

Redetermination of the crystal structure of di- μ_2 -hydroxido-bis[di-*tert*-butylchloridotin(IV)] at 100 K

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Received 9 January 2023

Accepted 23 January 2023

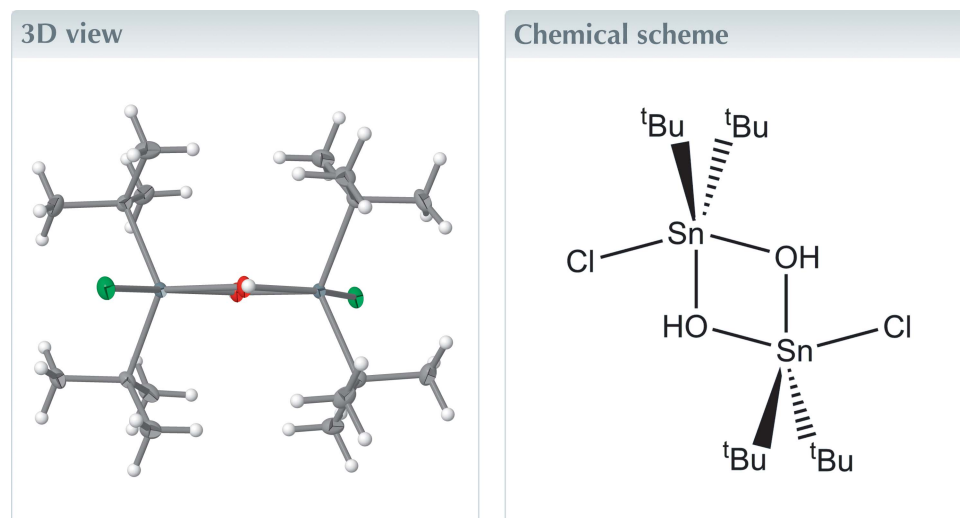
Edited by E. R. T. Tiekink, Sunway University, Malaysia

Keywords: crystal structure; redetermination; hydrolysis; diorganotin(IV)-hydroxide-halides; hydrogen bonding.

CCDC reference: 2237568

Structural data: full structural data are available from iucrdata.iucr.org

The structure of the dimeric title compound, $[\text{Sn}_2(\text{C}_4\text{H}_9)_4\text{Cl}_2(\text{OH})_2]$, was redetermined at 100 K by use of an area detector to provide new data to improve the structural parameters for detailed analysis. Noteworthy is the folding of the central, non-symmetric, four-membered $[\text{SnO}]_2$ ring [dihedral angle about the $\text{O} \cdots \text{O}$ axis = $1.09(3)^\circ$], as well as the elongation of the $\text{Sn}-\text{Cl}$ bonds [mean value = $2.5096(4) \text{ \AA}$], as a result of intermolecular $\text{O}-\text{H} \cdots \text{Cl}$ hydrogen bonds; the latter lead to a chain-like arrangement of dimeric molecules along $[101]$.



Structure description

The title compound, $[\text{tBu}_2\text{Sn}(\text{OH})\text{Cl}]_2$, belongs to the class of dimeric diorganotin(IV)-hydroxides-halides, $[\text{R}_2\text{Sn}(\text{OH})\text{X}]_2$, the first hydrolysis products of diorganotin(IV) dihalides, R_2SnX_2 . The structure of the title compound has been determined previously at room temperature using point detector data as part of a paper describing the series of dimeric di-*tert*-butyltin(IV) hydroxide halides, $[\text{tBu}_2\text{Sn}(\text{OH})\text{X}]_2$ with $\text{X} = \text{F}, \text{Cl}$ and Br (Puff *et al.*, 1985). This series was completed when a second modification of the title compound was reported (Di Nicola *et al.*, 2011) and more recently, when the crystal structures of the pure iodide compound, $[\text{tBu}_2\text{Sn}(\text{OH})\text{I}]_2$ (Reuter, 2022) and its DMSO-adduct (Reuter & Wilberts, 2014) were published. With two well-resolved, low-temperature crystal-structure determinations of the iodide derivative, it seemed reasonable to redetermine the structure of the chloride derivative using similar experimental conditions to enable a more valid comparison between structures.

As a result of the low-temperature measurement and the high data redundancy, combined with a multi-scan absorption correction, the new data improve the structural parameters of the title compound (Fig. 1) by an order of magnitude. In particular, the new data enable the confirmation of the exceptionally long $\text{Sn}-\text{C}$ bonds [range: $2.180(1)$ to

Table 1
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>
O1—H1···Cl2 ⁱ	0.96	2.30	3.2469 (10)	169
O2—H2···Cl1 ⁱⁱ	0.96	2.31	3.2482 (10)	166

Symmetry codes: (i) $x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$; (ii) $x - \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$.

2.184 (1) Å; mean value: 2.182 (2) Å] in accord with comparable values found in related [${}^t\text{Bu}_2\text{Sn}(\text{OH})\text{I}$]₂ compounds [pure state: $d(\text{Sn}-\text{C})_{\text{mean}} = 2.190$ (3) Å (Reuter, 2022), and DMSO-adduct: $d(\text{Sn}-\text{C})_{\text{mean}} = 2.193$ (10) Å (Reuter & Wilberts, 2014)].

The other structural features of note relate to the *tert*-butyl groups, which are characterized by C—C bond lengths in the range from 1.521 (2) to 1.532 (2) Å [mean value: 1.527 (4) Å], C_{methyl}—C—C_{methyl} angles in the range 107.1 (1) to 111.1 (1)° [mean value: 109.5 (11)°] and Sn—C—C angles of 107.1 (1) to 111.1 (1)° [mean value: 108.9 (12)°]. These new data are of the same precision and absolute values as those found in the iodide compound both in the pure state [$d(\text{C}-\text{C}) = 1.529$ (4) Å, $\langle(\text{C}_{\text{methyl}}-\text{C}-\text{C}_{\text{methyl}}) = 109.9$ (4)°, $d(\text{Sn}-\text{C}) = 2.193$ (10) Å and $\langle(\text{Sn}-\text{C}-\text{C}) = 109.4$ (7)° (Reuter, 2022)], and in the DMSO-adduct [$d(\text{C}-\text{C}) = 1.529$ (4) Å, $\langle(\text{C}_{\text{methyl}}-\text{C}-\text{C}_{\text{methyl}}) = 109.9$ (4)° and $\langle(\text{Sn}-\text{C}-\text{C}) = 109.4$ (7)° (Reuter & Wilberts, 2014)].

As the molecule belongs to point group *C*₁, the central, four-membered, rhombic [SnO]₂ ring is not exactly planar but folded along the O···O axis with an interplanar angle of 1.09 (3)°. As usual, the bond lengths and angles within the

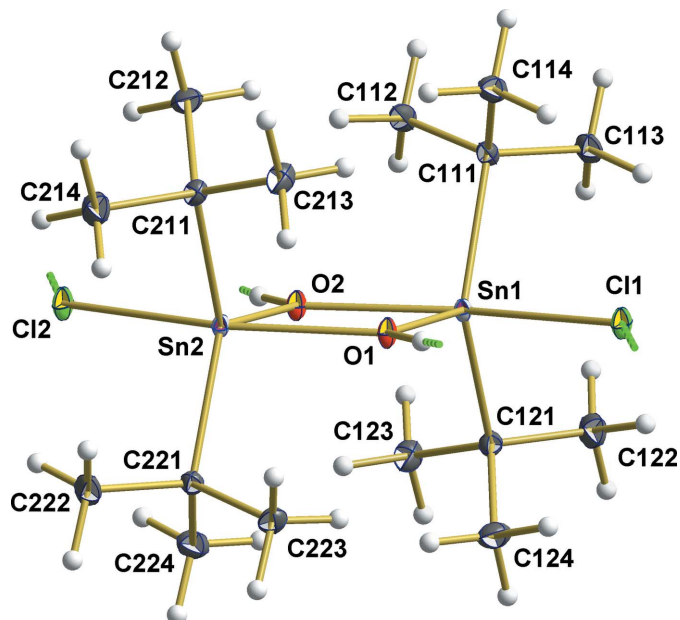


Figure 1
A representation of the dimeric, non-symmetric molecule found in the crystal of [${}^t\text{Bu}_2\text{Sn}(\text{OH})\text{Cl}$]₂, showing the atom numbering. With the exception of the hydrogen atoms, which are shown as spheres of arbitrary radius, all other atoms are drawn with displacement ellipsoids at the 40% probability level. Intermolecular O—H···Cl hydrogen bonds are indicated by dashed sticks in green.

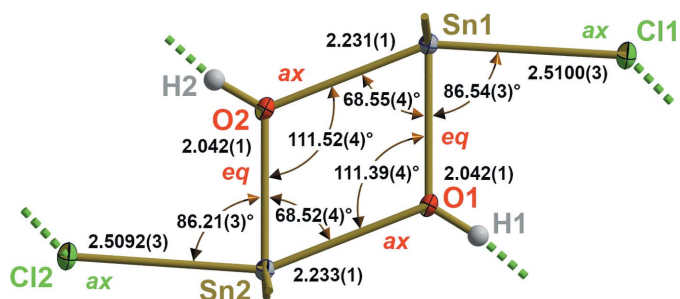


Figure 2
Ball-and-stick model of the inorganic framework of the [${}^t\text{Bu}_2\text{Sn}(\text{OH})\text{Cl}$]₂ molecule highlighting selected bond lengths (Å) and angles (°). Positions of oxygen and chloride atoms within the trigonal-bipyramidal coordination of the tin atoms are labelled by use of the abbreviation *ax* (= axial) and *eq* (= equatorial). For clarity, ^tBu groups are stripped down to the Sn—C bonds drawn as shortened sticks. Intermolecular O—H···Cl hydrogen bonds are indicated by dashed sticks in green.

inorganic part of the molecule (Fig. 2) are characteristic of tin(IV) in trigonal-bipyramidal coordination (*ax/eq*), and the size of the *tert*-butyl groups. A special feature of the title compound relates to the Sn—Cl distances [mean value: 2.5096 (4) Å], which are considerably longer in comparison with other Brønstedt-Base (BB) stabilized diorganotin(IV)-hydroxide-chlorides [*R* = Ph, BB = EtOH: $d(\text{Sn}-\text{Cl}) = 2.4748$ (6) Å (Barba *et al.*, 2007); *R* = Ph, BB = quinoline: $d(\text{Sn}-\text{Cl}) = 2.4648$ (11)/2.4353 (12) Å (Anaconda *et al.*, 2003)].

These unusually long Sn—Cl bonds in the title compound arise from the fact that the chloride atoms are involved in intermolecular O—H···Cl hydrogen bonds (Table 1), resulting in a chain-like arrangement of the [${}^t\text{Bu}_2\text{Sn}(\text{OH})\text{Cl}$]₂ molecules along [101], Fig. 3, a feature that had been recognized previously but now is confirmed unambiguously.

Synthesis and crystallization

For the synthesis of the title compound, see Puff *et al.* (1985).

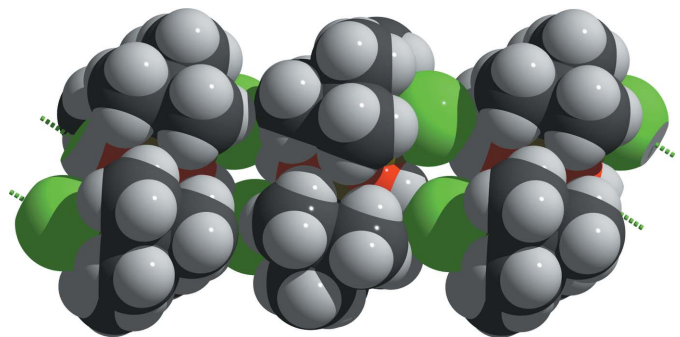


Figure 3
Space-filling model of the chain-like arrangement of the [${}^t\text{Bu}_2\text{Sn}(\text{OH})\text{Cl}$]₂ molecules along [101] encompassing intramolecular O—H···Cl hydrogen bonding. The image shows three complete molecules with their hydrogen bonds to neighbouring molecules. The corresponding atoms are visualized as truncated, two-coloured spheres and the hydrogen bonds are indicated by dashed sticks in green. Colour code of the atoms: Cl = green, H = white, C = grey, O = red, Sn = brass.

Table 2
Experimental details.

Crystal data	
Chemical formula	[Sn ₂ (C ₄ H ₉) ₄ Cl ₂ (OH) ₂]
<i>M_r</i>	570.74
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>n</i>
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	11.0632 (3), 16.9135 (5), 13.4178 (3)
β (°)	110.442 (1)
<i>V</i> (Å ³)	2352.60 (11)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	2.36
Crystal size (mm)	0.17 × 0.09 × 0.07
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T_{min}</i> , <i>T_{max}</i>	0.515, 0.745
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	114387, 5668, 5148
<i>R_{int}</i>	0.031
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.660
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.014, 0.034, 1.06
No. of reflections	5668
No. of parameters	224
H-atom treatment	Only H-atom displacement parameters refined
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.94, -0.49

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS97* (Sheldrick, 2008), *SHELXL2014/7* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 2006), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Six reflections were omitted from

the final cycles of refinement owing to poor agreement; details are given in the CIF.

Funding information

The Deutsche Forschungsgemeinschaft and the Government of Lower-Saxony are thanked for the funding of the diffractometer. Additional support by the Deutsche Forschungsgemeinschaft (DFG) is also acknowledged.

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full crystallographic data

IUCrData (2023). **8**, x230056 [https://doi.org/10.1107/S2414314623000561]

Redetermination of the crystal structure of di- μ_2 -hydroxido-bis[di-*tert*-butylchloridotin(IV)] at 100 K

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Di- μ_2 -hydroxido-bis[di-*tert*-butylchloridotin(IV)]

Crystal data

[Sn₂(C₄H₉)₄Cl₂(OH)₂]

$M_r = 570.74$

Monoclinic, $P2_1/n$

$a = 11.0632$ (3) Å

$b = 16.9135$ (5) Å

$c = 13.4178$ (3) Å

$\beta = 110.442$ (1)°

$V = 2352.60$ (11) Å³

$Z = 4$

$F(000) = 1136$

$D_x = 1.611$ Mg m⁻³

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

Cell parameters from 9559 reflections

$\theta = 3.0$ – 28.0 °

$\mu = 2.36$ mm⁻¹

$T = 100$ K

Bloc, colourless

$0.17 \times 0.09 \times 0.07$ mm

Data collection

Bruker APEXII CCD
diffractometer

φ and ω scans

Absorption correction: multi-scan
(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.515$, $T_{\max} = 0.745$

114387 measured reflections

5668 independent reflections

5148 reflections with $I > 2\sigma(I)$

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

$\theta_{\max} = 28.0$ °, $\theta_{\min} = 3.1$ °

$h = -14 \rightarrow 14$

$k = -22 \rightarrow 22$

$l = -17 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.014$

$wR(F^2) = 0.034$

$S = 1.06$

5668 reflections

224 parameters

0 restraints

Hydrogen site location: mixed

Only H-atom displacement parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0158P)^2 + 1.0738P]$

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

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 0.94$ e Å⁻³

$\Delta\rho_{\min} = -0.49$ e Å⁻³

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.

Refinement. Six reflections, i.e. (-1 1 1), (1 1 0), (0 2 1), (0 1 1), (1 0 1) and (0 0 2), were omitted from the final cycles of refinement owing to poor agreement.

The positions of all H 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 common $U_{\text{iso}}(\text{H})$ parameters for each of the methyl groups. The position of the H atoms of the OH groups were refined with a fixed O—H distance of 0.96 Å before they were fixed and allowed to ride on their parent atoms with a common $U_{\text{iso}}(\text{H})$ parameter.

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	0.73501 (2)	0.26288 (2)	0.64133 (2)	0.00989 (3)
Sn2	0.42676 (2)	0.22975 (2)	0.65688 (2)	0.01001 (3)
Cl1	0.92792 (3)	0.29807 (2)	0.80086 (3)	0.01622 (7)
Cl2	0.23245 (3)	0.20159 (2)	0.49523 (3)	0.01753 (7)
O1	0.63487 (9)	0.25652 (6)	0.74333 (7)	0.01351 (19)
H1	0.6748	0.2674	0.8179	0.039 (4)*
O2	0.52774 (9)	0.23420 (6)	0.55544 (8)	0.0136 (2)
H2	0.4839	0.2239	0.4812	0.039 (4)*
C111	0.72855 (13)	0.37640 (8)	0.56249 (11)	0.0143 (3)
C112	0.61905 (14)	0.37644 (9)	0.45494 (11)	0.0203 (3)
H11A	0.6206	0.4260	0.4177	0.025 (3)*
H11B	0.5363	0.3715	0.4658	0.025 (3)*
H11C	0.6299	0.3318	0.4123	0.025 (3)*
C113	0.85829 (14)	0.38736 (9)	0.54696 (12)	0.0201 (3)
H11D	0.8704	0.3449	0.5017	0.027 (3)*
H11E	0.9281	0.3857	0.6162	0.027 (3)*
H11F	0.8593	0.4385	0.5130	0.027 (3)*
C114	0.70965 (15)	0.44211 (9)	0.63384 (12)	0.0202 (3)
H11G	0.7103	0.4935	0.6004	0.033 (3)*
H11H	0.7797	0.4402	0.7030	0.033 (3)*
H11I	0.6268	0.4347	0.6439	0.033 (3)*
C121	0.81282 (13)	0.15162 (8)	0.60755 (11)	0.0149 (3)
C122	0.94120 (15)	0.16949 (10)	0.59347 (14)	0.0267 (4)
H12A	0.9778	0.1204	0.5774	0.025 (3)*
H12B	1.0011	0.1925	0.6592	0.025 (3)*
H12C	0.9271	0.2070	0.5348	0.025 (3)*
C123	0.71987 (15)	0.11464 (9)	0.50566 (12)	0.0217 (3)
H12D	0.7040	0.1520	0.4467	0.030 (3)*
H12E	0.6382	0.1021	0.5153	0.030 (3)*
H12F	0.7578	0.0661	0.4896	0.030 (3)*
C124	0.83528 (16)	0.09618 (9)	0.70159 (13)	0.0252 (3)
H12G	0.7532	0.0860	0.7118	0.034 (3)*
H12H	0.8958	0.1206	0.7659	0.034 (3)*
H12I	0.8713	0.0462	0.6877	0.034 (3)*
C211	0.35215 (13)	0.34122 (8)	0.69386 (11)	0.0148 (3)
C212	0.32310 (15)	0.39629 (9)	0.59874 (12)	0.0224 (3)
H21A	0.2627	0.3704	0.5355	0.031 (3)*
H21B	0.4033	0.4087	0.5865	0.031 (3)*

H21C	0.2845	0.4452	0.6129	0.031 (3)*
C213	0.44854 (15)	0.37962 (9)	0.79313 (12)	0.0216 (3)
H21D	0.5282	0.3922	0.7801	0.027 (3)*
H21E	0.4679	0.3430	0.8533	0.027 (3)*
H21F	0.4113	0.4283	0.8097	0.027 (3)*
C214	0.22696 (15)	0.32214 (10)	0.71335 (14)	0.0248 (3)
H21G	0.1663	0.2964	0.6502	0.036 (3)*
H21H	0.1888	0.3712	0.7277	0.036 (3)*
H21I	0.2457	0.2866	0.7746	0.036 (3)*
C221	0.42891 (13)	0.11423 (8)	0.72947 (11)	0.0153 (3)
C222	0.29620 (15)	0.10024 (10)	0.73817 (13)	0.0255 (4)
H22A	0.2296	0.1034	0.6673	0.037 (3)*
H22B	0.2799	0.1406	0.7843	0.037 (3)*
H22C	0.2942	0.0478	0.7685	0.037 (3)*
C223	0.53316 (14)	0.11266 (9)	0.84006 (11)	0.0199 (3)
H22D	0.6181	0.1192	0.8335	0.025 (3)*
H22E	0.5301	0.0620	0.8744	0.025 (3)*
H22F	0.5181	0.1558	0.8831	0.025 (3)*
C224	0.45453 (16)	0.05138 (9)	0.65775 (13)	0.0241 (3)
H22G	0.3885	0.0548	0.5867	0.031 (3)*
H22H	0.4518	-0.0011	0.6877	0.031 (3)*
H22I	0.5398	0.0601	0.6528	0.031 (3)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.00886 (5)	0.01220 (5)	0.00797 (5)	-0.00117 (3)	0.00212 (3)	0.00024 (3)
Sn2	0.00854 (5)	0.01264 (5)	0.00809 (5)	-0.00064 (3)	0.00195 (3)	0.00097 (3)
Cl1	0.01183 (14)	0.02417 (18)	0.00977 (14)	-0.00356 (13)	0.00015 (12)	0.00008 (13)
Cl2	0.01190 (14)	0.02750 (19)	0.00997 (15)	-0.00395 (13)	-0.00023 (12)	0.00079 (13)
O1	0.0099 (4)	0.0218 (5)	0.0079 (4)	-0.0028 (4)	0.0021 (4)	-0.0015 (4)
O2	0.0107 (4)	0.0209 (5)	0.0085 (4)	-0.0024 (4)	0.0025 (4)	-0.0011 (4)
C111	0.0147 (6)	0.0146 (7)	0.0125 (6)	-0.0035 (5)	0.0031 (5)	0.0011 (5)
C112	0.0209 (7)	0.0215 (8)	0.0138 (7)	-0.0043 (6)	0.0000 (6)	0.0042 (6)
C113	0.0190 (7)	0.0229 (8)	0.0198 (7)	-0.0036 (6)	0.0087 (6)	0.0044 (6)
C114	0.0228 (7)	0.0156 (7)	0.0213 (7)	-0.0016 (6)	0.0063 (6)	-0.0013 (6)
C121	0.0125 (6)	0.0151 (7)	0.0159 (7)	0.0001 (5)	0.0034 (5)	-0.0020 (5)
C122	0.0184 (7)	0.0250 (8)	0.0406 (10)	-0.0003 (6)	0.0153 (7)	-0.0069 (7)
C123	0.0201 (7)	0.0223 (8)	0.0199 (7)	0.0015 (6)	0.0036 (6)	-0.0080 (6)
C124	0.0274 (8)	0.0190 (8)	0.0243 (8)	0.0044 (6)	0.0030 (7)	0.0037 (6)
C211	0.0132 (6)	0.0162 (7)	0.0147 (7)	0.0016 (5)	0.0042 (5)	-0.0001 (5)
C212	0.0239 (8)	0.0178 (7)	0.0229 (8)	0.0038 (6)	0.0047 (6)	0.0042 (6)
C213	0.0192 (7)	0.0228 (8)	0.0197 (7)	0.0031 (6)	0.0028 (6)	-0.0066 (6)
C214	0.0189 (7)	0.0253 (8)	0.0343 (9)	0.0009 (6)	0.0143 (7)	-0.0034 (7)
C221	0.0134 (6)	0.0156 (7)	0.0156 (7)	-0.0016 (5)	0.0037 (5)	0.0036 (5)
C222	0.0182 (7)	0.0295 (9)	0.0288 (9)	-0.0037 (6)	0.0082 (7)	0.0122 (7)
C223	0.0190 (7)	0.0218 (8)	0.0163 (7)	0.0012 (6)	0.0029 (6)	0.0070 (6)
C224	0.0277 (8)	0.0172 (7)	0.0247 (8)	-0.0019 (6)	0.0059 (7)	-0.0017 (6)

Geometric parameters (Å, °)

Sn1—O1	2.0424 (10)	C123—H12D	0.9800
Sn1—C111	2.1813 (14)	C123—H12E	0.9800
Sn1—C121	2.1818 (14)	C123—H12F	0.9800
Sn1—O2	2.2306 (9)	C124—H12G	0.9800
Sn1—C11	2.5100 (3)	C124—H12H	0.9800
Sn2—O2	2.0416 (10)	C124—H12I	0.9800
Sn2—C221	2.1796 (14)	C211—C212	1.521 (2)
Sn2—C211	2.1836 (14)	C211—C213	1.5301 (19)
Sn2—O1	2.2329 (9)	C211—C214	1.531 (2)
Sn2—C12	2.5092 (3)	C212—H21A	0.9800
O1—H1	0.9600	C212—H21B	0.9800
O2—H2	0.9600	C212—H21C	0.9800
C111—C112	1.5261 (19)	C213—H21D	0.9800
C111—C114	1.528 (2)	C213—H21E	0.9800
C111—C113	1.532 (2)	C213—H21F	0.9800
C112—H11A	0.9800	C214—H21G	0.9800
C112—H11B	0.9800	C214—H21H	0.9800
C112—H11C	0.9800	C214—H21I	0.9800
C113—H11D	0.9800	C221—C224	1.525 (2)
C113—H11E	0.9800	C221—C223	1.5289 (19)
C113—H11F	0.9800	C221—C222	1.531 (2)
C114—H11G	0.9800	C222—H22A	0.9800
C114—H11H	0.9800	C222—H22B	0.9800
C114—H11I	0.9800	C222—H22C	0.9800
C121—C124	1.521 (2)	C223—H22D	0.9800
C121—C122	1.527 (2)	C223—H22E	0.9800
C121—C123	1.5283 (19)	C223—H22F	0.9800
C122—H12A	0.9800	C224—H22G	0.9800
C122—H12B	0.9800	C224—H22H	0.9800
C122—H12C	0.9800	C224—H22I	0.9800
O1—Sn1—C111	115.96 (5)	H12B—C122—H12C	109.5
O1—Sn1—C121	116.07 (5)	C121—C123—H12D	109.5
C111—Sn1—C121	127.37 (5)	C121—C123—H12E	109.5
O1—Sn1—O2	68.55 (4)	H12D—C123—H12E	109.5
C111—Sn1—O2	95.00 (4)	C121—C123—H12F	109.5
C121—Sn1—O2	96.55 (4)	H12D—C123—H12F	109.5
O1—Sn1—C11	86.54 (3)	H12E—C123—H12F	109.5
C111—Sn1—C11	94.53 (4)	C121—C124—H12G	109.5
C121—Sn1—C11	95.86 (4)	C121—C124—H12H	109.5
O2—Sn1—C11	155.04 (3)	H12G—C124—H12H	109.5
O2—Sn2—C221	114.07 (5)	C121—C124—H12I	109.5
O2—Sn2—C211	117.25 (5)	H12G—C124—H12I	109.5
C221—Sn2—C211	128.20 (5)	H12H—C124—H12I	109.5
O2—Sn2—O1	68.52 (4)	C212—C211—C213	110.44 (12)
C221—Sn2—O1	95.82 (4)	C212—C211—C214	109.50 (12)

C211—Sn2—O1	96.31 (4)	C213—C211—C214	109.74 (12)
O2—Sn2—Cl2	86.21 (3)	C212—C211—Sn2	108.90 (10)
C221—Sn2—Cl2	95.07 (4)	C213—C211—Sn2	111.13 (9)
C211—Sn2—Cl2	94.74 (4)	C214—C211—Sn2	107.05 (10)
O1—Sn2—Cl2	154.72 (3)	C211—C212—H21A	109.5
Sn1—O1—Sn2	111.39 (4)	C211—C212—H21B	109.5
Sn1—O1—H1	121.9	H21A—C212—H21B	109.5
Sn2—O1—H1	126.6	C211—C212—H21C	109.5
Sn2—O2—Sn1	111.52 (4)	H21A—C212—H21C	109.5
Sn2—O2—H2	119.3	H21B—C212—H21C	109.5
Sn1—O2—H2	129.2	C211—C213—H21D	109.5
C112—C111—C114	110.79 (12)	C211—C213—H21E	109.5
C112—C111—C113	110.09 (12)	H21D—C213—H21E	109.5
C114—C111—C113	109.69 (12)	C211—C213—H21F	109.5
C112—C111—Sn1	109.86 (9)	H21D—C213—H21F	109.5
C114—C111—Sn1	108.95 (9)	H21E—C213—H21F	109.5
C113—C111—Sn1	107.39 (9)	C211—C214—H21G	109.5
C111—C112—H11A	109.5	C211—C214—H21H	109.5
C111—C112—H11B	109.5	H21G—C214—H21H	109.5
H11A—C112—H11B	109.5	C211—C214—H21I	109.5
C111—C112—H11C	109.5	H21G—C214—H21I	109.5
H11A—C112—H11C	109.5	H21H—C214—H21I	109.5
H11B—C112—H11C	109.5	C224—C221—C223	110.91 (12)
C111—C113—H11D	109.5	C224—C221—C222	109.56 (13)
C111—C113—H11E	109.5	C223—C221—C222	109.98 (12)
H11D—C113—H11E	109.5	C224—C221—Sn2	108.55 (10)
C111—C113—H11F	109.5	C223—C221—Sn2	109.63 (9)
H11D—C113—H11F	109.5	C222—C221—Sn2	108.15 (10)
H11E—C113—H11F	109.5	C221—C222—H22A	109.5
C111—C114—H11G	109.5	C221—C222—H22B	109.5
C111—C114—H11H	109.5	H22A—C222—H22B	109.5
H11G—C114—H11H	109.5	C221—C222—H22C	109.5
C111—C114—H11I	109.5	H22A—C222—H22C	109.5
H11G—C114—H11I	109.5	H22B—C222—H22C	109.5
H11H—C114—H11I	109.5	C221—C223—H22D	109.5
C124—C121—C122	109.58 (13)	C221—C223—H22E	109.5
C124—C121—C123	110.72 (12)	H22D—C223—H22E	109.5
C122—C121—C123	109.55 (13)	C221—C223—H22F	109.5
C124—C121—Sn1	108.74 (10)	H22D—C223—H22F	109.5
C122—C121—Sn1	107.84 (10)	H22E—C223—H22F	109.5
C123—C121—Sn1	110.35 (9)	C221—C224—H22G	109.5
C121—C122—H12A	109.5	C221—C224—H22H	109.5
C121—C122—H12B	109.5	H22G—C224—H22H	109.5
H12A—C122—H12B	109.5	C221—C224—H22I	109.5
C121—C122—H12C	109.5	H22G—C224—H22I	109.5
H12A—C122—H12C	109.5	H22H—C224—H22I	109.5

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1—H1 \cdots Cl2 ⁱ	0.96	2.30	3.2469 (10)	169
O2—H2 \cdots Cl1 ⁱⁱ	0.96	2.31	3.2482 (10)	166

Symmetry codes: (i) $x+1/2, -y+1/2, z+1/2$; (ii) $x-1/2, -y+1/2, z-1/2$.