | 0.8445 | 0.8796 | 0.085* |
| C24 | 1.1862 (5) | 0.8026 (3) | 0.89768 (16) | 0.0585 (11) |
| H24 | 1.1268 | 0.7846 | 0.8616 | 0.070* |
| C25 | 0.7141 (4) | 0.8331 (3) | 0.86445 (15) | 0.0508 (10) |
| C26 | 0.6817 (5) | 0.9491 (4) | 0.87485 (19) | 0.0700 (12) |
| H26 | 0.7412 | 0.9868 | 0.9071 | 0.084* |
| C27 | 0.5624 (6) | 1.0113 (5) | 0.8384 (2) | 0.0913 (16) |
| H27 | 0.5436 | 1.0907 | 0.8459 | 0.110* |
| C28 | 0.4723 (6) | 0.9565 (7) | 0.7916 (2) | 0.0969 (19) |
| H28 | 0.3911 | 0.9980 | 0.7674 | 0.116* |
| C29 | 0.5006 (6) | 0.8424 (7) | 0.7803 (2) | 0.0976 (18) |
| H29 | 0.4386 | 0.8050 | 0.7484 | 0.117* |
| C30 | 0.6228 (5) | 0.7797 (4) | 0.81640 (18) | 0.0751 (13) |
| H30 | 0.6427 | 0.7013 | 0.8079 | 0.090* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|---------------|--------------|---------------|
| Sn1 | 0.05637 (18) | 0.04439 (15) | 0.04495 (15) | -0.01070 (14) | 0.01717 (12) | -0.00358 (12) |
| N1 | 0.058 (2) | 0.0411 (16) | 0.0412 (17) | -0.0028 (14) | 0.0175 (16) | -0.0055 (13) |
| N2 | 0.048 (2) | 0.0421 (16) | 0.0400 (17) | -0.0043 (14) | 0.0142 (15) | -0.0034 (13) |
| O1 | 0.094 (2) | 0.0545 (16) | 0.0572 (17) | -0.0219 (15) | 0.0407 (17) | -0.0132 (13) |
| O2 | 0.138 (3) | 0.0483 (16) | 0.079 (2) | -0.0149 (18) | 0.057 (2) | -0.0112 (15) |
| O3 | 0.080 (2) | 0.0532 (15) | 0.0504 (16) | -0.0166 (14) | 0.0309 (15) | -0.0128 (12) |
| C1 | 0.048 (3) | 0.046 (2) | 0.039 (2) | -0.0072 (18) | 0.0094 (18) | -0.0046 (16) |
| C2 | 0.054 (3) | 0.054 (2) | 0.036 (2) | -0.0022 (19) | 0.0113 (19) | -0.0059 (17) |
| C3 | 0.071 (3) | 0.053 (2) | 0.045 (2) | 0.008 (2) | 0.014 (2) | -0.0043 (18) |
| C4 | 0.114 (4) | 0.057 (3) | 0.067 (3) | 0.009 (3) | 0.029 (3) | -0.016 (2) |
| C5 | 0.120 (5) | 0.091 (4) | 0.065 (3) | 0.017 (3) | 0.032 (3) | -0.029 (3) |
| C6 | 0.142 (6) | 0.111 (4) | 0.064 (3) | -0.014 (4) | 0.056 (4) | -0.025 (3) |
| C7 | 0.097 (4) | 0.079 (3) | 0.057 (3) | -0.018 (3) | 0.037 (3) | -0.015 (2) |
| C8 | 0.051 (3) | 0.041 (2) | 0.044 (2) | 0.0003 (17) | 0.0162 (19) | 0.0026 (16) |
| C9 | 0.043 (2) | 0.045 (2) | 0.037 (2) | 0.0062 (17) | 0.0096 (17) | 0.0028 (15) |
| C10 | 0.047 (2) | 0.050 (2) | 0.044 (2) | 0.0035 (19) | 0.0112 (17) | -0.0021 (18) |
| C11 | 0.062 (3) | 0.050 (2) | 0.052 (2) | 0.002 (2) | 0.016 (2) | -0.0086 (18) |
| C12 | 0.068 (3) | 0.063 (3) | 0.053 (3) | 0.011 (2) | 0.021 (2) | -0.010 (2) |
| C13 | 0.060 (3) | 0.059 (2) | 0.052 (2) | 0.013 (2) | 0.023 (2) | 0.0021 (19) |
| C14 | 0.051 (3) | 0.052 (2) | 0.050 (2) | 0.0134 (19) | 0.018 (2) | 0.0057 (18) |
| C15 | 0.082 (4) | 0.058 (3) | 0.066 (3) | 0.005 (2) | 0.044 (3) | 0.003 (2) |
| C16 | 0.112 (5) | 0.071 (3) | 0.091 (4) | 0.001 (3) | 0.069 (3) | 0.007 (3) |
| C17 | 0.118 (5) | 0.089 (4) | 0.084 (4) | 0.014 (3) | 0.071 (4) | 0.014 (3) |
| C18 | 0.097 (4) | 0.077 (3) | 0.068 (3) | 0.016 (3) | 0.050 (3) | -0.003 (2) |
| C19 | 0.052 (2) | 0.0325 (18) | 0.047 (2) | -0.0046 (16) | 0.0141 (19) | 0.0030 (15) |
| C20 | 0.063 (3) | 0.062 (3) | 0.044 (2) | -0.007 (2) | 0.014 (2) | 0.0018 (18) |
| C21 | 0.059 (3) | 0.078 (3) | 0.068 (3) | -0.011 (3) | -0.004 (3) | -0.002 (2) |
| C22 | 0.055 (3) | 0.067 (3) | 0.106 (4) | -0.008 (2) | 0.027 (3) | -0.003 (3) |
| C23 | 0.076 (4) | 0.063 (3) | 0.089 (4) | -0.010 (2) | 0.048 (3) | 0.002 (2) |

| | | | | | | |
|-----|-----------|-----------|-----------|--------------|-------------|--------------|
| C24 | 0.067 (3) | 0.063 (2) | 0.047 (2) | -0.010 (2) | 0.022 (2) | -0.0004 (19) |
| C25 | 0.050 (3) | 0.056 (2) | 0.045 (2) | -0.0142 (19) | 0.0134 (19) | 0.0039 (17) |
| C26 | 0.059 (3) | 0.066 (3) | 0.077 (3) | -0.002 (2) | 0.012 (3) | 0.005 (2) |
| C27 | 0.080 (4) | 0.081 (4) | 0.106 (5) | 0.008 (3) | 0.021 (4) | 0.023 (3) |
| C28 | 0.058 (4) | 0.141 (6) | 0.088 (4) | 0.008 (4) | 0.019 (3) | 0.052 (4) |
| C29 | 0.070 (4) | 0.153 (6) | 0.055 (3) | -0.024 (4) | 0.001 (3) | 0.007 (4) |
| C30 | 0.076 (3) | 0.087 (3) | 0.054 (3) | -0.019 (3) | 0.011 (2) | -0.006 (2) |

Geometric parameters (Å, °)

| | | | |
|-------------|-------------|-------------|-----------|
| Sn1—O1 | 2.121 (2) | C13—C18 | 1.411 (5) |
| Sn1—O3 | 2.061 (2) | C13—C14 | 1.415 (5) |
| Sn1—N2 | 2.154 (3) | C14—C15 | 1.396 (5) |
| Sn1—C19 | 2.106 (4) | C15—C16 | 1.366 (5) |
| Sn1—C25 | 2.113 (4) | C15—H15 | 0.9300 |
| N1—C1 | 1.313 (4) | C16—C17 | 1.387 (6) |
| N1—N2 | 1.395 (4) | C16—H16 | 0.9300 |
| N2—C8 | 1.303 (4) | C17—C18 | 1.365 (6) |
| O1—C1 | 1.294 (4) | C17—H17 | 0.9300 |
| O2—C3 | 1.348 (5) | C18—H18 | 0.9300 |
| O2—H2 | 0.8200 | C19—C20 | 1.383 (5) |
| O3—C10 | 1.315 (4) | C19—C24 | 1.389 (5) |
| C1—C2 | 1.462 (5) | C20—C21 | 1.380 (6) |
| C2—C3 | 1.386 (5) | C20—H20 | 0.9300 |
| C2—C7 | 1.388 (5) | C21—C22 | 1.370 (6) |
| C3—C4 | 1.384 (5) | C21—H21 | 0.9300 |
| C4—C5 | 1.371 (6) | C22—C23 | 1.359 (6) |
| C4—H4 | 0.9300 | C22—H22 | 0.9300 |
| C5—C6 | 1.364 (7) | C23—C24 | 1.378 (6) |
| C5—H5 | 0.9300 | C23—H23 | 0.9300 |
| C6—C7 | 1.366 (6) | C24—H24 | 0.9300 |
| C6—H6 | 0.9300 | C25—C26 | 1.368 (5) |
| C7—H7 | 0.9300 | C25—C30 | 1.379 (5) |
| C8—C9 | 1.429 (5) | C26—C27 | 1.382 (6) |
| C8—H8 | 0.9300 | C26—H26 | 0.9300 |
| C9—C10 | 1.401 (5) | C27—C28 | 1.360 (7) |
| C9—C14 | 1.461 (5) | C27—H27 | 0.9300 |
| C10—C11 | 1.414 (5) | C28—C29 | 1.344 (8) |
| C11—C12 | 1.346 (5) | C28—H28 | 0.9300 |
| C11—H11 | 0.9300 | C29—C30 | 1.397 (7) |
| C12—C13 | 1.413 (6) | C29—H29 | 0.9300 |
| C12—H12 | 0.9300 | C30—H30 | 0.9300 |
| O3—Sn1—C19 | 94.31 (12) | C18—C13—C14 | 119.4 (4) |
| O3—Sn1—C25 | 99.45 (13) | C12—C13—C14 | 119.6 (3) |
| C19—Sn1—C25 | 123.88 (13) | C15—C14—C13 | 117.2 (3) |
| O3—Sn1—O1 | 155.42 (10) | C15—C14—C9 | 124.3 (3) |
| C19—Sn1—O1 | 93.27 (12) | C13—C14—C9 | 118.4 (3) |
| C25—Sn1—O1 | 95.61 (13) | C16—C15—C14 | 122.2 (4) |
| O3—Sn1—N2 | 82.61 (10) | C16—C15—H15 | 118.9 |

supplementary materials

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|--------------|-------------|-----------------|------------|
| C19—Sn1—N2 | 122.65 (12) | C14—C15—H15 | 118.9 |
| C25—Sn1—N2 | 113.00 (13) | C15—C16—C17 | 120.7 (4) |
| O1—Sn1—N2 | 73.63 (10) | C15—C16—H16 | 119.6 |
| C1—N1—N2 | 112.1 (3) | C17—C16—H16 | 119.6 |
| C8—N2—N1 | 115.9 (3) | C18—C17—C16 | 119.0 (4) |
| C8—N2—Sn1 | 128.2 (2) | C18—C17—H17 | 120.5 |
| N1—N2—Sn1 | 115.7 (2) | C16—C17—H17 | 120.5 |
| C1—O1—Sn1 | 115.0 (2) | C17—C18—C13 | 121.4 (4) |
| C3—O2—H2 | 109.5 | C17—C18—H18 | 119.3 |
| C10—O3—Sn1 | 133.8 (2) | C13—C18—H18 | 119.3 |
| O1—C1—N1 | 123.6 (3) | C20—C19—C24 | 117.7 (4) |
| O1—C1—C2 | 117.9 (3) | C20—C19—Sn1 | 122.6 (3) |
| N1—C1—C2 | 118.6 (3) | C24—C19—Sn1 | 119.7 (3) |
| C3—C2—C7 | 118.0 (3) | C21—C20—C19 | 120.6 (4) |
| C3—C2—C1 | 122.9 (3) | C21—C20—H20 | 119.7 |
| C7—C2—C1 | 119.1 (4) | C19—C20—H20 | 119.7 |
| O2—C3—C4 | 117.6 (4) | C22—C21—C20 | 120.5 (4) |
| O2—C3—C2 | 122.6 (3) | C22—C21—H21 | 119.8 |
| C4—C3—C2 | 119.9 (4) | C20—C21—H21 | 119.8 |
| C5—C4—C3 | 120.2 (5) | C23—C22—C21 | 119.9 (5) |
| C5—C4—H4 | 119.9 | C23—C22—H22 | 120.1 |
| C3—C4—H4 | 119.9 | C21—C22—H22 | 120.1 |
| C6—C5—C4 | 120.8 (4) | C22—C23—C24 | 120.0 (4) |
| C6—C5—H5 | 119.6 | C22—C23—H23 | 120.0 |
| C4—C5—H5 | 119.6 | C24—C23—H23 | 120.0 |
| C5—C6—C7 | 118.9 (5) | C23—C24—C19 | 121.3 (4) |
| C5—C6—H6 | 120.5 | C23—C24—H24 | 119.3 |
| C7—C6—H6 | 120.5 | C19—C24—H24 | 119.3 |
| C6—C7—C2 | 122.2 (5) | C26—C25—C30 | 117.7 (4) |
| C6—C7—H7 | 118.9 | C26—C25—Sn1 | 120.3 (3) |
| C2—C7—H7 | 118.9 | C30—C25—Sn1 | 121.9 (3) |
| N2—C8—C9 | 127.4 (3) | C25—C26—C27 | 121.4 (5) |
| N2—C8—H8 | 116.3 | C25—C26—H26 | 119.3 |
| C9—C8—H8 | 116.3 | C27—C26—H26 | 119.3 |
| C10—C9—C8 | 122.0 (3) | C28—C27—C26 | 120.0 (5) |
| C10—C9—C14 | 119.2 (3) | C28—C27—H27 | 120.0 |
| C8—C9—C14 | 118.8 (3) | C26—C27—H27 | 120.0 |
| O3—C10—C9 | 124.0 (3) | C29—C28—C27 | 120.1 (5) |
| O3—C10—C11 | 115.9 (3) | C29—C28—H28 | 120.0 |
| C9—C10—C11 | 120.0 (3) | C27—C28—H28 | 120.0 |
| C12—C11—C10 | 121.0 (4) | C28—C29—C30 | 120.3 (5) |
| C12—C11—H11 | 119.5 | C28—C29—H29 | 119.9 |
| C10—C11—H11 | 119.5 | C30—C29—H29 | 119.9 |
| C11—C12—C13 | 121.8 (4) | C25—C30—C29 | 120.5 (5) |
| C11—C12—H12 | 119.1 | C25—C30—H30 | 119.7 |
| C13—C12—H12 | 119.1 | C29—C30—H30 | 119.7 |
| C18—C13—C12 | 121.0 (4) | | |
| C1—N1—N2—C8 | 175.7 (3) | C11—C12—C13—C18 | -179.6 (4) |
| C1—N1—N2—Sn1 | -0.9 (4) | C11—C12—C13—C14 | 1.3 (6) |

| | | | |
|-----------------|------------|-----------------|------------|
| O3—Sn1—N2—C8 | 11.5 (3) | C18—C13—C14—C15 | 2.1 (6) |
| C19—Sn1—N2—C8 | 101.9 (3) | C12—C13—C14—C15 | -178.8 (4) |
| C25—Sn1—N2—C8 | -85.7 (3) | C18—C13—C14—C9 | -178.8 (4) |
| O1—Sn1—N2—C8 | -174.9 (3) | C12—C13—C14—C9 | 0.3 (6) |
| O3—Sn1—N2—N1 | -172.4 (2) | C10—C9—C14—C15 | 177.3 (4) |
| C19—Sn1—N2—N1 | -82.1 (3) | C8—C9—C14—C15 | -4.9 (6) |
| C25—Sn1—N2—N1 | 90.4 (3) | C10—C9—C14—C13 | -1.8 (5) |
| O1—Sn1—N2—N1 | 1.2 (2) | C8—C9—C14—C13 | 176.0 (3) |
| O3—Sn1—O1—C1 | 14.0 (5) | C13—C14—C15—C16 | -1.8 (7) |
| C19—Sn1—O1—C1 | 121.8 (3) | C9—C14—C15—C16 | 179.2 (4) |
| C25—Sn1—O1—C1 | -113.7 (3) | C14—C15—C16—C17 | 0.7 (8) |
| N2—Sn1—O1—C1 | -1.3 (3) | C15—C16—C17—C18 | 0.0 (8) |
| C19—Sn1—O3—C10 | -137.9 (3) | C16—C17—C18—C13 | 0.4 (8) |
| C25—Sn1—O3—C10 | 96.7 (3) | C12—C13—C18—C17 | 179.4 (5) |
| O1—Sn1—O3—C10 | -30.3 (5) | C14—C13—C18—C17 | -1.5 (7) |
| N2—Sn1—O3—C10 | -15.5 (3) | O3—Sn1—C19—C20 | 17.9 (3) |
| Sn1—O1—C1—N1 | 1.4 (5) | C25—Sn1—C19—C20 | 122.4 (3) |
| Sn1—O1—C1—C2 | -178.6 (3) | O1—Sn1—C19—C20 | -138.7 (3) |
| N2—N1—C1—O1 | -0.3 (5) | N2—Sn1—C19—C20 | -66.0 (3) |
| N2—N1—C1—C2 | 179.7 (3) | O3—Sn1—C19—C24 | -162.6 (3) |
| O1—C1—C2—C3 | -170.6 (4) | C25—Sn1—C19—C24 | -58.2 (3) |
| N1—C1—C2—C3 | 9.4 (6) | O1—Sn1—C19—C24 | 40.8 (3) |
| O1—C1—C2—C7 | 7.9 (6) | N2—Sn1—C19—C24 | 113.5 (3) |
| N1—C1—C2—C7 | -172.1 (4) | C24—C19—C20—C21 | -1.6 (6) |
| C7—C2—C3—O2 | 179.7 (4) | Sn1—C19—C20—C21 | 177.9 (3) |
| C1—C2—C3—O2 | -1.8 (6) | C19—C20—C21—C22 | 2.3 (7) |
| C7—C2—C3—C4 | -0.5 (6) | C20—C21—C22—C23 | -0.9 (7) |
| C1—C2—C3—C4 | 178.0 (4) | C21—C22—C23—C24 | -1.2 (7) |
| O2—C3—C4—C5 | 179.3 (5) | C22—C23—C24—C19 | 1.9 (7) |
| C2—C3—C4—C5 | -0.6 (7) | C20—C19—C24—C23 | -0.5 (6) |
| C3—C4—C5—C6 | 1.9 (8) | Sn1—C19—C24—C23 | 180.0 (3) |
| C4—C5—C6—C7 | -2.1 (9) | O3—Sn1—C25—C26 | 37.8 (3) |
| C5—C6—C7—C2 | 1.1 (9) | C19—Sn1—C25—C26 | -64.0 (4) |
| C3—C2—C7—C6 | 0.2 (7) | O1—Sn1—C25—C26 | -161.7 (3) |
| C1—C2—C7—C6 | -178.4 (5) | N2—Sn1—C25—C26 | 123.7 (3) |
| N1—N2—C8—C9 | 179.4 (3) | O3—Sn1—C25—C30 | -142.1 (3) |
| Sn1—N2—C8—C9 | -4.6 (6) | C19—Sn1—C25—C30 | 116.1 (3) |
| N2—C8—C9—C10 | -5.8 (6) | O1—Sn1—C25—C30 | 18.4 (3) |
| N2—C8—C9—C14 | 176.5 (4) | N2—Sn1—C25—C30 | -56.2 (4) |
| Sn1—O3—C10—C9 | 11.6 (6) | C30—C25—C26—C27 | -0.4 (7) |
| Sn1—O3—C10—C11 | -169.6 (3) | Sn1—C25—C26—C27 | 179.7 (4) |
| C8—C9—C10—O3 | 2.8 (6) | C25—C26—C27—C28 | 1.4 (8) |
| C14—C9—C10—O3 | -179.5 (3) | C26—C27—C28—C29 | -1.0 (8) |
| C8—C9—C10—C11 | -176.0 (3) | C27—C28—C29—C30 | -0.3 (8) |
| C14—C9—C10—C11 | 1.7 (5) | C26—C25—C30—C29 | -0.9 (7) |
| O3—C10—C11—C12 | -179.0 (4) | Sn1—C25—C30—C29 | 179.0 (4) |
| C9—C10—C11—C12 | -0.2 (6) | C28—C29—C30—C25 | 1.2 (8) |
| C10—C11—C12—C13 | -1.4 (6) | | |

supplementary materials

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> |
| O2—H2···N1 | 0.82 | 1.89 | 2.611 (5) | 146 |

Fig. 1

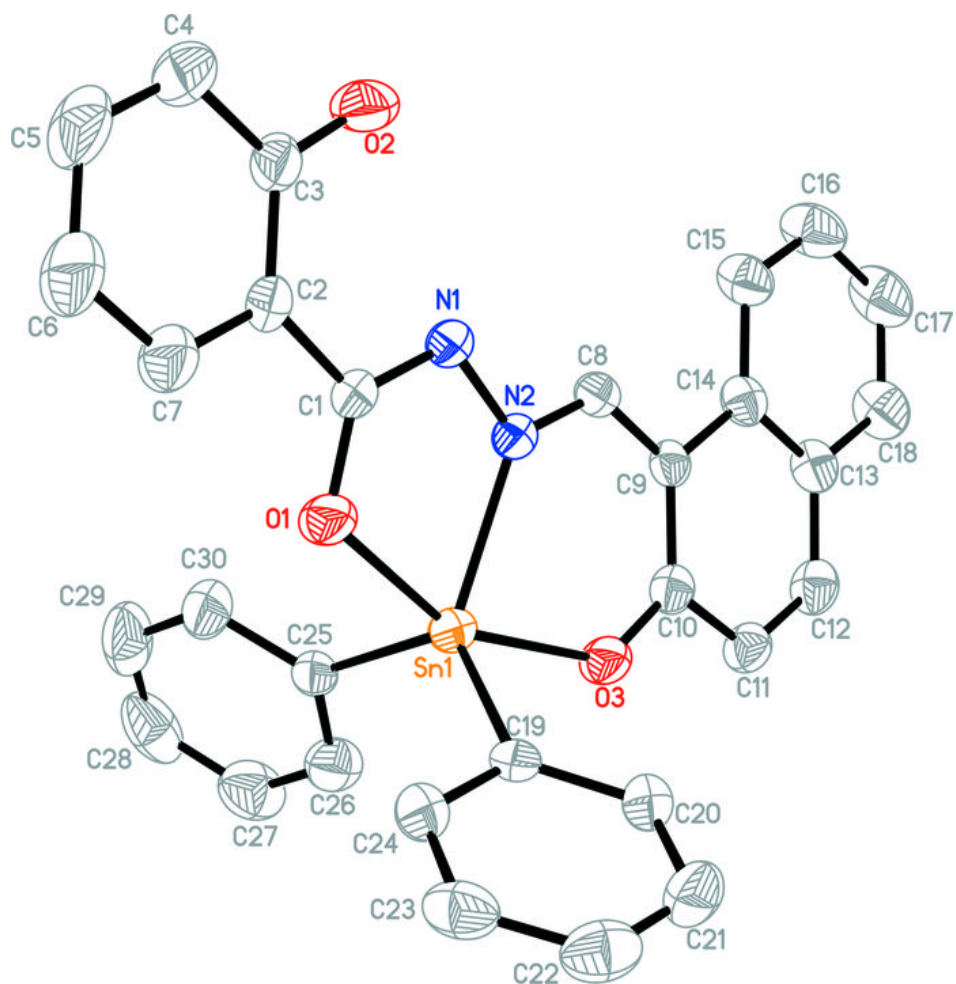


Fig. 2

