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Dichloridotriphenylantimony(V)–bis(pyrrolidin-1-ylthiocarbonyl) disulfide (1/1)

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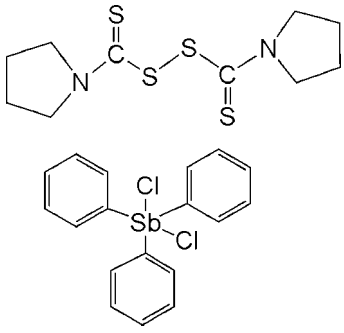
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.031; wR factor = 0.092; data-to-parameter ratio = 16.6.

The asymmetric unit of the title compound, $[Sb(C_6H_5)_3Cl_2]\cdot C_{10}H_{16}N_2S_4$, comprises a bis(pyrrolidinylthiocarbamoyl) molecule and a dichlorotriphenylantimony(V) complex. In the Sb complex, the central atom is coordinated by three C atoms of the three phenyl ligands and two Cl atoms in a slightly distorted trigonal-bipyramidal geometry. The thiocarbamoyl units, connected *via* the disulfide bond, are approximately perpendicular to each other. The molecules are connected by weak C—H···S and C—H···Cl hydrogen-bonding interactions into two one-dimensional supramolecular chains.

Related literature

For related structures, see: Williams *et al.* (1983); Feng Li *et al.* (2006). For discussion on C—H···S interactions, see: Srinivasan *et al.* (2007). For related literature, see: Kumar *et al.* (1990).



Experimental

Crystal data

$[Sb(C_6H_5)_3Cl_2]\cdot C_{10}H_{16}N_2S_4$
M_r = 716.48
Monoclinic, $P2_1/n$
a = 14.8138 (18) Å
b = 13.6440 (13) Å
c = 16.316 (3) Å
β = 105.509 (2)°
V = 3177.7 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.32 mm^{-1}
T = 298 (2) K
0.50 × 0.42 × 0.39 mm

Data collection

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.558, T_{max} = 0.627
14597 measured reflections
5560 independent reflections
4333 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.092
S = 1.00
5560 reflections
335 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15···S4^{i}	0.93	2.91	3.594 (5)	132
C13—H13···Cl2^{ii}	0.93	2.83	3.509 (4)	131
C8—H8A···Cl1^{iii}	0.97	2.84	3.719 (6)	151

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2063).

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supplementary materials

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Dichloridotriphenylantimony(V)-bis(pyrrolidin-1-ylthiocarbonyl) disulfide (1/1)

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Comment

In the title complex, the antimony atom is coordinated by three C atoms of three phenyl ligands and two Cl atoms in a slightly distorted trigonal-bipyramidal geometry. Atoms Cl1, Cl2 of the complex lie in axial positions (Fig. 1), with the axial angle Cl1—Sb1—Cl2 178.65 (4)°, deviating substantially from the linear value of 180°. The distances Sb—Cl also vary merely with the role they play in the structure: Sb1—Cl1 = 2.4720 (9) Å and Sb1—Cl2 = 2.4792 (10) Å. In the bis(pyrrolidinylthiocarbamoyl) molecule of the title compound, the thiocarbamoyl moieties, connected *via* the disulfide bond (S1—S3 = 2.0029 (17) Å), are approximately perpendicular to each other. A Newman projection, calculated with *PLATON*, with a view along the disulfide bond results in a dihedral angle of 87 ° for C1—S1—S3—C6 (Spek, 2003).

The Dipyrrolidylthiuram disulfide molecule, (which is another name of the organic part in our structure) shows a planar model with crystallographic inversion symmetry in the midpoint of the S—S bond (Williams *et al.*, 1983).

In the similar structure bis(*N*,*N*-dicyclohexylthiocarbamoyl) disulfide, a crystallographic twofold axis passes through the midpoint of the S—S bond (Li *et al.*, 2006). The disulfide S—S distance is close to the distances observed in free (uncoordinated) disulfides (Kumar *et al.*, 1990).

The S atoms of bis(pyrrolidinylthiocarbamoyl) and the Cl atoms of dichlorotriphenylantimony play a significant role in the crystal packing, linking the complex molecules by weak C—H···S and C—H···Cl (Table 1) hydrogen bonds to form two one-dimensional supramolecular chains (Fig. 2).

Experimental

Chlorotriphenylantimony (0.2 mmol) was dissolved in benzene (15 ml) and bis(pyrrolidinylthiocarbamoyl) (0.2 mmol) dissolved in methanol was added with stirring at room temperature for eight hours and then filtered. Orange crystals suitable for X-ray analysis were obtained by slow evaporation of a petroleum/dichloromethane (1:2 *v*/*v*) solution over a period of twenty days (yield 85%. m.p. 432k). Anal. Calcd (%) for $C_{28}H_{31}N_2S_4Cl_2Sb$(Mr = 716.48): C, 46.94; H, 4.36; N, 3.91. Found (%): C, 46.89; H, 4.31; N, 3.87.

Refinement

The H atoms bound to C of pyrrolidine were located in a difference map and were refined as riding on their respective C atoms with distances C—H = 0.97 Å and with U_{iso}(H) = 1.2U_{eq}(C). The other H atoms were constraint at calculated positions (riding mode), with C—H = 0.93 Å and U_{iso}(H) = 1.2 U_{eq}(C).

Figures

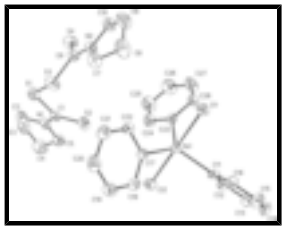

Fig. 1. The molecular structure of the title compound, with atom labels and 50% probability displacement ellipsoids for non-H atoms.

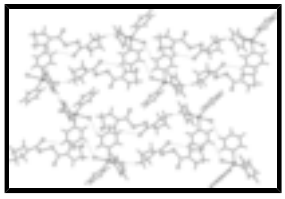

Fig. 2. Crystal packing of the title compound, showing catemer chains, linked by weak C15—H15···S4, C13—H13···Cl2, C8—H8A···Cl1 hydrogen bonding contacts, indicated by dashed lines. Symmetry codes are given in Table 1.

Dichloridotriphenylantimony(*V*)–bis(pyrrolidin-1-ylthiocarbonyl) disulfide (1/1)

Crystal data

$[Sb(C_6H_5)_3Cl_2]\cdot C_{10}H_{16}N_2S_4$	F_{000} = 1448
M_r = 716.48	D_x = 1.498 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 7025 reflections
a = 14.8138 (18) Å	θ = 2.2–27.8º
b = 13.6440 (13) Å	μ = 1.32 mm^{-1}
c = 16.316 (3) Å	T = 298 (2) K
β = 105.509 (2)º	Block, colorless
V = 3177.7 (8) Å^3	0.50 × 0.42 × 0.39 mm
Z = 4	

Data collection

Siemens SMART CCD diffractometer	5560 independent reflections
Radiation source: fine-focus sealed tube	4333 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.041
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −17→10
T_{min} = 0.558, T_{max} = 0.627	k = −16→16
14597 measured reflections	l = −19→19

Refinement

Refinement on f^2	Hydrogen site location: inferred from neighbouring sites

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.031$

$wR(F^2) = 0.092$

$S = 1.00$

5560 reflections

335 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.045P)^2 + 1.9404P]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 0.67$ e Å^{-3}

$\Delta\rho_{min} = -0.59$ e Å^{-3}

Extinction correction: SHELXL

Extinction coefficient: 0.0048 (3)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Sb1	0.018116 (16)	0.991080 (17)	0.234502 (14)	0.03657 (11)
Cl1	−0.07709 (7)	1.08719 (7)	0.11362 (6)	0.0508 (3)
Cl2	0.11117 (8)	0.89132 (8)	0.35457 (6)	0.0569 (3)
N1	0.6750 (2)	0.8384 (2)	0.3780 (2)	0.0516 (8)
N2	0.4034 (2)	1.0375 (2)	0.0796 (2)	0.0534 (9)
S1	0.59570 (9)	0.82805 (9)	0.21567 (7)	0.0664 (3)
S2	0.50821 (9)	0.92203 (9)	0.34589 (8)	0.0665 (3)
S3	0.46930 (9)	0.86974 (9)	0.14467 (7)	0.0704 (4)
S4	0.58682 (9)	1.05180 (10)	0.13631 (8)	0.0742 (4)
C1	0.5950 (3)	0.8643 (3)	0.3226 (2)	0.0479 (10)
C2	0.7541 (3)	0.7877 (3)	0.3599 (3)	0.0660 (12)
H2A	0.7718	0.8181	0.3127	0.079*
H2B	0.7396	0.7192	0.3467	0.079*
C3	0.8311 (4)	0.7985 (4)	0.4418 (3)	0.0879 (17)
H3A	0.8735	0.7429	0.4505	0.106*
H3B	0.8667	0.8580	0.4415	0.106*
C4	0.7802 (4)	0.8025 (5)	0.5087 (3)	0.0972 (19)
H4A	0.8174	0.8356	0.5591	0.117*
H4B	0.7654	0.7371	0.5243	0.117*
C5	0.6926 (3)	0.8589 (4)	0.4697 (3)	0.0685 (13)
H5A	0.6410	0.8362	0.4910	0.082*
H5B	0.7017	0.9285	0.4812	0.082*
C6	0.4843 (3)	0.9968 (3)	0.1173 (2)	0.0531 (11)
C7	0.3104 (3)	0.9904 (3)	0.0625 (3)	0.0732 (14)
H7A	0.3029	0.9567	0.1126	0.088*
H7B	0.3015	0.9438	0.0161	0.088*
C8	0.2428 (4)	1.0747 (4)	0.0389 (4)	0.100 (2)
H8A	0.1850	1.0541	−0.0012	0.120*
H8B	0.2283	1.1018	0.0889	0.120*
C9	0.2927 (4)	1.1471 (5)	−0.0001 (4)	0.104 (2)
H9A	0.2703	1.2128	0.0061	0.124*
H9B	0.2828	1.1334	−0.0602	0.124*
C10	0.3956 (4)	1.1383 (3)	0.0462 (3)	0.0739 (14)
H10A	0.4345	1.1476	0.0076	0.089*

H10B	0.4133	1.1858	0.0920	0.089*
C11	−0.0708 (2)	1.0332 (3)	0.3075 (2)	0.0377 (8)
C12	−0.0319 (3)	1.0717 (3)	0.3882 (2)	0.0496 (10)
H12	0.0328	1.0757	0.4095	0.059*
C13	−0.0893 (3)	1.1037 (3)	0.4366 (3)	0.0589 (11)
H13	−0.0632	1.1315	0.4897	0.071*
C14	−0.1851 (3)	1.0950 (3)	0.4067 (3)	0.0589 (11)
H14	−0.2235	1.1151	0.4403	0.071*
C15	−0.2239 (3)	1.0566 (3)	0.3274 (3)	0.0610 (11)
H15	−0.2886	1.0508	0.3075	0.073*
C16	−0.1680 (3)	1.0268 (3)	0.2772 (2)	0.0495 (10)
H16	−0.1950	1.0024	0.2230	0.059*
C17	−0.0118 (2)	0.8611 (3)	0.1610 (2)	0.0384 (8)
C18	−0.0404 (3)	0.7789 (3)	0.1959 (3)	0.0503 (10)
H18	−0.0478	0.7808	0.2507	0.060*
C19	−0.0580 (3)	0.6933 (3)	0.1490 (3)	0.0607 (12)
H19	−0.0773	0.6374	0.1723	0.073*
C20	−0.0469 (3)	0.6908 (3)	0.0685 (3)	0.0650 (12)
H20	−0.0581	0.6329	0.0373	0.078*
C21	−0.0195 (3)	0.7731 (3)	0.0336 (3)	0.0611 (11)
H21	−0.0127	0.7709	−0.0214	0.073*
C22	−0.0018 (3)	0.8593 (3)	0.0794 (2)	0.0491 (10)
H22	0.0166	0.9152	0.0556	0.059*
C23	0.1365 (3)	1.0813 (3)	0.2432 (2)	0.0428 (9)
C24	0.2261 (3)	1.0430 (4)	0.2705 (3)	0.0642 (12)
H24	0.2351	0.9765	0.2825	0.077*
C25	0.3018 (3)	1.1049 (4)	0.2797 (4)	0.0844 (16)
H25	0.3622	1.0795	0.2967	0.101*
C26	0.2892 (4)	1.2026 (4)	0.2643 (4)	0.0859 (16)
H26	0.3408	1.2437	0.2714	0.103*
C27	0.2006 (4)	1.2404 (3)	0.2382 (3)	0.0757 (14)
H27	0.1923	1.3072	0.2278	0.091*
C28	0.1236 (3)	1.1801 (3)	0.2271 (2)	0.0505 (10)
H28	0.0635	1.2060	0.2089	0.061*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sb1	0.03922 (16)	0.03827 (16)	0.03499 (15)	0.00222 (11)	0.01473 (11)	0.00279 (10)
Cl1	0.0587 (6)	0.0493 (6)	0.0422 (5)	0.0073 (5)	0.0095 (4)	0.0092 (4)
Cl2	0.0678 (7)	0.0605 (6)	0.0419 (5)	0.0145 (6)	0.0138 (5)	0.0138 (4)
N1	0.050 (2)	0.0453 (19)	0.0531 (19)	−0.0006 (17)	0.0033 (16)	0.0008 (15)
N2	0.059 (2)	0.0451 (19)	0.0507 (19)	−0.0064 (18)	0.0047 (17)	−0.0006 (15)
S1	0.0762 (8)	0.0609 (7)	0.0545 (6)	0.0119 (6)	0.0046 (6)	−0.0034 (5)
S2	0.0606 (7)	0.0570 (7)	0.0807 (8)	0.0096 (6)	0.0170 (6)	0.0004 (6)
S3	0.0749 (8)	0.0524 (7)	0.0655 (7)	−0.0139 (6)	−0.0136 (6)	0.0068 (5)
S4	0.0652 (8)	0.0727 (8)	0.0780 (8)	−0.0193 (7)	0.0074 (6)	0.0031 (6)
C1	0.053 (2)	0.034 (2)	0.054 (2)	−0.0035 (18)	0.0078 (19)	0.0020 (16)

C2	0.057 (3)	0.057 (3)	0.080 (3)	0.005 (2)	0.012 (2)	−0.004 (2)
C3	0.059 (3)	0.083 (4)	0.104 (4)	0.013 (3)	−0.010 (3)	−0.005 (3)
C4	0.085 (4)	0.111 (5)	0.076 (4)	0.005 (4)	−0.014 (3)	0.017 (3)
C5	0.072 (3)	0.072 (3)	0.055 (3)	−0.003 (3)	0.005 (2)	0.006 (2)
C6	0.066 (3)	0.048 (2)	0.040 (2)	−0.008 (2)	0.005 (2)	−0.0023 (17)
C7	0.059 (3)	0.066 (3)	0.085 (3)	−0.008 (3)	0.001 (3)	−0.005 (2)
C8	0.069 (4)	0.085 (4)	0.128 (5)	0.006 (3)	−0.001 (3)	−0.011 (4)
C9	0.095 (5)	0.091 (4)	0.116 (5)	0.031 (4)	0.014 (4)	0.029 (4)
C10	0.089 (4)	0.053 (3)	0.078 (3)	0.002 (3)	0.019 (3)	0.001 (2)
C11	0.039 (2)	0.047 (2)	0.0280 (17)	−0.0044 (18)	0.0112 (15)	0.0047 (15)
C12	0.047 (2)	0.059 (3)	0.045 (2)	0.001 (2)	0.0155 (18)	−0.0031 (18)
C13	0.066 (3)	0.068 (3)	0.046 (2)	−0.002 (2)	0.022 (2)	−0.011 (2)
C14	0.057 (3)	0.067 (3)	0.064 (3)	0.006 (2)	0.035 (2)	−0.008 (2)
C15	0.044 (2)	0.075 (3)	0.069 (3)	−0.001 (2)	0.025 (2)	−0.010 (2)
C16	0.047 (2)	0.060 (3)	0.041 (2)	−0.002 (2)	0.0133 (18)	−0.0061 (18)
C17	0.0344 (19)	0.038 (2)	0.0434 (19)	0.0001 (16)	0.0112 (16)	0.0024 (15)
C18	0.049 (2)	0.051 (2)	0.057 (2)	−0.001 (2)	0.0257 (19)	0.0049 (19)
C19	0.051 (3)	0.049 (3)	0.087 (3)	−0.011 (2)	0.026 (2)	0.004 (2)
C20	0.066 (3)	0.048 (3)	0.079 (3)	−0.002 (2)	0.017 (3)	−0.016 (2)
C21	0.078 (3)	0.059 (3)	0.050 (2)	0.003 (3)	0.024 (2)	−0.009 (2)
C22	0.065 (3)	0.045 (2)	0.043 (2)	0.003 (2)	0.0250 (19)	0.0023 (17)
C23	0.039 (2)	0.047 (2)	0.047 (2)	−0.0026 (18)	0.0181 (17)	−0.0019 (17)
C24	0.047 (3)	0.057 (3)	0.091 (3)	0.005 (2)	0.023 (2)	0.010 (2)
C25	0.038 (3)	0.081 (4)	0.131 (5)	0.000 (3)	0.017 (3)	0.013 (3)
C26	0.053 (3)	0.076 (4)	0.125 (5)	−0.022 (3)	0.018 (3)	0.004 (3)
C27	0.066 (3)	0.044 (3)	0.115 (4)	−0.010 (2)	0.021 (3)	0.004 (3)
C28	0.045 (2)	0.042 (2)	0.066 (3)	0.0014 (19)	0.017 (2)	0.0033 (19)

Geometric parameters (Å, °)

Sb1—C11	2.079 (4)	C10—H10A	0.9700
Sb1—C23	2.116 (4)	C10—H10B	0.9700
Sb1—C17	2.120 (3)	C11—C12	1.392 (5)
Sb1—Cl1	2.4720 (9)	C11—C16	1.394 (5)
Sb1—Cl2	2.4792 (10)	C12—C13	1.377 (5)
N1—C1	1.332 (5)	C12—H12	0.9300
N1—C2	1.457 (5)	C13—C14	1.377 (6)
N1—C5	1.476 (5)	C13—H13	0.9300
N2—C6	1.315 (5)	C14—C15	1.371 (6)
N2—C10	1.473 (5)	C14—H14	0.9300
N2—C7	1.477 (6)	C15—C16	1.372 (5)
S1—C1	1.817 (4)	C15—H15	0.9300
S1—S3	2.0029 (17)	C16—H16	0.9300
S2—C1	1.636 (4)	C17—C18	1.375 (5)
S3—C6	1.818 (4)	C17—C22	1.379 (5)
S4—C6	1.648 (5)	C18—C19	1.382 (6)
C2—C3	1.515 (6)	C18—H18	0.9300
C2—H2A	0.9700	C19—C20	1.368 (6)
C2—H2B	0.9700	C19—H19	0.9300

C3—C4	1.484 (8)	C20—C21	1.369 (6)
C3—H3A	0.9700	C20—H20	0.9300
C3—H3B	0.9700	C21—C22	1.381 (6)
C4—C5	1.496 (7)	C21—H21	0.9300
C4—H4A	0.9700	C22—H22	0.9300
C4—H4B	0.9700	C23—C28	1.378 (5)
C5—H5A	0.9700	C23—C24	1.384 (6)
C5—H5B	0.9700	C24—C25	1.380 (6)
C7—C8	1.507 (7)	C24—H24	0.9300
C7—H7A	0.9700	C25—C26	1.360 (7)
C7—H7B	0.9700	C25—H25	0.9300
C8—C9	1.476 (8)	C26—C27	1.367 (7)
C8—H8A	0.9700	C26—H26	0.9300
C8—H8B	0.9700	C27—C28	1.378 (6)
C9—C10	1.514 (7)	C27—H27	0.9300
C9—H9A	0.9700	C28—H28	0.9300
C9—H9B	0.9700		
C11—Sb1—C23	116.22 (14)	C8—C9—H9B	110.4
C11—Sb1—C17	119.09 (14)	C10—C9—H9B	110.4
C23—Sb1—C17	124.66 (14)	H9A—C9—H9B	108.6
C11—Sb1—Cl1	89.80 (10)	N2—C10—C9	103.2 (4)
C23—Sb1—Cl1	91.75 (10)	N2—C10—H10A	111.1
C17—Sb1—Cl1	90.23 (9)	C9—C10—H10A	111.1
C11—Sb1—Cl2	90.17 (10)	N2—C10—H10B	111.1
C23—Sb1—Cl2	89.47 (10)	C9—C10—H10B	111.1
C17—Sb1—Cl2	88.61 (9)	H10A—C10—H10B	109.1
Cl1—Sb1—Cl2	178.65 (4)	C12—C11—C16	119.1 (3)
C1—N1—C2	127.4 (3)	C12—C11—Sb1	118.7 (3)
C1—N1—C5	121.4 (4)	C16—C11—Sb1	122.2 (3)
C2—N1—C5	111.2 (3)	C13—C12—C11	119.9 (4)
C6—N2—C10	122.6 (4)	C13—C12—H12	120.0
C6—N2—C7	126.3 (4)	C11—C12—H12	120.0
C10—N2—C7	111.1 (4)	C12—C13—C14	120.4 (4)
C1—S1—S3	103.49 (15)	C12—C13—H13	119.8
C6—S3—S1	104.86 (16)	C14—C13—H13	119.8
N1—C1—S2	125.6 (3)	C15—C14—C13	119.9 (4)
N1—C1—S1	110.2 (3)	C15—C14—H14	120.1
S2—C1—S1	124.1 (2)	C13—C14—H14	120.1
N1—C2—C3	103.4 (4)	C14—C15—C16	120.6 (4)
N1—C2—H2A	111.1	C14—C15—H15	119.7
C3—C2—H2A	111.1	C16—C15—H15	119.7
N1—C2—H2B	111.1	C15—C16—C11	120.0 (4)
C3—C2—H2B	111.1	C15—C16—H16	120.0
H2A—C2—H2B	109.0	C11—C16—H16	120.0
C4—C3—C2	103.9 (4)	C18—C17—C22	120.6 (4)
C4—C3—H3A	111.0	C18—C17—Sb1	119.3 (3)
C2—C3—H3A	111.0	C22—C17—Sb1	120.1 (3)
C4—C3—H3B	111.0	C17—C18—C19	119.6 (4)
C2—C3—H3B	111.0	C17—C18—H18	120.2

H3A—C3—H3B	109.0	C19—C18—H18	120.2
C3—C4—C5	105.1 (4)	C20—C19—C18	120.0 (4)
C3—C4—H4A	110.7	C20—C19—H19	120.0
C5—C4—H4A	110.7	C18—C19—H19	120.0
C3—C4—H4B	110.7	C19—C20—C21	120.3 (4)
C5—C4—H4B	110.7	C19—C20—H20	119.9
H4A—C4—H4B	108.8	C21—C20—H20	119.9
N1—C5—C4	103.3 (4)	C20—C21—C22	120.5 (4)
N1—C5—H5A	111.1	C20—C21—H21	119.7
C4—C5—H5A	111.1	C22—C21—H21	119.7
N1—C5—H5B	111.1	C17—C22—C21	119.0 (4)
C4—C5—H5B	111.1	C17—C22—H22	120.5
H5A—C5—H5B	109.1	C21—C22—H22	120.5
N2—C6—S4	125.1 (3)	C28—C23—C24	120.2 (4)
N2—C6—S3	111.2 (3)	C28—C23—Sb1	119.1 (3)
S4—C6—S3	123.7 (3)	C24—C23—Sb1	120.5 (3)
N2—C7—C8	103.8 (4)	C25—C24—C23	119.0 (4)
N2—C7—H7A	111.0	C25—C24—H24	120.5
C8—C7—H7A	111.0	C23—C24—H24	120.5
N2—C7—H7B	111.0	C26—C25—C24	120.8 (5)
C8—C7—H7B	111.0	C26—C25—H25	119.6
H7A—C7—H7B	109.0	C24—C25—H25	119.6
C9—C8—C7	104.2 (5)	C25—C26—C27	120.0 (5)
C9—C8—H8A	110.9	C25—C26—H26	120.0
C7—C8—H8A	110.9	C27—C26—H26	120.0
C9—C8—H8B	110.9	C26—C27—C28	120.5 (4)
C7—C8—H8B	110.9	C26—C27—H27	119.7
H8A—C8—H8B	108.9	C28—C27—H27	119.7
C8—C9—C10	106.6 (4)	C27—C28—C23	119.5 (4)
C8—C9—H9A	110.4	C27—C28—H28	120.3
C10—C9—H9A	110.4	C23—C28—H28	120.3

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15···S4^{i}	0.93	2.91	3.594 (5)	132
C13—H13···Cl2^{ii}	0.93	2.83	3.509 (4)	131
C8—H8A···Cl1^{iii}	0.97	2.84	3.719 (6)	151

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) −*x*, −*y*+2, −*z*+1; (iii) −*x*, −*y*+2, −*z*.

Fig. 1

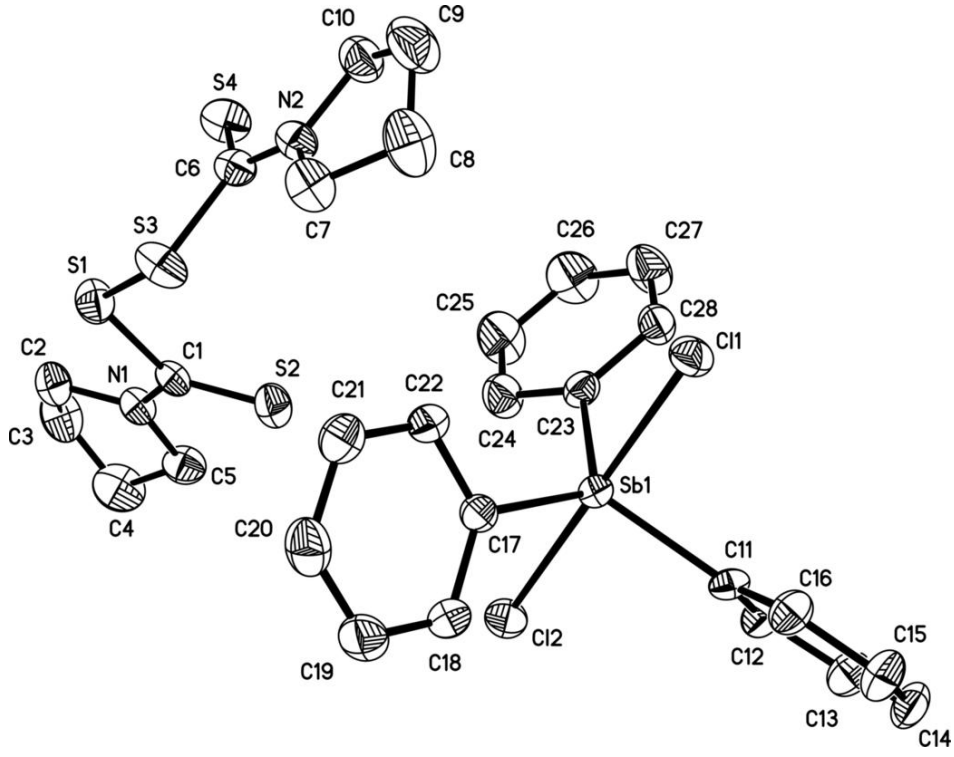
C10
C9
S4
N2
C6
C8
C7
S3
S1
C26
C27
C25
C28
Cl1
C2
N1
C1
S2
C21
C22
C24
C23
C3
C5
Sb1
C4
C20
C17
C11
C16
Cl2
C15
C12
C19
C18
C13
C14

Fig. 2