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[4-Chloro-*N*′-(3-methoxy-2-oxidobenzylidene)benzohydrazidato]diphenyltin(IV)

Jichun Cui, Handong Yin* and Yanling Qiao

College of Chemistry and Chemical Engineering, Liaocheng University, Shandong 252059, People's Republic of China
Correspondence e-mail: handongyin@163.com

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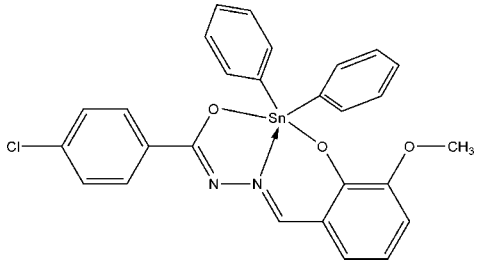
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.009 Å; R factor = 0.045; wR factor = 0.087; data-to-parameter ratio = 14.1.

The title compound, $[Sn(C_6H_5)_2(C_{15}H_{11}ClN_2O_3)]$, crystallizes with two independent molecules in the asymmetric unit with almost identical conformation. In each molecule, the Sn atom is coordinated by two O, one N and two C atoms in a distorted trigonal–bipyramidal geometry [Sn—O = 2.066 (3)–2.132 (4) Å, and Sn—N = 2.150 (4) and 2.141 (4) Å].

Related literature

For a related structure, see: Yin & Chen (2006).



Experimental

Crystal data

$[Sn(C_6H_5)_2(C_{15}H_{11}ClN_2O_3)]$
M_r = 575.60
Monoclinic, $P2_1/c$
a = 19.178 (2) Å
b = 27.968 (3) Å
c = 9.4230 (13) Å
β = 103.238 (2)°
V = 4920.1 (10) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.18 mm^{-1}
T = 298 (2) K
0.37 × 0.17 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.670, T_{max} = 0.872
20342 measured reflections
8658 independent reflections
5197 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.087
S = 1.01
8658 reflections
615 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.76 e Å^{-3}

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2284).

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supplementary materials

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[4-Chloro-*N*'-(3-methoxy-2-oxidobenzylidene)benzohydrazidato]diphenyltin(IV)

J. Cui, H. Yin and Y. Qiao

Comment

Recently, we have reported some organotin(IV) complexes with Schiff base of *o*-vanillin-2-thiophenoylhydrazone (Yin, Chen, 2006). As an extension of our work on the organotin(IV) Schiff bases chemistry, the title compound, (I), is reported here (Fig. 1).

In the title compound, (I), the Sn atom has a distorted trigonal-bipyramidal geometry, with atoms O1 (O4) and O2 (O5) in axial positions [O1—Sn1—O2 = 158.33 (13)°, O4—Sn2—O5 = 156.14 (15)°] and the atoms C16 (C43), C22 (C49)] and N1 (N3) in equatorial positions. The sum of the equatorial angles is 359.43 ° (359.86 °), indicating approximate coplanarity for these atoms. The Sn1—N1 (Sn2—N3) bond length is 2.150 (4) Å (2.141 (4) Å) close to the sum of the non-polar covalent radii 2.15 Å, indicate a strong Sn—N interaction. The O atoms coordinate to the Sn atom with one shorter and one longer Sn—O bond.

Experimental

The reaction was carried out under nitrogen atmosphere. *o*-vanillin 4-chlorobenzhydrazone(1 mmol) and sodium ethoxide (1.2 mmol) were added to the solution of benzene(30 ml) in a Schlenk flask and stirred for 0.5 h. Diphenyltin dichloride (1 mmol) was then added to the reactor and the reaction mixture was stirred for 4 h at 313 K·The resulting clear solution was evaporated under vacuum. The product was crystallized from a mixture of dichloromethane/methanol (1:1)·Analysis calculated for $C_{27}H_{21}ClN_2O_3Sn$ (Mr = 575.63): C, 56.34; H, 3.68; N, 4.87, found: C, 56.28; H, 3.61; N, 4.95.

Refinement

All H atoms attached to C atoms were fixed geometrically and treated as riding with aromatic C—H distances of 0.93 Å, methyl C—H distances of 0.96 Å. The U_{iso}(H) values were set at 1.5U_{iso}(C) for the methyl H atoms, and at 1.2U_{iso}(C) for the other H atoms.

Figures

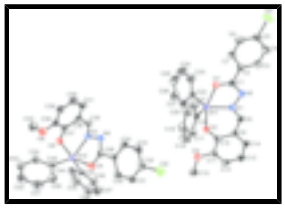


Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted for clarity.

[4-Chloro-*N*'-(3-methoxy-2-oxidobenzylidene)benzohydrazidato]diphenyltin(IV)

Crystal data

$[Sn(C_6H_5)_2(C_{15}H_{11}ClN_2O_3)]$	F_{000} = 2304
M_r = 575.60	D_x = 1.554 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 4610 reflections
a = 19.178 (2) Å	θ = 2.3–27.3º
b = 27.968 (3) Å	μ = 1.18 mm^{-1}
c = 9.4230 (13) Å	T = 298 (2) K
β = 103.238 (2)º	Block, orange
V = 4920.1 (10) Å^3	0.37 × 0.17 × 0.12 mm
Z = 8	

Data collection

CCD area-detector diffractometer	8658 independent reflections
Radiation source: fine-focus sealed tube	5197 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.045
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.3º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −22→22
T_{min} = 0.670, T_{max} = 0.872	k = −25→33
20342 measured reflections	l = −10→11

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.045	H-atom parameters constrained
$wR(F^2)$ = 0.087	$w = 1/[\sigma^2(F_o^2) + (0.0253P)^2 + 2.1263P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max}$ = 0.002
8658 reflections	$\Delta\rho_{max}$ = 0.54 e Å^{-3}
615 parameters	$\Delta\rho_{min}$ = −0.76 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.144802 (18)	0.519068 (13)	0.41711 (4)	0.04606 (12)
Sn2	0.501802 (19)	0.854204 (13)	0.48215 (4)	0.05022 (13)
Cl1	0.12874 (10)	0.25504 (6)	0.9118 (2)	0.1020 (6)
Cl2	0.14114 (9)	0.77336 (6)	0.8586 (2)	0.0956 (6)
N1	0.0499 (2)	0.47593 (15)	0.3566 (5)	0.0479 (11)
N2	0.0496 (2)	0.43350 (15)	0.4343 (5)	0.0559 (12)
N3	0.4951 (2)	0.78151 (15)	0.5491 (5)	0.0497 (12)
N4	0.4407 (2)	0.77048 (15)	0.6197 (5)	0.0547 (12)
O1	0.15977 (18)	0.45977 (12)	0.5633 (4)	0.0584 (10)
O2	0.09344 (17)	0.56387 (12)	0.2515 (4)	0.0527 (10)
O3	0.05732 (19)	0.63653 (14)	0.0770 (4)	0.0699 (12)
O4	0.40729 (17)	0.84888 (13)	0.5635 (4)	0.0620 (11)
O5	0.59883 (17)	0.83215 (13)	0.4450 (4)	0.0575 (10)
O6	0.7019 (2)	0.82949 (16)	0.3078 (5)	0.0771 (12)
C1	0.1073 (3)	0.4291 (2)	0.5375 (6)	0.0484 (14)
C2	0.1135 (3)	0.3856 (2)	0.6272 (6)	0.0508 (14)
C3	0.0614 (3)	0.3497 (2)	0.5990 (7)	0.0724 (18)
H3	0.0224	0.3526	0.5201	0.087*
C4	0.0673 (4)	0.3101 (2)	0.6865 (8)	0.0750 (19)
H4	0.0325	0.2864	0.6663	0.090*
C5	0.1236 (4)	0.3053 (2)	0.8025 (8)	0.0665 (18)
C6	0.1762 (3)	0.3391 (2)	0.8317 (7)	0.0737 (19)
H6	0.2155	0.3351	0.9095	0.088*
C7	0.1706 (3)	0.3793 (2)	0.7444 (7)	0.0630 (16)
H7	0.2061	0.4026	0.7654	0.076*
C8	−0.0062 (3)	0.48431 (19)	0.2528 (6)	0.0520 (14)
H8	−0.0416	0.4609	0.2375	0.062*
C9	−0.0202 (3)	0.52482 (19)	0.1600 (5)	0.0439 (13)
C10	0.0286 (3)	0.56267 (19)	0.1631 (6)	0.0472 (14)
C11	0.0074 (3)	0.6005 (2)	0.0660 (6)	0.0484 (14)
C12	−0.0584 (3)	0.6004 (2)	−0.0299 (6)	0.0636 (17)
H12	−0.0715	0.6258	−0.0941	0.076*
C13	−0.1056 (3)	0.5626 (2)	−0.0319 (7)	0.0667 (17)
H13	−0.1501	0.5628	−0.0969	0.080*
C14	−0.0870 (3)	0.5258 (2)	0.0593 (6)	0.0562 (15)
H14	−0.1187	0.5004	0.0563	0.067*
C15	0.0361 (3)	0.6782 (2)	−0.0083 (7)	0.089 (2)
H15A	0.0290	0.6703	−0.1098	0.133*

H15B	0.0728	0.7021	0.0168	0.133*
H15C	−0.0078	0.6903	0.0105	0.133*
C16	0.1542 (2)	0.57022 (19)	0.5832 (6)	0.0425 (13)
C17	0.1312 (3)	0.6159 (2)	0.5540 (6)	0.0654 (17)
H17	0.1108	0.6247	0.4584	0.078*
C18	0.1376 (4)	0.6494 (2)	0.6643 (8)	0.084 (2)
H18	0.1214	0.6805	0.6423	0.101*
C19	0.1677 (4)	0.6372 (2)	0.8048 (7)	0.0751 (19)
H19	0.1721	0.6597	0.8789	0.090*
C20	0.1911 (3)	0.5918 (3)	0.8352 (7)	0.080 (2)
H20	0.2110	0.5830	0.9312	0.096*
C21	0.1858 (3)	0.5588 (2)	0.7265 (7)	0.0636 (17)
H21	0.2037	0.5282	0.7491	0.076*
C22	0.2308 (3)	0.5003 (2)	0.3235 (6)	0.0464 (13)
C23	0.2741 (3)	0.4618 (2)	0.3749 (7)	0.0796 (19)
H23	0.2664	0.4440	0.4534	0.096*
C24	0.3291 (4)	0.4496 (3)	0.3086 (10)	0.112 (3)
H24	0.3578	0.4233	0.3425	0.134*
C25	0.3419 (4)	0.4752 (3)	0.1961 (9)	0.100 (3)
H25	0.3793	0.4666	0.1533	0.120*
C26	0.3006 (4)	0.5131 (3)	0.1460 (8)	0.090 (2)
H26	0.3095	0.5309	0.0688	0.108*
C27	0.2453 (3)	0.5254 (2)	0.2085 (7)	0.0681 (17)
H27	0.2167	0.5516	0.1720	0.082*
C28	0.3999 (3)	0.8073 (2)	0.6217 (6)	0.0497 (14)
C29	0.3380 (3)	0.80035 (18)	0.6884 (6)	0.0450 (13)
C30	0.2846 (3)	0.83445 (19)	0.6718 (6)	0.0517 (15)
H30	0.2893	0.8629	0.6237	0.062*
C31	0.2243 (3)	0.82690 (19)	0.7259 (6)	0.0546 (15)
H31	0.1885	0.8500	0.7147	0.065*
C32	0.2182 (3)	0.7847 (2)	0.7965 (6)	0.0587 (16)
C33	0.2704 (3)	0.7508 (2)	0.8147 (7)	0.0763 (19)
H33	0.2657	0.7225	0.8632	0.092*
C34	0.3297 (3)	0.7589 (2)	0.7611 (7)	0.0689 (18)
H34	0.3653	0.7357	0.7740	0.083*
C35	0.5305 (3)	0.7454 (2)	0.5154 (6)	0.0590 (16)
H35	0.5175	0.7154	0.5433	0.071*
C36	0.5869 (3)	0.7465 (2)	0.4408 (6)	0.0554 (15)
C37	0.6176 (3)	0.7894 (2)	0.4070 (6)	0.0512 (15)
C38	0.6743 (3)	0.7866 (2)	0.3343 (6)	0.0590 (16)
C39	0.6974 (3)	0.7431 (3)	0.2950 (7)	0.0726 (19)
H39	0.7342	0.7419	0.2459	0.087*
C40	0.6663 (4)	0.7012 (3)	0.3279 (7)	0.082 (2)
H40	0.6826	0.6720	0.3012	0.099*
C41	0.6117 (3)	0.7024 (2)	0.3992 (7)	0.0727 (19)
H41	0.5909	0.6740	0.4203	0.087*
C42	0.7613 (3)	0.8289 (2)	0.2383 (8)	0.099 (2)
H42A	0.7992	0.8097	0.2945	0.149*
H42B	0.7783	0.8610	0.2319	0.149*

H42C	0.7461	0.8157	0.1421	0.149*
C43	0.4510 (3)	0.86868 (17)	0.2621 (6)	0.0517 (15)
C44	0.4930 (3)	0.87867 (19)	0.1658 (7)	0.0666 (17)
H44	0.5425	0.8767	0.1969	0.080*
C45	0.4628 (4)	0.8915 (2)	0.0243 (8)	0.084 (2)
H45	0.4920	0.8991	−0.0389	0.101*
C46	0.3906 (5)	0.8930 (3)	−0.0232 (8)	0.101 (3)
H46	0.3704	0.9014	−0.1193	0.121*
C47	0.3473 (4)	0.8823 (2)	0.0689 (10)	0.091 (2)
H47	0.2977	0.8828	0.0354	0.109*
C48	0.3776 (3)	0.8707 (2)	0.2124 (8)	0.0718 (18)
H48	0.3482	0.8641	0.2760	0.086*
C49	0.5474 (3)	0.91054 (18)	0.6191 (6)	0.0481 (14)
C50	0.5057 (3)	0.9406 (2)	0.6795 (7)	0.080 (2)
H50	0.4570	0.9343	0.6659	0.096*
C51	0.5347 (5)	0.9802 (3)	0.7605 (8)	0.105 (3)
H51	0.5057	0.9999	0.8016	0.126*
C52	0.6051 (5)	0.9899 (3)	0.7797 (9)	0.108 (3)
H52	0.6243	1.0167	0.8327	0.130*
C53	0.6480 (4)	0.9606 (3)	0.7221 (8)	0.097 (2)
H53	0.6966	0.9674	0.7363	0.117*
C54	0.6196 (3)	0.9211 (2)	0.6425 (7)	0.0704 (18)
H54	0.6493	0.9011	0.6039	0.084*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0419 (2)	0.0469 (2)	0.0478 (2)	−0.00302 (17)	0.00702 (17)	0.0001 (2)
Sn2	0.0486 (2)	0.0417 (2)	0.0617 (3)	−0.00054 (18)	0.01537 (19)	0.0007 (2)
Cl1	0.1256 (16)	0.0735 (13)	0.1236 (16)	0.0273 (10)	0.0628 (13)	0.0444 (12)
Cl2	0.0946 (13)	0.0798 (13)	0.1330 (17)	−0.0108 (10)	0.0691 (12)	0.0045 (11)
N1	0.044 (3)	0.047 (3)	0.051 (3)	−0.004 (2)	0.009 (2)	0.002 (2)
N2	0.056 (3)	0.048 (3)	0.063 (3)	−0.008 (2)	0.012 (3)	0.010 (3)
N3	0.048 (3)	0.037 (3)	0.064 (3)	0.003 (2)	0.013 (2)	0.007 (2)
N4	0.049 (3)	0.038 (3)	0.079 (4)	0.002 (2)	0.019 (3)	0.009 (2)
O1	0.051 (2)	0.053 (2)	0.064 (3)	−0.0073 (19)	−0.0029 (19)	0.013 (2)
O2	0.043 (2)	0.057 (2)	0.053 (2)	−0.0029 (17)	0.0003 (19)	0.0101 (19)
O3	0.063 (3)	0.064 (3)	0.079 (3)	−0.001 (2)	0.008 (2)	0.021 (2)
O4	0.060 (2)	0.040 (2)	0.095 (3)	0.0040 (18)	0.037 (2)	0.014 (2)
O5	0.051 (2)	0.046 (2)	0.080 (3)	0.0015 (17)	0.022 (2)	−0.008 (2)
O6	0.063 (3)	0.083 (3)	0.093 (3)	−0.001 (2)	0.032 (2)	−0.012 (3)
C1	0.044 (3)	0.058 (4)	0.046 (4)	−0.001 (3)	0.016 (3)	0.004 (3)
C2	0.055 (4)	0.048 (4)	0.054 (4)	0.001 (3)	0.022 (3)	−0.001 (3)
C3	0.068 (4)	0.063 (5)	0.083 (5)	0.001 (4)	0.011 (4)	0.011 (4)
C4	0.091 (5)	0.045 (4)	0.098 (6)	−0.005 (4)	0.040 (5)	0.014 (4)
C5	0.074 (5)	0.055 (4)	0.079 (5)	0.019 (4)	0.033 (4)	0.014 (4)
C6	0.072 (5)	0.075 (5)	0.076 (5)	0.020 (4)	0.020 (4)	0.015 (4)
C7	0.067 (4)	0.055 (4)	0.066 (4)	0.001 (3)	0.013 (4)	0.008 (4)

C8	0.043 (3)	0.051 (4)	0.062 (4)	0.001 (3)	0.012 (3)	−0.008 (3)
C9	0.044 (3)	0.047 (4)	0.039 (3)	0.009 (3)	0.006 (3)	−0.007 (3)
C10	0.047 (3)	0.055 (4)	0.041 (3)	0.008 (3)	0.012 (3)	−0.002 (3)
C11	0.051 (4)	0.048 (4)	0.046 (4)	0.002 (3)	0.010 (3)	0.000 (3)
C12	0.070 (4)	0.066 (5)	0.052 (4)	0.020 (4)	0.007 (3)	0.004 (3)
C13	0.053 (4)	0.070 (5)	0.069 (5)	0.000 (4)	−0.003 (3)	−0.011 (4)
C14	0.047 (4)	0.062 (4)	0.053 (4)	0.003 (3)	−0.001 (3)	−0.006 (3)
C15	0.076 (5)	0.078 (5)	0.113 (6)	0.008 (4)	0.024 (4)	0.037 (5)
C16	0.039 (3)	0.044 (4)	0.047 (4)	−0.004 (2)	0.015 (3)	0.000 (3)
C17	0.085 (5)	0.061 (5)	0.043 (4)	0.009 (3)	0.000 (3)	−0.005 (3)
C18	0.123 (6)	0.058 (5)	0.066 (5)	0.024 (4)	0.012 (4)	−0.002 (4)
C19	0.102 (5)	0.064 (5)	0.060 (5)	−0.013 (4)	0.018 (4)	−0.018 (4)
C20	0.113 (6)	0.080 (6)	0.044 (4)	−0.005 (4)	0.010 (4)	0.005 (4)
C21	0.077 (4)	0.053 (4)	0.056 (4)	0.013 (3)	0.004 (3)	−0.002 (3)
C22	0.041 (3)	0.055 (4)	0.042 (3)	0.004 (3)	0.006 (3)	−0.007 (3)
C23	0.075 (5)	0.085 (5)	0.082 (5)	0.020 (4)	0.024 (4)	0.007 (4)
C24	0.103 (6)	0.111 (7)	0.135 (8)	0.053 (5)	0.056 (6)	0.013 (6)
C25	0.067 (5)	0.134 (8)	0.105 (7)	0.022 (5)	0.034 (5)	−0.025 (6)
C26	0.075 (5)	0.124 (7)	0.082 (5)	0.004 (5)	0.041 (4)	0.010 (5)
C27	0.056 (4)	0.077 (5)	0.073 (5)	0.009 (3)	0.021 (3)	0.005 (4)
C28	0.050 (3)	0.042 (4)	0.055 (4)	−0.007 (3)	0.010 (3)	0.000 (3)
C29	0.044 (3)	0.039 (4)	0.050 (4)	−0.006 (3)	0.006 (3)	0.005 (3)
C30	0.057 (4)	0.044 (4)	0.054 (4)	0.002 (3)	0.013 (3)	0.014 (3)
C31	0.057 (4)	0.040 (4)	0.068 (4)	0.009 (3)	0.019 (3)	−0.003 (3)
C32	0.056 (4)	0.055 (4)	0.066 (4)	−0.006 (3)	0.015 (3)	0.000 (3)
C33	0.084 (5)	0.060 (4)	0.094 (5)	−0.001 (4)	0.039 (4)	0.034 (4)
C34	0.055 (4)	0.060 (4)	0.090 (5)	0.008 (3)	0.014 (3)	0.033 (4)
C35	0.058 (4)	0.044 (4)	0.071 (4)	0.006 (3)	0.006 (3)	0.003 (3)
C36	0.049 (4)	0.056 (4)	0.056 (4)	0.009 (3)	0.002 (3)	−0.008 (3)
C37	0.040 (3)	0.056 (4)	0.050 (4)	0.010 (3)	−0.004 (3)	−0.007 (3)
C38	0.051 (4)	0.055 (5)	0.069 (4)	−0.001 (3)	0.009 (3)	−0.014 (3)
C39	0.063 (4)	0.078 (5)	0.075 (5)	0.010 (4)	0.013 (3)	−0.018 (4)
C40	0.087 (5)	0.065 (5)	0.096 (6)	0.019 (4)	0.022 (4)	−0.024 (4)
C41	0.073 (4)	0.052 (4)	0.089 (5)	0.013 (3)	0.008 (4)	−0.004 (4)
C42	0.084 (5)	0.108 (6)	0.121 (7)	−0.001 (4)	0.057 (5)	−0.006 (5)
C43	0.055 (4)	0.033 (3)	0.065 (4)	−0.004 (3)	0.010 (3)	−0.008 (3)
C44	0.070 (4)	0.059 (4)	0.070 (5)	−0.006 (3)	0.014 (4)	0.002 (4)
C45	0.112 (6)	0.088 (6)	0.053 (5)	0.008 (5)	0.019 (4)	0.009 (4)
C46	0.129 (8)	0.094 (6)	0.065 (6)	0.010 (6)	−0.009 (6)	−0.008 (5)
C47	0.070 (5)	0.092 (6)	0.092 (6)	−0.001 (4)	−0.023 (5)	−0.013 (5)
C48	0.058 (4)	0.066 (5)	0.086 (5)	−0.006 (3)	0.005 (4)	−0.008 (4)
C49	0.052 (4)	0.037 (3)	0.055 (4)	0.005 (3)	0.012 (3)	0.005 (3)
C50	0.071 (4)	0.075 (5)	0.090 (5)	0.004 (4)	0.010 (4)	−0.027 (4)
C51	0.117 (7)	0.083 (6)	0.109 (7)	0.029 (5)	0.012 (5)	−0.036 (5)
C52	0.122 (7)	0.063 (6)	0.119 (7)	−0.002 (5)	−0.014 (6)	−0.032 (5)
C53	0.078 (5)	0.072 (6)	0.130 (7)	−0.014 (4)	−0.003 (5)	−0.022 (5)
C54	0.061 (4)	0.057 (4)	0.090 (5)	−0.003 (3)	0.013 (4)	−0.010 (4)

Geometric parameters (Å, °)

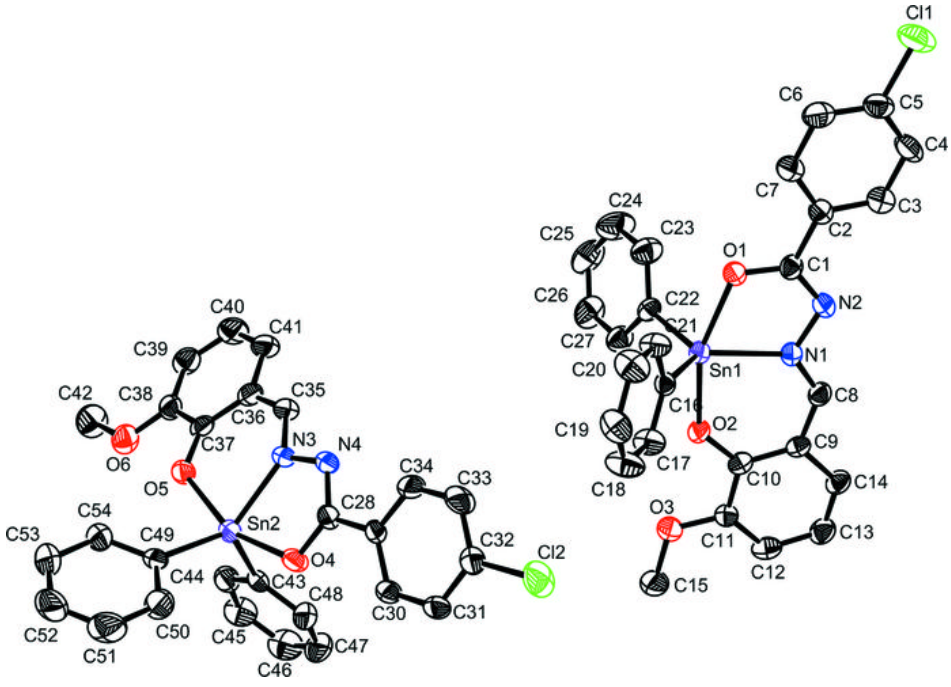
Sn1—O2	2.067 (3)	C20—H20	0.9300
Sn1—C16	2.097 (5)	C21—H21	0.9300
Sn1—C22	2.107 (5)	C22—C27	1.372 (7)
Sn1—O1	2.133 (3)	C22—C23	1.379 (7)
Sn1—N1	2.149 (4)	C23—C24	1.387 (8)
Sn2—O5	2.065 (3)	C23—H23	0.9300
Sn2—C49	2.097 (5)	C24—C25	1.347 (9)
Sn2—C43	2.119 (6)	C24—H24	0.9300
Sn2—O4	2.129 (3)	C25—C26	1.343 (9)
Sn2—N3	2.141 (4)	C25—H25	0.9300
Cl1—C5	1.733 (6)	C26—C27	1.370 (8)
Cl2—C32	1.739 (6)	C26—H26	0.9300
N1—C8	1.299 (6)	C27—H27	0.9300
N1—N2	1.395 (5)	C28—C29	1.477 (7)
N2—C1	1.301 (6)	C29—C34	1.375 (7)
N3—C35	1.296 (6)	C29—C30	1.382 (6)
N3—N4	1.395 (5)	C30—C31	1.383 (7)
N4—C28	1.297 (6)	C30—H30	0.9300
O1—C1	1.303 (6)	C31—C32	1.372 (7)
O2—C10	1.330 (5)	C31—H31	0.9300
O3—C11	1.377 (6)	C32—C33	1.361 (7)
O3—C15	1.421 (6)	C33—C34	1.364 (7)
O4—C28	1.307 (6)	C33—H33	0.9300
O5—C37	1.321 (6)	C34—H34	0.9300
O6—C38	1.358 (6)	C35—C36	1.418 (7)
O6—C42	1.439 (6)	C35—H35	0.9300
C1—C2	1.469 (7)	C36—C37	1.406 (7)
C2—C7	1.377 (7)	C36—C41	1.410 (7)
C2—C3	1.400 (7)	C37—C38	1.413 (7)
C3—C4	1.368 (7)	C38—C39	1.373 (7)
C3—H3	0.9300	C39—C40	1.382 (8)
C4—C5	1.355 (8)	C39—H39	0.9300
C4—H4	0.9300	C40—C41	1.367 (8)
C5—C6	1.363 (8)	C40—H40	0.9300
C6—C7	1.383 (7)	C41—H41	0.9300
C6—H6	0.9300	C42—H42A	0.9600
C7—H7	0.9300	C42—H42B	0.9600
C8—C9	1.419 (7)	C42—H42C	0.9600
C8—H8	0.9300	C43—C44	1.373 (7)
C9—C10	1.408 (7)	C43—C48	1.379 (7)
C9—C14	1.409 (6)	C44—C45	1.374 (8)
C10—C11	1.398 (7)	C44—H44	0.9300
C11—C12	1.374 (7)	C45—C46	1.355 (9)
C12—C13	1.389 (7)	C45—H45	0.9300
C12—H12	0.9300	C46—C47	1.365 (9)
C13—C14	1.335 (7)	C46—H46	0.9300

C13—H13	0.9300	C47—C48	1.383 (9)
C14—H14	0.9300	C47—H47	0.9300
C15—H15A	0.9600	C48—H48	0.9300
C15—H15B	0.9600	C49—C50	1.371 (7)
C15—H15C	0.9600	C49—C54	1.382 (7)
C16—C17	1.358 (7)	C50—C51	1.386 (8)
C16—C21	1.385 (7)	C50—H50	0.9300
C17—C18	1.385 (7)	C51—C52	1.347 (9)
C17—H17	0.9300	C51—H51	0.9300
C18—C19	1.361 (8)	C52—C53	1.360 (9)
C18—H18	0.9300	C52—H52	0.9300
C19—C20	1.355 (8)	C53—C54	1.377 (8)
C19—H19	0.9300	C53—H53	0.9300
C20—C21	1.364 (8)	C54—H54	0.9300
O2—Sn1—C16	95.42 (18)	C27—C22—Sn1	121.5 (4)
O2—Sn1—C22	96.78 (18)	C23—C22—Sn1	120.9 (4)
C16—Sn1—C22	122.71 (18)	C22—C23—C24	119.5 (7)
O2—Sn1—O1	158.35 (13)	C22—C23—H23	120.2
C16—Sn1—O1	94.18 (18)	C24—C23—H23	120.2
C22—Sn1—O1	94.26 (18)	C25—C24—C23	121.2 (7)
O2—Sn1—N1	84.94 (15)	C25—C24—H24	119.4
C16—Sn1—N1	120.24 (16)	C23—C24—H24	119.4
C22—Sn1—N1	116.48 (17)	C26—C25—C24	119.8 (7)
O1—Sn1—N1	73.46 (15)	C26—C25—H25	120.1
O5—Sn2—C49	93.66 (17)	C24—C25—H25	120.1
O5—Sn2—C43	96.99 (19)	C25—C26—C27	120.1 (7)
C49—Sn2—C43	119.50 (19)	C25—C26—H26	120.0
O5—Sn2—O4	156.18 (14)	C27—C26—H26	120.0
C49—Sn2—O4	95.77 (18)	C26—C27—C22	121.8 (6)
C43—Sn2—O4	97.29 (19)	C26—C27—H27	119.1
O5—Sn2—N3	83.29 (15)	C22—C27—H27	119.1
C49—Sn2—N3	125.24 (18)	N4—C28—O4	125.2 (5)
C43—Sn2—N3	115.12 (17)	N4—C28—C29	116.6 (5)
O4—Sn2—N3	73.40 (15)	O4—C28—C29	118.1 (5)
C8—N1—N2	116.5 (4)	C34—C29—C30	118.1 (5)
C8—N1—Sn1	127.1 (4)	C34—C29—C28	121.3 (5)
N2—N1—Sn1	116.3 (3)	C30—C29—C28	120.5 (5)
C1—N2—N1	111.6 (4)	C29—C30—C31	120.9 (5)
C35—N3—N4	115.8 (4)	C29—C30—H30	119.5
C35—N3—Sn2	126.7 (4)	C31—C30—H30	119.5
N4—N3—Sn2	116.9 (3)	C32—C31—C30	118.7 (5)
C28—N4—N3	110.6 (4)	C32—C31—H31	120.6
C1—O1—Sn1	114.1 (3)	C30—C31—H31	120.6
C10—O2—Sn1	132.3 (3)	C33—C32—C31	121.3 (5)
C11—O3—C15	116.9 (4)	C33—C32—Cl2	119.1 (5)
C28—O4—Sn2	113.4 (3)	C31—C32—Cl2	119.6 (5)
C37—O5—Sn2	129.0 (3)	C32—C33—C34	119.2 (6)
C38—O6—C42	117.2 (5)	C32—C33—H33	120.4
N2—C1—O1	124.4 (5)	C34—C33—H33	120.4

N2—C1—C2	116.9 (5)	C33—C34—C29	121.7 (5)
O1—C1—C2	118.7 (5)	C33—C34—H34	119.1
C7—C2—C3	117.5 (6)	C29—C34—H34	119.1
C7—C2—C1	120.8 (5)	N3—C35—C36	127.3 (5)
C3—C2—C1	121.7 (6)	N3—C35—H35	116.4
C4—C3—C2	120.6 (6)	C36—C35—H35	116.4
C4—C3—H3	119.7	C37—C36—C41	119.9 (6)
C2—C3—H3	119.7	C37—C36—C35	122.5 (5)
C5—C4—C3	120.5 (6)	C41—C36—C35	117.6 (6)
C5—C4—H4	119.8	O5—C37—C36	123.8 (5)
C3—C4—H4	119.8	O5—C37—C38	118.1 (5)
C4—C5—C6	120.7 (6)	C36—C37—C38	118.0 (5)
C4—C5—Cl1	119.1 (6)	O6—C38—C39	124.7 (6)
C6—C5—Cl1	120.2 (6)	O6—C38—C37	114.5 (5)
C5—C6—C7	119.4 (6)	C39—C38—C37	120.8 (6)
C5—C6—H6	120.3	C38—C39—C40	120.5 (6)
C7—C6—H6	120.3	C38—C39—H39	119.7
C2—C7—C6	121.3 (6)	C40—C39—H39	119.7
C2—C7—H7	119.3	C41—C40—C39	120.6 (6)
C6—C7—H7	119.3	C41—C40—H40	119.7
N1—C8—C9	128.0 (5)	C39—C40—H40	119.7
N1—C8—H8	116.0	C40—C41—C36	120.1 (6)
C9—C8—H8	116.0	C40—C41—H41	119.9
C10—C9—C14	119.8 (5)	C36—C41—H41	119.9
C10—C9—C8	123.8 (5)	O6—C42—H42A	109.5
C14—C9—C8	116.4 (5)	O6—C42—H42B	109.5
O2—C10—C11	118.8 (5)	H42A—C42—H42B	109.5
O2—C10—C9	123.6 (5)	O6—C42—H42C	109.5
C11—C10—C9	117.6 (5)	H42A—C42—H42C	109.5
C12—C11—O3	124.7 (5)	H42B—C42—H42C	109.5
C12—C11—C10	121.0 (5)	C44—C43—C48	118.4 (6)
O3—C11—C10	114.3 (5)	C44—C43—Sn2	118.5 (4)
C11—C12—C13	120.5 (6)	C48—C43—Sn2	123.0 (5)
C11—C12—H12	119.7	C43—C44—C45	120.9 (6)
C13—C12—H12	119.7	C43—C44—H44	119.5
C14—C13—C12	120.1 (6)	C45—C44—H44	119.5
C14—C13—H13	120.0	C46—C45—C44	120.0 (7)
C12—C13—H13	120.0	C46—C45—H45	120.0
C13—C14—C9	121.0 (6)	C44—C45—H45	120.0
C13—C14—H14	119.5	C45—C46—C47	120.5 (7)
C9—C14—H14	119.5	C45—C46—H46	119.7
O3—C15—H15A	109.5	C47—C46—H46	119.7
O3—C15—H15B	109.5	C46—C47—C48	119.5 (7)
H15A—C15—H15B	109.5	C46—C47—H47	120.2
O3—C15—H15C	109.5	C48—C47—H47	120.2
H15A—C15—H15C	109.5	C43—C48—C47	120.6 (7)
H15B—C15—H15C	109.5	C43—C48—H48	119.7
C17—C16—C21	117.5 (5)	C47—C48—H48	119.7
C17—C16—Sn1	121.5 (4)	C50—C49—C54	117.4 (5)

C21—C16—Sn1	121.0 (4)	C50—C49—Sn2	121.0 (4)
C16—C17—C18	121.1 (6)	C54—C49—Sn2	121.3 (4)
C16—C17—H17	119.5	C49—C50—C51	121.3 (6)
C18—C17—H17	119.5	C49—C50—H50	119.3
C19—C18—C17	120.3 (6)	C51—C50—H50	119.3
C19—C18—H18	119.8	C52—C51—C50	119.9 (7)
C17—C18—H18	119.8	C52—C51—H51	120.1
C20—C19—C18	119.2 (6)	C50—C51—H51	120.1
C20—C19—H19	120.4	C51—C52—C53	120.3 (7)
C18—C19—H19	120.4	C51—C52—H52	119.8
C19—C20—C21	120.6 (6)	C53—C52—H52	119.8
C19—C20—H20	119.7	C52—C53—C54	120.0 (7)
C21—C20—H20	119.7	C52—C53—H53	120.0
C20—C21—C16	121.2 (6)	C54—C53—H53	120.0
C20—C21—H21	119.4	C53—C54—C49	121.0 (6)
C16—C21—H21	119.4	C53—C54—H54	119.5
C27—C22—C23	117.6 (5)	C49—C54—H54	119.5

Fig. 1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