



Di-*tert*-butyltin(IV)–hydroxide–iodide, $t\text{Bu}_2\text{Sn}(\text{OH})\text{I}$, the last missing member in the series of pure di-*tert*-butyltin(IV)–hydroxide–halides

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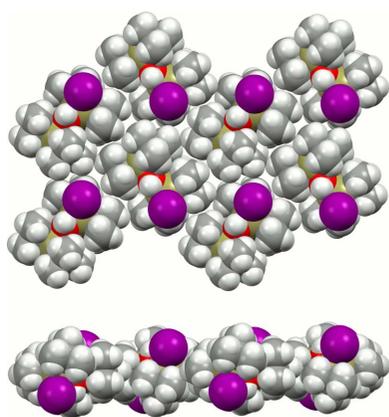
The crystal structure of di-*tert*-butylhydroxidoiodidotin(IV), $[\text{Sn}(\text{C}_4\text{H}_9)_2\text{I}(\text{OH})]$ or $t\text{Bu}_2\text{Sn}(\text{OH})\text{I}$, consists of dimeric, centrosymmetric molecules exhibiting the typical structural features of diorganotin(IV)-hydroxide-halides, $R_2\text{Sn}(\text{OH})\text{Hal}$. Two trigonal-bipyramidally coordinated tin(IV) atoms are bridged *via* two hydroxyl groups, resulting in a planar, four-membered $\{\text{Sn}-\text{O}\}_2$ ring of rhombic shape, with acute angles at tin, obtuse angles at oxygen and two different Sn–O distances depending whether the oxygen atom adopts an axial or equatorial position at the tin(IV) atom. In contrast to its fluorine, chlorine and bromine homologues, no hydrogen bonds between the OH group and the halide atom exist, confining the intermolecular interactions to van der Waals forces.

1. Chemical context

During the hydrolysis of diorganotin(IV)-dihalides, $R_2\text{SnHal}_2$, to diorganotin(IV) oxides, $R_2\text{SnO}$, various intermediates are formed. The most prominent ones are the diorganotin-hydroxide-halides, $R_2\text{Sn}(\text{OH})\text{Hal}$, the tetraorgano-dihalo-genide-distannoxanes, $(R_2\text{SnHal})_2\text{O}$, the tetraorgano-hydroxide-halide-distannoxanes, $(R_2\text{SnHal})\text{O}(R_2\text{SnOH})$, and the tetraorgano-dihydroxide-distannoxanes, $(R_2\text{SnOH})_2\text{O}$. In solution as well as in the crystalline state, all these compounds are comprised of dimeric molecules, and their compositions and structures result from a sequence of different hydrolysis, aggregation and condensation reactions.

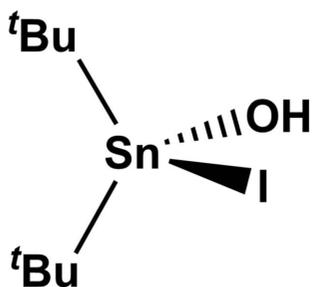
In all three different classes of tetraorgano-distannoxanes, numerous compounds have been structurally characterized. All of them exhibit a ladder-type arrangement of the Sn–O–Hal/OH framework [e.g. *dihalogenides*: $R = \text{Ph}$, $\text{Hal} = \text{Cl}$ (Vollano *et al.*, 1984), $R = t\text{Pr}$, $\text{Hal} = \text{Br}$ (Beckmann *et al.*, 2002a); *hydroxide-halides*: $R = \text{Et}$, $\text{Hal} = \text{Cl}$ (Momeni *et al.*, 2019), $R = \text{Ph}$, $\text{Hal} = \text{Br}$ (Yap *et al.*, 2010); *dihydroxides*: $R = \text{neophyl}$ (Reuter & Pawlak, 2000), $R = \text{trimethylsilylmethyl}$ (Beckmann *et al.*, 2002b)].

Pure *hydroxide halides* have been prepared and structurally characterized for $t\text{Bu}_2\text{Sn}(\text{OH})\text{Hal}$ with $\text{Hal} = \text{F}$, Br (Puff *et al.*, 1985), $\text{Hal} = \text{Cl}$ (α -modification: Puff *et al.*, 1985; β -modification: Di Nicola *et al.*, 2011) and for $R = p\text{-tolyl}$ and $\text{Hal} = \text{Br}$ (Lo & Ng, 2009). Their structures are dominated by various –OH \cdots Hal bridges between neighbouring molecules, resulting in their chain-like arrangements. *Hydroxide halides* can be isolated when their hydroxyl groups are involved in hydrogen bonds to Brønsted bases (*BB*). Such adducts of formula $[R_2\text{Sn}(\text{OH})\text{Hal}]\cdot 2\text{BB}$ have been described for $R = \text{Ph}$, $\text{Hal} = \text{Cl}$ with $\text{BB} = \text{EtOH}$ (Barba *et al.*, 2007), and $\text{BB} = \text{quinoline}$ (Anaconda *et al.*, 2003).



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Here we present the molecular and crystal structure of the last missing member in the series of pure di-*tert*-butyltin hydroxide halides where *Hal* = I. The analogous molecule with DMSO as a hydrogen-bonded Brønsted base was formerly found as part of co-crystals with [(*t*Bu₂Sn)₃O(OH)₂I] (Reuter & Wilberts, 2014).

2. Structural commentary

The asymmetric unit of the title compound comprises one *t*Bu₂Sn(OH)I moiety that dimerizes to form a centrosymmetric molecule (Fig. 1). As in all other *hydroxide halides*, dimerization occurs *via* the two hydroxyl groups that act as bridges between two trigonal-bipyramidally (tbpy) coordinated Sn^{IV} atoms.

The anisotropic displacement parameters as well as the small isotropic displacement parameters of the hydrogen atoms (see *Refinement*) indicate a negligibly small rotation of the *tert*-butyl groups as a whole and a small rotation of the methyl groups in particular, giving rise to very precise infor-

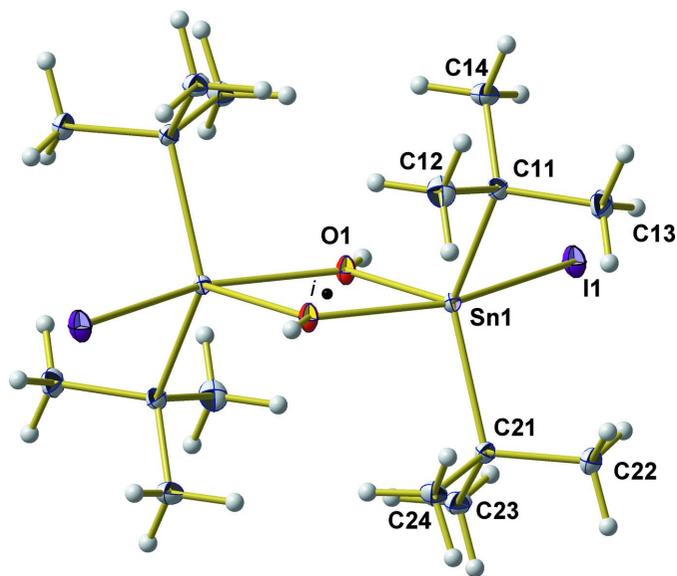


Figure 1

Ball-and-stick model of the dimeric, centrosymmetric molecule found in the crystal of *t*Bu₂Sn(OH)I, with atom numbering of the asymmetric unit. With the exception of the hydrogen atoms that are shown as spheres of arbitrary radius, all other atoms are drawn as displacement ellipsoids at the 40% probability level. The black dot labelled *i* indicates the position of the centre of symmetry.

mation on bond lengths and angles. The structural features of the *tert*-butyl groups are characterized by C–C bond lengths in the range 1.524 (3) to 1.533 (3) Å [mean value: 1.529 (3) Å], C–C–C angles in the range 109.5 (2) to 111.3 (2)° [mean value: 110.2 (7)°], Sn–C bond lengths between 2.187 (2) and 2.193 (2) Å [mean value: 2.190 (3) Å], and Sn–C–C angles of 107.8 (1)° to 109.6 (1)° [mean value: 108.8 (9)°]. All these values are more precise in comparison with those of the formerly determined di-*tert*-butyltin hydroxide halides (Puff *et al.*, 1985; Di Nicola *et al.*, 2011), especially as a result of low-temperature measurement and high data redundancy combined with multi-scan absorption correction, but are of the same accuracy and absolute value as those of the DMSO adduct [(*t*Bu₂Sn)₃O(OH)₂I] [$d(\text{C}–\text{C}) = 1.529(4)$ Å, $\langle(\text{C}–\text{C}–\text{C}) = 109.9(4)^\circ$, $d(\text{Sn}–\text{C}) = 2.193(10)$, $\langle(\text{Sn}–\text{C}–\text{C}) = 109.4(7)^\circ$; Reuter & Wilberts, 2014]. These data are confirmed by a redetermination of the crystal structure of the α -modification of [*t*Bu₂Sn(OH)Cl]₂ (Reuter, 2022) performed with similar experimental conditions as for the title compound and its co-crystallate. In this context, Sn–C distances are of special interest as they belong to the longest ones observed in case of Sn in a trigonal-bipyramidal coordination. In the other hydroxide halides mentioned above, the following bond lengths have been found: $d(\text{Sn}–\text{C})_{\text{mean}} = 2.120(8)$ Å for *R* = *p*-tolyl, *Hal* = Br; $d(\text{Sn}–\text{C})_{\text{mean}} = 2.121(10)/2.117(4)$ Å for *R* = Ph, *Hal* = Cl, *BB* = quinoline/EtOH.

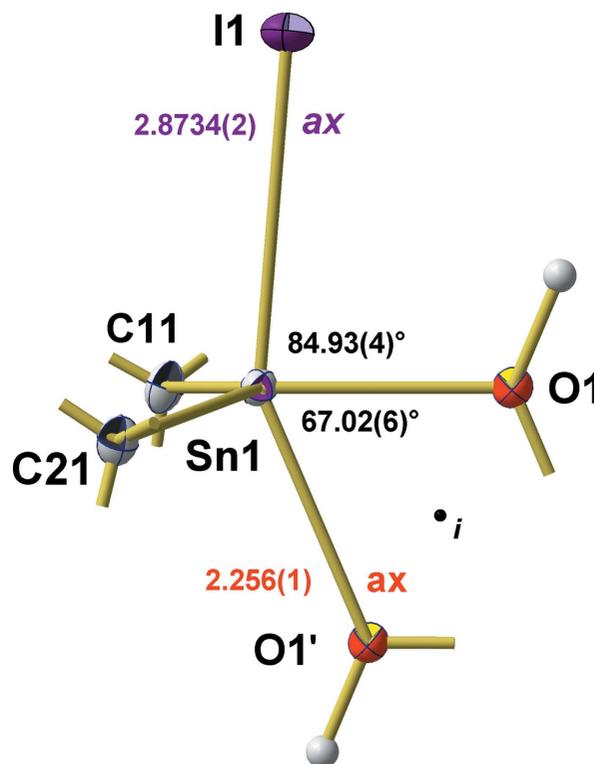


Figure 2

Ball-and-stick model of the trigonal-bipyramidal coordination environment of the tin atom in the dimeric molecule of *t*Bu₂Sn(OH)I with bond lengths (Å) and angles (°) characterizing the polyhedron axes. For clarity, methyl groups of the *t*Bu ligands are stripped down to the carbon–carbon bonds drawn as shortened sticks. Atom O1' is generated by symmetry code $-x, -y + 1, -z + 1$.

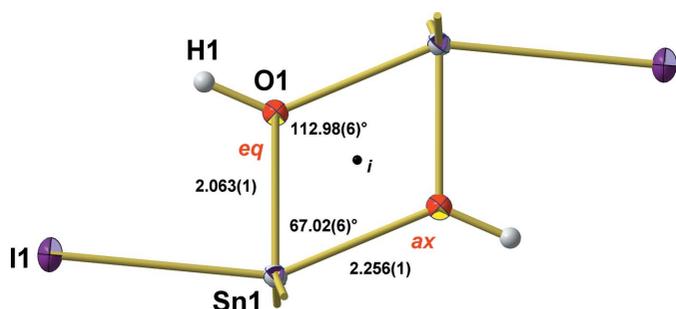


Figure 3
Ball-and-stick model of the four-membered, centrosymmetric $\{\text{Sn}-\text{O}\}_2$ ring in the dimeric molecule of ${}^t\text{Bu}_2\text{Sn}(\text{OH})\text{I}$ with bond lengths (\AA) and angles ($^\circ$) underlining its rhombic shape as the result of axially (ax) and equatorially (eq) bonded O atoms.

Within the trigonal-bipyramidal coordination of the Sn^{IV} atom (Fig. 2), both *tert*-butyl groups are in equatorial (eq) positions in correspondence with the predictions of the VSEPR concept. The bond angle enclosed by the two *tert*-butyl groups of $126.81(8)^\circ$ is identical with the value $[126.89(9)^\circ]$ in the co-crystal and lies in the range $122.0(2)$ to $129.3(1)^\circ$ of $\text{C}-\text{Sn}-\text{C}$ angles found in the other *hydroxide-halides*. The iodine atom adopts an axial (ax) position and one of the bridging hydroxyl groups is in an equatorial, the other in an axial position. As a result of dimerization *via* the hydroxyl groups, the axis of the trigonal bipyramid strongly deviates from linearity [$\text{I}_{\text{ax}}-\text{Sn}-(\text{OH})_{\text{ax}} = 151.94(4)^\circ$]. In addition, the $\text{Sn}-\text{I}$ distance of $2.8734(2) \text{\AA}$ is only marginally shorter than in the co-crystal [$\text{Sn}-\text{I} = 2.8852(2) \text{\AA}$], both being significantly longer than the sum (2.78\AA) of the covalent radii (Cordero *et al.*, 2008) of tin (1.39\AA) and iodine (1.39\AA) and much longer than the mean $\text{Sn}-\text{I}$ distance of $2.661(2)$ (Reuter & Pawlak, 2001) in tin(IV) iodide, SnI_4 , with tetrahedrally coordinated tin.

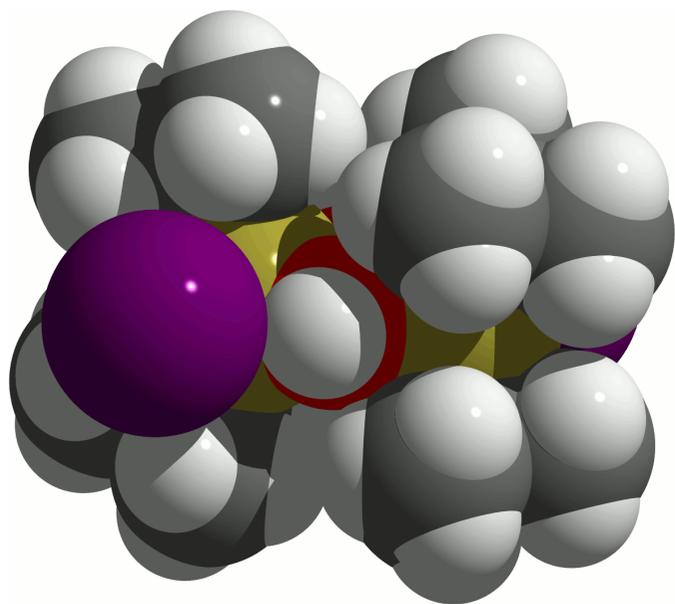


Figure 4
Space-filling model of the dimeric molecule of ${}^t\text{Bu}_2\text{Sn}(\text{OH})\text{I}$ showing the OH group wedged in between the iodine atom and the *tert*-butyl groups. Colour code: I = violet, H = white, C = grey, O = red, Sn = brass-coloured.

Because of the centrosymmetric nature of the dimer, the central four-membered $\{\text{Sn}-\text{O}\}_2$ ring is exactly planar. Its rhombic shape (Fig. 3) is characterized by acute angles $[67.02(6)^\circ]$ at tin and obtuse ones $[112.98(6)^\circ]$ at oxygen. Moreover, these rings exhibit two different $\text{Sn}-\text{O}$ distances depending on the position (ax/eq) of the oxygen atom in the trigonal-bipyramidal coordination environment of tin(IV): $\text{Sn}-(\text{OH})_{\text{ax}} = 2.256(1) \text{\AA}$ versus $\text{Sn}-(\text{OH})_{\text{eq}} = 2.063(1) \text{\AA}$. All these structural features are typical. For example, for the other four-membered $\{\text{Sn}-\text{O}\}_2$ rings of *hydroxide halides* with $R = {}^t\text{Bu}$, $\text{Hal} = \text{F}, \text{Cl}, \text{Br}$, the $\text{Sn}-\text{O}-\text{Sn}$ angles range from $109.9(2)$ to $112.5(3)^\circ$, the $\text{O}-\text{Sn}-\text{O}$ angles from $67.9(3)$ to $70.1(2)^\circ$, the $\text{Sn}-(\text{OH})_{\text{eq}}$ distances from $2.012(5)$ to $2.048(10) \text{\AA}$, and the $\text{Sn}-(\text{OH})_{\text{ax}}$ distances from $2.199(5)$ to $2.257(16) \text{\AA}$ (Puff *et al.*, 1985).

3. Supramolecular features

While the hydroxyl groups of the $[{}^t\text{Bu}_2\text{Sn}(\text{OH})\text{I}]_2$ molecules of the co-crystallate (Reuter & Wilberts, 2014) are involved in $\text{OH}\cdots\text{O}$ hydrogen-bonding to DMSO molecules, those of all other $[{}^t\text{Bu}_2\text{Sn}(\text{OH})\text{Hal}]_2$ molecules develop intermolecular $\text{O}-\text{H}\cdots\text{Hal}$ bonds resulting in a chain-like arrangement of the corresponding molecules in the crystal. In contrast, there are no hydrogen bonds in the crystal structure of the title compound as the voluminous iodine atoms (Fig. 4) prevent significant intermolecular $\text{OH}\cdots\text{I}$ interactions (Table 1). Hence, only van der Waals forces exist between the individual molecules, resulting in a layer-like arrangement (Fig. 5) with

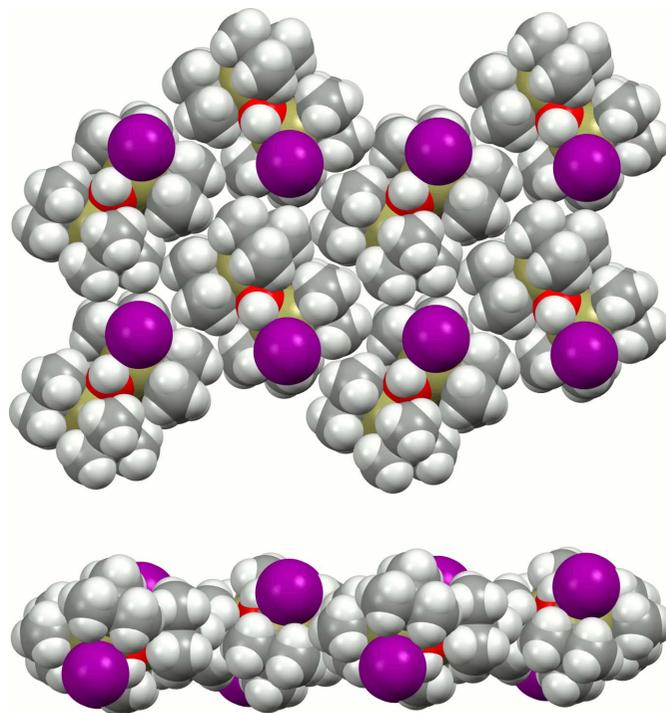


Figure 5
Space-filling model showing the layer-like arrangement of the dimeric $[{}^t\text{Bu}_2\text{Sn}(\text{OH})\text{I}]_2$ molecules in the crystal structure. Top: top view; bottom: side view; colour code as in Fig. 4.

Table 1
Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 \cdots I1	0.96	2.93	3.3862 (14)	111

the Sn—I bonds perpendicular to the layer plane. These layers expand perpendicular to the [101] direction (Fig. 6).

4. Synthesis and crystallization

Yellow block-like single crystals of the title compound were obtained after several years of storage in a sample of (tBu₂Sn)₂I₂ originally prepared by the reaction of the cyclo-tetrastannane (tBu₂Sn)₄ with I₂ in toluene at elevated temperature in a molar ratio of 1:2. As other molar ratios and temperatures result in the formation of (tBu₂Sn)₄I₂ or tBu₂SnI₂ (Farrar & Skinner, 1964; Adams & Dräger, 1985; Puff *et al.*, 1989), it seems possible that the sample was contaminated with the latter one, which reacts over the long time of storage with atmospheric moisture to give the title compound.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All hydrogen atoms were clearly identified in difference-Fourier syntheses. Those of the *tert*-butyl groups were refined with calculated positions (C—H = 0.98 Å) and a common $U_{\text{iso}}(\text{H})$ parameter for each of the methyl groups. The position of the H atom of the OH group was refined with a fixed O—H distance of 0.96 Å and the $U_{\text{iso}}(\text{H})$ parameter refined freely.

Acknowledgements

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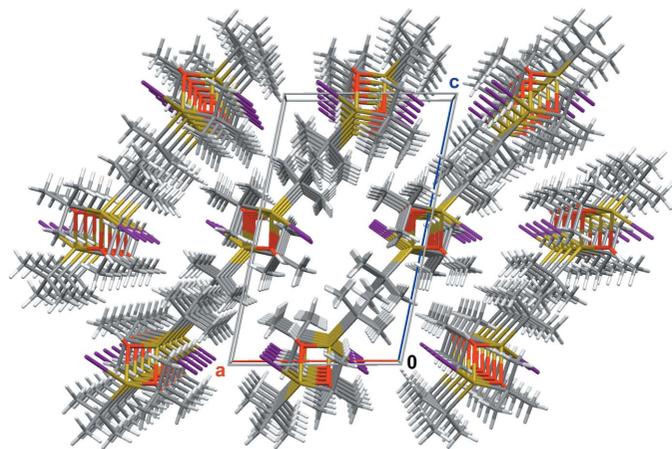


Figure 6
Stick-model showing the arrangement of layers with respect to the unit cell; colour code as in Fig. 4.

Table 2
Experimental details.

Crystal data	[Sn(C ₄ H ₉) ₂ I(OH)]
Chemical formula	376.82
M_r	Monoclinic, $P2_1/n$
Crystal system, space group	100
Temperature (K)	8.4903 (4), 10.8848 (5), 13.5107 (6)
a, b, c (Å)	101.881 (2)
β (°)	1221.85 (10)
V (Å ³)	4
Z	Mo $K\alpha$
Radiation type	4.58
μ (mm ⁻¹)	0.24 × 0.12 × 0.09
Crystal size (mm)	
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (SADABS; Krause <i>et al.</i> , 2015)
$T_{\text{min}}, T_{\text{max}}$	0.457, 0.715
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	48755, 2950, 2761
R_{int}	0.064
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.661
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.016, 0.037, 1.08
No. of reflections	2950
No. of parameters	114
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.85, -0.49

Computer programs: APEX2 and SAINT (Bruker, 2009), SHELXS (Sheldrick, 2008), SHELXL (Sheldrick, 2015), DIAMOND (Brandenburg, 2006), Mercury (Macrae *et al.*, 2020) and publCIF (Westrip, 2010).

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supporting information

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Di-*tert*-butyltin(IV)–hydroxide–iodide, $\text{Bu}_2\text{Sn}(\text{OH})\text{I}$, the last missing member in the series of pure di-*tert*-butyltin(IV)–hydroxide–halides

Hans Reuter

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINTE* (Bruker, 2009); data reduction: *SAINTE* (Bruker, 2009); program(s) used to solve structure: *SHELXS* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2006) and *Mercury* (Macrae *et al.*, 2020); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Di-*tert*-butylhydroxidoiodidotin(IV)

Crystal data

$[\text{Sn}(\text{C}_4\text{H}_9)_2\text{I}(\text{OH})]$
 $M_r = 376.82$
 Monoclinic, $P2_1/n$
 $a = 8.4903$ (4) Å
 $b = 10.8848$ (5) Å
 $c = 13.5107$ (6) Å
 $\beta = 101.881$ (2)°
 $V = 1221.85$ (10) Å³
 $Z = 4$

$F(000) = 712$
 $D_x = 2.048$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 9771 reflections
 $\theta = 2.4$ – 29.2 °
 $\mu = 4.58$ mm⁻¹
 $T = 100$ K
 Block, yellow
 $0.24 \times 0.12 \times 0.09$ mm

Data collection

Bruker APEXII CCD
 diffractometer
 φ and ω scans
 Absorption correction: multi-scan
 (*SADABS*; Krause *et al.*, 2015)
 $T_{\min} = 0.457$, $T_{\max} = 0.715$
 48755 measured reflections

2950 independent reflections
 2761 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.064$
 $\theta_{\max} = 28.0$ °, $\theta_{\min} = 2.6$ °
 $h = -11 \rightarrow 11$
 $k = -14 \rightarrow 13$
 $l = -17 \rightarrow 17$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.016$
 $wR(F^2) = 0.037$
 $S = 1.08$
 2950 reflections
 114 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods
 Hydrogen site location: mixed

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0075P)^2 + 1.3137P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.003$
 $\Delta\rho_{\max} = 0.85$ e Å⁻³
 $\Delta\rho_{\min} = -0.49$ e Å⁻³
 Extinction correction: SHELXL-2014/7
 (Sheldrick 2015,
 $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$)
 Extinction coefficient: 0.00139 (11)

Special details

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

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Il	0.31459 (2)	0.21150 (2)	0.53430 (2)	0.01973 (5)
Sn1	0.06240 (2)	0.37120 (2)	0.43364 (2)	0.01006 (5)
C21	0.1879 (2)	0.44568 (19)	0.32082 (15)	0.0137 (4)
C22	0.2375 (3)	0.3375 (2)	0.26155 (17)	0.0193 (5)
H22A	0.1409	0.2956	0.2247	0.032 (4)*
H22B	0.3027	0.2798	0.3086	0.032 (4)*
H22C	0.3004	0.3679	0.2135	0.032 (4)*
C23	0.3377 (3)	0.5141 (2)	0.37485 (17)	0.0190 (4)
H23A	0.3972	0.5445	0.3249	0.023 (4)*
H23B	0.4064	0.4582	0.4218	0.023 (4)*
H23C	0.3059	0.5835	0.4126	0.023 (4)*
C24	0.0749 (3)	0.5304 (2)	0.24902 (16)	0.0190 (4)
H24A	0.1273	0.5569	0.1944	0.027 (4)*
H24B	0.0495	0.6025	0.2863	0.027 (4)*
H24C	-0.0246	0.4863	0.2203	0.027 (4)*
C11	-0.1328 (3)	0.23567 (19)	0.40781 (16)	0.0153 (4)
C12	-0.2895 (3)	0.2973 (2)	0.35517 (19)	0.0233 (5)
H12A	-0.2754	0.3331	0.2910	0.029 (4)*
H12B	-0.3175	0.3623	0.3987	0.029 (4)*
H12C	-0.3759	0.2362	0.3421	0.029 (4)*
C13	-0.0867 (3)	0.1346 (2)	0.34001 (18)	0.0214 (5)
H13A	-0.0798	0.1697	0.2742	0.028 (4)*
H13B	-0.1687	0.0699	0.3304	0.028 (4)*
H13C	0.0178	0.0997	0.3721	0.028 (4)*
C14	-0.1500 (3)	0.1809 (2)	0.50925 (18)	0.0236 (5)
H14A	-0.2351	0.1185	0.4979	0.029 (4)*
H14B	-0.1781	0.2461	0.5526	0.029 (4)*
H14C	-0.0480	0.1431	0.5423	0.029 (4)*
O1	0.09927 (17)	0.46366 (13)	0.56977 (10)	0.0150 (3)
H1	0.1841	0.4272	0.6190	0.070 (12)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Il	0.02092 (9)	0.01756 (8)	0.01844 (8)	0.00750 (5)	-0.00125 (6)	0.00161 (5)
Sn1	0.01100 (8)	0.00881 (8)	0.01046 (7)	0.00010 (5)	0.00239 (5)	-0.00050 (5)
C21	0.0164 (10)	0.0130 (10)	0.0128 (9)	-0.0014 (8)	0.0051 (8)	-0.0012 (8)
C22	0.0235 (12)	0.0175 (11)	0.0188 (11)	-0.0001 (9)	0.0085 (9)	-0.0039 (9)
C23	0.0180 (11)	0.0196 (11)	0.0206 (11)	-0.0048 (9)	0.0067 (9)	-0.0020 (9)

C24	0.0236 (11)	0.0176 (11)	0.0158 (10)	0.0020 (9)	0.0040 (9)	0.0041 (8)
C11	0.0170 (10)	0.0131 (10)	0.0171 (10)	-0.0037 (8)	0.0064 (8)	-0.0040 (8)
C12	0.0153 (11)	0.0226 (12)	0.0308 (13)	-0.0029 (9)	0.0018 (9)	-0.0057 (10)
C13	0.0223 (12)	0.0173 (11)	0.0255 (12)	-0.0036 (9)	0.0070 (9)	-0.0083 (9)
C14	0.0295 (13)	0.0198 (12)	0.0250 (12)	-0.0054 (10)	0.0135 (10)	0.0012 (9)
O1	0.0166 (7)	0.0147 (7)	0.0126 (7)	0.0047 (6)	0.0004 (6)	-0.0021 (6)

Geometric parameters (Å, °)

Il—Sn1	2.8734 (2)	C24—H24C	0.9800
Sn1—O1	2.0631 (1)	C11—C12	1.528 (3)
Sn1—C21	2.187 (2)	C11—C14	1.529 (3)
Sn1—C11	2.193 (2)	C11—C13	1.533 (3)
Sn1—O1 ⁱ	2.2564 (1)	C12—H12A	0.9800
C21—C23	1.524 (3)	C12—H12B	0.9800
C21—C24	1.526 (3)	C12—H12C	0.9800
C21—C22	1.531 (3)	C13—H13A	0.9800
C22—H22A	0.9800	C13—H13B	0.9800
C22—H22B	0.9800	C13—H13C	0.9800
C22—H22C	0.9800	C14—H14A	0.9800
C23—H23A	0.9800	C14—H14B	0.9800
C23—H23B	0.9800	C14—H14C	0.9800
C23—H23C	0.9800	O1—Sn1 ⁱ	2.2563 (14)
C24—H24A	0.9800	O1—H1	0.9600
C24—H24B	0.9800		
O1—Sn1—C21	115.73 (7)	C21—C24—H24C	109.5
O1—Sn1—C11	116.17 (7)	H24A—C24—H24C	109.5
C21—Sn1—C11	126.81 (8)	H24B—C24—H24C	109.5
O1—Sn1—O1 ⁱ	67.02 (6)	C12—C11—C14	110.71 (19)
C21—Sn1—O1 ⁱ	94.13 (7)	C12—C11—C13	109.99 (18)
C11—Sn1—O1 ⁱ	95.51 (7)	C14—C11—C13	109.84 (19)
O1—Sn1—I1	84.93 (4)	C12—C11—Sn1	109.60 (14)
C21—Sn1—I1	97.57 (5)	C14—C11—Sn1	109.16 (14)
C11—Sn1—I1	97.67 (6)	C13—C11—Sn1	107.47 (14)
O1 ⁱ —Sn1—I1	151.94 (4)	C11—C12—H12A	109.5
C23—C21—C24	111.25 (18)	C11—C12—H12B	109.5
C23—C21—C22	109.50 (17)	H12A—C12—H12B	109.5
C24—C21—C22	109.69 (17)	C11—C12—H12C	109.5
C23—C21—Sn1	109.00 (13)	H12A—C12—H12C	109.5
C24—C21—Sn1	109.55 (13)	H12B—C12—H12C	109.5
C22—C21—Sn1	107.78 (14)	C11—C13—H13A	109.5
C21—C22—H22A	109.5	C11—C13—H13B	109.5
C21—C22—H22B	109.5	H13A—C13—H13B	109.5
H22A—C22—H22B	109.5	C11—C13—H13C	109.5
C21—C22—H22C	109.5	H13A—C13—H13C	109.5
H22A—C22—H22C	109.5	H13B—C13—H13C	109.5
H22B—C22—H22C	109.5	C11—C14—H14A	109.5

C21—C23—H23A	109.5	C11—C14—H14B	109.5
C21—C23—H23B	109.5	H14A—C14—H14B	109.5
H23A—C23—H23B	109.5	C11—C14—H14C	109.5
C21—C23—H23C	109.5	H14A—C14—H14C	109.5
H23A—C23—H23C	109.5	H14B—C14—H14C	109.5
H23B—C23—H23C	109.5	Sn1—O1—Sn1 ⁱ	112.98 (6)
C21—C24—H24A	109.5	Sn1—O1—H1	111.7
C21—C24—H24B	109.5	Sn1 ⁱ —O1—H1	135.3
H24A—C24—H24B	109.5		

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

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
O1—H1...I1	0.96	2.93	3.3862 (14)	111