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

**Li Quan, Handong Yin,* Jun Zhai and Daqi Wang**

College of Chemistry and Chemical Engineering, Liaocheng University, Shandong 252059, People's Republic of China
Correspondence e-mail: handongyin@163.com

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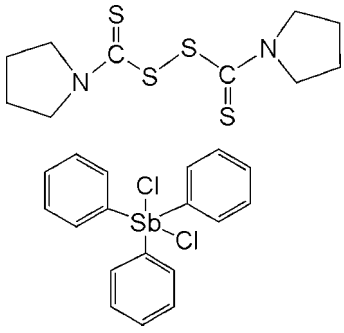
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.007 Å; $R$ factor = 0.031; $wR$ factor = 0.092; data-to-parameter ratio = 16.6.

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
$\beta$ = 105.509 (2)°
$V$ = 3177.7 (8) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 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—H8$A$···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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# supporting information

*Acta Cryst.* (2008). E**64**, m108 [https://doi.org/10.1107/S1600536807063830]

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

**Li Quan, Handong Yin, Jun Zhai and Daqi Wang**

### S1. 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).

### S2. 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.

### S3. 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) = 1.2$U_{eq}$(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).

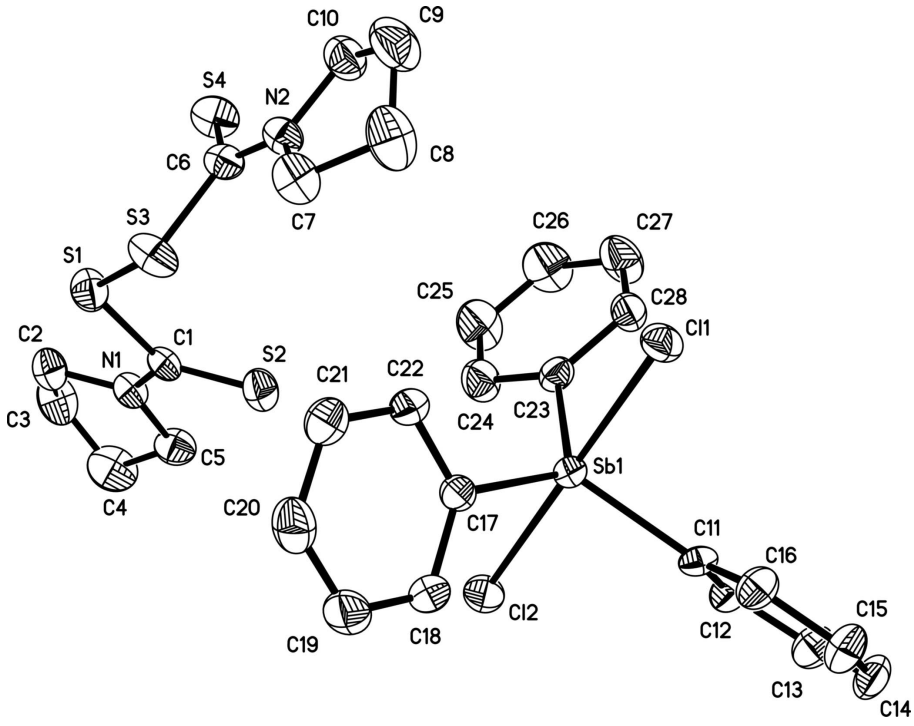


**Figure 1**

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

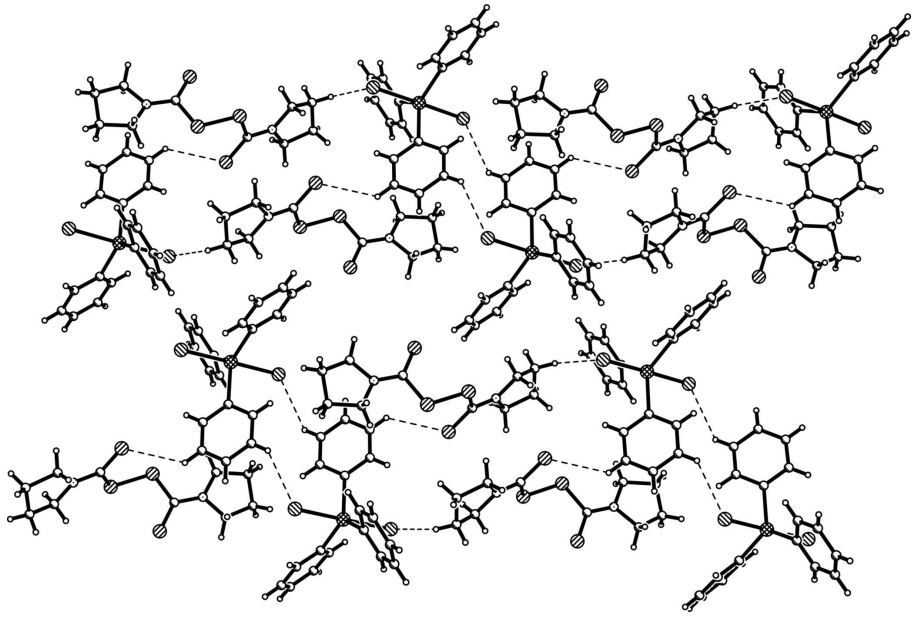

**Figure 2**

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*

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

*Data collection*

Siemens SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.558$, $T_{max} = 0.627$
14597 measured reflections
5560 independent reflections
4333 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.0°$
$h = -17\rightarrow10$
$k = -16\rightarrow16$
$l = -19\rightarrow19$

*Refinement*

Refinement on f$^2$
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
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
$w = 1/[\sigma^2(F_o^2) + (0.045P)^2 + 1.9404P]$ 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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, º)*

| | | | |
|---|---|---|---|
| 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 | | |

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| 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 |

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| 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) |

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| 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, º)*

| *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—H8*A*···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*.