Refinement of the crystal structure of bis[(di-*n*-propyldithiocarbamato)gold(I)], C₇H₁₄AuNS₂

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Received September 18, 2002; accepted and available on-line November 11, 2002; CCDC-No. 1267931

Abstract

C₇H₁₄AuNS₂, tetragonal, $P\bar{4}b2$ (No. 117), $a = 13.1178(7)$ Å, $c = 6.0819(6)$ Å, $V = 1046.6$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.029$, $wR_{\text{ref}}(F^2) = 0.079$, $T = 183$ K.

Source of material

Bis[(di-*n*-propyldithiocarbamato)gold(I)], a known species [1], was isolated as yellow needles from the attempted recrystallization of (furyl)₃PAu(S₂CN_nPr₂) from an acetonitrile solution of the compound.

Experimental details

The H atoms were placed in their geometrically calculated positions and included in the final refinement in the riding model approximation.

Discussion

The crystal structure of [Au(S₂CN_nPr₂)]₂ was reported from photographic data [1]. The new X-ray analysis confirms the original description but with geometric parameters of greater precision. The molecule is highly symmetric with the Au atom situated on a mirror plane and the C1 & N1 atoms lying on a perpendicular mirror plane so that the asymmetric unit is $1/2 \times (\text{AuS}_2\text{CN}_n\text{Pr}_2)$. The structure comprises dimeric units stabilised by transannular Au...Au interactions with $d(\text{Au}\cdots\text{Au}) = 2.8071(5)$ Å. As illustrated in the figure, dimeric units are linked into a chain running parallel to the *c*-axis by somewhat weaker intermolecular Au...Au contacts of $3.2748(6)$ Å. Other important geometric parameters are $d(\text{Au}-\text{S}) = 2.285(1)$ Å, $d(\text{S1}-\text{C1}) = 1.738(3)$ Å, $d(\text{C1}-\text{N1}) = 1.312(9)$ Å and $\angle \text{S1}-\text{Au}-\text{S1} = 178.04(6)^\circ$.

Table 1. Data collection and handling.

Crystal:	yellow needle, size 0.05 × 0.07 × 0.26 mm
Wavelength:	Mo K α radiation (0.7107 Å)
μ :	143.99 cm ⁻¹
Diffraction, scan mode:	Bruker AXS SMART CCD, ω
$2\theta_{\text{max}}$:	60°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	8506, 1544
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1180
$N(\text{param})_{\text{refined}}$:	53
Programs:	teXsan [2], SHELXL-97 [3], ORTEP [4]

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(2a)	8i	0.1753	0.3131	0.1922	0.048
H(2b)	8i	0.2296	0.2216	0.3210	0.048
H(3a)	8i	0.0695	0.1945	0.0090	0.054
H(3b)	8i	0.1236	0.1032	0.1395	0.054
H(4a)	8i	-0.0323	0.1468	0.3099	0.117
H(4b)	8i	0.0078	0.2607	0.3468	0.117
H(4c)	8i	0.0604	0.1680	0.4749	0.117

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Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Au	4f	1/2	0	0.23077(4)	0.0267(2)	0.0225(2)	0.0155(1)	0.0006(1)	0.0	0.0
S(1)	8i	0.3438(1)	0.0771(1)	0.2244(2)	0.0286(6)	0.0345(7)	0.0184(5)	0.0052(6)	0.0052(6)	0.0064(5)
N(1)	4g	0.2701(3)	1/2 - x	0	0.032(2)	U ₁₁	0.022(3)	0.004(3)	0.003(2)	U ₁₃
C(1)	4g	0.3409(4)	1/2 - x	0	0.026(2)	U ₁₁	0.017(3)	-0.004(3)	0.000(3)	U ₁₃
C(2)	8i	0.1963(5)	0.2407(4)	0.1810(8)	0.059(4)	0.039(3)	0.022(3)	0.027(3)	0.009(3)	-0.003(3)
C(3)	8i	0.1031(4)	0.1757(5)	0.149(1)	0.033(3)	0.057(4)	0.046(4)	0.012(3)	0.010(3)	0.011(3)
C(4)	8i	0.0281(6)	0.1890(8)	0.337(2)	0.069(5)	0.095(7)	0.071(7)	0.046(5)	0.043(5)	0.035(5)

Acknowledgment. The National University of Singapore is thanked for support (R-143-000-139-112).

References

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