0.022 Å [M—Cl(1)($-x$, $1-y$, $1-z$)] to 0.040 Å (M—O etheric, capping) and average 0.03 Å. Similar average distances in the related complex $[PrCl(OH_2)_3(EO4)]Cl_2.H_2O$ (Rogers, Etzenhouser, Murdoch & Reyes, 1991) are an average 0.07 Å shorter as a consequence of the reduced number of tight ion pairs compared to the title complex.

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Structure of Bis(*N*,*N*-diethyldithiocarbamato)gold(III) Hexafluoroantimonate

BY MAOCHUN HONG,* ZHIYING HUANG, XINJIAN LEI, FEILONG JIANG AND HANQIN LIU

Fujian Institute of Research on the Structure of Matter and Fuzhou Laboratory of Structural Chemistry, Chinese Academy of Sciences, Fuzhou, Fujian 350002, *People's Republic of China*

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Abstract. $[Au\{S_2CN(C_2H_5)_2\}_2]SbF_6$, $M_r = 1458.55$, triclinic, $P\bar{1}$, $a = 14.533$ (3), $b = 18.004$ (5), $c = 8.538$ (2) Å, $\alpha = 100.37$ (4), $\beta = 105.92$ (5), $\gamma = 74.69$ (3)°, $V = 2058.06$ Å^3, $Z = 4$, $D_x = 2.353$ g cm^{-3}, Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å, $\mu = 88.7$ cm^{-1}, $F(000) = 1368$, $T = 296$ (1) K, $R = 0.048$ and $wR = 0.056$ for 4323 reflections with $I > 3\sigma(I)$. Each Au atom is four coordinated in a plane. The Au—S bond distances fall in the range 2.318–2.330 Å.

Experimental. The title compound was prepared by reaction of Ph_2PAuCl, $NaS_2CNEt_2.3H_2O$ and $NaSbF_6$ in EtOH solution and a crystal suitable for X-ray analysis was grown by evaporation of the reaction solution in air.

Diffraction intensities were collected from a prismatic pale-yellow crystal 0.30 × 0.30 × 0.60 mm in the θ–2θ scan mode on a Rigaku AFC5R diffractometer using graphite-monochromatized Mo $K\alpha$ radiation. Cell constants were obtained from least-squares refinement of 20 reflections (θ from 8 to 10°). A total of 7399 reflections were collected in the range $3 < 2\theta < 50°$ ($0 < h < 15$, $-21 < k < 21$, $-10 < l < 10$). The intensities were monitored by three representative reflections. The data were corrected for the fluctuation of the monitored reflections (between 1.000 and 0.981), the Lp factor, and empirical absorption (between 1.112 and 0.905), but no extinction correction was made. 4323 unique reflections with $I > 3\sigma(I)$ were used for structure solution and refinement. Calculations were performed on a VAX 11/785 computer with the *SDP* program package (Frenz, 1978). All metal atoms were located from the E map. A Fourier map phased by the metal atoms contained most of the remaining non-H atoms. H atoms were not included in the calculation. 433 variables were used in the refinement. $R_{int} = 0.067$. Full-matrix least-squares refinement with anisotropic thermal parameters for all non-H atoms led to convergence with $R = 0.048$ and $wR = 0.056$. Function minimized was $\sum w(|F_o| - |F_c|)^2$, where $w^{-1} = 1 + \{[(F_o)^2 + 2\sigma(F_o)|F_o|]^{1/2} - |F_o|\}^2 + (0.01F_o)^2$. Atomic scattering factors were taken from *International Tables for X-ray Crystallography* (Cromer & Waber, 1974). The goodness of fit (S) is 2.01. The largest Δ/σ value in the final cycle is 0.40 while the extreme peaks in the difference electron density map are 1.95 and -1.67 e Å^{-3}. Final positional parameters given in Table 1, and atomic distances and bond angles are list in Table 2.† The atomic labelling scheme and the structure of the cation are shown in Fig. 1, and the cell packing is shown in Fig. 2.

Related literature. Crystal structures of related compounds have been studied: $[Au(S_2CNBu_2)_2]$-$[AuBr_2]$ (Beurskens, Blaauw, Cras & Steggerda, 1968), $[Au(S_2CNBu_2)_2]Br$ (Beurskens, Cras & van der Linden, 1970), [3,3′-Au(1,2-$C_2B_9H_{11})_2$][Au-$(S_2CNEt_2)_2$] (Colquhoun, Greenhough & Wallbridge, 1977).

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† Tables of anisotropic thermal parameters and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54810 (13 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AS0529]

* To whom correspondence should be addressed.

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Table 1. *Positional parameters and equivalent isotropic displacement parameters with e.s.d.'s in parentheses*

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as: $(4/3) \times [a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + bc(\cos\beta)B(1,3) + ac(\cos\alpha)B(2,3)]$.

	x	y	z	B_{eq} (Å^2)
Au(1)	0.94780 (5)	0.60835 (4)	0.65278 (9)	2.87 (2)
Au(2)	0.35591 (5)	−0.10628 (4)	0.53398 (8)	2.48 (1)
Sb(1)	0.5635 (1)	0.34575 (8)	0.8224 (2)	3.10 (3)
Sb(2)	0.1572 (1)	0.13515 (9)	1.0282 (2)	3.75 (3)
S(1)	1.1055 (4)	0.6304 (3)	0.7275 (6)	3.5 (1)
S(2)	0.7873 (4)	0.5928 (3)	0.5806 (6)	3.1 (1)
S(3)	0.9869 (4)	0.6066 (3)	0.4050 (6)	3.5 (1)
S(4)	0.9109 (4)	0.6105 (3)	0.9015 (6)	3.9 (1)
S(5)	0.1858 (4)	−0.0749 (3)	0.4922 (6)	3.4 (1)
S(6)	0.3276 (3)	−0.1498 (3)	0.7533 (6)	3.3 (1)
S(7)	0.5258 (3)	−0.1327 (3)	0.5857 (5)	2.8 (1)
S(8)	0.3869 (4)	−0.0656 (3)	0.3133 (6)	3.1 (1)
F(11)	0.498 (1)	0.408 (1)	0.974 (2)	7.9 (5)
F(12)	0.665 (2)	0.317 (2)	0.977 (2)	20.8 (9)
F(13)	0.510 (1)	0.271 (1)	0.827 (2)	20.6 (5)
F(14)	0.611 (1)	0.422 (1)	0.803 (2)	16.4 (5)
F(15)	0.630 (1)	0.2818 (9)	0.674 (2)	7.5 (4)
F(16)	0.463 (2)	0.379 (2)	0.661 (3)	19 (1)
F(21)	0.244 (1)	0.1878 (9)	1.169 (2)	7.9 (5)
F(22)	0.258 (1)	0.061 (1)	0.968 (2)	10.6 (5)
F(23)	0.168 (1)	0.0775 (9)	1.197 (2)	7.1 (4)
F(24)	0.054 (1)	0.2063 (9)	1.095 (2)	8.3 (5)
F(25)	0.148 (1)	0.194 (1)	0.867 (2)	9.3 (5)
F(26)	0.068 (1)	0.082 (1)	0.890 (2)	10.3 (6)
N(10)	1.170 (1)	0.6306 (9)	0.460 (2)	3.3 (4)
N(20)	0.721 (1)	0.6086 (9)	0.850 (2)	3.0 (4)
N(30)	0.135 (1)	−0.1208 (8)	0.735 (2)	3.0 (4)
N(40)	0.582 (1)	−0.0966 (8)	0.342 (2)	2.8 (3)
C(10)	1.099 (1)	0.622 (1)	0.520 (2)	3.0 (4)
C(11)	1.263 (1)	0.649 (1)	0.575 (3)	4.0 (5)
C(12)	1.342 (2)	0.575 (1)	0.608 (3)	5.3 (6)
C(13)	1.162 (2)	0.619 (1)	0.282 (3)	4.4 (6)
C(14)	1.120 (2)	0.699 (2)	0.211 (3)	6.2 (8)
C(20)	0.793 (1)	0.605 (1)	0.789 (2)	2.3 (4)
C(21)	0.620 (1)	0.604 (1)	0.748 (2)	2.9 (4)
C(22)	0.554 (2)	0.684 (2)	0.731 (3)	5.6 (7)
C(23)	0.730 (2)	0.625 (1)	1.037 (2)	4.0 (5)
C(24)	0.762 (2)	0.546 (1)	1.106 (3)	6.1 (7)
C(30)	0.202 (1)	−0.116 (1)	0.671 (2)	2.4 (4)
C(31)	0.157 (1)	−0.163 (1)	0.883 (2)	3.6 (4)
C(32)	0.159 (2)	−0.104 (1)	1.036 (3)	5.4 (7)
C(33)	0.030 (1)	−0.087 (1)	0.658 (2)	3.4 (5)
C(34)	−0.016 (2)	−0.148 (2)	0.536 (3)	5.3 (7)
C(40)	0.511 (1)	−0.097 (1)	0.402 (2)	2.7 (4)
C(41)	0.562 (1)	−0.066 (1)	0.178 (2)	3.3 (5)
C(42)	0.559 (2)	−0.135 (1)	0.040 (2)	4.8 (6)
C(43)	0.686 (1)	−0.123 (1)	0.430 (2)	3.2 (4)
C(44)	0.724 (2)	−0.211 (1)	0.400 (3)	4.9 (6)

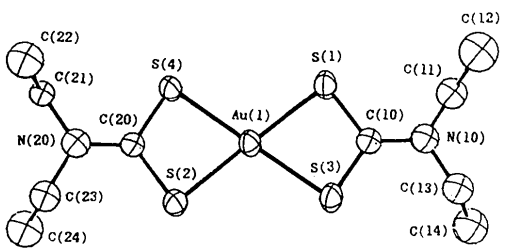

Fig. 1. Molecular structure and atomic labelling scheme for the cation.

Table 2. *Selected bond distances* (Å) *and angles* (°)

Au(1)—S(1)	2.326 (6)	N(10)—C(13)	1.47 (3)
Au(1)—S(2)	2.323 (5)	N(20)—C(20)	1.27 (3)
Au(1)—S(3)	2.330 (6)	N(20)—C(21)	1.50 (2)
Au(1)—S(4)	2.320 (6)	N(20)—C(23)	1.54 (3)
Au(2)—S(5)	2.326 (5)	N(30)—C(30)	1.27 (3)
Au(2)—S(6)	2.326 (6)	N(30)—C(31)	1.51 (3)
Au(2)—S(7)	2.318 (5)	N(30)—C(33)	1.49 (2)
Au(2)—S(8)	2.330 (6)	N(40)—C(40)	1.28 (3)
S(1)—C(10)	1.73 (2)	N(40)—C(41)	1.51 (3)
S(2)—C(20)	1.74 (2)	N(40)—C(43)	1.49 (3)
S(3)—C(10)	1.72 (2)	C(11)—C(12)	1.52 (3)
S(4)—C(20)	1.74 (2)	C(13)—C(14)	1.57 (4)
S(5)—C(30)	1.75 (2)	C(21)—C(22)	1.52 (3)
S(6)—C(30)	1.75 (1)	C(23)—C(24)	1.55 (3)
S(7)—C(40)	1.74 (2)	C(31)—C(32)	1.52 (3)
S(8)—C(40)	1.74 (1)	C(33)—C(34)	1.53 (3)
N(10)—C(10)	1.32 (3)	C(41)—C(42)	1.55 (3)
N(10)—C(11)	1.52 (2)	C(43)—C(44)	1.53 (3)

S(1)—Au(1)—S(2)	177.3 (2)	Au(1)—S(1)—C(10)	86.5 (7)
S(1)—Au(1)—S(3)	75.4 (2)	Au(1)—S(2)—C(20)	87.0 (6)
S(1)—Au(1)—S(4)	103.8 (2)	Au(1)—S(3)—C(10)	86.7 (7)
S(2)—Au(1)—S(3)	105.1 (2)	Au(1)—S(4)—C(20)	87.0 (7)
S(2)—Au(1)—S(4)	75.8 (2)	Au(2)—S(5)—C(30)	87.4 (6)
S(3)—Au(1)—S(4)	179.2 (2)	Au(2)—S(6)—C(30)	87.4 (7)
S(5)—Au(2)—S(6)	75.6 (2)	Au(2)—S(7)—C(40)	87.2 (7)
S(5)—Au(2)—S(7)	177.2 (2)	Au(2)—S(8)—C(40)	86.9 (7)
S(5)—Au(2)—S(8)	105.4 (2)	S(1)—C(10)—S(3)	111 (1)
S(6)—Au(2)—S(7)	103.6 (2)	S(2)—C(20)—S(4)	110 (1)
S(6)—Au(2)—S(8)	178.7 (2)	S(5)—C(30)—S(6)	110 (1)
S(7)—Au(2)—S(8)	75.5 (2)	S(7)—C(40)—S(8)	110 (1)

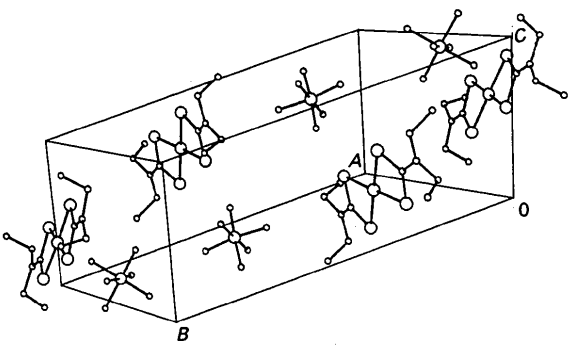

Fig. 2. Cell packing for $[Au\{S_2CN(C_2H_5)_2\}_2]SbF_6$.

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