The interstack contacts are shown in Fig. 2. There exist one Se—Se and two S—S contacts shorter than the sum of the van der Waals radii. These contacts lie between molecules related by a translation of *a* along the *a* axis, in contrast to TMTSF salts (Thorup, Rindorf, Soling & Bechgaard, 1981). The ethylenedithio group contributes to the S—S interstack contacts. The interstack contacts in $(DMET)_2Au(CN)_2$ are related to the appearance of superconductivity. The detailed comparison of crystal structures will be helpful in clarifying this point. The crystal structures of other DMET salts will be published shortly.

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Structure of Phenylbis[2-pyridinethiolato(1−)]antimony(III)

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Abstract. $[Sb(C_5H_4NS)_2(C_6H_5)]$, $M_r = 419{\cdot}2$, monoclinic, $P2_1/c$, $a = 11{\cdot}123\,(9)$, $b = 15{\cdot}649\,(5)$, $c = 10{\cdot}165\,(14)$ Å, $\beta = 115{\cdot}27\,(9)°$, $V = 1600{\cdot}0$ Å^3, $Z = 4$, $D_x = 1{\cdot}740$ Mg m^{-3}, $F(000) = 824$, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71069$ Å, $\mu = 1{\cdot}98$ mm^{-1}, $T = 291\,(1)$ K. Final $R = 0{\cdot}016$ for 2279 unique observed $[I \geq 1{\cdot}96\sigma(I)]$ X-ray diffractometer data. In the distorted tetragonal pyramidal (pseudo-octahedral) coordination polyhedron around Sb the two S and the two N atoms [Sb—S 2·503 (1), 2·500 (1) Å; S—Sb—S 85·00 (2)°; Sb—N 2·633 (2), 2·725 (2) Å; N—Sb—N 152·76 (6)°] are in *cis*-position, the phenyl group is in apical position. Intermolecular distances exceed van der Waals distances.

Experimental. The compound was prepared from $C_6H_5SbCl_2$ and sodium 2-pyridinethiolate in ethanol at 343 K. Colorless crystals from DMF. M.p. 443–445 K. Crystal size ~0·3 × 0·4 × 0·4 mm, $\omega/2\theta$ scan, scan speed 1·1–3·3° min^{-1} in θ, Nonius CAD-4 diffractometer, graphite-monochromated Mo $K\alpha$; lattice parameters from least-squares fit with 25 reflections up to $2\theta = 26{\cdot}2°$; six standard reflections recorded every 2·5 h, only random deviations; 9293 reflections measured; $1{\cdot}5 \leq \theta \leq 25{\cdot}0°$, $-12 \leq h \leq 12$,

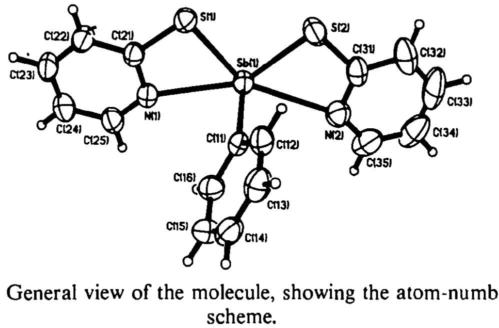

Fig. 1. General view of the molecule, showing the atom-numbering scheme.

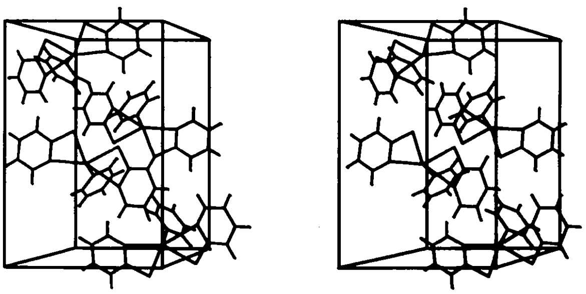

Fig. 2. Stereoscopic view of the unit cell (*b* vertical, *c* horizontal).

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$-18 \le k \le 18$, $-13 \le l \le 5$; after averaging ($R_{\rm int}$ = 0·016): 2926 unique reflections, 2279 with $I \ge 1{\cdot}96\sigma(I)$; Lorentz–polarization correction and absorption correction *via* ψ scans; max./min. transmission 1·00/0·80; systematic absences ($h0l$) $l = 2n + 1$, ($0k0$) $k = 2n + 1$ conform to space group $P2_1/c$; structure solution *via* direct methods, ΔF syntheses and full-matrix least-squares refinement with anisotropic temperature factors for all non-H atoms and a common isotropic temperature factor for H atoms, which were placed in geometrically calculated positions (C—H 0·95 Å); refinement on F with 2279 reflections and 191 refined parameters; $w = 4F_o^2/[\sigma^2(F_o^2) + (0{\cdot}02F_o^2)^2]$; S = 0·90, R = 0·016, wR = 0·020, $(\Delta/\sigma)_{\rm max}$ = 0·01, no extinction correction; largest peak in final ΔF map ±0·3 (1) e Å^{-3}, complex neutral-atom scattering factors from *International Tables for X-ray Crystallography* (1974); programs: Enraf–Nonius *Structure Determination Package* (Frenz, 1981), *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980), *ORTEP*II (Johnson, 1976), *POP*1 (van de Waal, 1976).

Table 1. *Atomic coordinates and equivalent isotropic thermal parameters* (Å^2 × 10^3)

$$U_{\rm eq} = (1/6\pi^2)\textstyle\sum_i\sum_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
Sb(1)	0·16029 (1)	−0·08229 (1)	0·05609 (1)	36
S(1)	0·25177 (6)	0·05855 (4)	0·17232 (6)	43
S(2)	0·11151 (7)	−0·00684 (4)	−0·17807 (7)	52
N(1)	0·2701 (2)	−0·0710 (1)	0·3419 (2)	41
N(2)	0·0664 (2)	−0·1722 (1)	−0·1977 (2)	51
C(11)	0·3513 (2)	−0·1337 (1)	0·0884 (2)	36
C(12)	0·4201 (2)	−0·1042 (2)	0·0118 (2)	48
C(13)	0·5424 (2)	−0·1382 (2)	0·0359 (3)	55
C(14)	0·5967 (2)	−0·2029 (2)	0·1369 (3)	56
C(15)	0·5297 (3)	−0·2325 (2)	0·2133 (3)	57
C(16)	0·4074 (2)	−0·1980 (2)	0·1895 (3)	47
C(21)	0·2957 (2)	0·0124 (2)	0·3439 (2)	37
C(22)	0·3527 (2)	0·0583 (2)	0·4736 (3)	49
C(23)	0·3784 (3)	0·0170 (2)	0·6011 (3)	55
C(24)	0·3485 (3)	−0·0688 (2)	0·5992 (3)	58
C(25)	0·2965 (3)	−0·1106 (2)	0·4682 (3)	50
C(31)	0·0396 (2)	−0·1009 (2)	−0·2755 (2)	47
C(32)	−0·0433 (3)	−0·0991 (2)	−0·4231 (3)	69
C(33)	−0·0964 (3)	−0·1750 (3)	−0·4902 (3)	88
C(34)	−0·0685 (3)	−0·2492 (2)	−0·4121 (3)	80
C(35)	0·0120 (3)	−0·2454 (2)	−0·2662 (3)	66

Table 2. *Bond distances* (Å) *and angles* (°)

Sb(1)—C(11)	2·162 (1)	N(2)—C(31)	1·325 (3)
Sb(1)—S(2)	2·500 (1)	C(21)—C(22)	1·394 (3)
Sb(1)—S(1)	2·503 (1)	C(22)—C(23)	1·366 (3)
Sb(1)—N(1)	2·633 (2)	C(23)—C(24)	1·382 (4)
Sb(1)—N(2)	2·725 (2)	C(24)—C(25)	1·371 (3)
S(1)—C(21)	1·753 (2)	C(31)—C(32)	1·386 (3)
S(2)—C(31)	1·764 (3)	C(32)—C(33)	1·372 (5)
N(1)—C(21)	1·334 (3)	C(33)—C(34)	1·366 (5)
N(1)—C(25)	1·340 (3)	C(34)—C(35)	1·369 (4)
N(2)—C(35)	1·342 (4)		

C(11)—Sb(1)—S(2)	96·89 (5)	C(35)—N(2)—Sb(1)	146·8 (1)
C(11)—Sb(1)—S(1)	94·63 (6)	C(12)—C(11)—Sb(1)	122·4 (2)
C(11)—Sb(1)—N(1)	83·96 (6)	C(16)—C(11)—Sb(1)	119·1 (1)
C(11)—Sb(1)—N(2)	84·63 (6)	N(1)—C(21)—C(22)	121·8 (2)
N(1)—Sb(1)—N(2)	152·76 (6)	N(1)—C(21)—S(1)	114·9 (2)
S(2)—Sb(1)—S(1)	85·00 (2)	C(22)—C(21)—S(1)	123·3 (2)
S(2)—Sb(1)—N(1)	145·95 (4)	C(23)—C(22)—C(21)	118·7 (2)
S(2)—Sb(1)—N(2)	60·18 (5)	C(22)—C(23)—C(24)	119·7 (2)
S(1)—Sb(1)—N(1)	61·08 (4)	C(25)—C(24)—C(23)	118·5 (2)
S(1)—Sb(1)—N(2)	144·68 (4)	N(1)—C(25)—C(24)	122·6 (2)
C(31)—S(2)—Sb(1)	90·14 (8)	N(2)—C(31)—C(32)	122·6 (3)
C(21)—S(1)—Sb(1)	89·51 (8)	N(2)—C(31)—S(2)	115·8 (2)
C(21)—N(1)—C(25)	118·7 (2)	N(2)—C(35)—C(34)	122·8 (3)
C(25)—N(1)—Sb(1)	146·5 (2)	C(32)—C(31)—S(2)	121·6 (2)
C(21)—N(1)—Sb(1)	94·5 (1)	C(33)—C(32)—C(31)	117·8 (3)
C(31)—N(2)—Sb(1)	91·6 (1)	C(33)—C(34)—C(35)	118·3 (3)
C(31)—N(2)—C(35)	118·2 (2)	C(34)—C(33)—C(32)	120·4 (3)

C—C distances and C—C—C angles of the phenyl ring are in the range 1·367 (3) to 1·385 (3) Å, mean value 1·381 (4) Å, and 118·6 (2) and 120·8 (2)°, mean value 120·0 (2)°.

Discussion. The structure of the title compound and the numbering scheme are shown in Fig. 1 and a stereoscopic view of the unit cell in Fig. 2. Positional parameters and the equivalent values of the anisotropic temperature factors for the non-H atoms are given in Table 1.* Bond lengths and angles are given in Table 2. The asymmetric unit contains one molecule. Both 2-pyridinethiolato ligands extend the equatorial plane of a distorted tetragonal pyramidal (pseudo-octahedral) polyhedron around Sb, the two S atoms as well as the two N atoms being in *cis* position. The Sb—N distances are appreciably shorter, the Sb—S distances are only slightly longer than in tris[2-pyridinethiolato(1−)]antimony(III) (Bozopoulos, Kokkou & Rentzeperis, 1984). In contrast to the latter compound and to diphenyl[8-quinolinethiolato(1−)-*S*]antimony(III) (Preut, Praeckel & Huber, 1986) the intermolecular Sb···Sb distance of 4·145 (1) Å is longer than the van der Waals distance, excluding Sb···Sb interaction in the title compound.

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* Lists of H-atom coordinates, anisotropic thermal parameters and structure-factor amplitudes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44531 (19 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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