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{4-Hydroxy-*N*′-[(2*E*,3*Z*)-4-oxido-4-phenylbut-3-en-2-ylidene]benzohydrazidato}diphenyltin(IV) methanol monosolvate

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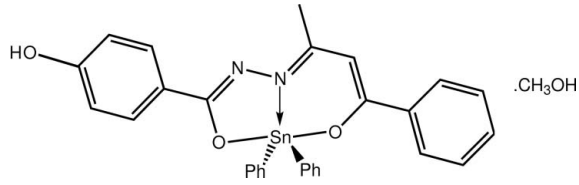
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.005 Å; R factor = 0.032; wR factor = 0.079; data-to-parameter ratio = 13.6.

Two independent diphenyltin molecules and two independent methanol molecules comprise the asymmetric unit of the title compound, $[Sn(C_6H_5)_2(C_{17}H_{14}N_2O_3)]\cdot CH_3OH$. The Sn atom in each is five-coordinated by a tridentate ligand and the *ipso*-C atoms of the Sn-bound benzene substituents. The resulting C_2N_2O donor set defines a coordination geometry that is intermediate between trigonal-bipyramidal (TP) and square-pyramidal (SP), with one molecule slightly tending towards TP and the other slightly towards SP. The molecules differ in terms of the relative orientations of the terminal benzene rings [dihedral angles = 45.71 (18) and 53.98 (17)°] and of the Sn-bound benzene substituents [dihedral angles = 59.5 (2) and 45.77 (18)°, respectively]. The most prominent feature of the crystal packing is the formation of four-molecule aggregates *via* O—H···O and O—H···N hydrogen bonds, in which the hydroxy group is connected to a methanol molecule which, in turn, is linked to a non-coordinating N atom. Weak C—H···π interactions also occur.

Related literature

For background to the biological interest in related compounds, see: Affan *et al.* (2010). For related structures, see: Affan *et al.* (2009, 2011). For additional structural analysis, see: Addison *et al.* (1984).



Experimental

Crystal data

$[Sn(C_6H_5)_2(C_{17}H_{14}N_2O_3)]\cdot CH_4O$
M_r = 599.23
Monoclinic, $P2_1/c$
a = 18.6824 (2) Å
b = 28.7280 (4) Å
c = 10.3369 (1) Å
β = 99.856 (1)°
V = 5466.02 (11) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 7.74 mm^{-1}
T = 150 K
0.37 × 0.29 × 0.17 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: analytical (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.231, T_{max} = 0.611
17500 measured reflections
9175 independent reflections
8138 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.079
S = 1.00
9175 reflections
675 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}

Table 1
Selected bond lengths (Å).

Sn1—O1	2.124 (2)	Sn2—O4	2.123 (2)
Sn1—O3	2.102 (2)	Sn2—O6	2.094 (2)
Sn1—N2	2.133 (2)	Sn2—N4	2.141 (3)
Sn1—C18	2.118 (4)	Sn2—C47	2.116 (3)
Sn1—C24	2.117 (3)	Sn2—C53	2.124 (3)

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

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the C31–C36, C18–C23 and C12–C17 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2o···O8^{i}	0.84	1.81	2.650 (4)	175
O5—H5o···O7^{ii}	0.84	1.85	2.681 (4)	170
O7—H7o···N3^{iii}	0.84	2.02	2.830 (4)	163
O8—H8o···N1^{iv}	0.84	1.98	2.821 (4)	175
C50—H50···*Cg*1^{v}	0.95	2.91	3.440 (5)	116
C57—H57···*Cg*2	0.95	2.84	3.664 (4)	145
C60—H60a···*Cg*3^{vi}	0.98	2.98	3.886 (6)	155

Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $x, y, z+1$; (iii) $-x+1, -y+1, -z+1$; (iv) $x-1, y, z-1$; (v) $x, y, z-1$; (vi) $x-1, y, z$.

Data collection: *CrysAlis PRO* (Agilent, 2011); 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), *DIAMOND* (Brandenburg, 2006) and Qmol (Gans & Shalloway, 2001); software used to prepare material for publication: *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

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