Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tetrakis(4-chloroanilinium) hexachloridostannate(IV) dichloride

Benhua Zhou* and Hongxia Liu

School of Chemical and Biological Engineering, Yancheng Institute of Technology, Yancheng 224051, People's Republic of China
Correspondence e-mail: rongtao198806@163.com

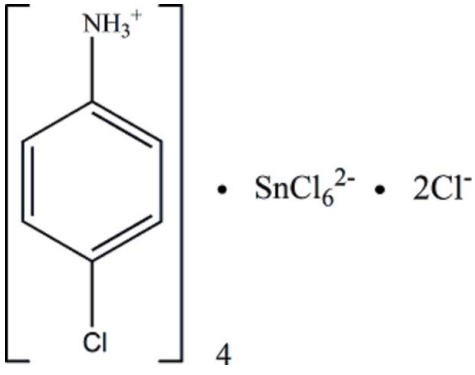
Received 23 April 2012; accepted 13 May 2012

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.030; wR factor = 0.067; data-to-parameter ratio = 21.9.

The asymmetric unit of the title compound, $(C_6H_7ClN)_4[SnCl_6]Cl_2$, comprises two 4-chloroanilinium cations, half of an $[SnCl_6]^{2-}$ anion and a Cl^- anion. The Sn^{IV} atom, located on a special position on a twofold rotation axis, exhibits an octahedral environment. In the crystal, molecules are linked by N—H···Cl hydrogen bonds between the 4-chloroanilinium cations, $[SnCl_6]^{2-}$ anions and Cl^- anions.

Related literature

For general background to ferroelectric metal-organic frameworks, see: Ye *et al.* (2009); Fu *et al.* (2007). For phase transitions in ferroelectric materials, see: Zhang *et al.* (2008); Zhao *et al.* (2008); Ye *et al.* (2006).



Experimental

Crystal data

$(C_6H_7ClN)_4[SnCl_6]Cl_2$
M_r = 916.59
Monoclinic, $C2/c$
a = 27.855 (6) Å
b = 7.2061 (14) Å
c = 21.895 (4) Å
β = 125.03 (3)°
V = 3598.8 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.63 mm^{-1}
T = 293 K
0.20 × 0.20 × 0.20 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.715, T_{max} = 0.730
17870 measured reflections
4122 independent reflections
3581 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.067
S = 1.10
4122 reflections
188 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cl3—Sn1	2.4205 (11)	Cl5—Sn1	2.4356 (7)
Cl4—Sn1	2.4076 (7)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···Cl5^{i}	0.89	2.64	3.522 (2)	172
N1—H1A···Cl3^{i}	0.89	2.98	3.424 (2)	112
N1—H1B···Cl6^{ii}	0.89	2.25	3.123 (3)	165
N1—H1C···Cl6^{iii}	0.89	2.26	3.120 (3)	162
N2—H2A···Cl3^{iv}	0.89	2.75	3.455 (2)	137
N2—H2A···Cl4^{v}	0.89	2.79	3.567 (2)	147
N2—H2A···Cl4^{iv}	0.89	2.92	3.344 (3)	111
N2—H2B···Cl6^{vi}	0.89	2.20	3.085 (3)	175
N2—H2C···Cl5^{vii}	0.89	2.61	3.424 (3)	153

Symmetry codes: (i) $x-1, y, z$; (ii) $x, y-1, z$; (iii) $-x, -y+1, -z$; (iv) $x-\frac{1}{2}, y+\frac{1}{2}, z$; (v) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (vi) $x+\frac{1}{2}, y-\frac{1}{2}, z$; (vii) $x-\frac{1}{2}, y-\frac{1}{2}, z$.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *SHELXL97*.

The authors are grateful to the starter fund of Southeast University, Nanjing, People's Republic of China.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2409).

References

Brandenburg, K. & Putz, H. (2005). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Fu, D.-W., Song, Y.-M., Wang, G.-X., Ye, Q., Xiong, R.-G., Akutagawa, T., Nakamura, T., Chan, P. W. H. & Huang, S. D. (2007). *J. Am. Chem. Soc.* **129**, 5346–5347.
Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Ye, H.-Y., Fu, D.-W., Zhang, Y., Zhang, W., Xiong, R.-G. & Huang, S. D. (2009). *J. Am. Chem. Soc.* **131**, 42–43.
Ye, Q., Song, Y.-M., Wang, G.-X., Fu, D.-W. & Xiong, R.-G. (2006). *J. Am. Chem. Soc.* **128**, 6554–6555.
Zhang, W., Xiong, R.-G. & Huang, S.-P. D. (2008). *J. Am. Chem. Soc.* **130**, 10468–10469.
Zhao, H., Qu, Z.-R., Ye, H.-Y. & Xiong, R.-G. (2008). *Chem. Soc. Rev.* **37**, 84–100.

supporting information

Acta Cryst. (2012). E**68**, m782 [doi:10.1107/S1600536812021666]

Tetrakis(4-chloroanilinium) hexachloridostannate(IV) dichloride

Benhua Zhou and Hongxia Liu

S1. Comment

The study of ferroelectric materials has received much attention; some of them have predominantly dielectric–ferroelectric performance (Ye *et al.*, 2006; Fu *et al.*, 2007; Zhao *et al.* 2008; Zhang *et al.*, 2008; Ye *et al.*, 2009). As a part of our work to obtain potential ferroelectric phase-transition material, we report herein on the crystal structure of title compound. Unluckily, the title compound has no dielectric anomalies in the temperature range 93–453 K, suggesting that it might be only a paraelectric.

The asymmetric unit of the title compound is shown in Fig. 1 and Sn-Cl bonds are listed in Table 1. The crystal packing (Fig. 2) is stabilised by intermolecular N—H···Cl hydrogen bonds between the $[C_6H_7ClN]^+$cations and $SnCl_6^{2-}$anions and Cl^- anions (Table 2).

S2. Experimental

For the preparation of the title compound, the water solution of the hydrochloric acid (10 mmol) was added to the ethanol solution of the 4-chlorobenzenamine(10 mmol), then the water solution of the $SnCl_4$(5 mmol) was added into a reaction mixture. The resulting precipitate was filtered. Colourless crystals suitable for X-ray analysis were formed after several weeks by slow evaporation of the solvent at room temperature.

S3. Refinement

Positional parameters of all the H atoms bonded to C atoms were calculated geometrically and were allowed to ride on the C atoms to which they are bonded, with U_{iso}(H) = 1.2Ueq(C) and U_{iso}(H) = 1.5Ueq(C) for the methyl group. The other H bonded to N atoms were calculated geometrically and were allowed to ride on the N atoms with U_{iso}(H) = 1.5Ueq(O).

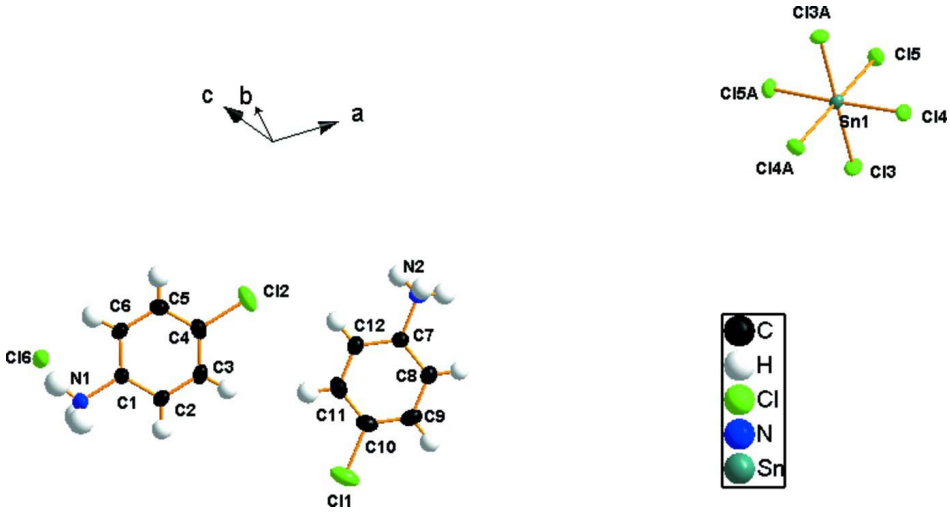


Figure 1

The molecular structure of the title compound with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.[The suffix A denotes the symmetry code: 2-*x* *y* 1/2 - *z*.]

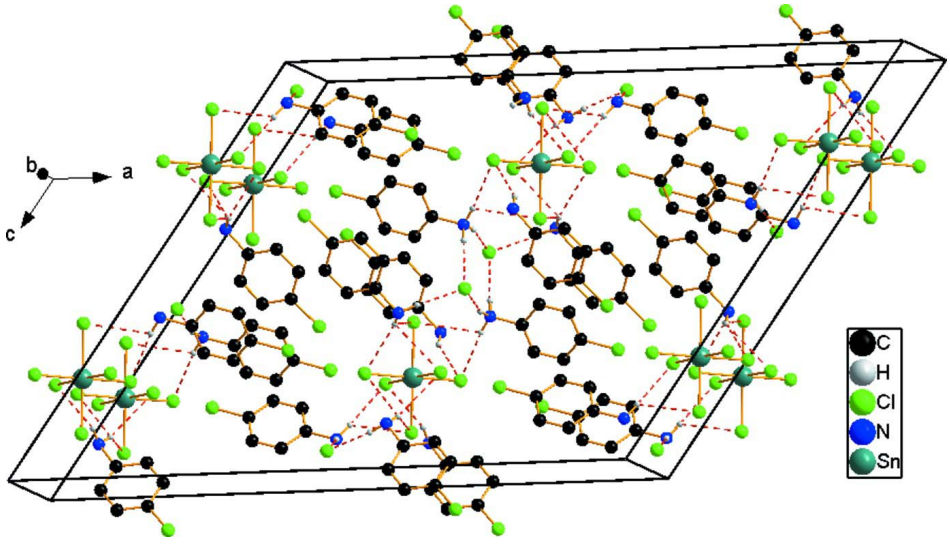


Figure 2

Crystal packing of the title compound. Dashed lines indicate hydrogen bonds.

Tetrakis(4-chloroanilinium) hexachloridostannate(IV) dichloride

Crystal data

$(C_6H_7ClN)_4[SnCl_6]Cl_2$
$M_r = 916.59$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 27.855$ (6) Å
$b = 7.2061$ (14) Å
$c = 21.895$ (4) Å
$\beta = 125.03$ (3)°
$V = 3598.8$ (18) Å^3
$Z = 4$
$F(000) = 1816$
$D_x = 1.692$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4122 reflections
$\theta = 3.4$–27.5°
$\mu = 1.63$ mm^{-1}
$T = 293$ K
Prism, colourless
0.20 × 0.20 × 0.20 mm

Data collection

Rigaku SCXmini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
CCD_Profile_fitting scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.715, T_{max} = 0.730
17870 measured reflections
4122 independent reflections
3581 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 27.5°, θ_{min} = 3.4°
h = −36→35
k = −9→9
l = −28→28

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.067
S = 1.10
4122 reflections
188 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
$w = 1/[\sigma^2(F_o^2) + (0.0236P)^2 + 4.0429P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e 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	y	z	U_{iso}*/U_{eq}
C1	0.12061 (12)	0.1500 (4)	0.12876 (15)	0.0503 (6)
C2	0.13487 (13)	0.0639 (4)	0.08532 (16)	0.0540 (7)
H2	0.1066	−0.0001	0.0425	0.065*
C3	0.19188 (13)	0.0738 (4)	0.10633 (16)	0.0535 (7)
H3	0.2025	0.0155	0.0779	0.064*
C4	0.23257 (12)	0.1696 (4)	0.16906 (17)	0.0507 (7)
C5	0.21803 (13)	0.2551 (5)	0.21162 (17)	0.0632 (8)
H5	0.2463	0.3194	0.2544	0.076*
C6	0.16093 (14)	0.2459 (5)	0.19102 (17)	0.0661 (9)
H6	0.1503	0.3047	0.2195	0.079*
C7	0.39010 (11)	0.0792 (3)	0.05568 (13)	0.0401 (5)
C8	0.38139 (12)	−0.0100 (3)	−0.00526 (14)	0.0470 (6)
H8	0.4121	−0.0253	−0.0103	0.056*
C9	0.32612 (14)	−0.0767 (4)	−0.05904 (15)	0.0556 (7)
H9	0.3192	−0.1366	−0.1010	0.067*
C10	0.28179 (12)	−0.0544 (4)	−0.05054 (16)	0.0554 (7)

C11	0.29063 (13)	0.0384 (5)	0.00988 (18)	0.0634 (8)
H11	0.2597	0.0554	0.0144	0.076*
C12	0.34538 (13)	0.1062 (4)	0.06368 (16)	0.0559 (7)
H12	0.3519	0.1694	0.1049	0.067*
Cl1	0.21316 (4)	−0.14614 (15)	−0.11590 (6)	0.0983 (3)
Cl2	0.30443 (4)	0.17986 (14)	0.19641 (6)	0.0843 (3)
Cl3	0.94108 (3)	0.11974 (9)	0.11503 (3)	0.04947 (16)
Cl4	1.06231 (3)	−0.11341 (9)	0.25190 (4)	0.04712 (15)
Cl5	1.06027 (3)	0.36499 (8)	0.24919 (4)	0.04846 (15)
Cl6	0.02508 (4)	0.72478 (14)	0.05762 (5)	0.0808 (3)
N1	0.05994 (11)	0.1377 (4)	0.10653 (15)	0.0707 (8)
H1A	0.0577	0.1853	0.1423	0.106*
H1B	0.0488	0.0193	0.0993	0.106*
H1C	0.0365	0.2010	0.0645	0.106*
N2	0.44908 (10)	0.1413 (3)	0.11539 (12)	0.0525 (5)
H2A	0.4466	0.2420	0.1370	0.079*
H2B	0.4692	0.1682	0.0964	0.079*
H2C	0.4674	0.0515	0.1492	0.079*
Sn1	1.0000	0.12149 (3)	0.2500	0.03220 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0478 (15)	0.0652 (17)	0.0503 (15)	−0.0127 (13)	0.0353 (13)	−0.0134 (13)
C2	0.0628 (18)	0.0596 (17)	0.0540 (16)	−0.0140 (14)	0.0419 (15)	−0.0158 (13)
C3	0.0664 (18)	0.0497 (15)	0.0680 (18)	−0.0019 (13)	0.0524 (17)	−0.0038 (13)
C4	0.0492 (15)	0.0470 (15)	0.0678 (18)	0.0016 (12)	0.0405 (15)	0.0108 (13)
C5	0.0535 (17)	0.075 (2)	0.0566 (17)	−0.0164 (15)	0.0292 (15)	−0.0175 (15)
C6	0.0631 (19)	0.086 (2)	0.0632 (19)	−0.0188 (17)	0.0446 (17)	−0.0322 (17)
C7	0.0448 (13)	0.0332 (12)	0.0393 (12)	0.0021 (10)	0.0223 (11)	0.0041 (9)
C8	0.0551 (16)	0.0395 (13)	0.0508 (15)	0.0061 (11)	0.0329 (13)	0.0027 (11)
C9	0.072 (2)	0.0416 (14)	0.0429 (14)	−0.0030 (13)	0.0270 (15)	−0.0031 (11)
C10	0.0507 (16)	0.0471 (15)	0.0483 (15)	−0.0062 (12)	0.0167 (13)	0.0083 (12)
C11	0.0526 (17)	0.074 (2)	0.071 (2)	0.0020 (15)	0.0404 (17)	0.0082 (17)
C12	0.0602 (18)	0.0636 (18)	0.0546 (16)	0.0014 (14)	0.0392 (15)	−0.0034 (14)
Cl1	0.0635 (5)	0.0962 (7)	0.0859 (7)	−0.0256 (5)	0.0140 (5)	0.0026 (5)
Cl2	0.0541 (5)	0.0922 (6)	0.1164 (8)	0.0013 (4)	0.0548 (5)	0.0153 (6)
Cl3	0.0565 (4)	0.0537 (4)	0.0338 (3)	0.0105 (3)	0.0233 (3)	0.0055 (3)
Cl4	0.0442 (3)	0.0433 (3)	0.0505 (3)	0.0109 (3)	0.0252 (3)	−0.0019 (3)
Cl5	0.0575 (4)	0.0401 (3)	0.0623 (4)	−0.0089 (3)	0.0428 (3)	−0.0001 (3)
Cl6	0.0672 (5)	0.1076 (7)	0.0878 (6)	−0.0289 (5)	0.0563 (5)	−0.0438 (5)
N1	0.0547 (15)	0.110 (2)	0.0647 (16)	−0.0254 (14)	0.0443 (14)	−0.0329 (15)
N2	0.0499 (13)	0.0521 (13)	0.0477 (12)	0.0004 (10)	0.0234 (11)	−0.0010 (10)
Sn1	0.04091 (13)	0.02673 (11)	0.03437 (12)	0.000	0.02476 (10)	0.000

Geometric parameters (Å, º)

C1—C6	1.356 (4)	C9—H9	0.9300
C1—C2	1.372 (4)	C10—C11	1.373 (4)
C1—N1	1.468 (3)	C10—Cl1	1.732 (3)
C2—C3	1.378 (4)	C11—C12	1.374 (4)
C2—H2	0.9300	C11—H11	0.9300
C3—C4	1.364 (4)	C12—H12	0.9300
C3—H3	0.9300	Cl3—Sn1	2.4205 (11)
C4—C5	1.359 (4)	Cl4—Sn1	2.4076 (7)
C4—Cl2	1.731 (3)	Cl5—Sn1	2.4356 (7)
C5—C6	1.383 (4)	N1—H1A	0.8900
C5—H5	0.9300	N1—H1B	0.8900
C6—H6	0.9300	N1—H1C	0.8900
C7—C12	1.368 (4)	N2—H2A	0.8900
C7—C8	1.371 (3)	N2—H2B	0.8900
C7—N2	1.464 (3)	N2—H2C	0.8900
C8—C9	1.381 (4)	Sn1—Cl4^{i}	2.4076 (7)
C8—H8	0.9300	Sn1—Cl3^{i}	2.4205 (11)
C9—C10	1.360 (4)	Sn1—Cl5^{i}	2.4356 (7)
C6—C1—C2	121.7 (3)	C12—C11—H11	120.1
C6—C1—N1	119.7 (2)	C7—C12—C11	118.9 (3)
C2—C1—N1	118.6 (2)	C7—C12—H12	120.5
C1—C2—C3	118.8 (3)	C11—C12—H12	120.5
C1—C2—H2	120.6	C1—N1—H1A	109.5
C3—C2—H2	120.6	C1—N1—H1B	109.5
C4—C3—C2	119.6 (3)	H1A—N1—H1B	109.5
C4—C3—H3	120.2	C1—N1—H1C	109.5
C2—C3—H3	120.2	H1A—N1—H1C	109.5
C5—C4—C3	121.2 (3)	H1B—N1—H1C	109.5
C5—C4—Cl2	119.0 (2)	C7—N2—H2A	109.5
C3—C4—Cl2	119.9 (2)	C7—N2—H2B	109.5
C4—C5—C6	119.6 (3)	H2A—N2—H2B	109.5
C4—C5—H5	120.2	C7—N2—H2C	109.5
C6—C5—H5	120.2	H2A—N2—H2C	109.5
C1—C6—C5	119.1 (3)	H2B—N2—H2C	109.5
C1—C6—H6	120.5	Cl4^{i}—Sn1—Cl4	90.65 (4)
C5—C6—H6	120.5	Cl4^{i}—Sn1—Cl3	89.91 (3)
C12—C7—C8	121.7 (2)	Cl4—Sn1—Cl3	89.67 (3)
C12—C7—N2	118.7 (2)	Cl4^{i}—Sn1—Cl3^{i}	89.67 (3)
C8—C7—N2	119.6 (2)	Cl4—Sn1—Cl3^{i}	89.91 (3)
C7—C8—C9	118.7 (3)	Cl3—Sn1—Cl3^{i}	179.40 (3)
C7—C8—H8	120.6	Cl4^{i}—Sn1—Cl5	178.18 (2)
C9—C8—H8	120.6	Cl4—Sn1—Cl5	90.77 (3)
C10—C9—C8	119.9 (3)	Cl3—Sn1—Cl5	88.97 (3)
C10—C9—H9	120.1	Cl3^{i}—Sn1—Cl5	91.46 (3)
C8—C9—H9	120.1	Cl4^{i}—Sn1—Cl5^{i}	90.77 (3)

C9—C10—C11	121.0 (3)	Cl4—Sn1—Cl5^{i}	178.18 (2)
C9—C10—Cl1	120.0 (2)	Cl3—Sn1—Cl5^{i}	91.46 (3)
C11—C10—Cl1	119.0 (3)	Cl3^{i}—Sn1—Cl5^{i}	88.97 (3)
C10—C11—C12	119.7 (3)	Cl5—Sn1—Cl5^{i}	87.82 (4)
C10—C11—H11	120.1		
C6—C1—C2—C3	0.8 (5)	C12—C7—C8—C9	−1.1 (4)
N1—C1—C2—C3	−179.5 (3)	N2—C7—C8—C9	176.5 (2)
C1—C2—C3—C4	−0.5 (4)	C7—C8—C9—C10	−0.5 (4)
C2—C3—C4—C5	0.3 (5)	C8—C9—C10—C11	1.9 (4)
C2—C3—C4—Cl2	179.1 (2)	C8—C9—C10—Cl1	−177.3 (2)
C3—C4—C5—C6	−0.3 (5)	C9—C10—C11—C12	−1.6 (5)
Cl2—C4—C5—C6	−179.1 (3)	Cl1—C10—C11—C12	177.6 (2)
C2—C1—C6—C5	−0.8 (5)	C8—C7—C12—C11	1.4 (4)
N1—C1—C6—C5	179.5 (3)	N2—C7—C12—C11	−176.2 (3)
C4—C5—C6—C1	0.5 (5)	C10—C11—C12—C7	0.0 (5)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···Cl5^{ii}	0.89	2.64	3.522 (2)	172
N1—H1*A*···Cl3^{ii}	0.89	2.98	3.424 (2)	112
N1—H1*B*···Cl6^{iii}	0.89	2.25	3.123 (3)	165
N1—H1*C*···Cl6^{iv}	0.89	2.26	3.120 (3)	162
N2—H2*A*···Cl3^{v}	0.89	2.75	3.455 (2)	137
N2—H2*A*···Cl4^{vi}	0.89	2.79	3.567 (2)	147
N2—H2*A*···Cl4^{v}	0.89	2.92	3.344 (3)	111
N2—H2*B*···Cl6^{vii}	0.89	2.20	3.085 (3)	175
N2—H2*C*···Cl5^{viii}	0.89	2.61	3.424 (3)	153

Symmetry codes: (ii) $x-1, y, z$; (iii) $x, y-1, z$; (iv) $-x, -y+1, -z$; (v) $x-1/2, y+1/2, z$; (vi) $-x+3/2, y+1/2, -z+1/2$; (vii) $x+1/2, y-1/2, z$; (viii) $x-1/2, y-1/2, z$.