Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Triphenyl-*n*-propylphosphonium bis(2-thioxo-1,3-dithiole-4,5-dithiolato)aurate(III)

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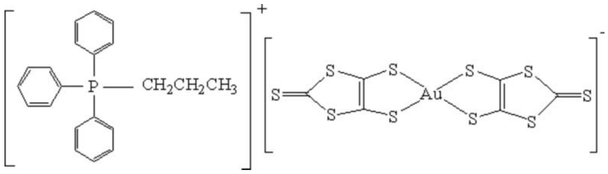
Received 27 August 2007; accepted 7 September 2007

Key indicators: single-crystal X-ray study; *T* = 296 K; mean σ(C–C) = 0.005 Å; *R* factor = 0.025; *wR* factor = 0.060; data-to-parameter ratio = 21.0.

In the title complex, $(C_{21}H_{22}P)[Au(C_3S_5)_2]$ or $(Ph_3C_3H_7P)[Au(dmit)_2]$ (where $Ph_3C_3H_7P$ is the triphenyl-*n*-propylphosphonium cation and dmit is the 2-thioxo-1,3-dithiole-4,5-dithiolate anion), the Au^{III} atom exhibits a square-planar coordination involving four S atoms from two dmit ligands. The $[Au(dmit)_2]^-$ anions form discrete pairs with a long intermolecular Au⋯S interaction for each Au atom in the crystal structure.

Related literature

For related literature, see: Allen *et al.* (1987); Cassoux (1999); Coe (2004); Kuang *et al.* (2003); Li *et al.* (2005, 2006); Liu *et al.* (2002); Matsubayashi & Yokozawa (1990); Miura *et al.* (2004); Pauling (1960); Pullen & Olk (1999); Robertson & Cronin (2002); Sheik-Bahae *et al.* (1989, 1990); Steimeck & Kirmse (1979); Sun *et al.* (2006); Svenstrup & Becher (1995); Wang *et al.* (1999, 2005); Yang *et al.* (2005).



Experimental

Crystal data

$(C_{21}H_{22}P)[Au(C_3S_5)_2]$
M_r = 894.98
Monoclinic, $P2_1/n$
a = 8.4916 (1) Å
b = 25.8266 (3) Å
c = 14.9202 (2) Å
β = 97.979 (1)°
V = 3240.46 (7) Å^3
Z = 4
Mo *K*α radiation
μ = 5.25 mm^{-1}
T = 296 (2) K
0.23 × 0.19 × 0.17 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*APEX2*; Bruker, 2005)
T_{min} = 0.378, T_{max} = 0.469 (expected range = 0.330–0.409)
28396 measured reflections
7419 independent reflections
6100 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.060
S = 1.04
7419 reflections
353 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.87 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Au1—S6	2.3160 (8)	Au1—S4	2.3212 (8)
Au1—S7	2.3182 (9)	Au1—S5	2.3221 (8)
S6—Au1—S7	91.34 (3)	S6—Au1—S5	178.54 (3)
S6—Au1—S4	88.22 (3)	S7—Au1—S5	88.64 (3)
S7—Au1—S4	178.58 (4)	S4—Au1—S5	91.83 (3)

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

This work was supported by the Foundation for the Author of National Excellent Doctoral Dissertation of the People's Republic of China (grant No. 200539) and by the National Natural Science Foundation of China (grant Nos. 60476020, 60608010 and 50672049).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2133).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–S19.
Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
Bruker (1997). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2005). *APEX2*. Version 2.0-2. Bruker AXS Inc., Madison, Wisconsin, USA.
Cassoux, P. (1999). *Coord. Chem. Rev.* **185**, 213–232.
Coe, B. J. (2004). *Comprehensive Coordination Chemistry II*, Vol. 9, edited by J. A. McCleverty & T. J. Meyer, pp. 621–687. Oxford: Elsevier–Pergamon.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Kuang, L., Chen, Q. Y., Sargent, E. H. & Wang, Z. Y. (2003). *J. Am. Chem. Soc.* **125**, 13648–13649.
Li, T. B., Yu, W. T., Xu, D., Ren, Q., Zhang, G. H. & Wang, X. Q. (2005). *Z. Kristallogr. New Cryst. Struct.* **220**, 625–626.
Li, T. B., Yu, W. T., Xu, D., Zhang, G. H. & Wang, X. Q. (2006). *Z. Kristallogr. New Cryst. Struct.* **221**, 55–56.
Liu, C. M., Zhang, D. Q., Song, Y. L., Zhang, C. L., Li, Y. L. & Zhu, D. B. (2002). *Eur. J. Inorg. Chem.* pp. 1591–1594.
Matsubayashi, G. & Yokozawa, A. (1990). *J. Chem. Soc. Dalton Trans.* pp. 3535–3539.
Miura, Y. F., Horikiri, M., Honda, K., Shiro, M., Sasaki, K. & Sugi, M. (2004). *Jpn J. Appl. Phys.* **43**, 2628–2629.

Pauling, L. (1960). In *The Nature of the Chemical Bond*, 3rd ed. Ithaca, New York: Cornell University Press.

Pullen, A. E. & Olk, R. M. (1999). *Coord. Chem. Rev.* **188**, 211–262.

Robertson, N. & Cronin, L. (2002). *Coord. Chem. Rev.* **227**, 93–127.

Sheik-Bahae, M., Said, A. A. & Van Stryland, E. W. (1989). *Opt. Lett.* **14**, 955–957.

Sheik-Bahae, M., Said, A. A., Wei, T. H., Hagan, D. J. & Van Stryland, E. W. (1990). *IEEE J. Quantum Electron.* **26**, 760–769.

Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.

Steimeck, G. & Kirmse, R. (1979). *Phosphorus Sulfur*, **7**, 49–55.

Sun, X. B., Ren, Q., Wang, X. Q., Zhang, G. H., Yang, H. L., Feng, L., Xu, D. & Liu, Z. B. (2006). *Chin. Phys.* **15**, 2618–2622.

Svenstrup, N. & Becher, J. (1995). *Synthesis*, pp. 215–235.

Wang, S. F., Huang, W. T., Zhang, T. Q., Yang, H., Gong, Q. H., Okuma, Y., Horikiri, M. & Miura, Y. F. (1999). *Appl. Phys. Lett.* **75**, 1845–1847.

Wang, X.-Q., Yu, W.-T., Xu, D., Wang, Y.-L., Li, T.-B. & Guo, W.-F. (2005). *Acta Cryst.* C**61**, o583–o585.

Yang, H. L., Wang, X. Q., Ren, Q., Zhang, G. H., Sun, X. B., Feng, L., Wang, S. F. & Wang, Z. W. (2005). *J. Opt. A: Pure Appl. Opt.* **7**, 510–513.

m2530 Wang *et al.* • $(C_{21}H_{22}P)[Au(C_3S_5)_2]$ *Acta Cryst.* (2007). E**63**, m2529–m2530

supplementary materials

Acta Cryst. (2007). E**63**, m2529-m2530 [**doi:10.1107/S1600536807043929**]

Triphenyl-*n*-propylphosphonium bis(2-thioxo-1,3-dithiole-4,5-dithiolato)aurate(III)

X. Q. Wang, J. D. Fan, D. Xu, W. T. Yu and **J. Sun**

Comment

In modern communications, all-optical switching is one of the important ways to realise all-optical networks. For realisation of all-optical switching devices, the following material requirements have to be met: $W>>1$ and $T<<1$. The two figures of merit are defined as $W=n_2I/(\alpha\lambda)$ and $T=\beta\lambda/n_2$, where n_2 is the non-linear refractive index, α is the linear absorption coefficient, β is the non-linear absorption coefficient, λ is the wavelength, and I is the light intensity. Furthermore, ultrafast response times are required for the non-linear processes involved. Therefore, to be practically useful for all-optical switching, materials should have a large n_2 at the operating wavelength, small α and β, ultrafast response time, together with good physicochemical properties, such as environmental stability, processability *etc* (Kuang *et al.*, 2003).

Since their discovery nearly three decades ago (Steimeck & Kirmse, 1979), 2-thioxo-1,3-dithiole-4,5-dithiolate (dmit) complexes and related analogues have been of considerable interest as the building units for electrical conductors and superconductors (Svenstrup & Becher, 1995; Cassoux, 1999; Pullen & Olk, 1999; Robertson & Cronin, 2002) and potential candidates of ultrafast optical response capabilities and large third-order non-linear optical (TONLO) effects as special π-electron conjugated systems (Wang *et al.*, 1999; Liu *et al.*, 2002; Coe, 2004). In our recent reports, the TONLO properties of a series of such complexes have been presented; they possess large TONLO properties with sub-picosecond response times (Yang *et al.*, 2005; Sun *et al.*, 2006). Among them, Au-dmit complexes have been found to possess a large n_2 and nearly zero absorption with good W and T for all-optical switching applications at 1064 nm. Therefore, they are good candidates for all-optical switching device application. As a continuation of this work, a new Au-dmit complex, the title compound, (I), has been prepared and its crystal structure is reported here.

In the structure of (I), there are one $[Au(dmit)_2]^-$ anion and one $Ph_3C_3H_7P^+$ counter-cation in the asymmetric unit. The dmit ligand shows its typical behaviour as a bidentate ligand and coordinates the Au^{3+} ion through S atoms. It is similar to Au-dmit complexes with other large counter-cations (Miura *et al.*, 2004; Li *et al.*, 2006), and different from those with small counter-cations (Matsubayashi & Yokozawa, 1990; Li *et al.*, 2005) in which there are two crystallographically independent $[Au(dmit)_2]^-$ anions. The S—Au—S bond angles for the vicinal S atoms are almost exact right angles. The other two S—Au—S angles are nearly 180°. The Au—S bond lengths are slightly smaller than the sum of the single-bond covalent radii (1.36 Å; Pauling, 1960) and are in accordance with those observed elsewhere for Au-dmit complexes (Matsubayashi & Yokozawa, 1990; Miura *et al.*, 2004; Li *et al.*, 2005; Li *et al.*, 2006). The C═S double bond is much longer than the typical C═S bond length (1.599 Å; Allen *et al.*, 1987). The other C—S bonds span the range 1.721 (3) to 1.748 (3) Å. They are all shorter than the typical C—S single bond (1.819 Å; Allen *et al.*, 1987) and are essentially single bonds with some double-bond character. The two C═C bond lengths of the dmit ion are are very close to the corresponding double-bond value of 1.34 Å.

In short, $[Au(dmit)_2]^-$, comprising the central Au^{3+} ion, four S atoms and the adjacent C═C units in the quasi-square plane, is the extended electronically delocalized core of (I). The unfilled d electron shell of Au^{3+} allowing the possibility of low-energy charge-transfer transitions is an important contribution to optical non-linearity. In particular, the 3p orbitals of S and 3 d orbitals of Au^{3+} can overlap to form a highly delocalized system. The delocalization will greatly enhance the hyperpolarizability and the non-linear susceptibility, and lead to large TONLO properties. The TONLO properties of (I) were measured by the *Z*-scan technique (Sheik-Bahae *et al.*, 1989, 1990) in m*M* solutions of both acetone and acetonitrile at 1064 nm. These revealed that the non-linear refractive index n_2 of (I) was superior to that of CS_2.

Experimental

4,5-Bis(furoylsulfanyl)-1,3-dithiole-2-thione (1.211 g) (Wang *et al.*, 2005) was suspended in methanol (15 ml). Under a nitrogen atmosphere, a sodium methoxide solution obtained from Na (0.145 g) in methanol (15 ml) was added to the above-mentioned mixture at room temperature to give a dark-red solution. To this solution, separate solutions of $NaAuCl_4·2H_2O$ (0.597 g) dissolved in methanol (5 ml), and $C_{21}H_{22}PBr$ (0.606 g) in methanol (5 ml) were added consecutively with stirring at room temperature. The reaction mixture was stirred for about 30 min. The product was collected by filtration and washed with methanol to afford a dark-brown precipitate of (I). An acetone solution of (I) was left standing at room temperature; thereby brown crystals (I) used for the structure determination were obtained. Thermal analysis (Diamond TGA/DTA Perkin Elmer instrument): m.p. 399.2 K. Electronic absorption (Hitachi model U-3500 recording spectrophotometer; nm): 288 and 330 (π-π* transition of the dmit ligand), 466 (Au←S charge transfer transition).

Refinement

H atoms were placed in geometrically calculated positions and refined using a riding model with C—H = 0.96%A (for CH_2 groups), 0.97%A (for CH_3 groups) and 0.93%A (for C_6H_5 groups); $U_{iso}(H)$ was set to 1.2 (1.5 for CH_3 groups) times $U_{eq}(C)$.

Figures

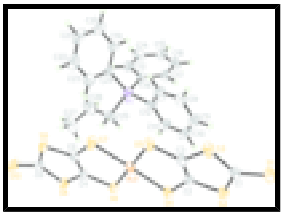


Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids. H atoms have been omitted for clarity.

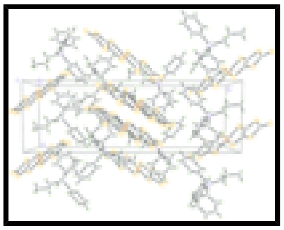


Fig. 2. The crystal packing in (I), viewed along the *b* axis. H atoms have been omitted.

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Crystal data

$(C_{21}H_{22}P)[Au(C_3S_5)_2]$	$F_{000} = 1752$
$M_r = 894.98$	$D_x = 1.834$ Mg m^{-3}

Monoclinic, $P2_1/n$

a = 8.4916 (1) Å

b = 25.8266 (3) Å

c = 14.9202 (2) Å

β = 97.979 (1)°

V = 3240.46 (7) Å^3

Z = 4

Mo $K\alpha$ radiation
λ = 0.71073 Å

Cell parameters from 5335 reflections

θ = 2.7–27.4°

μ = 5.25 mm^{-1}

T = 296 (2) K

Prism, brown

0.23 × 0.19 × 0.17 mm

Data collection

Bruker APEXII CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 296(2) K

φ and ω scans

Absorption correction: multi-scan
APEX2 (Bruker, 2005)

$T_{\min}$ = 0.378, $T_{\max}$ = 0.469

28396 measured reflections

7419 independent reflections

6100 reflections with $I > 2\sigma(I)$

R_{int} = 0.024

$\theta_{\max}$ = 27.5°

$\theta_{\min}$ = 1.6°

$h = -11 \rightarrow 11$

$k = -33 \rightarrow 25$

$l = -19 \rightarrow 19$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.025

$wR(F^2)$ = 0.060

S = 1.04

7419 reflections

353 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.030P)^2 + 0.7621P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max}$ = 0.005

$\Delta\rho_{\max}$ = 0.87 e Å^{-3}

$\Delta\rho_{\min}$ = −0.46 e Å^{-3}

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of F^2 > 2sigma(F^2) is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\AA^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
Au1	0.156935 (13)	0.033241 (4)	0.417388 (8)	0.04162 (5)
C1	−0.0529 (4)	0.16080 (12)	0.6775 (2)	0.0495 (8)
C2	0.0957 (3)	0.09287 (12)	0.5911 (2)	0.0433 (7)
C3	−0.0135 (4)	0.11295 (12)	0.5279 (2)	0.0475 (8)
C4	0.3257 (4)	−0.04787 (12)	0.3078 (2)	0.0420 (7)
C5	0.2135 (4)	−0.02857 (12)	0.2449 (2)	0.0474 (7)
C6	0.3537 (4)	−0.10056 (13)	0.1615 (2)	0.0529 (8)
C7	0.2905 (4)	0.18091 (14)	0.3191 (2)	0.0572 (9)
H7	0.2393	0.1903	0.2623	0.069*
C8	0.2322 (5)	0.19795 (16)	0.3954 (3)	0.0694 (10)
H8	0.1423	0.2189	0.3906	0.083*
C9	0.3091 (5)	0.18353 (16)	0.4793 (3)	0.0696 (11)
H9	0.2718	0.1954	0.5312	0.083*
C10	0.4391 (5)	0.15204 (18)	0.4869 (2)	0.0766 (12)
H10	0.4881	0.1421	0.5439	0.092*
C11	0.4987 (4)	0.13483 (17)	0.4108 (2)	0.0671 (10)
H11	0.5875	0.1134	0.4162	0.081*
C12	0.4244 (4)	0.14997 (13)	0.3258 (2)	0.0489 (8)
C13	0.7643 (5)	0.17737 (15)	0.1504 (3)	0.0671 (10)
H13	0.7414	0.1528	0.1049	0.080*
C14	0.8862 (5)	0.21229 (18)	0.1470 (3)	0.0784 (12)
H14	0.9459	0.2109	0.0993	0.094*
C15	0.9200 (5)	0.24880 (16)	0.2129 (3)	0.0696 (11)
H15	1.0036	0.2718	0.2107	0.084*
C16	0.8318 (4)	0.25141 (15)	0.2815 (3)	0.0682 (10)
H16	0.8528	0.2771	0.3252	0.082*
C17	0.7111 (4)	0.21651 (13)	0.2873 (2)	0.0551 (8)
H17	0.6530	0.2183	0.3356	0.066*
C18	0.6757 (4)	0.17896 (12)	0.2220 (2)	0.0444 (7)
C19	0.3567 (4)	0.18961 (16)	0.0829 (2)	0.0602 (9)
H19	0.4265	0.2166	0.1011	0.072*
C20	0.2388 (5)	0.19604 (19)	0.0095 (3)	0.0755 (12)
H20	0.2288	0.2277	−0.0205	0.091*
C21	0.1388 (5)	0.1572 (2)	−0.0186 (3)	0.0904 (16)
H21	0.0617	0.1618	−0.0687	0.109*
C22	0.1506 (6)	0.1115 (2)	0.0259 (4)	0.1092 (18)
H22	0.0813	0.0847	0.0063	0.131*
C23	0.2659 (5)	0.10439 (18)	0.1008 (3)	0.0869 (14)
H23	0.2721	0.0731	0.1320	0.104*
C24	0.3701 (4)	0.14356 (13)	0.1283 (2)	0.0485 (8)
C25	0.5824 (5)	0.06864 (14)	0.2317 (3)	0.0704 (11)
H25A	0.6584	0.0641	0.2859	0.084*
H25B	0.4927	0.0461	0.2365	0.084*
C26	0.6612 (6)	0.05169 (18)	0.1486 (4)	0.0969 (15)
H26A	0.6012	0.0665	0.0946	0.116*

H26B	0.7677	0.0661	0.1547	0.116*
C27	0.6717 (8)	−0.0050 (2)	0.1361 (4)	0.126 (2)
H27A	0.7232	−0.0205	0.1909	0.188*
H27B	0.7320	−0.0122	0.0877	0.188*
H27C	0.5666	−0.0191	0.1216	0.188*
P1	0.51405 (10)	0.13479 (3)	0.22710 (5)	0.0471 (2)
S1	−0.11931 (12)	0.19761 (4)	0.75427 (7)	0.0643 (2)
S2	0.10232 (11)	0.11750 (4)	0.70039 (6)	0.0542 (2)
S3	−0.13337 (10)	0.16097 (4)	0.56477 (7)	0.0599 (2)
S4	0.23101 (11)	0.04451 (3)	0.57183 (6)	0.0508 (2)
S5	−0.04207 (10)	0.09517 (4)	0.41390 (6)	0.0561 (2)
S6	0.35984 (10)	−0.02690 (3)	0.41999 (5)	0.0508 (2)
S7	0.08042 (12)	0.01999 (4)	0.26385 (6)	0.0645 (3)
S8	0.44341 (11)	−0.09704 (4)	0.27207 (5)	0.0531 (2)
S9	0.20122 (11)	−0.05625 (4)	0.13737 (6)	0.0596 (2)
S10	0.40964 (17)	−0.14087 (5)	0.08663 (6)	0.0822 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.03750 (7)	0.04197 (8)	0.04511 (8)	−0.00021 (5)	0.00474 (5)	−0.00546 (5)
C1	0.0454 (17)	0.0439 (18)	0.060 (2)	−0.0044 (14)	0.0109 (15)	−0.0071 (15)
C2	0.0408 (15)	0.0412 (17)	0.0490 (18)	−0.0015 (13)	0.0100 (13)	−0.0062 (14)
C3	0.0397 (16)	0.0447 (18)	0.058 (2)	−0.0001 (14)	0.0074 (15)	−0.0118 (15)
C4	0.0410 (16)	0.0459 (17)	0.0381 (16)	0.0016 (13)	0.0020 (13)	−0.0075 (13)
C5	0.0476 (18)	0.053 (2)	0.0398 (17)	−0.0002 (15)	0.0011 (14)	−0.0084 (14)
C6	0.062 (2)	0.057 (2)	0.0392 (17)	−0.0013 (17)	0.0052 (15)	−0.0068 (15)
C7	0.064 (2)	0.065 (2)	0.0406 (18)	−0.0034 (18)	−0.0003 (16)	0.0083 (16)
C8	0.074 (3)	0.078 (3)	0.056 (2)	0.000 (2)	0.009 (2)	0.004 (2)
C9	0.073 (3)	0.085 (3)	0.052 (2)	−0.025 (2)	0.0140 (19)	−0.005 (2)
C10	0.074 (3)	0.112 (4)	0.039 (2)	−0.017 (3)	−0.0067 (18)	0.018 (2)
C11	0.056 (2)	0.096 (3)	0.047 (2)	−0.002 (2)	−0.0034 (16)	0.019 (2)
C12	0.0472 (18)	0.055 (2)	0.0422 (17)	−0.0133 (15)	−0.0038 (14)	0.0088 (15)
C13	0.078 (3)	0.070 (3)	0.056 (2)	−0.008 (2)	0.0192 (19)	−0.0129 (19)
C14	0.071 (3)	0.090 (3)	0.082 (3)	−0.006 (2)	0.040 (2)	0.001 (3)
C15	0.054 (2)	0.072 (3)	0.083 (3)	−0.0133 (19)	0.011 (2)	0.007 (2)
C16	0.060 (2)	0.071 (3)	0.073 (3)	−0.018 (2)	0.007 (2)	−0.014 (2)
C17	0.0540 (19)	0.059 (2)	0.053 (2)	−0.0087 (17)	0.0106 (16)	−0.0079 (16)
C18	0.0432 (16)	0.0476 (18)	0.0408 (17)	0.0029 (14)	0.0003 (13)	0.0034 (14)
C19	0.062 (2)	0.070 (3)	0.047 (2)	0.0070 (18)	0.0015 (17)	0.0071 (17)
C20	0.079 (3)	0.104 (3)	0.042 (2)	0.026 (3)	0.0028 (19)	0.012 (2)
C21	0.075 (3)	0.143 (5)	0.046 (2)	0.033 (3)	−0.019 (2)	−0.017 (3)
C22	0.089 (3)	0.116 (4)	0.106 (4)	−0.016 (3)	−0.046 (3)	−0.020 (3)
C23	0.085 (3)	0.078 (3)	0.085 (3)	−0.014 (2)	−0.034 (2)	0.005 (2)
C24	0.0508 (18)	0.054 (2)	0.0372 (17)	0.0027 (15)	−0.0049 (14)	−0.0040 (14)
C25	0.067 (2)	0.051 (2)	0.086 (3)	−0.0014 (19)	−0.017 (2)	0.0052 (19)
C26	0.092 (3)	0.068 (3)	0.134 (5)	0.017 (3)	0.025 (3)	−0.001 (3)
C27	0.129 (5)	0.085 (4)	0.163 (6)	−0.023 (4)	0.023 (4)	−0.027 (4)

P1	0.0484 (5)	0.0460 (5)	0.0431 (5)	−0.0044 (4)	−0.0069 (4)	0.0035 (4)
S1	0.0658 (6)	0.0614 (6)	0.0679 (6)	0.0083 (5)	0.0171 (5)	−0.0170 (5)
S2	0.0576 (5)	0.0557 (5)	0.0496 (5)	0.0107 (4)	0.0085 (4)	−0.0060 (4)
S3	0.0511 (5)	0.0594 (6)	0.0664 (6)	0.0156 (4)	−0.0017 (4)	−0.0171 (4)
S4	0.0542 (5)	0.0519 (5)	0.0462 (5)	0.0147 (4)	0.0062 (4)	−0.0038 (4)
S5	0.0487 (4)	0.0603 (5)	0.0555 (5)	0.0124 (4)	−0.0056 (4)	−0.0133 (4)
S6	0.0536 (5)	0.0595 (5)	0.0369 (4)	0.0149 (4)	−0.0027 (3)	−0.0108 (4)
S7	0.0595 (5)	0.0776 (6)	0.0515 (5)	0.0244 (5)	−0.0094 (4)	−0.0103 (5)
S8	0.0614 (5)	0.0590 (5)	0.0377 (4)	0.0137 (4)	0.0024 (4)	−0.0080 (4)
S9	0.0642 (5)	0.0722 (6)	0.0385 (4)	0.0068 (5)	−0.0074 (4)	−0.0119 (4)
S10	0.1166 (9)	0.0858 (8)	0.0442 (5)	0.0266 (7)	0.0109 (5)	−0.0180 (5)

Geometric parameters (Å, °)

Au1—S6	2.3160 (8)	C13—C18	1.390 (4)
Au1—S7	2.3182 (9)	C13—H13	0.930
Au1—S4	2.3212 (8)	C14—C15	1.364 (6)
Au1—S5	2.3221 (8)	C14—H14	0.930
C1—S1	1.647 (3)	C15—C16	1.351 (5)
C1—S3	1.725 (3)	C15—H15	0.930
C1—S2	1.726 (3)	C16—C17	1.377 (5)
C2—C3	1.332 (4)	C16—H16	0.930
C2—S2	1.744 (3)	C17—C18	1.378 (4)
C2—S4	1.748 (3)	C17—H17	0.930
C3—S3	1.741 (3)	C18—P1	1.794 (3)
C3—S5	1.746 (3)	C19—C24	1.366 (5)
C4—C5	1.337 (4)	C19—C20	1.387 (5)
C4—S8	1.744 (3)	C19—H19	0.930
C4—S6	1.745 (3)	C20—C21	1.343 (6)
C5—S7	1.737 (3)	C20—H20	0.930
C5—S9	1.747 (3)	C21—C22	1.351 (7)
C6—S10	1.644 (3)	C21—H21	0.930
C6—S8	1.721 (3)	C22—C23	1.392 (6)
C6—S9	1.728 (4)	C22—H22	0.930
C7—C8	1.376 (5)	C23—C24	1.369 (5)
C7—C12	1.381 (5)	C23—H23	0.930
C7—H7	0.930	C24—P1	1.794 (3)
C8—C9	1.379 (5)	C25—C26	1.550 (6)
C8—H8	0.930	C25—P1	1.802 (4)
C9—C10	1.363 (6)	C25—H25A	0.970
C9—H9	0.930	C25—H25B	0.970
C10—C11	1.379 (5)	C26—C27	1.481 (7)
C10—H10	0.930	C26—H26A	0.970
C11—C12	1.392 (4)	C26—H26B	0.970
C11—H11	0.930	C27—H27A	0.960
C12—P1	1.792 (3)	C27—H27B	0.960
C13—C14	1.379 (5)	C27—H27C	0.960
S6—Au1—S7	91.34 (3)	C16—C17—H17	119.8
S6—Au1—S4	88.22 (3)	C18—C17—H17	119.8

S7—Au1—S4	178.58 (4)	C17—C18—C13	118.4 (3)
S6—Au1—S5	178.54 (3)	C17—C18—P1	120.7 (2)
S7—Au1—S5	88.64 (3)	C13—C18—P1	120.8 (3)
S4—Au1—S5	91.83 (3)	C24—C19—C20	119.8 (4)
S1—C1—S3	123.3 (2)	C24—C19—H19	120.1
S1—C1—S2	124.2 (2)	C20—C19—H19	120.1
S3—C1—S2	112.52 (18)	C21—C20—C19	120.9 (4)
C3—C2—S2	116.6 (2)	C21—C20—H20	119.6
C3—C2—S4	124.8 (2)	C19—C20—H20	119.6
S2—C2—S4	118.54 (18)	C20—C21—C22	119.8 (4)
C2—C3—S3	115.7 (2)	C20—C21—H21	120.1
C2—C3—S5	125.2 (2)	C22—C21—H21	120.1
S3—C3—S5	119.12 (19)	C21—C22—C23	120.4 (5)
C5—C4—S8	116.1 (2)	C21—C22—H22	119.8
C5—C4—S6	124.4 (2)	C23—C22—H22	119.8
S8—C4—S6	119.54 (18)	C24—C23—C22	119.7 (4)
C4—C5—S7	124.8 (2)	C24—C23—H23	120.1
C4—C5—S9	116.0 (2)	C22—C23—H23	120.1
S7—C5—S9	119.19 (19)	C19—C24—C23	119.3 (3)
S10—C6—S8	123.6 (2)	C19—C24—P1	121.2 (3)
S10—C6—S9	123.8 (2)	C23—C24—P1	119.4 (3)
S8—C6—S9	112.57 (18)	C26—C25—P1	114.2 (3)
C8—C7—C12	120.8 (3)	C26—C25—H25A	108.7
C8—C7—H7	119.6	P1—C25—H25A	108.7
C12—C7—H7	119.6	C26—C25—H25B	108.7
C7—C8—C9	119.0 (4)	P1—C25—H25B	108.7
C7—C8—H8	120.5	H25A—C25—H25B	107.6
C9—C8—H8	120.5	C27—C26—C25	114.9 (4)
C10—C9—C8	120.8 (4)	C27—C26—H26A	108.6
C10—C9—H9	119.6	C25—C26—H26A	108.6
C8—C9—H9	119.6	C27—C26—H26B	108.6
C9—C10—C11	120.6 (3)	C25—C26—H26B	108.6
C9—C10—H10	119.7	H26A—C26—H26B	107.5
C11—C10—H10	119.7	C26—C27—H27A	109.5
C10—C11—C12	119.2 (4)	C26—C27—H27B	109.5
C10—C11—H11	120.4	H27A—C27—H27B	109.5
C12—C11—H11	120.4	C26—C27—H27C	109.5
C7—C12—C11	119.5 (3)	H27A—C27—H27C	109.5
C7—C12—P1	120.4 (2)	H27B—C27—H27C	109.5
C11—C12—P1	119.8 (3)	C12—P1—C24	109.16 (15)
C14—C13—C18	119.9 (3)	C12—P1—C18	108.09 (15)
C14—C13—H13	120.1	C24—P1—C18	108.85 (15)
C18—C13—H13	120.1	C12—P1—C25	110.34 (18)
C15—C14—C13	120.6 (4)	C24—P1—C25	109.26 (17)
C15—C14—H14	119.7	C18—P1—C25	111.10 (17)
C13—C14—H14	119.7	C1—S2—C2	97.27 (15)
C16—C15—C14	119.8 (4)	C1—S3—C3	97.82 (16)
C16—C15—H15	120.1	C2—S4—Au1	99.15 (11)
C14—C15—H15	120.1	C3—S5—Au1	99.04 (11)

C15—C16—C17	120.7 (4)	C4—S6—Au1	99.67 (11)
C15—C16—H16	119.6	C5—S7—Au1	99.66 (11)
C17—C16—H16	119.6	C6—S8—C4	97.77 (16)
C16—C17—C18	120.5 (3)	C6—S9—C5	97.60 (15)

S2—C2—C3—S3	0.0 (3)	C19—C24—P1—C25	−147.0 (3)
S4—C2—C3—S3	−179.71 (17)	C23—C24—P1—C25	36.6 (4)
S2—C2—C3—S5	179.37 (18)	C17—C18—P1—C12	−0.3 (3)
S4—C2—C3—S5	−0.3 (4)	C13—C18—P1—C12	−177.9 (3)
S8—C4—C5—S7	179.35 (19)	C17—C18—P1—C24	118.1 (3)
S6—C4—C5—S7	−0.9 (5)	C13—C18—P1—C24	−59.4 (3)
S8—C4—C5—S9	0.7 (4)	C17—C18—P1—C25	−121.5 (3)
S6—C4—C5—S9	−179.52 (19)	C13—C18—P1—C25	60.9 (3)
C12—C7—C8—C9	−0.2 (6)	C26—C25—P1—C12	179.7 (3)
C7—C8—C9—C10	−1.3 (6)	C26—C25—P1—C24	59.6 (4)
C8—C9—C10—C11	1.4 (6)	C26—C25—P1—C18	−60.5 (3)
C9—C10—C11—C12	0.0 (6)	S1—C1—S2—C2	177.8 (2)
C8—C7—C12—C11	1.6 (5)	S3—C1—S2—C2	−1.5 (2)
C8—C7—C12—P1	−172.0 (3)	C3—C2—S2—C1	1.0 (3)
C10—C11—C12—C7	−1.4 (5)	S4—C2—S2—C1	−179.31 (19)
C10—C11—C12—P1	172.2 (3)	S1—C1—S3—C3	−177.8 (2)
C18—C13—C14—C15	−0.6 (6)	S2—C1—S3—C3	1.6 (2)
C13—C14—C15—C16	−1.1 (7)	C2—C3—S3—C1	−1.0 (3)
C14—C15—C16—C17	2.1 (6)	S5—C3—S3—C1	179.6 (2)
C15—C16—C17—C18	−1.5 (6)	C3—C2—S4—Au1	0.9 (3)
C16—C17—C18—C13	−0.2 (5)	S2—C2—S4—Au1	−178.80 (15)
C16—C17—C18—P1	−177.8 (3)	S6—Au1—S4—C2	177.69 (11)
C14—C13—C18—C17	1.2 (5)	S5—Au1—S4—C2	−0.85 (11)
C14—C13—C18—P1	178.8 (3)	C2—C3—S5—Au1	−0.5 (3)
C24—C19—C20—C21	−1.2 (6)	S3—C3—S5—Au1	178.91 (16)
C19—C20—C21—C22	1.3 (7)	S7—Au1—S5—C3	179.40 (11)
C20—C21—C22—C23	0.0 (8)	S4—Au1—S5—C3	0.74 (11)
C21—C22—C23—C24	−1.4 (8)	C5—C4—S6—Au1	3.0 (3)
C20—C19—C24—C23	−0.3 (6)	S8—C4—S6—Au1	−177.26 (17)
C20—C19—C24—P1	−176.7 (3)	S7—Au1—S6—C4	−2.97 (12)
C22—C23—C24—C19	1.5 (7)	S4—Au1—S6—C4	175.68 (11)
C22—C23—C24—P1	178.0 (4)	C4—C5—S7—Au1	−1.8 (3)
P1—C25—C26—C27	−161.6 (4)	S9—C5—S7—Au1	176.79 (17)
C7—C12—P1—C24	−21.4 (3)	S6—Au1—S7—C5	2.67 (12)
C11—C12—P1—C24	165.0 (3)	S5—Au1—S7—C5	−178.79 (12)
C7—C12—P1—C18	96.9 (3)	S10—C6—S8—C4	179.8 (2)
C11—C12—P1—C18	−76.7 (3)	S9—C6—S8—C4	1.0 (2)
C7—C12—P1—C25	−141.4 (3)	C5—C4—S8—C6	−1.1 (3)
C11—C12—P1—C25	45.0 (3)	S6—C4—S8—C6	179.2 (2)
C19—C24—P1—C12	92.3 (3)	S10—C6—S9—C5	−179.5 (2)
C23—C24—P1—C12	−84.1 (4)	S8—C6—S9—C5	−0.7 (2)
C19—C24—P1—C18	−25.5 (3)	C4—C5—S9—C6	0.0 (3)
C23—C24—P1—C18	158.1 (3)	S7—C5—S9—C6	−178.7 (2)

Fig. 1

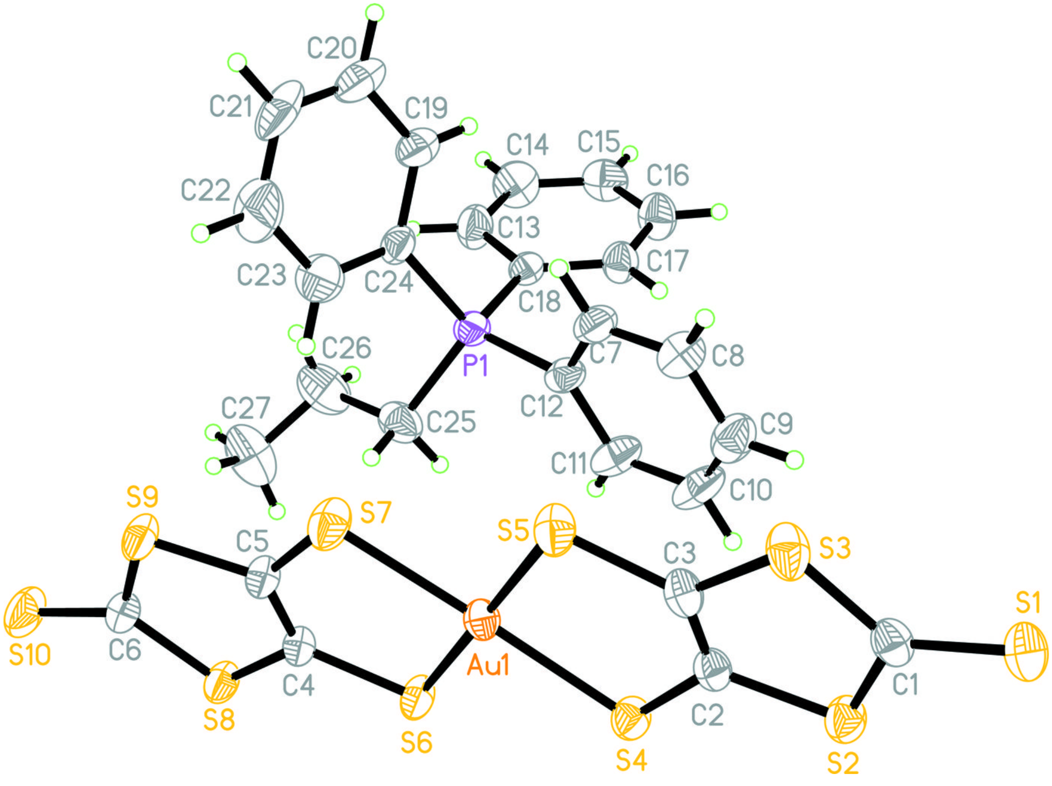
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Fig. 2