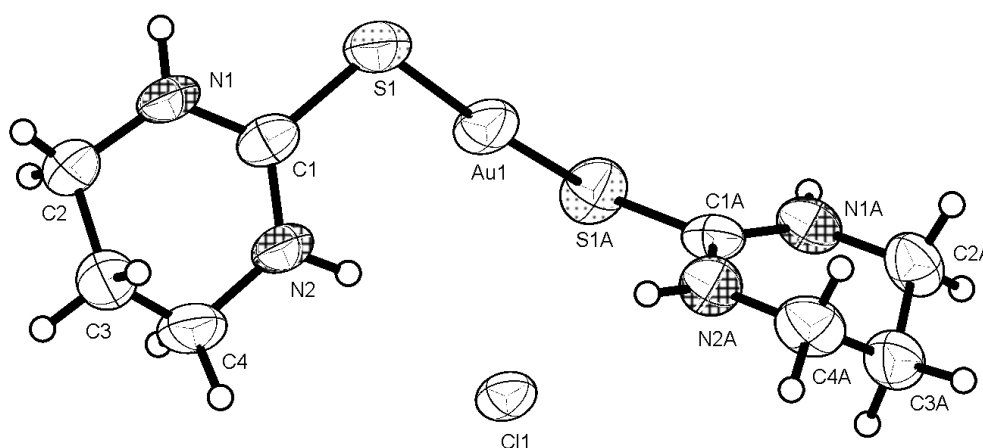


Crystal structure of bis(3,4,5,6-tetrahydropyrimidine-2(1*H*)-thione-*S*)gold(I) chloride, [Au(C₄H₈N₂S)₂]Cl

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Abstract

C₈H₁₆AuClN₄S₂, orthorhombic, *Pbcn* (no. 60),
 $a = 11.906(1) \text{ \AA}$, $b = 11.751(1) \text{ \AA}$, $c = 10.062(1) \text{ \AA}$,
 $V = 1407.6 \text{ \AA}^3$, $Z = 4$, $R_{\text{gt}}(F) = 0.031$, $wR_{\text{ref}}(F^2) = 0.077$,
 $T = 294 \text{ K}$.

Source of material

The title complex was prepared according to the procedure reported earlier [1]. Colorless parallelepipedic crystals were obtained by slow evaporation from a methanol solution.

Discussion

Gold(I) complexes are of current interest for instance because of their potential antirheumatic activity [2]. In this context, bis-(thione)gold(I) complexes present a variety of geometrical differences. The structural and computational data show that the hydrogen bonding scheme of the coordinated thione ligands is the main determining factor of the geometry of the complex [3].

In the title compound, the gold metal ion is two coordinated and located on a two-fold rotation axis. It is bound to the S atoms of two symmetry-related tetrahydropyrimidinethione ligand molecules ($d(\text{Au1}-\text{S1}) = 2.2769 \text{ \AA}$). The Au—S bond distances reported for related complexes bis(dimethylthiourea)gold(I) and bis(imidazolinethione)gold(I) are 2.285 Å and 2.304 Å [4] as well as 2.318 Å [5]. The coordination deviates from perfect linearity ($\angle \text{S1}-\text{Au1}-\text{S1A} = 174.57^\circ$). The shortest Au...Au distance is 5.041 Å, ruling out any metal-metal interaction. The SCN₂ moiety of the ligand molecule is essentially planar (mean deviation of 0.0033 Å) with following bond lengths $d(\text{S1}-\text{C1}) = 1.739 \text{ \AA}$, $d(\text{C1}-\text{N1}) = 1.323 \text{ \AA}$, $d(\text{C1}-\text{N2}) = 1.311 \text{ \AA}$. The corresponding bond lengths reported for the free ligand are $d(\text{S}-\text{C}) = 1.720 \text{ \AA}$ and $d(\text{C}-\text{N}) = 1.331 \text{ \AA}$ [6]. Within the ligand molecule, the two

S—C—N bond angles differ by approximately 5°, a very close value to that observed in bis(thiourea)Au(I) chloride [7] while only about half the difference has been reported for the bromide salt [8]. The chloride ion is also located on the two-fold rotation axis and has non-bonding contacts with the N atoms of the ligand molecule. The N...Cl⁻ shortest distances are in the range of 3.226 Å – 3.229 Å, suggesting hydrogen bonding.

Table 1. Data collection and handling.

Crystal:	colorless parallelepiped, size 0.32 × 0.35 × 0.46 mm
Wavelength:	Mo <i>K</i> _α radiation (0.71073 Å)
μ :	109.19 cm ⁻¹
Diffractometer, scan mode:	Bruker SMART Apex CCD, ω
$2\theta_{\text{max}}$:	56.58°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	11352, 1707
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1380
$N(\text{param})_{\text{refined}}$:	75
Programs:	SADABS [9], SHELXTL [10]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(1)	8 <i>d</i>	0.8822	0.4942	0.2035	0.056
H(2)	8 <i>d</i>	0.6429	0.7001	0.1767	0.060
H(2A)	8 <i>d</i>	0.9192	0.5896	-0.0094	0.064
H(2B)	8 <i>d</i>	1.0044	0.6132	0.1067	0.064
H(3A)	8 <i>d</i>	0.9100	0.7769	0.1664	0.067
H(3B)	8 <i>d</i>	0.9326	0.7845	0.0127	0.067
H(4A)	8 <i>d</i>	0.7441	0.8305	0.0654	0.069
H(4B)	8 <i>d</i>	0.7511	0.7271	-0.0334	0.069

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