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μ-Ethane-1,2-diylbis(diphenylphosphine oxide)-κ^2O:O'-bis[dibenzyldichlorotin(IV)]: a centrosymmetric complex containing trigonal-bipyramidal tin(IV), linked into chains of rings by C—H$\cdots\pi$(arene) hydrogen bonds

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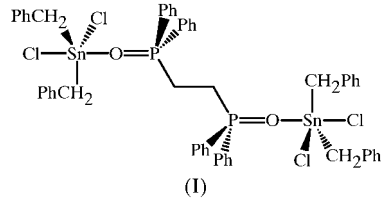
The title compound, $[Sn_2Cl_4(C_7H_7)_4(C_{26}H_{24}O_2P_2)]$, (I), was isolated from the reaction of 1,2-bis(diphenylphosphino)ethane with dibenzyltin(IV) dichloride in the presence of air. The molecules of (I) lie across centres of inversion in space group *C*2/*c* and contain five-coordinate Sn atoms. The molecules are linked into chains of rings by a single C—H$\cdots\pi$(arene) hydrogen bond.

Comment

The interaction of chelating bisphosphines with tin(IV) halides has been the subject of several investigations. Reaction of both simple phosphines and 1,2-bis(diphenylphosphino)ethane, $Ph_2PCH_2CH_2PPh_2$, with SnX_4 (X = Cl or Br) gave products characterized on the basis of spectral data only as 1:1 adducts containing six-coordinate tin (Reutov *et al.*, 1988). On the other hand, the reaction of the same bisphosphine with Me_2SnCl_2 in the presence of air gave a 1:1 adduct characterized by X-ray diffraction as a continuous-chain polymer containing the oxidized ligand $Ph_2P(O)CH_2CH_2P(O)Ph_2$ bridging pairs of six-coordinate Sn atoms (Pettinari *et al.*, 2001). The analogous product from Ph_2SnCl_2 was assigned a similar structure, but in the absence of air, no reaction was observed with R_2SnCl_2 (R = Me or Ph). We have now investigated the reaction of 1,2-bis(diphenylphosphino)ethane with dibenzyltin(IV) dichloride, $(PhCH_2)_2SnCl_2$, and report here the molecular and supramolecular structure of the product, (I), a 2:1 complex containing the oxidized ligand $Ph_2P(O)CH_2CH_2P(O)Ph_2$ bridging pairs of five-coordinate Sn atoms. The oxidation of the bisphosphine can be readily diagnosed both from the IR absorption characteristics of P=O bonds and from the ^{31}P NMR spectrum.



(I)

Complex (I) is centrosymmetric; it lies across a centre of inversion in space group *C*2/*c*, chosen for the sake of convenience as that at ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$). Accordingly, the P—C—C—P fragment of the phosphine oxide ligand has a *trans*-planar conformation. The five-coordinate Sn atom has a trigonal-bipyramidal configuration, with the O atom and one of the chloro ligands (Cl1) in axial sites, and the other chloro ligand and the two benzyl ligands in equatorial sites (Fig. 1); the interbond angles are close to idealized values (Table 1). The axial Sn—Cl bond is longer than the equatorial Sn—Cl bond by ~0.12 Å, and the P—O—Sn fragment is nearly linear. The remaining bond lengths and angles show no unusual values.

The complexes are linked by a single C—H$\cdots\pi$(arene) hydrogen bond (Table 2), in which the same benzyl group provides both the donor and the acceptor. Benzyl atom C3 in the reference complex centred at ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$) acts as a hydrogen-bond donor, *via* atom H3*A*, to the C31–C36 ring at ($1-x$, y, $\frac{1}{2}-z$), which forms part of the complex centred at ($\frac{1}{2}$, $\frac{1}{2}$, 0). Propagation of this interaction by the space group then generates a chain of rings running parallel to the [001] direction (Fig. 2).

Since no coordination of unoxidized bisphosphine was observed in the absence of air by Pettinari *et al.* (2001), it seems probable that the bulk of the oxidation occurs before

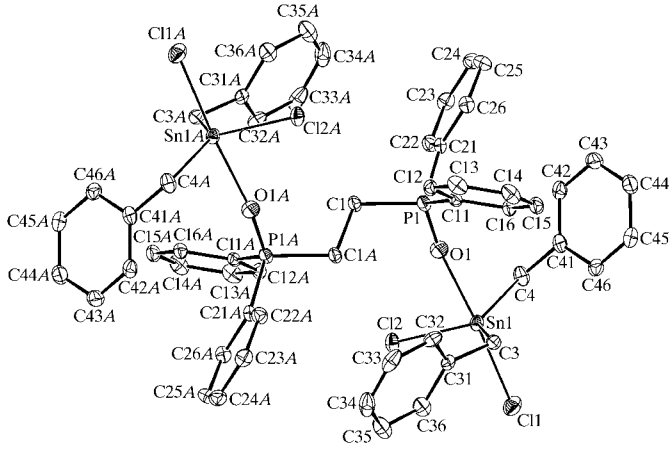


Figure 1
A view of complex (I), showing the atom-labelling scheme. Atoms labelled with the suffix '*A*' are at the symmetry position ($1-x$, $1-y$, $1-z$). Displacement ellipsoids are drawn at the 30% probability level. For the sake of clarity, H atoms have been omitted.

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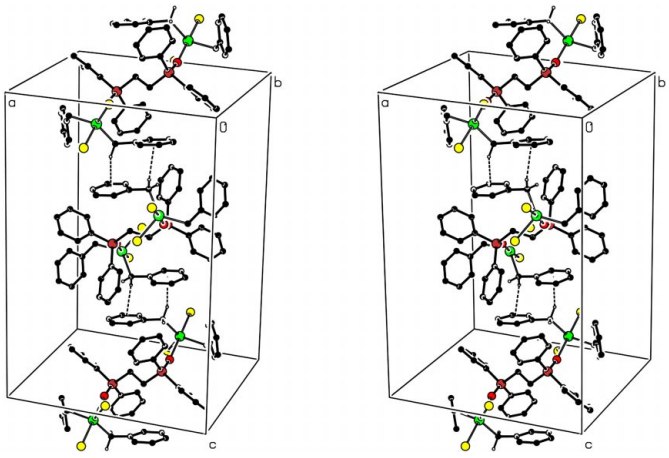

Figure 2
A stereoview of part of the crystal structure of (I), showing the formation of a chain of rings along the [001] direction. For clarity, H atoms other than those bonded to the C atom involved in the motif shown have been omitted.

the formation of the final product; however, the detailed mechanism of this process remains unknown.

Experimental

For the synthesis of (I), a dilute solution of dibenzyltin(IV) chloride [prepared according to Sisido *et al.* (1961)] in chloroform was added dropwise to an equimolar quantity of 1,2-bis(diphenylphosphino)-ethane, also in chloroform solution, and the mixture was stirred overnight. After removal of the solvent *in vacuo*, a pale yellow solid was obtained; vapour diffusion of light petroleum into a solution of this solid in benzene gave colourless crystals of (I) suitable for single-crystal X-ray diffraction (m.p. 445–447 K). IR (KBr disk): 1191 and 1153 cm^{-1} [ν(P═O)]; ^{1}H NMR ($CDCl_3$): δ 2.26 (*br*, 4H, 2 × CH_2P), 2.93 (*s* with Sn satellites, $^2J_{Sn-H}$ = 93.6 Hz, 8H, 4 × CH_2Ph), 6.85–6.98 (*m*, 20H, 4 × Ph), 7.18–7.55 (*m*, 20H, 4 × Ph); ^{31}P NMR ($CDCl_3$): δ 38.7; ^{119}Sn NMR ($CDCl_3$): δ −137.5.

Crystal data

$[Sn_2Cl_4(C_7H_7)_4(C_{26}H_{24}O_2P_2)]$
M_r = 1174.12
Monoclinic, *C*2/*c*
a = 15.0100 (5) Å
b = 14.7055 (6) Å
c = 22.6909 (6) Å
β = 91.571 (2)°
V = 5006.7 (3) Å^3
Z = 4
D_x = 1.558 Mg m^{-3}
Mo *K*α radiation
Cell parameters from 5716 reflections
θ = 3.2–27.5°
μ = 1.32 mm^{-1}
T = 120 (2) K
Needle, colourless
0.20 × 0.07 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
φ scans, and ω scans with κ offsets
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995, 1997)
T_{min} = 0.731, T_{max} = 0.940
31 842 measured reflections
5716 independent reflections
3778 reflections with $I > 2\sigma(I)$
R_{int} = 0.082
θ_{max} = 27.5°
h = −19 → 19
k = −18 → 19
l = −29 → 29

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.083
S = 0.96
5716 reflections
289 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0368P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—Cl1	2.4788 (10)	Sn1—C3	2.132 (3)
Sn1—Cl2	2.3597 (8)	Sn1—C4	2.137 (4)
Sn1—O1	2.242 (2)	P1—O1	1.467 (3)
Cl2—Sn1—C3	116.68 (9)	O1—Sn1—Cl1	175.87 (6)
Cl2—Sn1—C4	114.37 (9)	P1—O1—Sn1	164.8 (2)
C3—Sn1—C4	128.0 (2)		

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

*Cg*1 is the centroid of the C31–C36 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3*A*···*Cg*1^{i}	0.99	2.67	3.466 (3)	137

Symmetry code: (i) $1-x, y, \frac{1}{2}-z$.

Crystals of (I) are monoclinic and the systematic absences permitted *C*2/*c* and *Cc* as possible space groups; *C*2/*c* was selected and confirmed by the subsequent analysis. All H atoms were located from difference maps and treated as riding atoms, with C—H distances of 0.95 (aromatic) or 0.99 Å (CH_2).

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO–SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO–SMN*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL*97 and *PRPKAPPA* (Ferguson, 1999).

X-ray data were collected at the EPSRC X-ray Crystallographic Service, University of Southampton, England; the authors thank the staff for all their help and advice. JNL thanks NCR Self-Service, Dundee, for grants that have provided computing facilities for this work.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1706). Services for accessing these data are described at the back of the journal.

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Computing details

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO*–SMN (Otwinowski & Minor, 1997); data reduction: *DENZO*–SMN; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* (Sheldrick, 1997) and *PRPKAPPA* (Ferguson, 1999).

μ-ethane-1,2-diylbis(diphenylphosphine oxide)-κ^2O:O'- bis[dibenzyldichlorotin(IV)]

Crystal data

$C_{54}H_{52}Cl_4O_2P_2Sn_2$
$M_r = 1174.12$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 15.0100\ (5)$ Å
$b = 14.7055\ (6)$ Å
$c = 22.6909\ (6)$ Å
$\beta = 91.571\ (2)°$
$V = 5006.7\ (3)$ Å^3
$Z = 4$
$F(000) = 2360$
$D_x = 1.558$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5716 reflections
$\theta = 3.2–27.5°$
$\mu = 1.32$ mm^{-1}
$T = 120$ K
Needle, colourless
0.20 × 0.07 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: rotating anode
Graphite monochromator
φ scans, and ω scans with κ offsets
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995; Blessing, 1997)
$T_{min} = 0.731$, $T_{max} = 0.940$
31842 measured reflections
5716 independent reflections
3778 reflections with $I > 2\sigma(I)$
$R_{int} = 0.082$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.2°$
$h = -19\rightarrow19$
$k = -18\rightarrow19$
$l = -29\rightarrow29$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.083$
$S = 0.96$
5716 reflections
289 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0368P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.20$ e Å^{-3}
$\Delta\rho_{min} = -0.68$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.341728 (15)	0.293892 (16)	0.383758 (9)	0.02403 (9)
Cl1	0.33173 (7)	0.14724 (6)	0.33012 (4)	0.0418 (3)
Cl2	0.42566 (6)	0.22832 (6)	0.46228 (4)	0.0326 (2)
O1	0.35524 (16)	0.42107 (17)	0.43776 (10)	0.0373 (6)
P1	0.36645 (6)	0.51543 (6)	0.45765 (4)	0.0251 (2)
C1	0.4573 (2)	0.5223 (3)	0.51083 (13)	0.0270 (8)
C3	0.4150 (2)	0.3585 (2)	0.31629 (13)	0.0249 (8)
C4	0.2017 (2)	0.3007 (3)	0.39790 (16)	0.0346 (9)
C11	0.3876 (2)	0.5926 (2)	0.39847 (13)	0.0231 (8)
C12	0.4530 (2)	0.6587 (2)	0.40075 (14)	0.0271 (8)
C13	0.4649 (2)	0.7158 (2)	0.35356 (16)	0.0360 (9)
C14	0.4101 (3)	0.7076 (3)	0.30358 (16)	0.0388 (10)
C15	0.3448 (2)	0.6430 (3)	0.30059 (15)	0.0325 (9)
C16	0.3326 (2)	0.5854 (2)	0.34792 (13)	0.0273 (8)
C21	0.2677 (2)	0.5538 (2)	0.49210 (13)	0.0238 (8)
C22	0.2253 (2)	0.4961 (3)	0.53128 (14)	0.0304 (9)
C23	0.1449 (2)	0.5203 (3)	0.55530 (15)	0.0329 (9)
C24	0.1073 (2)	0.6027 (3)	0.53999 (15)	0.0338 (9)
C25	0.1478 (2)	0.6601 (3)	0.50128 (15)	0.0330 (9)
C26	0.2280 (2)	0.6368 (2)	0.47775 (14)	0.0285 (9)
C31	0.5138 (2)	0.3634 (2)	0.32797 (13)	0.0241 (8)
C32	0.5592 (3)	0.4455 (3)	0.32751 (14)	0.0329 (9)
C33	0.6520 (3)	0.4470 (3)	0.33559 (15)	0.0464 (12)
C34	0.6977 (3)	0.3671 (4)	0.34417 (16)	0.0520 (13)
C35	0.6536 (3)	0.2859 (3)	0.34459 (16)	0.0496 (12)
C36	0.5626 (3)	0.2838 (3)	0.33685 (14)	0.0370 (10)
C41	0.1612 (2)	0.3801 (2)	0.36526 (15)	0.0280 (8)
C42	0.1166 (2)	0.4476 (3)	0.39409 (15)	0.0310 (9)
C43	0.0811 (2)	0.5212 (3)	0.36405 (16)	0.0370 (10)
C44	0.0902 (3)	0.5291 (3)	0.30359 (17)	0.0392 (10)
C45	0.1346 (2)	0.4621 (3)	0.27407 (16)	0.0368 (10)
C46	0.1706 (2)	0.3881 (2)	0.30399 (15)	0.0316 (9)
H1A	0.4695	0.5870	0.5199	0.032*
H1B	0.4396	0.4922	0.5477	0.032*

H12	0.4901	0.6647	0.4351	0.032*
H13	0.5104	0.7607	0.3552	0.043*
H14	0.4181	0.7473	0.2711	0.047*
H15	0.3078	0.6376	0.2661	0.039*
H16	0.2867	0.5409	0.3461	0.033*
H22	0.2519	0.4394	0.5416	0.037*
H23	0.1162	0.4808	0.5819	0.040*
H24	0.0524	0.6200	0.5565	0.041*
H25	0.1202	0.7162	0.4907	0.040*
H26	0.2565	0.6774	0.4517	0.034*
H3A	0.4038	0.3252	0.2789	0.030*
H3B	0.3919	0.4210	0.3108	0.030*
H32	0.5274	0.5008	0.3217	0.039*
H33	0.6833	0.5031	0.3351	0.056*
H34	0.7606	0.3683	0.3499	0.062*
H35	0.6860	0.2309	0.3502	0.060*
H36	0.5324	0.2270	0.3376	0.044*
H4A	0.1729	0.2437	0.3841	0.042*
H4B	0.1912	0.3072	0.4406	0.042*
H42	0.1100	0.4434	0.4355	0.037*
H43	0.0501	0.5668	0.3849	0.044*
H44	0.0661	0.5801	0.2829	0.047*
H45	0.1406	0.4666	0.2326	0.044*
H46	0.2017	0.3427	0.2831	0.038*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.02342 (15)	0.02919 (16)	0.01947 (13)	−0.00203 (12)	0.00056 (9)	0.00214 (11)
Cl1	0.0565 (7)	0.0328 (6)	0.0358 (5)	−0.0057 (5)	−0.0067 (5)	−0.0017 (4)
Cl2	0.0317 (5)	0.0416 (6)	0.0240 (4)	−0.0010 (4)	−0.0048 (4)	0.0073 (4)
O1	0.0389 (16)	0.0397 (17)	0.0333 (14)	0.0020 (13)	0.0023 (12)	−0.0014 (12)
P1	0.0216 (5)	0.0295 (6)	0.0242 (5)	0.0032 (4)	−0.0006 (4)	0.0039 (4)
C1	0.023 (2)	0.038 (2)	0.0196 (18)	0.0079 (16)	−0.0006 (14)	0.0030 (15)
C3	0.026 (2)	0.028 (2)	0.0203 (17)	0.0022 (16)	0.0035 (14)	0.0017 (15)
C4	0.022 (2)	0.042 (3)	0.039 (2)	−0.0033 (18)	−0.0026 (16)	0.0067 (19)
C11	0.0193 (19)	0.029 (2)	0.0214 (17)	0.0044 (16)	0.0009 (14)	0.0000 (15)
C12	0.020 (2)	0.035 (2)	0.0262 (19)	−0.0009 (17)	−0.0020 (15)	−0.0020 (17)
C13	0.027 (2)	0.033 (2)	0.049 (2)	−0.0029 (18)	0.0087 (18)	0.0105 (19)
C14	0.035 (2)	0.047 (3)	0.035 (2)	0.009 (2)	0.0098 (18)	0.0193 (19)
C15	0.030 (2)	0.044 (3)	0.0234 (19)	0.0088 (19)	−0.0019 (16)	0.0022 (17)
C16	0.027 (2)	0.030 (2)	0.0243 (19)	0.0032 (17)	−0.0029 (15)	0.0020 (16)
C21	0.021 (2)	0.027 (2)	0.0227 (18)	−0.0007 (16)	−0.0051 (15)	0.0016 (16)
C22	0.031 (2)	0.032 (2)	0.029 (2)	0.0022 (18)	0.0005 (16)	0.0032 (17)
C23	0.029 (2)	0.042 (3)	0.028 (2)	−0.0062 (19)	0.0078 (16)	−0.0014 (17)
C24	0.028 (2)	0.039 (3)	0.035 (2)	0.0017 (19)	0.0047 (17)	−0.0071 (18)
C25	0.028 (2)	0.028 (2)	0.043 (2)	0.0065 (18)	0.0040 (18)	0.0001 (18)
C26	0.028 (2)	0.027 (2)	0.0308 (19)	−0.0023 (17)	−0.0015 (16)	0.0034 (16)

C31	0.026 (2)	0.035 (2)	0.0111 (16)	0.0010 (17)	0.0051 (13)	0.0024 (15)
C32	0.040 (3)	0.036 (2)	0.0240 (19)	−0.0034 (19)	0.0099 (16)	−0.0060 (17)
C33	0.045 (3)	0.067 (3)	0.028 (2)	−0.024 (3)	0.0080 (19)	−0.012 (2)
C34	0.025 (2)	0.102 (4)	0.029 (2)	0.000 (3)	0.0006 (18)	0.000 (2)
C35	0.038 (3)	0.077 (4)	0.035 (2)	0.020 (3)	0.0069 (19)	0.015 (2)
C36	0.036 (2)	0.047 (3)	0.028 (2)	0.003 (2)	0.0071 (17)	0.0093 (18)
C41	0.0166 (19)	0.032 (2)	0.036 (2)	−0.0080 (17)	−0.0035 (15)	0.0041 (17)
C42	0.018 (2)	0.047 (3)	0.0279 (19)	−0.0054 (18)	0.0004 (15)	−0.0001 (18)
C43	0.026 (2)	0.038 (3)	0.046 (2)	0.0015 (18)	−0.0027 (18)	−0.0093 (19)
C44	0.035 (2)	0.036 (3)	0.046 (3)	0.0023 (19)	−0.0114 (19)	0.000 (2)
C45	0.038 (2)	0.043 (3)	0.029 (2)	−0.005 (2)	−0.0091 (18)	0.0003 (19)
C46	0.028 (2)	0.033 (2)	0.033 (2)	−0.0047 (18)	−0.0026 (16)	−0.0043 (17)

Geometric parameters (Å, º)

Sn1—Cl1	2.4788 (10)	C25—C26	1.374 (5)
Sn1—Cl2	2.3597 (8)	C25—H25	0.95
Sn1—O1	2.242 (2)	C26—H26	0.95
Sn1—C3	2.132 (3)	C3—C31	1.501 (5)
Sn1—C4	2.137 (4)	C3—H3A	0.99
P1—O1	1.467 (3)	C3—H3B	0.99
P1—C21	1.787 (3)	C31—C32	1.388 (5)
P1—C11	1.793 (3)	C31—C36	1.393 (5)
P1—C1	1.799 (3)	C32—C33	1.400 (5)
C1—C1^{i}	1.533 (6)	C32—H32	0.95
C1—H1A	0.99	C33—C34	1.371 (6)
C1—H1B	0.99	C33—H33	0.95
C11—C12	1.381 (5)	C34—C35	1.365 (6)
C11—C16	1.399 (4)	C34—H34	0.95
C12—C13	1.377 (5)	C35—C36	1.374 (5)
C12—H12	0.95	C35—H35	0.95
C13—C14	1.388 (5)	C36—H36	0.95
C13—H13	0.95	C4—C41	1.502 (5)
C14—C15	1.366 (5)	C4—H4A	0.99
C14—H14	0.95	C4—H4B	0.99
C15—C16	1.384 (5)	C41—C42	1.373 (5)
C15—H15	0.95	C41—C46	1.406 (5)
C16—H16	0.95	C42—C43	1.378 (5)
C21—C26	1.393 (5)	C42—H42	0.95
C21—C22	1.396 (5)	C43—C44	1.387 (5)
C22—C23	1.384 (5)	C43—H43	0.95
C22—H22	0.95	C44—C45	1.374 (5)
C23—C24	1.377 (5)	C44—H44	0.95
C23—H23	0.95	C45—C46	1.385 (5)
C24—C25	1.372 (5)	C45—H45	0.95
C24—H24	0.95	C46—H46	0.95
Cl2—Sn1—C3	116.68 (9)	C24—C25—H25	119.9

Cl2—Sn1—C4	114.37 (9)	C26—C25—H25	119.9
C3—Sn1—C4	128.0 (2)	C25—C26—C21	120.0 (3)
C3—Sn1—O1	88.87 (11)	C25—C26—H26	120.0
C4—Sn1—O1	87.32 (12)	C21—C26—H26	120.0
O1—Sn1—Cl2	83.67 (6)	C31—C3—Sn1	114.9 (2)
C3—Sn1—Cl1	93.46 (9)	C31—C3—H3A	108.5
C4—Sn1—Cl1	93.90 (11)	Sn1—C3—H3A	108.5
O1—Sn1—Cl1	175.87 (6)	C31—C3—H3B	108.5
Cl2—Sn1—Cl1	92.24 (3)	Sn1—C3—H3B	108.5
P1—O1—Sn1	164.8 (2)	H3A—C3—H3B	107.5
O1—P1—C21	110.10 (16)	C32—C31—C36	118.4 (3)
O1—P1—C11	112.91 (14)	C32—C31—C3	121.6 (3)
C21—P1—C11	107.10 (15)	C36—C31—C3	119.9 (3)
O1—P1—C1	109.74 (16)	C31—C32—C33	120.0 (4)
C21—P1—C1	108.17 (15)	C31—C32—H32	120.0
C11—P1—C1	108.68 (16)	C33—C32—H32	120.0
C1^{i}—C1—P1	112.7 (3)	C34—C33—C32	119.8 (4)
C1^{i}—C1—H1A	109.0	C34—C33—H33	120.1
P1—C1—H1A	109.0	C32—C33—H33	120.1
C1^{i}—C1—H1B	109.0	C35—C34—C33	120.6 (4)
P1—C1—H1B	109.0	C35—C34—H34	119.7
H1A—C1—H1B	107.8	C33—C34—H34	119.7
C12—C11—C16	119.1 (3)	C34—C35—C36	120.0 (4)
C12—C11—P1	123.9 (2)	C34—C35—H35	120.0
C16—C11—P1	117.0 (3)	C36—C35—H35	120.0
C13—C12—C11	120.5 (3)	C35—C36—C31	121.1 (4)
C13—C12—H12	119.7	C35—C36—H36	119.4
C11—C12—H12	119.7	C31—C36—H36	119.4
C12—C13—C14	119.7 (3)	C41—C4—Sn1	110.4 (2)
C12—C13—H13	120.1	C41—C4—H4A	109.6
C14—C13—H13	120.1	Sn1—C4—H4A	109.6
C15—C14—C13	120.6 (3)	C41—C4—H4B	109.6
C15—C14—H14	119.7	Sn1—C4—H4B	109.6
C13—C14—H14	119.7	H4A—C4—H4B	108.1
C14—C15—C16	119.8 (3)	C42—C41—C46	118.3 (3)
C14—C15—H15	120.1	C42—C41—C4	121.5 (3)
C16—C15—H15	120.1	C46—C41—C4	120.2 (3)
C15—C16—C11	120.2 (3)	C41—C42—C43	121.2 (3)
C15—C16—H16	119.9	C41—C42—H42	119.4
C11—C16—H16	119.9	C43—C42—H42	119.4
C26—C21—C22	118.9 (3)	C42—C43—C44	120.5 (4)
C26—C21—P1	121.9 (3)	C42—C43—H43	119.7
C22—C21—P1	119.0 (3)	C44—C43—H43	119.7
C23—C22—C21	120.8 (3)	C45—C44—C43	119.0 (4)
C23—C22—H22	119.6	C45—C44—H44	120.5
C21—C22—H22	119.6	C43—C44—H44	120.5
C24—C23—C22	118.9 (4)	C44—C45—C46	120.8 (4)
C24—C23—H23	120.5	C44—C45—H45	119.6

C22—C23—H23	120.5	C46—C45—H45	119.6
C25—C24—C23	121.1 (4)	C45—C46—C41	120.1 (4)
C25—C24—H24	119.4	C45—C46—H46	119.9
C23—C24—H24	119.4	C41—C46—H46	119.9
C24—C25—C26	120.2 (3)		

C3—Sn1—O1—P1	25.1 (6)	C23—C24—C25—C26	−1.1 (5)
C4—Sn1—O1—P1	−103.1 (6)	C24—C25—C26—C21	1.4 (5)
Cl2—Sn1—O1—P1	142.1 (6)	C22—C21—C26—C25	−1.1 (5)
Sn1—O1—P1—C21	115.7 (6)	P1—C21—C26—C25	174.1 (3)
Sn1—O1—P1—C11	−3.9 (7)	C4—Sn1—C3—C31	162.8 (2)
Sn1—O1—P1—C1	−125.3 (6)	O1—Sn1—C3—C31	77.1 (2)
O1—P1—C1—C1^{i}	51.2 (4)	Cl2—Sn1—C3—C31	−5.2 (3)
C21—P1—C1—C1^{i}	171.4 (3)	Cl1—Sn1—C3—C31	−99.5 (2)
C11—P1—C1—C1^{i}	−72.7 (4)	Sn1—C3—C31—C32	−124.3 (3)
O1—P1—C11—C12	−134.4 (3)	Sn1—C3—C31—C36	58.7 (4)
C21—P1—C11—C12	104.2 (3)	C36—C31—C32—C33	0.3 (5)
C1—P1—C11—C12	−12.4 (3)	C3—C31—C32—C33	−176.7 (3)
O1—P1—C11—C16	47.0 (3)	C31—C32—C33—C34	−0.3 (5)
C21—P1—C11—C16	−74.4 (3)	C32—C33—C34—C35	0.4 (6)
C1—P1—C11—C16	169.0 (3)	C33—C34—C35—C36	−0.5 (6)
C16—C11—C12—C13	−1.0 (5)	C34—C35—C36—C31	0.6 (6)
P1—C11—C12—C13	−179.6 (3)	C32—C31—C36—C35	−0.5 (5)
C11—C12—C13—C14	0.7 (5)	C3—C31—C36—C35	176.6 (3)
C12—C13—C14—C15	−0.4 (6)	C3—Sn1—C4—C41	−17.3 (3)
C13—C14—C15—C16	0.4 (6)	O1—Sn1—C4—C41	69.1 (2)
C14—C15—C16—C11	−0.7 (5)	Cl2—Sn1—C4—C41	151.0 (2)
C12—C11—C16—C15	1.1 (5)	Cl1—Sn1—C4—C41	−114.8 (2)
P1—C11—C16—C15	179.7 (3)	Sn1—C4—C41—C42	−121.6 (3)
O1—P1—C21—C26	−131.7 (3)	Sn1—C4—C41—C46	56.7 (4)
C11—P1—C21—C26	−8.6 (3)	C46—C41—C42—C43	0.4 (5)
C1—P1—C21—C26	108.3 (3)	C4—C41—C42—C43	178.7 (3)
O1—P1—C21—C22	43.4 (3)	C41—C42—C43—C44	−0.4 (5)
C11—P1—C21—C22	166.5 (3)	C42—C43—C44—C45	0.5 (6)
C1—P1—C21—C22	−76.5 (3)	C43—C44—C45—C46	−0.7 (6)
C26—C21—C22—C23	0.4 (5)	C44—C45—C46—C41	0.7 (5)
P1—C21—C22—C23	−174.9 (3)	C42—C41—C46—C45	−0.6 (5)
C21—C22—C23—C24	−0.1 (5)	C4—C41—C46—C45	−178.9 (3)
C22—C23—C24—C25	0.5 (5)		

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3*A*···*Cg*1^{ii}	0.99	2.67	3.466 (3)	137

Symmetry code: (ii) −*x*+1, *y*, −*z*+1/2.