

Acta Crystallographica Section E Structure Reports Online

ISSN 1600-5368

Trimethylammonium dichloridotriphenylstannate(IV)

Tidiane Diop,^a* Libasse Diop,^a Jerry P. Jasinski^b and Amanda C. Keeley^b

^aLaboratoire de Chimie Minerale et Analytique, Département de Chimie, Faculté des Sciences et Techniques, Université Cheikh Anta Diop, Dakar, Senegal, and ^bDepartment of Chemistry, Keene State College 229 Main Street Keene, NH 03435-2001, USA

Correspondence e-mail: tijchimia@yahoo.fr

Received 30 July 2012; accepted 7 September 2012

Key indicators: single-crystal X-ray study; T = 173 K; mean σ (C–C) = 0.005 Å; R factor = 0.030; wR factor = 0.083; data-to-parameter ratio = 18.1.

In the structure of the title monomeric coordination salt, $(C_3H_{10}N)[Sn(C_6H_5)_3Cl_2]$, the Sn^{IV} atom is five coordinate, with the SnC₃Cl₂ entity in a *trans* trigonal-bipyramidal arrangement and the chlorine atoms in apical positions. In the crystal, the cations and anions are connected by N-H···Cl hydrogen bonds.

Related literature

For medical applications of tin(IV) compounds, see: Evans & Karpel (1985); Gielen (2002); Davies *et al.* (2008). For literature on organotin(IV) compounds, see: Chandrasekhar & Baskar (2003); Samuel *et al.* (2002); Nath *et al.* (2003). For related structures, see: Ng (1999, 1995); Harrison *et al.* (1978); Nayek *et al.* (2010); Sow *et al.* (2012); De Lorentiis *et al.* (2011).



Experimental

Crystal data $(C_3H_{10}N)[Sn(C_6H_5)Cl_2]$ $M_r = 481.01$ Monoclinic, $P2_1/n$ a = 9.2650 (2) Å

b = 15.6882 (4) Å c = 14.7891 (3) Å $\beta = 90.941 (2)^{\circ}$ $V = 2149.32 (8) \text{ Å}^{3}$ Z = 4Cu *K* α radiation $\mu = 11.75 \text{ mm}^{-1}$

Data collection

Oxford Diffraction Xcalibur Eos Gemini diffractometer Absorption correction: multi-scan (*CrysAlis PRO* and *CrysAlis RED*; Oxford Diffraction, 2010) $T_{min} = 0.328, T_{max} = 1.000$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.030$ $wR(F^2) = 0.083$ S = 1.064143 reflections

Table 1

Hydrogen-bond geometry (Å, °).

 $D-H\cdots A$ D-H $H\cdots A$ $D\cdots A$ $D-H\cdots A$ $N1-H1\cdots Cl1^i$ 0.912.213.087 (3)161

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

JPJ acknowledges the NSF–MRI program (grant No. CHE1039027) for funds to purchase the X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2438).

References

- Chandrasekhar, V. & Baskar, V. (2003). Indian J. Chem. Sect. A Inorg. Bioinorg. Phys. Theor. Anal. Chem. 42, 2376–2381.
- Davies, A. G., Gielen, M., Pannell, K. H. & Tiekink, E. R. T. (2008). Editors. *Tin Chemistry*. Chichester: Wiley.
- De Lorentiis, L., Graiff, C. & Predieri, G. (2011). Acta Cryst. E67, m1356.
- Evans, C. J. & Karpel, S. (1985). Organotin Compounds in Modern Technology, J. Organomet. Chem. Library, Vol. 16. Amsterdam: Elsevier. Gielen, M. (2002). Appl. Organomet. Chem. 16, 481–494.
- Harrison, P. G., Molloy, K., Phillips, R. C., Smith, P. J. & Crowe, A. J. (1978). J.
- Organomet. Chem. 160, 421–434. Nath, M., Pokharia, S., Song, X., Eng, G., Gielen, M., Kemmer, M., Biesemans,

M., Willem, R. & Vos, D. D. (2003). Appl. Organomet. Chem. **17**, 305–314. Navek, H. P., Massa, W. & Dehnen, S. (2010). Inorg. Chem. **49**, 144–149.

- Nayek, H. P., Massa, W. & Dennen, S. (2010). In Ng, S. W. (1995). Acta Cryst. C**51**, 1124–1125.
- Ng, S. W. (1999). Acta Cryst. C51, 1124–111. Ng, S. W. (1999). Acta Cryst. C55, 523–531.
- Ng, S. W. (1999). Actu Cryst. C55, 525–551.
- Oxford Diffraction (2010). CrysAlis PRO and CrysAlis RED. Oxford Diffraction Ltd, Abingdon, England.
- Samuel, P. M., De Vos, D., Raveendra, D., Sarma, J. A. R. P. & Roy, S. (2002). Bioorg. Med. Chem. Lett. 12, 61–64.
- Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.
- Sow, Y., Diop, L., Kociok-Kohn, G. & Molloy, K. C. (2012). Acta Cryst. E68, m1015-m1016.

metal-organic compounds

 $0.34 \times 0.22 \times 0.16 \text{ mm}$

13300 measured reflections

4143 independent reflections

3739 reflections with $I > 2\sigma(I)$

H-atom parameters constrained

T = 173 K

 $R_{\rm int}=0.054$

229 parameters

 $\Delta \rho_{\rm max} = 0.53 \ {\rm e} \ {\rm \AA}^-$

 $\Delta \rho_{\rm min} = -0.53 \text{ e } \text{\AA}^{-3}$

supporting information

Acta Cryst. (2012). E68, m1279 [https://doi.org/10.1107/S1600536812038457] Trimethylammonium dichloridotriphenylstannate(IV) Tidiane Diop, Libasse Diop, Jerry P. Jasinski and Amanda C. Keeley

S1. Comment

The interest in synthesis of new organotin(IV) derivatives is related to their applications in different fields (agrochemicals, surface disinfectants and marine antifouling paints) (Evans & Karpel, 1985; Gielen, 2002; Davies et al., 2008) and explains the involvement of many groups in the search for new organotin compounds (Chandrasekhar & Baskar, 2003; Samuel et al., 2002; Nath et al., 2003). Many compounds containing the [SnPh₃Cl₂]⁻ ion in the trans conformation have been reported (Ng, 1995, 1999; Harrison et al., 1978; Nayek et al., 2010; Sow et al., 2012). In our search for new organotin(IV) compounds we have initiated here the study of the interactions between $(CH_3)_3N.HCl$ and $SnPh_3Cl$, which led to the title compound. In the $[SnPh_3Cl_2]^2$ anion, the tin atom is located on a centre of inversion and is bonded to two Cl atoms and three phenyl groups giving a trigonal bipyramidal geometry with the chloride atoms in transpositions (Fig. 1). The sum of the angles at atom Sn by the *ipso*-carbons $[128.08 (12)^\circ, 113.70 (12)^\circ, 117.83 (12)^\circ]$ is 359.61° . The corresponding axial Cl₁—Sn—Cl₂ angle is 171.62 (3)°, indicating a slight deviation from linearity. The Sn -C bond distances (2.135 (3) Å, 2.142 (3) Å and 2.151 (3) Å) are similar to those reported for bis(triphenylphosphanylidene)iminium dichloridotriphenylstannate(IV) (2.134 (3) Å, 2.1476 (19) Å and 2.1476 (19) Å) (De Lorentiis et al., 2011). The two axial Sn-Cl distances, [Sn-Cl 2.5227 (7) Å and 2.6983 (8) Å], are very close to those reported (Sow et al., 2012). The two types of Sn-Cl binding are due to disruption of NH ... Cl hydrogen bonding on one of the chlorine atoms. The C–N–C angles of the cation are close to 109° , in agreement with the expected sp^{3} hybridization. The cation and the anion are connected by N-H...Cl hydrogen bonds (Fig. 2).

S2. Experimental

Crystals of the title compound, $[C_3H_{10}N^+]$ [Sn(C₆H₅)₃Cl₂⁻], were obtained by reacting SnPh₃Cl with (CH₃)₃N.HCl in ethanol in a 1/1 ratio. (CH₃)₃N.HCl (Merck) and SnPh₃Cl (Aldrich) were used without further purification. The title compound was obtained by mixing in a 1/1 ratio (CH₃)₃N.HCl dissolved in methanol and a minimum of water and SnPh₃Cl dissolved in methanol. The mixture was stirred for around two hours at room temperature and upon slow solvent evaporation gave prismatic crystals suitable for X-ray diffraction analysis.

S3. Refinement

All of the H atoms were placed in calculated positions and then refined using a riding model with C—H lengths of 0.95 Å (CH) or 0.98 Å (CH₃) and N—H lengths of 0.90 Å (NH). The isotropic displacement parameters for these atoms were set to 1.2 (CH, NH), or 1.5 (CH₃) times U_{eq} of the parent atom.





Molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level.



Figure 2

The packing of the structure viewed along the c axis. N—H···Cl hydrogen bonds are shown as dashed lines. The remaining H atoms have been removed for clarity.

Trimethylammonium dichloridotriphenylstannate(IV)

Crystal data

 $\begin{array}{l} (C_{3}H_{10}N)[Sn(C_{6}H_{5})Cl_{2}]\\ M_{r} = 481.01\\ Monoclinic, P2_{1}/n\\ Hall symbol: -P 2yn\\ a = 9.2650 \ (2) \ \text{\AA}\\ b = 15.6882 \ (4) \ \text{\AA}\\ c = 14.7891 \ (3) \ \text{\AA}\\ \beta = 90.941 \ (2)^{\circ}\\ V = 2149.32 \ (8) \ \text{\AA}^{3}\\ Z = 4 \end{array}$

F(000) = 968 $D_x = 1.486 \text{ Mg m}^{-3}$ Cu K\alpha radiation, $\lambda = 1.5418 \text{ Å}$ Cell parameters from 6465 reflections $\theta = 3.0-71.4^{\circ}$ $\mu = 11.75 \text{ mm}^{-1}$ T = 173 KChunk, colorless $0.34 \times 0.22 \times 0.16 \text{ mm}$ Data collection

Oxford Diffraction Xcalibur Eos Gemini diffractometer Radiation source: Enhance (Cu) X-ray Source Graphite monochromator Detector resolution: 16.15 pixels mm ⁻¹ ω scans Absorption correction: multi-scan (<i>CrysAlis PRO</i> and <i>CrysAlis RED</i> ; Oxford Diffraction, 2010)	$T_{\min} = 0.328, T_{\max} = 1.000$ 13300 measured reflections 4143 independent reflections 3739 reflections with $I > 2\sigma(I)$ $R_{int} = 0.054$ $\theta_{\max} = 71.6^{\circ}, \theta_{\min} = 4.1^{\circ}$ $h = -11 \rightarrow 11$ $k = 0 \rightarrow 19$ $l = 0 \rightarrow 17$
Refinement	
Refinement on F^2 Least-squares matrix: full $R[F^2 > 2\sigma(F^2)] = 0.030$ $wR(F^2) = 0.083$ S = 1.06 4143 reflections 229 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 $w = 1/[\sigma^2(F_o^2) + (0.0407P)^2 + 0.8952P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{max} = 0.002$ $\Delta\rho_{max} = 0.53 \text{ e } \text{Å}^{-3}$ $\Delta\rho_{min} = -0.53 \text{ e } \text{Å}^{-3}$

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2 , conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	У	Ζ	$U_{ m iso}$ */ $U_{ m eq}$	
Sn1	0.25216 (2)	0.438102 (12)	0.741033 (13)	0.01599 (8)	
C11	0.34357 (9)	0.51960 (5)	0.59185 (5)	0.02688 (18)	
Cl2	0.18198 (9)	0.34254 (5)	0.87027 (5)	0.02576 (18)	
N1	0.3823 (3)	0.37067 (17)	0.38252 (19)	0.0258 (6)	
H1	0.4476	0.4132	0.3918	0.031*	
C1	0.1366 (3)	0.5479 (2)	0.7884 (2)	0.0208 (7)	
C2	0.1101 (4)	0.6179 (2)	0.7323 (2)	0.0288 (8)	
H2	0.1510	0.6199	0.6738	0.035*	
C3	0.0234 (4)	0.6853 (2)	0.7619 (3)	0.0358 (9)	
Н3	0.0051	0.7324	0.7231	0.043*	
C4	-0.0352 (5)	0.6838 (2)	0.8462 (3)	0.0402 (10)	
H4	-0.0947	0.7294	0.8654	0.048*	
C5	-0.0079 (5)	0.6165 (3)	0.9030 (3)	0.0481 (12)	
Н5	-0.0469	0.6159	0.9620	0.058*	
C6	0.0780 (5)	0.5481 (2)	0.8737 (3)	0.0369 (9)	
H6	0.0960	0.5014	0.9132	0.044*	

C7	0.1311 (3)	0.36151 (19)	0.64762 (19)	0.0174 (6)
C8	0.0298 (4)	0.4005 (2)	0.5905 (2)	0.0276 (7)
H8	0.0208	0.4608	0.5908	0.033*
C9	-0.0578 (4)	0.3526 (3)	0.5332 (2)	0.0404 (10)
H9	-0.1287	0.3799	0.4962	0.048*
C10	-0.0417 (5)	0.2640 (3)	0.5299 (3)	0.0459 (11)
H10	-0.0998	0.2309	0.4897	0.055*
C11	0.0582 (5)	0.2257 (3)	0.5850 (3)	0.0434 (10)
H11	0.0697	0.1655	0.5827	0.052*
C12	0.1433 (4)	0.2732 (2)	0.6441 (2)	0.0287 (8)
H12	0.2108	0.2451	0.6828	0.034*
C13	0.4751 (3)	0.42610 (19)	0.7796 (2)	0.0203 (7)
C14	0.5815 (4)	0.4029 (2)	0.7194 (3)	0.0314 (8)
H14	0.5568	0.3940	0.6575	0.038*
C15	0.7231 (4)	0.3926 (3)	0.7486 (3)	0.0469 (11)
H15	0.7940	0.3747	0.7070	0.056*
C16	0.7619 (5)	0.4079 (3)	0.8363 (4)	0.0518 (12)
H16	0.8597	0.4017	0.8553	0.062*
C17	0.6597 (5)	0.4321 (3)	0.8969 (4)	0.0592 (14)
H17	0.6867	0.4428	0.9582	0.071*
C18	0.5153 (4)	0.4413 (3)	0.8688 (3)	0.0416 (10)
H18	0.4446	0.4581	0.9111	0.050*
C19	0.4022 (6)	0.3087 (3)	0.4570 (3)	0.0486 (12)
H19A	0.3296	0.2635	0.4512	0.073*
H19B	0.3913	0.3378	0.5151	0.073*
H19C	0.4989	0.2837	0.4540	0.073*
C20	0.4135 (6)	0.3326 (3)	0.2933 (3)	0.0504 (11)
H20A	0.5078	0.3043	0.2960	0.076*
H20B	0.4149	0.3776	0.2473	0.076*
H20C	0.3386	0.2908	0.2775	0.076*
C21	0.2380 (4)	0.4099 (3)	0.3837 (3)	0.0465 (11)
H21A	0.1643	0.3652	0.3835	0.070*
H21B	0.2248	0.4460	0.3301	0.070*
H21C	0.2290	0.4448	0.4383	0.070*

Atomic displacement parameters (\mathring{A}^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.01316 (13)	0.01873 (12)	0.01599 (12)	-0.00260 (7)	-0.00193 (8)	-0.00006 (7)
C11	0.0250 (4)	0.0310 (4)	0.0247 (4)	-0.0069(3)	0.0019 (3)	0.0076 (3)
Cl2	0.0272 (4)	0.0299 (4)	0.0201 (4)	-0.0032 (3)	-0.0008(3)	0.0082 (3)
N1	0.0266 (16)	0.0215 (13)	0.0292 (15)	-0.0046 (12)	0.0047 (12)	-0.0017 (11)
C1	0.0162 (16)	0.0226 (15)	0.0236 (17)	-0.0008 (12)	-0.0050 (13)	-0.0098 (12)
C2	0.033 (2)	0.0266 (17)	0.0270 (18)	0.0065 (15)	-0.0098 (15)	-0.0050 (14)
C3	0.039 (2)	0.0297 (19)	0.038 (2)	0.0097 (16)	-0.0127 (18)	-0.0103 (15)
C4	0.038 (2)	0.0291 (19)	0.054 (3)	0.0014 (16)	0.005 (2)	-0.0202 (17)
C5	0.062 (3)	0.038 (2)	0.045 (2)	-0.007(2)	0.030 (2)	-0.0145 (18)
C6	0.056 (3)	0.0246 (17)	0.031 (2)	-0.0022 (17)	0.0143 (18)	-0.0039 (15)

supporting information

C7	0.0150 (15)	0.0246 (15)	0.0127 (14)	-0.0037 (12)	0.0012 (11)	-0.0020 (11)
C8	0.0255 (19)	0.0328 (18)	0.0243 (17)	-0.0009 (14)	-0.0011 (14)	0.0038 (14)
C9	0.027 (2)	0.069 (3)	0.0252 (19)	-0.0121 (19)	-0.0130 (15)	0.0065 (18)
C10	0.048 (3)	0.062 (3)	0.027 (2)	-0.030 (2)	-0.0060 (18)	-0.0113 (19)
C11	0.062 (3)	0.034 (2)	0.035 (2)	-0.018 (2)	-0.001 (2)	-0.0107 (17)
C12	0.033 (2)	0.0268 (17)	0.0266 (18)	0.0011 (15)	-0.0024 (15)	-0.0019 (14)
C13	0.0119 (15)	0.0214 (15)	0.0276 (18)	-0.0009 (12)	-0.0016 (13)	0.0015 (12)
C14	0.0238 (19)	0.0297 (18)	0.041 (2)	0.0000 (14)	0.0016 (16)	0.0007 (15)
C15	0.020 (2)	0.047 (3)	0.073 (3)	0.0009 (18)	0.009 (2)	0.016 (2)
C16	0.019 (2)	0.057 (3)	0.078 (4)	-0.0007 (19)	-0.014 (2)	0.020 (3)
C17	0.038 (3)	0.089 (4)	0.049 (3)	-0.009 (2)	-0.028 (2)	0.006 (2)
C18	0.024 (2)	0.065 (3)	0.036 (2)	-0.0048 (18)	-0.0083 (17)	-0.0027 (18)
C19	0.075 (4)	0.033 (2)	0.037 (2)	0.008 (2)	0.007 (2)	0.0056 (17)
C20	0.061 (3)	0.058 (3)	0.032 (2)	0.009 (2)	0.013 (2)	-0.004 (2)
C21	0.030 (2)	0.055 (3)	0.054 (3)	0.004 (2)	-0.0066 (19)	-0.016 (2)

Geometric parameters (Å, °)

Sn1—C7	2.135 (3)	C10-C11	1.363 (6)
Sn1—C13	2.142 (3)	C10—H10	0.9500
Sn1—C1	2.151 (3)	C11—C12	1.385 (5)
Sn1—Cl2	2.5227 (7)	C11—H11	0.9500
Sn1—Cl1	2.6983 (8)	C12—H12	0.9500
N1—C21	1.472 (5)	C13—C18	1.385 (5)
N1—C19	1.478 (5)	C13—C14	1.388 (5)
N1—C20	1.481 (5)	C14—C15	1.384 (5)
N1—H1	0.9099	C14—H14	0.9500
C1—C6	1.381 (5)	C15—C16	1.361 (7)
C1—C2	1.396 (5)	C15—H15	0.9500
C2—C3	1.403 (5)	C16—C17	1.369 (7)
С2—Н2	0.9500	C16—H16	0.9500
C3—C4	1.368 (6)	C17—C18	1.403 (6)
С3—Н3	0.9500	С17—Н17	0.9500
C4—C5	1.370 (6)	C18—H18	0.9500
C4—H4	0.9500	С19—Н19А	0.9800
C5—C6	1.409 (5)	C19—H19B	0.9800
С5—Н5	0.9500	С19—Н19С	0.9800
С6—Н6	0.9500	C20—H20A	0.9800
C7—C12	1.391 (5)	C20—H20B	0.9800
C7—C8	1.394 (4)	C20—H20C	0.9800
C8—C9	1.385 (5)	C21—H21A	0.9800
С8—Н8	0.9500	C21—H21B	0.9800
C9—C10	1.399 (6)	C21—H21C	0.9800
С9—Н9	0.9500		
C7—Sn1—C13	128.08 (12)	С11—С10—Н10	120.3
C7—Sn1—C1	113.70 (12)	С9—С10—Н10	120.3
C13—Sn1—C1	117.83 (12)	C10-C11-C12	120.9 (4)

C7—Sn1—Cl2	90.95 (8)	C10-C11-H11	119.6
C13—Sn1—Cl2	90.30 (9)	C12—C11—H11	119.6
C1—Sn1—Cl2	95.35 (10)	C11—C12—C7	120.9 (3)
C7—Sn1—Cl1	84.62 (8)	C11—C12—H12	119.5
C13—Sn1—Cl1	86.86 (9)	C7—C12—H12	119.5
C1— $Sn1$ — $C11$	92.95 (10)	C18 - C13 - C14	118.3 (3)
Cl2— $Sn1$ — $Cl1$	171.62.(3)	$C_{18} - C_{13} - S_{n1}$	118.8(3)
C_{21} N1-C19	1116(3)	C14— $C13$ — $Sn1$	122.9(3)
C_{21} N_{1} C_{20}	111.0(3) 111.7(3)	C_{15} C_{14} C_{13}	122.9(3) 120.6(4)
C19 - N1 - C20	1120(3)	C_{15} C_{14} H_{14}	119.7
C21_N1_H1	107.0	C_{13} C_{14} H_{14}	119.7
C19 N1 H1	107.2	C16-C15-C14	120.7 (4)
C_{20} N1 H1	107.0	$C_{10} = C_{15} = C_{14}$	110.6
C_{20} C_{1} C_{2}	107.0 118.2 (3)	$C_{10} = C_{15} = H_{15}$	119.0
$C_0 = C_1 = C_2$	110.2(3)	$C_{14} = C_{15} = 1115$	119.0
$C_0 = C_1 = S_{n1}$	120.3(3) 121.2(3)	C15 - C16 - U17	119.9 (4)
$C_2 = C_1 = S_{111}$	121.3(3)	C15—C10—H10	120.0
C1 = C2 = C3	120.2 (4)	C1/-C10-H10	120.0
C1 - C2 - H2	119.9	C16 - C17 - C18	120.0 (5)
$C_3 = C_2 = H_2$	119.9	C10-C17-H17	120.0
C4 - C3 - C2	120.7 (4)	C18 - C17 - H17	120.0
C4 - C3 - H3	119.7		120.4 (4)
C2—C3—H3	119.7	C13-C18-H18	119.8
$C_3 = C_4 = C_5$	120.0 (4)	C1/C18H18	119.8
C3—C4—H4	120.0	NI	109.5
C5—C4—H4	120.0	NI—CI9—HI9B	109.5
C4—C5—C6	119.8 (4)	Н19А—С19—Н19В	109.5
C4—C5—H5	120.1	N1—C19—H19C	109.5
С6—С5—Н5	120.1	H19A—C19—H19C	109.5
C1—C6—C5	121.0 (4)	H19B—C19—H19C	109.5
C1—C6—H6	119.5	N1—C20—H20A	109.5
С5—С6—Н6	119.5	N1—C20—H20B	109.5
C12—C7—C8	117.9 (3)	H20A—C20—H20B	109.5
C12—C7—Sn1	122.9 (2)	N1—C20—H20C	109.5
C8—C7—Sn1	119.1 (2)	H20A—C20—H20C	109.5
C9—C8—C7	121.0 (3)	H20B—C20—H20C	109.5
С9—С8—Н8	119.5	N1—C21—H21A	109.5
С7—С8—Н8	119.5	N1—C21—H21B	109.5
C8—C9—C10	119.9 (4)	H21A—C21—H21B	109.5
С8—С9—Н9	120.1	N1—C21—H21C	109.5
С10—С9—Н9	120.1	H21A—C21—H21C	109.5
C11—C10—C9	119.3 (3)	H21B—C21—H21C	109.5
C7—Sn1—C1—C6	103.1 (3)	C12—C7—C8—C9	1.2 (5)
C13—Sn1—C1—C6	-83.4 (3)	Sn1—C7—C8—C9	-175.6(3)
Cl2— $Sn1$ — $C1$ — $C6$	9.7 (3)	C7—C8—C9—C10	-2.3 (6)
Cl1—Sn1—C1—C6	-171.4 (3)	C8-C9-C10-C11	1.5 (6)
C7-Sn1-C1-C2	-72.4 (3)	C9-C10-C11-C12	0.3 (7)
C13—Sn1—C1—C2	101.0 (3)	C10-C11-C12-C7	-1.3(6)

	1(5.0.(2))	G0 G7 G10 G11	
Cl2— $Sn1$ — Cl — $C2$	-165.8 (3)	C8—C7—C12—C11	0.6 (5)
Cl1— $Sn1$ — $C1$ — $C2$	13.0 (3)	Sn1—C7—C12—C11	177.3 (3)
C6—C1—C2—C3	-1.5 (5)	C7—Sn1—C13—C18	-142.3 (3)
Sn1—C1—C2—C3	174.2 (3)	C1—Sn1—C13—C18	45.3 (3)
C1—C2—C3—C4	0.7 (6)	Cl2—Sn1—C13—C18	-50.9 (3)
C2-C3-C4-C5	0.7 (6)	Cl1—Sn1—C13—C18	137.0 (3)
C3—C4—C5—C6	-1.3 (7)	C7—Sn1—C13—C14	37.0 (3)
C2-C1-C6-C5	0.9 (6)	C1—Sn1—C13—C14	-135.3 (3)
Sn1—C1—C6—C5	-174.8 (3)	Cl2—Sn1—C13—C14	128.5 (3)
C4—C5—C6—C1	0.4 (7)	Cl1—Sn1—C13—C14	-43.6 (3)
C13—Sn1—C7—C12	42.1 (3)	C18—C13—C14—C15	2.1 (5)
C1—Sn1—C7—C12	-145.3 (3)	Sn1—C13—C14—C15	-177.3 (3)
Cl2—Sn1—C7—C12	-49.0 (3)	C13—C14—C15—C16	-2.3 (6)
Cl1—Sn1—C7—C12	123.8 (3)	C14-C15-C16-C17	1.2 (7)
C13—Sn1—C7—C8	-141.3 (2)	C15—C16—C17—C18	0.0 (8)
C1—Sn1—C7—C8	31.3 (3)	C14—C13—C18—C17	-0.9 (6)
Cl2—Sn1—C7—C8	127.6 (2)	Sn1—C13—C18—C17	178.5 (3)
Cl1—Sn1—C7—C8	-59.6 (2)	C16—C17—C18—C13	-0.1 (7)

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D····A	D—H···A
N1—H1···Cl1 ⁱ	0.91	2.21	3.087 (3)	161

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