



catena-Poly[bis(1,3-benzothiazol-3-ium) [[di-chloridoantimonate(III)]-di- μ -chlorido- μ -oxido-[chloridoantimonate(III)]- μ -chlorido]]

Oussama Chebout,^a Mhamed Boudraa,^a Sofiane Bouacida,^{a,b,*} Hocine Merazig^a and Chaouki Boudaren^a

Received 31 December 2015

Accepted 14 January 2016

Edited by P. C. Healy, Griffith University, Australia

Keywords: crystal structure; organic–inorganic hybrid compound; antimony; hydrogen bonding; π – π stacking

CCDC reference: 1447413

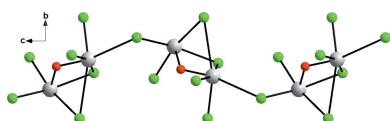
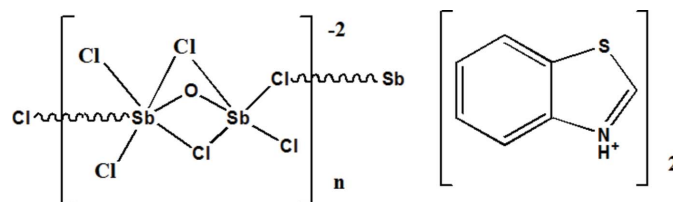
Supporting information: this article has supporting information at journals.iucr.org/e

^aUnité de Recherche de Chimie de l'Environnement et Moléculaire Structurale, CHEMS, Université Frères Montouri Constantine, 25000, Algeria, and ^bDépartement Sciences de la Matière, Faculté des Sciences Exactes et Sciences de la Nature et de la Vie, Université Oum El Bouaghi, Algeria. *Correspondence e-mail: Bouacida_Sofiane@yahoo.fr

The title compound, $\{(C_7H_6NS)_2[Sb_2Cl_6O]\}_n$, contains two benzothiazolidium cations and one tri- μ -chlorido-trichlorido- μ -oxido-diantimonate(III) anion. The structure of the inorganic cation may be described as being built up from two polyhedra, *i.e.* a square-pyramidal $SbCl_4O$ and a distorted octahedral $SbOCl_5$ unit, sharing a common face (comprising the O atom and two Cl atoms). The two benzothiazole cations are quasi-planar and subtend a dihedral angle of 19.93 (5)°. The crystal packing can be described by alternating (100) layers and [001] chains of the organic cations and inorganic anions connected through an extensive three-dimensional network of N–H...Cl, C–H...O and C–H...Cl hydrogen bonds. This is consolidated by slipped π – π stacking, with centroid-to-centroid distances between the benzothiazole rings of 3.7111 (18)–3.8452 (16) Å. These interactions link the molecules within the layers and also link the layers together and reinforce the cohesion of the ionic structure.

1. Chemical context

The coordination chemistry of antimony has both a practical and theoretical interest (Abboud *et al.*, 2007; Bujak & Angel, 2006). Recently, the use of antimony complexes in cancer chemotherapy has become a topic of interest (Demicheli *et al.*, 2006; Rais *et al.*, 2000). As part of our ongoing studies of benzothiazole-based coordination networks (Bouchareb *et al.*, 2014), we now report the polymeric structure of new organic–inorganic hybrid compound $\{(C_7H_6NS)_2[Sb_2Cl_6O]\}_n$, (I).



2. Structural commentary

The title compound contains two benzothiazolidium cations and one tri- μ -chlorido-trichlorido- μ -oxido-diantimonate(III) anion ($Sb_2Cl_6O^{2-}$). The molecular geometry and the atom-numbering scheme are shown in Fig. 1.

The structure of the inorganic anion may be described as two polyhedra, square-pyramidal $SbCl_4O$ and distorted octahedral $SbOCl_5$, sharing a common face (O1, Cl5 and Cl6). In

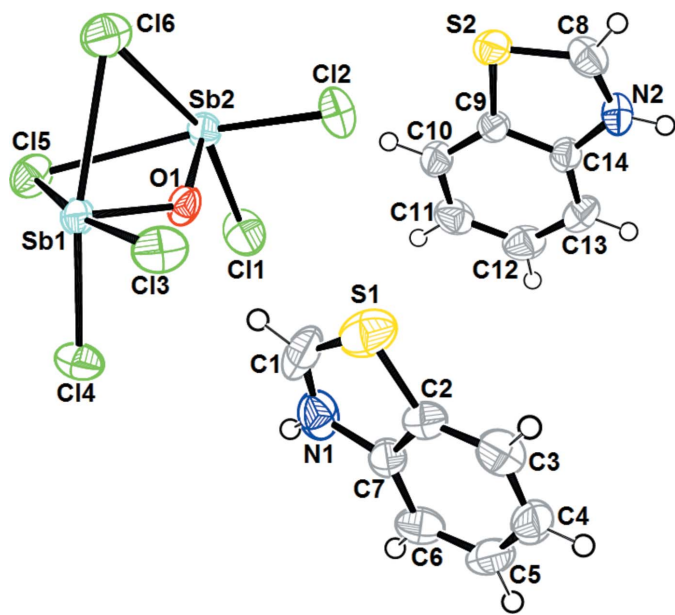


Figure 1
The asymmetric unit of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

the first polyhedron, four Cl atoms (Cl3–Cl4–Cl5–Cl6) form a basal plane with the Sb1 atom lying 0.3011 (2) Å below the plane. The apical position is occupied by the O1 atom. In the second polyhedron, the O1 atom occupies the apical position and four Cl atoms (Cl1–Cl2–Cl5–Cl6) form the base equatorial plane with Sb2 displaced by 0.4168 (1) Å from it. The geometry of the Sb2 atom can be described as distorted octahedral, a sixth coordination is observed at a longer distance, with Sb2 coordinated by the adjacent Cl3ⁱ atom at a distance of 3.546 (4) Å [symmetry code: (i) $\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$], forming an infinite chain parallel to [001] (Fig. 2). This distance is significantly shorter than the sum of the relevant van der Waals radii of 4.01 Å ($r_{\text{Sb}} = 2.1$ Å and $r_{\text{Cl}} = 1.91$ Å) and in good agreement with those found in [SbCl₃(C₂₅H₂₂O₂P₂)] (Razak *et al.*, 1999) and in [(CH₃)₂NH(CH₂)₂NH₃][SbCl₅] (Bujak & Angel, 2006). In this molecule, the angle between the two equatorial planes is 75.86 (2)°.

The Sb–O bridge distances of 1.9404 (16) and 1.9460 (17) Å are similar to those found in the Sb₂Cl₆O₂ moiety (Abboud *et al.*, 2007). Excluding the longest bond (Sb2–Cl3ⁱ), the terminal Sb–Cl bonds are in the range

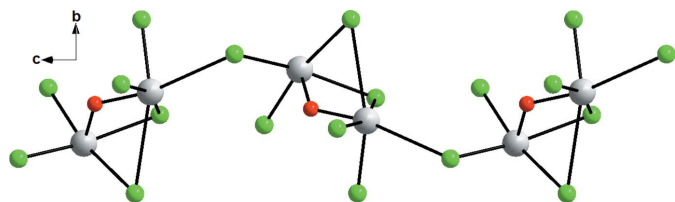


Figure 2
View of a polymeric chain of Sb₂Cl₆O along the *c* axis.

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>
N1–H1N···Cl6 ⁱ	0.86	2.37	3.200 (3)	162
N2–H2N···Cl6 ⁱⁱ	0.86	2.35	3.145 (3)	153
C1–H1···O1	0.93	2.27	3.152 (4)	159
C8–H8···Cl5 ⁱⁱⁱ	0.93	2.72	3.327 (3)	124
C10–H10···Cl3 ^{iv}	0.93	2.78	3.612 (3)	150
C13–H13···Cl2 ⁱⁱ	0.93	2.76	3.524 (3)	140

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

2.3974 (8)–2.4982 (8) Å and are shorter than the bridging bonds [2.7522 (8)–3.3244 (9) Å] and are in good agreement with those found in C₂₆H₂₈N₈O₆Sb₄Cl₁₀ (Abboud *et al.*, 2007). However, the Sb–O–Sb bond angle is 123.56 (9)° which is very different to that observed in Cs₂Sb₂O₂(OH)₈ (Mikhaylov *et al.*, 2011) and the Sb₂Cl₆O₂ moiety (Abboud *et al.*, 2007). The dihedral angle between the mean planes of the two benzothiazole cations is 19.93 (5)°.

3. Supramolecular features

The crystal packing can be described by alternating (100) layers and [001] chains of organic cations and inorganic anions connected through an extensive network of N–H···Cl, C–H···O and C–H···Cl hydrogen bonds, leading to the formation of a three-dimensional network (Table 1, Fig. 3). The packing is consolidated by slipped π – π stacking with centroid-to-centroid distances of 3.7111 (18)–3.8452 (16) Å between the benzothiazole rings. These interactions link the molecules within the layers and also link the layers together, reinforcing the cohesion of the ionic structure.

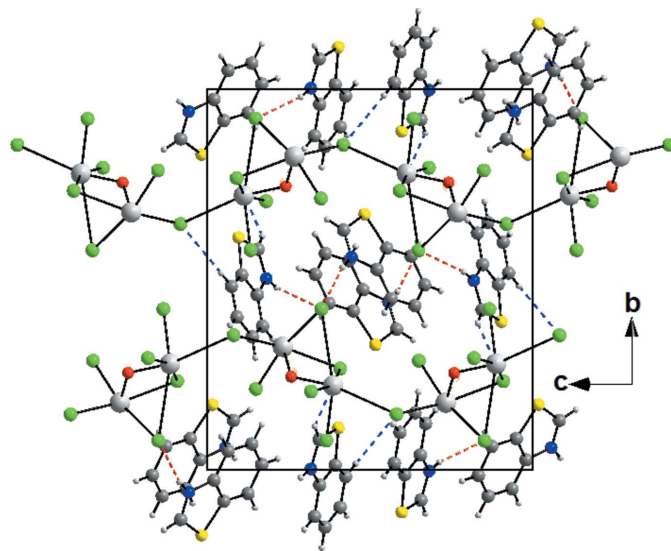


Figure 3
Part of diagram packing of the title compound, viewed along the *a* axis, showing alternating chains and layers connected by N–H···Cl and C–H···Cl hydrogen bonds (shown as dashed lines).

4. Synthesis and crystallization

A solution of SbCl_3 (45.6 mg, 0.2 mmol) in water (10 ml) was added dropwise to a solution of benzothiazole (0.5 ml, 4.6 mmol) in ethanol (10 ml). The mixture was then refluxed with stirring for 3 h and the resulting solution was left to stand at room temperature. Colorless crystals were obtained after several days.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Approximate positions for all H atoms were first obtained from the difference electron density map. However, the H atoms were placed into idealized positions and refined using the riding-atom approximation. The applied constraints were: C—H = 0.93 Å and N—H = 0.86 Å, $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C or N})$.

Acknowledgements

This work is supported by the 'Unité de recherche de Chimie de l'Environnement et Moléculaire Structurale', CHEMS, Université de Constantine, Algeria. Thanks are due to MESRS and ATRST (Ministère de l'Enseignement Supérieur et de la Recherche Scientifique et l'Agence Thématique de Recherche en Sciences et Technologie – Algérie).

References

Abboud, K. A., Palenik, R. C., Palenik, G. J. & Wood, R. M. (2007). *Inorg. Chim. Acta*, **360**, 3642–3646.
 Bouchareb, H., Benmebarek, S., Bouacida, S., Merazig, H. & Boudraa, M. (2014). *Acta Cryst. E* **70**, m275.
 Brandenburg, K. & Berndt, M. (2001). *DIAMOND*. Crystal Impact, Bonn, Germany.
 Bruker (2011). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Bujak, M. & Angel, R. J. (2006). *J. Phys. Chem. B*, **110**, 10322–10331.
 Burla, M. C., Caliendo, R., Camalli, M., Carrozzini, B., Cascarano, G. L., De Caro, L., Giacovazzo, C., Polidori, G. & Spagna, R. (2005). *J. Appl. Cryst.* **38**, 381–388.
 Demicheli, C., Santos, L. S., Ferreira, C. S., Bouchemal, N., Hantz, E., Eberlin, M. N. & Frézard, F. (2006). *Inorg. Chim. Acta*, **359**, 159–167.

Table 2

Experimental details.

Crystal data	
Chemical formula	$(\text{C}_7\text{H}_6\text{NS})_2[\text{Sb}_2\text{Cl}_6\text{O}]$
M_r	744.58
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	295
a, b, c (Å)	10.2826 (2), 16.2448 (3), 14.9849 (3)
β (°)	111.674 (1)
V (Å ³)	2326.09 (8)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	3.20
Crystal size (mm)	0.17 × 0.13 × 0.11
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Sheldrick, 2002)
$T_{\text{min}}, T_{\text{max}}$	0.630, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	20349, 5344, 4627
R_{int}	0.026
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.651
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.022, 0.050, 1.02
No. of reflections	5344
No. of parameters	244
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.54, -0.77

Computer programs: *APEX2* and *SAINT* (Bruker, 2011), *SIR2002* (Burla *et al.*, 2005), *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *DIAMOND* (Brandenburg & Berndt, 2001).

Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
 Mikhaylov, A. A., Mel'nik, E. A., Churakov, A. V., Novotortsev, V. M., Howard, J. A. K., Sladkevich, S., Gun, J., Bharathi, S., Lev, O. & Prikhodchenko, P. V. (2011). *Inorg. Chim. Acta*, **378**, 24–29.
 Rais, S., Perianin, A., Lenoir, M., Sadak, A., Rivollet, D., Paul, M. & Deniau, M. (2000). *Antimicrob. Agents Chemother.* **44**, 2406–2410.
 Razak, I. A., Fun, H.-K., Yamin, B. M., Chinnakali, K., Zakaria, H. & Ismail, N. B. (1999). *Acta Cryst. C* **55**, 172–174.
 Sheldrick, G. M. (2002). *SADABS*. University of Göttingen, Germany.
 Sheldrick, G. M. (2008). *Acta Cryst. A* **64**, 112–122.

supporting information

Acta Cryst. (2016). E72, 212-214 [doi:10.1107/S2056989016000785]

catena-Poly[bis(1,3-benzothiazol-3-ium) [[dichloridoantimonate(III)]-di- μ -chlorido- μ -oxido-[chloridoantimonate(III)]- μ -chlorido]]

Oussama Chebout, Mhamed Boudraa, Sofiane Bouacida, Hocine Merazig and Chaouki Boudaren

Computing details

Data collection: *APEX2* (Bruker, 2011); cell refinement: *S SAINT* (Bruker, 2011); data reduction: *S SAINT* (Bruker, 2011); program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg & Berndt, 2001); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

catena-Poly[1,3-benzothiazol-3-ium [[dichloridoantimonate(III)]-di- μ -chlorido- μ -oxido-[chloridoantimonate(III)]- μ -chlorido]]

Crystal data

(C₇H₆NS)₂[Sb₂Cl₆O]
M_r = 744.58
 Monoclinic, *P2₁/c*
 Hall symbol: -P 2ybc
a = 10.2826 (2) Å
b = 16.2448 (3) Å
c = 14.9849 (3) Å
 β = 111.674 (1)°
V = 2326.09 (8) Å³
Z = 4

F(000) = 1416
D_x = 2.126 Mg m⁻³
 Mo *K* α radiation, λ = 0.71073 Å
 Cell parameters from 8790 reflections
 θ = 2.5–27.5°
 μ = 3.20 mm⁻¹
T = 295 K
 Block, colorless
 0.17 × 0.13 × 0.11 mm

Data collection

Bruker APEXII CCD
 diffractometer
 Radiation source: sealed tube
 Graphite monochromator
 φ and ω scans
 Absorption correction: multi-scan
 (*SADABS*; Sheldrick, 2002)
T_{min} = 0.630, *T_{max}* = 0.746

20349 measured reflections
 5344 independent reflections
 4627 reflections with *I* > 2 σ (*I*)
R_{int} = 0.026
 θ_{\max} = 27.5°, θ_{\min} = 2.9°
h = -11→13
k = -19→21
l = -19→18

Refinement

Refinement on *F*²
 Least-squares matrix: full
R[*F*² > 2 σ (*F*²)] = 0.022
wR(*F*²) = 0.050
S = 1.02
 5344 reflections

244 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

$$w = 1/[\sigma^2(F_o^2) + (0.0186P)^2 + 1.5448P]$$

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

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 0.54 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.77 \text{ e } \text{\AA}^{-3}$$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.36748 (12)	0.17148 (5)	0.98344 (7)	0.0662 (3)
N1	0.1904 (3)	0.05865 (18)	0.94373 (19)	0.0539 (7)
H1N	0.114	0.0319	0.9156	0.065*
C1	0.2113 (4)	0.1303 (2)	0.9189 (2)	0.0653 (10)
H1	0.1448	0.1582	0.8683	0.078*
C2	0.4125 (3)	0.08232 (16)	1.05140 (19)	0.0386 (6)
C3	0.5374 (3)	0.0621 (2)	1.1261 (2)	0.0509 (8)
H3	0.612	0.0988	1.147	0.061*
C4	0.5459 (3)	-0.0141 (2)	1.1676 (2)	0.0528 (8)
H4	0.6282	-0.0293	1.2172	0.063*
C5	0.4350 (4)	-0.0684 (2)	1.1374 (2)	0.0516 (8)
H5	0.4439	-0.1191	1.1678	0.062*
C6	0.3131 (3)	-0.04978 (18)	1.0645 (2)	0.0474 (7)
H6	0.2391	-0.087	1.0443	0.057*
C7	0.3030 (3)	0.02653 (17)	1.02135 (19)	0.0372 (6)
S2	0.52690 (8)	0.11063 (4)	0.59703 (6)	0.04448 (17)
N2	0.7036 (2)	0.00265 (15)	0.68158 (18)	0.0436 (6)
H2N	0.7828	-0.0203	0.7127	0.052*
C8	0.6923 (3)	0.07956 (18)	0.6561 (2)	0.0465 (7)
H8	0.769	0.1143	0.6695	0.056*
C9	0.4653 (3)	0.01241 (16)	0.60657 (18)	0.0339 (6)
C10	0.3292 (3)	-0.01737 (19)	0.5748 (2)	0.0431 (7)
H10	0.2533	0.0166	0.5433	0.052*
C11	0.3111 (3)	-0.0985 (2)	0.5917 (2)	0.0501 (7)
H11	0.2208	-0.1199	0.5712	0.06*
C12	0.4237 (3)	-0.15006 (19)	0.6385 (2)	0.0530 (8)
H12	0.4069	-0.205	0.6482	0.064*
C13	0.5579 (3)	-0.12215 (18)	0.6705 (2)	0.0481 (7)
H13	0.6331	-0.1567	0.7016	0.058*
C14	0.5770 (3)	-0.03964 (16)	0.65440 (19)	0.0359 (6)

Sb1	−0.067085 (18)	0.323213 (10)	0.767483 (12)	0.03143 (5)
Sb2	0.053422 (18)	0.221298 (11)	0.613337 (12)	0.03397 (5)
C11	0.01992 (9)	0.07748 (5)	0.63368 (7)	0.0589 (2)
C12	0.30403 (7)	0.20616 (5)	0.68094 (6)	0.05062 (18)
C13	0.13613 (8)	0.35386 (5)	0.91846 (5)	0.05065 (18)
C14	−0.14276 (8)	0.21318 (5)	0.84967 (6)	0.05007 (18)
C15	−0.24438 (8)	0.26668 (4)	0.59142 (6)	0.04931 (18)
O1	0.05721 (19)	0.24501 (12)	0.74157 (12)	0.0391 (4)
Cl6	0.04721 (8)	0.42304 (5)	0.64881 (6)	0.0558 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0921 (7)	0.0379 (4)	0.0703 (6)	0.0017 (4)	0.0319 (5)	0.0061 (4)
N1	0.0376 (13)	0.0731 (19)	0.0455 (15)	0.0001 (13)	0.0092 (12)	−0.0065 (14)
C1	0.073 (2)	0.071 (2)	0.0456 (19)	0.042 (2)	0.0148 (18)	0.0111 (17)
C2	0.0497 (16)	0.0334 (13)	0.0350 (15)	−0.0018 (12)	0.0181 (13)	−0.0021 (11)
C3	0.0474 (17)	0.062 (2)	0.0414 (17)	−0.0141 (15)	0.0139 (14)	−0.0112 (15)
C4	0.0485 (18)	0.076 (2)	0.0313 (15)	0.0127 (17)	0.0116 (14)	0.0045 (15)
C5	0.070 (2)	0.0477 (17)	0.0422 (17)	0.0085 (16)	0.0267 (17)	0.0122 (14)
C6	0.0581 (19)	0.0430 (16)	0.0458 (17)	−0.0131 (14)	0.0247 (15)	−0.0014 (13)
C7	0.0363 (14)	0.0440 (15)	0.0308 (14)	0.0019 (12)	0.0117 (12)	−0.0024 (11)
S2	0.0533 (4)	0.0327 (3)	0.0566 (5)	0.0085 (3)	0.0310 (4)	0.0065 (3)
N2	0.0318 (12)	0.0456 (13)	0.0510 (15)	0.0069 (11)	0.0125 (11)	−0.0009 (11)
C8	0.0454 (17)	0.0419 (16)	0.060 (2)	−0.0037 (13)	0.0282 (15)	−0.0071 (14)
C9	0.0385 (14)	0.0333 (13)	0.0329 (14)	0.0054 (11)	0.0168 (12)	0.0027 (11)
C10	0.0368 (15)	0.0549 (18)	0.0368 (15)	0.0077 (13)	0.0125 (12)	0.0067 (13)
C11	0.0422 (16)	0.061 (2)	0.0444 (17)	−0.0152 (15)	0.0135 (14)	−0.0025 (15)
C12	0.062 (2)	0.0387 (16)	0.058 (2)	−0.0107 (15)	0.0214 (17)	0.0041 (14)
C13	0.0533 (18)	0.0384 (15)	0.0495 (18)	0.0097 (14)	0.0153 (15)	0.0106 (13)
C14	0.0344 (13)	0.0375 (14)	0.0357 (14)	0.0054 (11)	0.0127 (12)	0.0011 (11)
Sb1	0.03409 (9)	0.02825 (9)	0.03458 (10)	0.00560 (7)	0.01575 (7)	−0.00018 (7)
Sb2	0.03473 (10)	0.04105 (10)	0.02678 (9)	0.00516 (8)	0.01211 (7)	−0.00064 (7)
C11	0.0568 (5)	0.0425 (4)	0.0830 (6)	−0.0050 (4)	0.0325 (4)	−0.0093 (4)
C12	0.0351 (4)	0.0611 (5)	0.0567 (5)	0.0025 (3)	0.0181 (3)	−0.0138 (4)
C13	0.0601 (5)	0.0487 (4)	0.0381 (4)	−0.0131 (4)	0.0122 (3)	−0.0065 (3)
C14	0.0570 (4)	0.0486 (4)	0.0529 (4)	−0.0093 (3)	0.0301 (4)	0.0031 (3)
C15	0.0457 (4)	0.0430 (4)	0.0491 (4)	−0.0024 (3)	0.0057 (3)	0.0020 (3)
O1	0.0460 (11)	0.0463 (11)	0.0271 (9)	0.0225 (9)	0.0160 (8)	0.0044 (8)
Cl6	0.0466 (4)	0.0579 (5)	0.0518 (5)	−0.0107 (4)	0.0051 (4)	0.0103 (4)

Geometric parameters (Å, °)

S1—C1	1.678 (4)	C8—H8	0.93
S1—C2	1.732 (3)	C9—C10	1.388 (4)
N1—C1	1.265 (4)	C9—C14	1.393 (3)
N1—C7	1.404 (4)	C10—C11	1.368 (4)
N1—H1N	0.8599	C10—H10	0.93

C1—H1	0.93	C11—C12	1.391 (4)
C2—C7	1.385 (4)	C11—H11	0.93
C2—C3	1.396 (4)	C12—C13	1.360 (4)
C3—C4	1.373 (5)	C12—H12	0.93
C3—H3	0.93	C13—C14	1.389 (4)
C4—C5	1.379 (4)	C13—H13	0.93
C4—H4	0.93	Sb1—O1	1.9404 (16)
C5—C6	1.358 (4)	Sb1—C14	2.4545 (7)
C5—H5	0.93	Sb1—C13	2.4982 (8)
C6—C7	1.384 (4)	Sb1—C15	2.7522 (8)
C6—H6	0.93	Sb1—C16	2.9524 (8)
S2—C8	1.679 (3)	Sb2—O1	1.9460 (17)
S2—C9	1.742 (3)	Sb2—C11	2.3974 (8)
N2—C8	1.299 (4)	Sb2—C12	2.4081 (7)
N2—C14	1.392 (3)	Sb2—C15	3.0473 (8)
N2—H2N	0.8599	Sb2—C16	3.3244 (9)
C1—S1—C2	89.81 (16)	C9—C10—H10	121.2
C1—N1—C7	114.1 (3)	C10—C11—C12	121.9 (3)
C1—N1—H1N	123	C10—C11—H11	119.1
C7—N1—H1N	122.9	C12—C11—H11	119.1
N1—C1—S1	115.3 (3)	C13—C12—C11	121.6 (3)
N1—C1—H1	122.3	C13—C12—H12	119.2
S1—C1—H1	122.3	C11—C12—H12	119.2
C7—C2—C3	120.2 (3)	C12—C13—C14	116.8 (3)
C7—C2—S1	110.3 (2)	C12—C13—H13	121.6
C3—C2—S1	129.4 (2)	C14—C13—H13	121.6
C4—C3—C2	117.5 (3)	C13—C14—N2	127.1 (3)
C4—C3—H3	121.3	C13—C14—C9	122.1 (3)
C2—C3—H3	121.3	N2—C14—C9	110.8 (2)
C3—C4—C5	121.4 (3)	O1—Sb1—C14	88.74 (6)
C3—C4—H4	119.3	O1—Sb1—C13	85.37 (6)
C5—C4—H4	119.3	C14—Sb1—C13	90.28 (3)
C6—C5—C4	121.8 (3)	O1—Sb1—C15	80.90 (6)
C6—C5—H5	119.1	C14—Sb1—C15	91.00 (3)
C4—C5—H5	119.1	C13—Sb1—C15	166.17 (3)
C5—C6—C7	117.6 (3)	O1—Sb1—C16	78.52 (6)
C5—C6—H6	121.2	C14—Sb1—C16	166.56 (3)
C7—C6—H6	121.2	C13—Sb1—C16	92.87 (2)
C6—C7—C2	121.5 (3)	C15—Sb1—C16	82.88 (2)
C6—C7—N1	128.1 (3)	O1—Sb2—C11	91.07 (6)
C2—C7—N1	110.4 (3)	O1—Sb2—C12	88.67 (6)
C8—S2—C9	90.54 (14)	C11—Sb2—C12	91.64 (3)
C8—N2—C14	114.6 (2)	O1—Sb2—C15	73.22 (5)
C8—N2—H2N	122.7	C11—Sb2—C15	93.65 (2)
C14—N2—H2N	122.7	C12—Sb2—C15	161.21 (2)
N2—C8—S2	114.0 (2)	O1—Sb2—C16	69.00 (6)
N2—C8—H8	123	C11—Sb2—C16	158.15 (3)

S2—C8—H8	123	Cl2—Sb2—Cl6	96.56 (2)
C10—C9—C14	120.0 (2)	Cl5—Sb2—Cl6	72.59 (2)
C10—C9—S2	130.0 (2)	Sb1—Cl5—Sb2	72.175 (18)
C14—C9—S2	110.0 (2)	Sb1—O1—Sb2	123.56 (9)
C11—C10—C9	117.5 (3)	Sb1—Cl6—Sb2	65.814 (16)
C11—C10—H10	121.2		
C7—N1—C1—S1	-0.1 (4)	C8—N2—C14—C9	-1.1 (3)
C2—S1—C1—N1	0.8 (3)	C10—C9—C14—C13	1.2 (4)
C1—S1—C2—C7	-1.2 (2)	S2—C9—C14—C13	-178.9 (2)
C1—S1—C2—C3	178.1 (3)	C10—C9—C14—N2	-178.8 (2)
C7—C2—C3—C4	-0.2 (4)	S2—C9—C14—N2	1.1 (3)
S1—C2—C3—C4	-179.4 (2)	O1—Sb1—Cl5—Sb2	-17.75 (6)
C2—C3—C4—C5	-0.6 (5)	Cl4—Sb1—Cl5—Sb2	-106.31 (2)
C3—C4—C5—C6	1.0 (5)	Cl3—Sb1—Cl5—Sb2	-11.07 (11)
C4—C5—C6—C7	-0.5 (4)	Cl6—Sb1—Cl5—Sb2	61.70 (2)
C5—C6—C7—C2	-0.3 (4)	O1—Sb2—Cl5—Sb1	18.27 (6)
C5—C6—C7—N1	178.1 (3)	Cl1—Sb2—Cl5—Sb1	108.29 (3)
C3—C2—C7—C6	0.7 (4)	Cl2—Sb2—Cl5—Sb1	2.25 (9)
S1—C2—C7—C6	180.0 (2)	Cl6—Sb2—Cl5—Sb1	-54.403 (18)
C3—C2—C7—N1	-178.0 (3)	Cl4—Sb1—O1—Sb2	124.26 (11)
S1—C2—C7—N1	1.3 (3)	Cl3—Sb1—O1—Sb2	-145.35 (12)
C1—N1—C7—C6	-179.4 (3)	Cl5—Sb1—O1—Sb2	33.05 (11)
C1—N1—C7—C2	-0.8 (4)	Cl6—Sb1—O1—Sb2	-51.47 (11)
C14—N2—C8—S2	0.6 (3)	Cl1—Sb2—O1—Sb1	-124.01 (11)
C9—S2—C8—N2	0.1 (2)	Cl2—Sb2—O1—Sb1	144.37 (12)
C8—S2—C9—C10	179.2 (3)	Cl5—Sb2—O1—Sb1	-30.53 (10)
C8—S2—C9—C14	-0.7 (2)	Cl6—Sb2—O1—Sb1	46.83 (10)
C14—C9—C10—C11	-0.6 (4)	O1—Sb1—Cl6—Sb2	24.73 (6)
S2—C9—C10—C11	179.5 (2)	Cl4—Sb1—Cl6—Sb2	6.05 (11)
C9—C10—C11—C12	-0.1 (4)	Cl3—Sb1—Cl6—Sb2	109.41 (2)
C10—C11—C12—C13	0.4 (5)	Cl5—Sb1—Cl6—Sb2	-57.378 (18)
C11—C12—C13—C14	0.2 (5)	O1—Sb2—Cl6—Sb1	-25.97 (6)
C12—C13—C14—N2	179.1 (3)	Cl1—Sb2—Cl6—Sb1	-0.64 (7)
C12—C13—C14—C9	-1.0 (4)	Cl2—Sb2—Cl6—Sb1	-112.00 (2)
C8—N2—C14—C13	178.9 (3)	Cl5—Sb2—Cl6—Sb1	52.283 (18)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1N \cdots Cl6 ⁱ	0.86	2.37	3.200 (3)	162
N2—H2N \cdots Cl6 ⁱⁱ	0.86	2.35	3.145 (3)	153
C1—H1 \cdots O1	0.93	2.27	3.152 (4)	159
C8—H8 \cdots Cl5 ⁱⁱⁱ	0.93	2.72	3.327 (3)	124
C10—H10 \cdots Cl3 ^{iv}	0.93	2.78	3.612 (3)	150
C13—H13 \cdots Cl2 ⁱⁱ	0.93	2.76	3.524 (3)	140

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