Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

[(*Z*)-*O*-Ethyl-*N*-(*o*-tolyl)thiocarbamato-*κS*](triphenylphosphine-*κP*)gold(I)

Primjira P. Tadbuppa[a] and Edward R. T. Tiekink[b]*

[a]Department of Chemistry, National University of Singapore, Singapore 117543, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: edward.tiekink@gmail.com

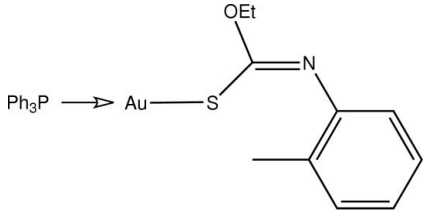
Received 13 November 2009; accepted 15 November 2009

Key indicators: single-crystal X-ray study; T = 223 K; mean σ(C–C) = 0.008 Å; R factor = 0.031; wR factor = 0.104; data-to-parameter ratio = 19.3.

The title compound, [Au($C_{10}H_{12}NOS$)($C_{18}H_{15}P$)], features a linear geometry for the Au atom defined by the S and P donor atoms. A small deviation from the ideal geometry is noted and is ascribed to an intramolecular Au···O contact [2.936 (4) Å]. Inversion dimers are formed in the crystal structure mediated by C—H···π interactions between centrosymmetrically related *o*-tolyl residues [C···*Cg* = 3.532 (6) Å].

Related literature

For structural systematics and luminescence properties of phosphinegold(I) carbonimidothioates, see: Ho *et al.* (2006); Ho & Tiekink (2007); Kuan *et al.* (2008). For the synthesis, see Hall *et al.* (1993).



Experimental

Crystal data

[Au($C_{10}H_{12}NOS$)($C_{18}H_{15}P$)]
M_r = 653.50
Triclinic, $P\overline{1}$
a = 9.3378 (6) Å
b = 10.1665 (6) Å
c = 13.9711 (8) Å
α = 95.514 (1)°
β = 103.371 (1)°
γ = 98.334 (1)°
V = 1265.11 (13) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 5.98 mm^{-1}
T = 223 K
0.24 × 0.13 × 0.03 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.311, T_{max} = 1
8823 measured reflections
5772 independent reflections
5279 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.104
S = 1.07
5772 reflections
299 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.62 e Å^{-3}
$\Delta\rho_{min}$ = −1.26 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Au—S1	2.3105 (11)	Au—P1	2.2509 (11)
P1—Au—S1	177.00 (4)		

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *PATTY* in *DIRDIF92* (Beurskens *et al.*, 1992); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2009).

The National University of Singapore (grant No. R-143–000–213–112) is thanked for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2686).

References

Beurskens, P. T., Admiraal, G., Beurskens, G., Bosman, W. P., Garcia-Granda, S., Gould, R. O., Smits, J. M. M. & Smykalla, C. (1992). *The DIRDIF Program System*. Technical Report. Crystallography Laboratory, University of Nijmegen, The Netherlands.
Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2000). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, U. S. A.
Hall, V. J., Siasios, G. & Tiekink, E. R. T. (1993). *Aust. J. Chem.* **46**, 561–570.
Ho, S. Y., Cheng, E. C.-C., Tiekink, E. R. T. & Yam, V. W.-W. (2006). *Inorg. Chem.* **45**, 8165–8174.
Ho, S. Y. & Tiekink, E. R. T. (2007). *CrystEngComm*, **9**, 368–378.
Kuan, F. S., Ho, S. Y., Tadbuppa, P. P. & Tiekink, E. R. T. (2008). *CrystEngComm*, **10**, 548–564.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2009). *publCIF*. In preparation.

supplementary materials

Acta Cryst. (2009). E**65**, m1612 [**doi:10.1107/S1600536809048466**]

[(*Z*)-*O*-Ethyl-*N*-(*o*-tolyl)thiocarbamato-κ*S*](triphenylphosphine-κ*P*)gold(I)

P. P. Tadbuppa and E. R. T. Tiekink

Comment

The title compound, Ph_3Au[SC(OEt)*N*(*o*-tolyl), (I), was synthesized during the course of systematic studies of phosphinegold(I) thiocarbamides (Ho *et al.* 2006; Ho & Tiekink, 2007; Kuan *et al.*, 2008)..

The gold atom in (I) exists in a linear geometry defined by an *S*,*P* donor set, Table 1 and Fig. 1. The small deviation from linearity is due to the close approach of the O1 atom to Au [Au···O = 2.936 (4) Å]. The anion, having C1—S1 = 1.768 (5) Å and C1N1 = 1.254 (6) Å, coordinates as a thiolate ligand. The configuration about the C1N1 double bond is *Z*.

In the crystal structure of (I), supramolecular dimers are formed between centrosymmetric pairs of *o*-tolyl residues owing to the presence of C—H···π interactions whereby the π system is defined by the (C2–C7) ring; C8–H8c···Cg^{i} = 2.67 Å, C8···Cg^{i} = 3.532 (6) Å with an angle at H8c = 148 ° for *i*: -1 - *x*, 1 - *y*, -*z*.

Experimental

Compound (I) was prepared following the standard literature procedure from the reaction of Ph_3AuCl and EtOC(*S*)*N*(*H*)(*o*-tolyl) in the presence of base (Hall *et al.*, 1993).

Refinement

The H atoms were geometrically placed (C—H = 0.94–0.98 Å) and refined as riding with U_{iso}(H) = 1.2–1.5U_{eq}(C). The maximum and minimum residual electron density peaks of 1.62 and 1.26 e Å^{-3}, respectively, were located 0.81 Å and 0.92 Å from the Au atom.

Figures

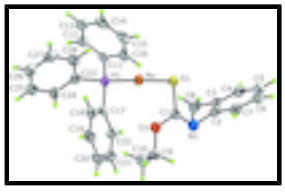


Fig. 1. Molecular structure of (I) showing atom-labelling scheme and displacement ellipsoids at the 50% probability level.

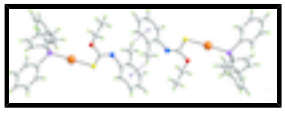


Fig. 2. The supramolecular dimer in (I) mediated by C—H···π contacts (purple dashed lines). Colour code: Au, orange; S, yellow; P, pink; O, red; N, blue; C, grey; and H, green.

[(*Z*)-*O*-Ethyl-*N*-(*o*-tolyl)thiocarbamato- κ*S*](triphenylphosphine-κ*P*)gold(I)

Crystal data

$[Au(C_{10}H_{12}NOS)(C_{18}H_{15}P)]$	$Z = 2$
$M_r = 653.50$	$F_{000} = 640$
Triclinic, $P\overline{1}$	$D_x = 1.716$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
$a = 9.3378$ (6) Å	Cell parameters from 5740 reflections
$b = 10.1665$ (6) Å	$\theta = 2.3$–29.9º
$c = 13.9711$ (8) Å	$\mu = 5.98$ mm^{-1}
$\alpha = 95.514$ (1)º	$T = 223$ K
$\beta = 103.371$ (1)º	Block, colourless
$\gamma = 98.334$ (1)º	0.24 × 0.13 × 0.03 mm
$V = 1265.11$ (13) Å^3	

Data collection

Bruker SMART CCD diffractometer	5772 independent reflections
Radiation source: fine-focus sealed tube	5279 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.023$
$T = 223$ K	$\theta_{max} = 27.5$º
ω scans	$\theta_{min} = 1.5$º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$h = -12 \rightarrow 11$
$T_{min} = 0.311$, $T_{max} = 1$	$k = -10 \rightarrow 13$
8823 measured reflections	$l = -17 \rightarrow 18$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.031$	H-atom parameters constrained
$wR(F^2) = 0.104$	$w = 1/[\sigma^2(F_o^2) + (0.0692P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} = 0.001$
5772 reflections	$\Delta\rho_{max} = 1.62$ e Å^{-3}
299 parameters	$\Delta\rho_{min} = -1.26$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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 ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
Au	0.147930 (18)	0.358507 (16)	0.308910 (12)	0.03424 (8)
S1	−0.00461 (14)	0.49405 (12)	0.22765 (9)	0.0352 (2)
P1	0.28887 (13)	0.21714 (12)	0.38273 (9)	0.0305 (2)
O1	−0.1318 (4)	0.2462 (3)	0.1600 (3)	0.0419 (8)
N1	−0.2434 (5)	0.3967 (4)	0.0724 (3)	0.0392 (9)
C1	−0.1424 (5)	0.3740 (5)	0.1420 (3)	0.0340 (9)
C2	−0.2509 (5)	0.5300 (5)	0.0506 (4)	0.0368 (10)
C3	−0.3452 (5)	0.6059 (5)	0.0885 (3)	0.0375 (10)
C4	−0.3575 (6)	0.7297 (5)	0.0590 (4)	0.0435 (11)
H4	−0.4198	0.7813	0.0840	0.052*
C5	−0.2799 (6)	0.7804 (6)	−0.0070 (4)	0.0483 (13)
H5	−0.2893	0.8658	−0.0256	0.058*
C6	−0.1902 (6)	0.7060 (6)	−0.0448 (4)	0.0447 (12)
H6	−0.1390	0.7395	−0.0903	0.054*
C7	−0.1747 (5)	0.5813 (6)	−0.0160 (4)	0.0412 (11)
H7	−0.1120	0.5307	−0.0417	0.049*
C8	−0.4332 (6)	0.5472 (6)	0.1575 (4)	0.0461 (12)
H8A	−0.4931	0.6107	0.1765	0.069*
H8B	−0.3648	0.5289	0.2164	0.069*
H8C	−0.4981	0.4645	0.1238	0.069*
C9	−0.2431 (6)	0.1389 (5)	0.0974 (4)	0.0476 (12)
H9A	−0.1996	0.0572	0.0923	0.057*
H9B	−0.2735	0.1637	0.0305	0.057*
C10	−0.3760 (7)	0.1122 (7)	0.1382 (5)	0.0568 (15)
H10A	−0.4484	0.0400	0.0952	0.085*
H10B	−0.4203	0.1925	0.1420	0.085*
H10C	−0.3462	0.0866	0.2040	0.085*
C11	0.4873 (5)	0.2811 (5)	0.4272 (4)	0.0336 (9)
C12	0.5675 (6)	0.2763 (5)	0.5233 (4)	0.0425 (11)
H12	0.5166	0.2442	0.5694	0.051*
C13	0.7199 (6)	0.3175 (6)	0.5527 (4)	0.0490 (13)
H13	0.7724	0.3139	0.6182	0.059*
C14	0.7945 (6)	0.3639 (6)	0.4854 (5)	0.0523 (14)

H14	0.8989	0.3902	0.5047	0.063*
C15	0.7178 (6)	0.3723 (6)	0.3895 (5)	0.0509 (13)
H15	0.7697	0.4056	0.3443	0.061*
C16	0.5622 (6)	0.3310 (5)	0.3600 (4)	0.0449 (11)
H16	0.5092	0.3372	0.2951	0.054*
C17	0.2775 (5)	0.0655 (4)	0.2989 (3)	0.0317 (9)
C18	0.3943 (6)	−0.0073 (5)	0.3093 (4)	0.0413 (11)
H18	0.4832	0.0241	0.3587	0.050*
C19	0.3800 (7)	−0.1259 (6)	0.2472 (4)	0.0479 (13)
H19	0.4599	−0.1736	0.2534	0.058*
C20	0.2469 (8)	−0.1739 (6)	0.1757 (5)	0.0550 (14)
H20	0.2355	−0.2559	0.1351	0.066*
C21	0.1319 (7)	−0.1011 (7)	0.1645 (5)	0.0578 (15)
H21	0.0427	−0.1331	0.1155	0.069*
C22	0.1467 (6)	0.0183 (6)	0.2245 (4)	0.0436 (11)
H22	0.0685	0.0682	0.2153	0.052*
C23	0.2305 (5)	0.1605 (5)	0.4895 (3)	0.0328 (9)
C24	0.2240 (6)	0.0302 (5)	0.5088 (4)	0.0389 (10)
H24	0.2465	−0.0348	0.4647	0.047*
C25	0.1840 (6)	−0.0054 (6)	0.5941 (4)	0.0478 (12)
H25	0.1777	−0.0949	0.6068	0.057*
C26	0.1532 (6)	0.0910 (6)	0.6604 (4)	0.0467 (12)
H26	0.1288	0.0670	0.7188	0.056*
C27	0.1583 (7)	0.2195 (6)	0.6411 (4)	0.0502 (13)
H27	0.1370	0.2843	0.6860	0.060*
C28	0.1950 (6)	0.2562 (5)	0.5551 (4)	0.0425 (11)
H28	0.1959	0.3449	0.5412	0.051*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au	0.03477 (12)	0.03251 (12)	0.03386 (12)	0.01184 (8)	0.00062 (8)	0.00697 (7)
S1	0.0354 (6)	0.0300 (5)	0.0369 (6)	0.0114 (4)	−0.0012 (5)	0.0052 (4)
P1	0.0305 (5)	0.0294 (6)	0.0300 (6)	0.0095 (4)	0.0012 (4)	0.0054 (4)
O1	0.0446 (19)	0.0308 (17)	0.0437 (19)	0.0065 (14)	−0.0023 (15)	0.0060 (14)
N1	0.038 (2)	0.037 (2)	0.041 (2)	0.0108 (17)	0.0020 (17)	0.0072 (17)
C1	0.035 (2)	0.030 (2)	0.036 (2)	0.0089 (18)	0.0053 (19)	0.0039 (18)
C2	0.028 (2)	0.040 (3)	0.036 (2)	0.0070 (19)	−0.0033 (18)	0.0013 (19)
C3	0.039 (2)	0.041 (3)	0.030 (2)	0.011 (2)	0.0010 (19)	0.0030 (19)
C4	0.044 (3)	0.044 (3)	0.040 (3)	0.012 (2)	0.005 (2)	−0.001 (2)
C5	0.052 (3)	0.038 (3)	0.047 (3)	0.003 (2)	0.000 (2)	0.008 (2)
C6	0.044 (3)	0.045 (3)	0.043 (3)	0.004 (2)	0.004 (2)	0.012 (2)
C7	0.034 (2)	0.047 (3)	0.043 (3)	0.016 (2)	0.004 (2)	0.007 (2)
C8	0.048 (3)	0.053 (3)	0.039 (3)	0.015 (2)	0.011 (2)	0.005 (2)
C9	0.053 (3)	0.031 (2)	0.050 (3)	0.007 (2)	−0.002 (2)	−0.001 (2)
C10	0.047 (3)	0.053 (3)	0.065 (4)	0.005 (3)	0.002 (3)	0.013 (3)
C11	0.030 (2)	0.029 (2)	0.038 (2)	0.0040 (17)	0.0017 (18)	0.0047 (18)
C12	0.042 (3)	0.038 (3)	0.041 (3)	0.000 (2)	0.002 (2)	0.005 (2)

C13	0.039 (3)	0.042 (3)	0.052 (3)	0.005 (2)	−0.013 (2)	0.001 (2)
C14	0.034 (3)	0.038 (3)	0.077 (4)	0.000 (2)	0.002 (3)	0.004 (3)
C15	0.046 (3)	0.040 (3)	0.068 (4)	−0.002 (2)	0.023 (3)	0.007 (3)
C16	0.047 (3)	0.041 (3)	0.047 (3)	0.010 (2)	0.010 (2)	0.010 (2)
C17	0.033 (2)	0.028 (2)	0.034 (2)	0.0051 (17)	0.0085 (18)	0.0054 (17)
C18	0.046 (3)	0.041 (3)	0.036 (2)	0.009 (2)	0.008 (2)	0.003 (2)
C19	0.063 (4)	0.039 (3)	0.049 (3)	0.016 (3)	0.023 (3)	0.007 (2)
C20	0.075 (4)	0.039 (3)	0.051 (3)	0.005 (3)	0.023 (3)	−0.006 (2)
C21	0.057 (3)	0.058 (4)	0.047 (3)	−0.002 (3)	0.002 (3)	−0.007 (3)
C22	0.036 (2)	0.049 (3)	0.037 (3)	0.001 (2)	0.000 (2)	−0.001 (2)
C23	0.032 (2)	0.036 (2)	0.031 (2)	0.0124 (18)	0.0045 (17)	0.0039 (18)
C24	0.044 (3)	0.037 (2)	0.039 (3)	0.014 (2)	0.009 (2)	0.010 (2)
C25	0.056 (3)	0.045 (3)	0.046 (3)	0.010 (2)	0.015 (2)	0.013 (2)
C26	0.044 (3)	0.058 (3)	0.041 (3)	0.010 (2)	0.014 (2)	0.010 (2)
C27	0.050 (3)	0.059 (4)	0.042 (3)	0.014 (3)	0.016 (2)	−0.007 (3)
C28	0.047 (3)	0.037 (3)	0.045 (3)	0.015 (2)	0.011 (2)	−0.001 (2)

Geometric parameters (Å, °)

Au—S1	2.3105 (11)	C12—C13	1.375 (7)
Au—P1	2.2509 (11)	C12—H12	0.9400
S1—C1	1.768 (5)	C13—C14	1.373 (9)
P1—C11	1.812 (5)	C13—H13	0.9400
P1—C23	1.817 (5)	C14—C15	1.382 (9)
P1—C17	1.819 (5)	C14—H14	0.9400
O1—C1	1.360 (6)	C15—C16	1.403 (8)
O1—C9	1.450 (6)	C15—H15	0.9400
N1—C1	1.254 (6)	C16—H16	0.9400
N1—C2	1.425 (6)	C17—C18	1.392 (7)
C2—C7	1.391 (7)	C17—C22	1.396 (6)
C2—C3	1.410 (7)	C18—C19	1.386 (8)
C3—C4	1.374 (7)	C18—H18	0.9400
C3—C8	1.514 (7)	C19—C20	1.392 (9)
C4—C5	1.390 (8)	C19—H19	0.9400
C4—H4	0.9400	C20—C21	1.379 (9)
C5—C6	1.366 (8)	C20—H20	0.9400
C5—H5	0.9400	C21—C22	1.377 (8)
C6—C7	1.384 (7)	C21—H21	0.9400
C6—H6	0.9400	C22—H22	0.9400
C7—H7	0.9400	C23—C24	1.372 (7)
C8—H8A	0.9700	C23—C28	1.401 (7)
C8—H8B	0.9700	C24—C25	1.393 (7)
C8—H8C	0.9700	C24—H24	0.9400
C9—C10	1.482 (9)	C25—C26	1.390 (8)
C9—H9A	0.9800	C25—H25	0.9400
C9—H9B	0.9800	C26—C27	1.356 (9)
C10—H10A	0.9700	C26—H26	0.9400
C10—H10B	0.9700	C27—C28	1.392 (8)
C10—H10C	0.9700	C27—H27	0.9400

C11—C16	1.387 (7)	C28—H28	0.9400
C11—C12	1.387 (7)		
P1—Au—S1	177.00 (4)	C13—C12—C11	121.4 (5)
C1—S1—Au	101.39 (16)	C13—C12—H12	119.3
C11—P1—C23	105.3 (2)	C11—C12—H12	119.3
C11—P1—C17	104.4 (2)	C14—C13—C12	119.4 (5)
C23—P1—C17	105.6 (2)	C14—C13—H13	120.3
C11—P1—Au	116.15 (15)	C12—C13—H13	120.3
C23—P1—Au	112.80 (15)	C13—C14—C15	120.7 (5)
C17—P1—Au	111.68 (15)	C13—C14—H14	119.6
C1—O1—C9	117.5 (4)	C15—C14—H14	119.6
C1—N1—C2	120.8 (4)	C14—C15—C16	119.7 (5)
N1—C1—O1	120.6 (4)	C14—C15—H15	120.1
N1—C1—S1	127.0 (4)	C16—C15—H15	120.1
O1—C1—S1	112.4 (3)	C11—C16—C15	119.5 (5)
C7—C2—C3	119.5 (5)	C11—C16—H16	120.2
C7—C2—N1	119.5 (5)	C15—C16—H16	120.2
C3—C2—N1	120.7 (5)	C18—C17—C22	119.2 (5)
C4—C3—C2	118.4 (5)	C18—C17—P1	121.5 (4)
C4—C3—C8	122.2 (5)	C22—C17—P1	119.3 (4)
C2—C3—C8	119.3 (5)	C19—C18—C17	120.4 (5)
C3—C4—C5	121.6 (5)	C19—C18—H18	119.8
C3—C4—H4	119.2	C17—C18—H18	119.8
C5—C4—H4	119.2	C18—C19—C20	119.8 (6)
C6—C5—C4	119.9 (5)	C18—C19—H19	120.1
C6—C5—H5	120.1	C20—C19—H19	120.1
C4—C5—H5	120.1	C21—C20—C19	119.9 (5)
C5—C6—C7	120.0 (5)	C21—C20—H20	120.0
C5—C6—H6	120.0	C19—C20—H20	120.0
C7—C6—H6	120.0	C22—C21—C20	120.5 (6)
C6—C7—C2	120.6 (5)	C22—C21—H21	119.7
C6—C7—H7	119.7	C20—C21—H21	119.7
C2—C7—H7	119.7	C21—C22—C17	120.2 (5)
C3—C8—H8A	109.5	C21—C22—H22	119.9
C3—C8—H8B	109.5	C17—C22—H22	119.9
H8A—C8—H8B	109.5	C24—C23—C28	119.6 (5)
C3—C8—H8C	109.5	C24—C23—P1	122.8 (4)
H8A—C8—H8C	109.5	C28—C23—P1	117.6 (4)
H8B—C8—H8C	109.5	C23—C24—C25	119.9 (5)
O1—C9—C10	111.1 (5)	C23—C24—H24	120.1
O1—C9—H9A	109.4	C25—C24—H24	120.1
C10—C9—H9A	109.4	C26—C25—C24	120.2 (5)
O1—C9—H9B	109.4	C26—C25—H25	119.9
C10—C9—H9B	109.4	C24—C25—H25	119.9
H9A—C9—H9B	108.0	C27—C26—C25	120.1 (5)
C9—C10—H10A	109.5	C27—C26—H26	119.9
C9—C10—H10B	109.5	C25—C26—H26	119.9
H10A—C10—H10B	109.5	C26—C27—C28	120.4 (5)
C9—C10—H10C	109.5	C26—C27—H27	119.8

H10A—C10—H10C	109.5	C28—C27—H27	119.8
H10B—C10—H10C	109.5	C27—C28—C23	119.8 (5)
C16—C11—C12	119.2 (5)	C27—C28—H28	120.1
C16—C11—P1	117.8 (4)	C23—C28—H28	120.1
C12—C11—P1	123.0 (4)		
C2—N1—C1—O1	−177.2 (4)	C12—C11—C16—C15	1.7 (8)
C2—N1—C1—S1	4.3 (7)	P1—C11—C16—C15	−175.3 (4)
C9—O1—C1—N1	−1.4 (7)	C14—C15—C16—C11	−0.5 (8)
C9—O1—C1—S1	177.3 (4)	C11—P1—C17—C18	26.2 (4)
Au—S1—C1—N1	−171.6 (4)	C23—P1—C17—C18	−84.6 (4)
Au—S1—C1—O1	9.8 (4)	Au—P1—C17—C18	152.4 (4)
C1—N1—C2—C7	89.5 (6)	C11—P1—C17—C22	−156.2 (4)
C1—N1—C2—C3	−96.3 (6)	C23—P1—C17—C22	93.0 (4)
C7—C2—C3—C4	−0.7 (7)	Au—P1—C17—C22	−29.9 (4)
N1—C2—C3—C4	−174.9 (4)	C22—C17—C18—C19	−0.7 (7)
C7—C2—C3—C8	177.4 (5)	P1—C17—C18—C19	177.0 (4)
N1—C2—C3—C8	3.1 (7)	C17—C18—C19—C20	−1.5 (8)
C2—C3—C4—C5	0.2 (8)	C18—C19—C20—C21	2.3 (9)
C8—C3—C4—C5	−177.8 (5)	C19—C20—C21—C22	−0.9 (10)
C3—C4—C5—C6	0.7 (8)	C20—C21—C22—C17	−1.3 (9)
C4—C5—C6—C7	−1.1 (8)	C18—C17—C22—C21	2.1 (8)
C5—C6—C7—C2	0.6 (8)	P1—C17—C22—C21	−175.6 (4)
C3—C2—C7—C6	0.3 (7)	C11—P1—C23—C24	−93.8 (4)
N1—C2—C7—C6	174.6 (5)	C17—P1—C23—C24	16.3 (5)
C1—O1—C9—C10	−88.1 (6)	Au—P1—C23—C24	138.5 (4)
C23—P1—C11—C16	179.7 (4)	C11—P1—C23—C28	84.5 (4)
C17—P1—C11—C16	68.7 (4)	C17—P1—C23—C28	−165.4 (4)
Au—P1—C11—C16	−54.7 (4)	Au—P1—C23—C28	−43.2 (4)
C23—P1—C11—C12	2.8 (5)	C28—C23—C24—C25	−0.8 (8)
C17—P1—C11—C12	−108.2 (4)	P1—C23—C24—C25	177.5 (4)
Au—P1—C11—C12	128.4 (4)	C23—C24—C25—C26	−1.1 (8)
C16—C11—C12—C13	−1.3 (8)	C24—C25—C26—C27	1.7 (9)
P1—C11—C12—C13	175.5 (4)	C25—C26—C27—C28	−0.3 (9)
C11—C12—C13—C14	−0.3 (9)	C26—C27—C28—C23	−1.6 (9)
C12—C13—C14—C15	1.4 (9)	C24—C23—C28—C27	2.2 (8)
C13—C14—C15—C16	−1.0 (9)	P1—C23—C28—C27	−176.2 (4)

Fig. 1

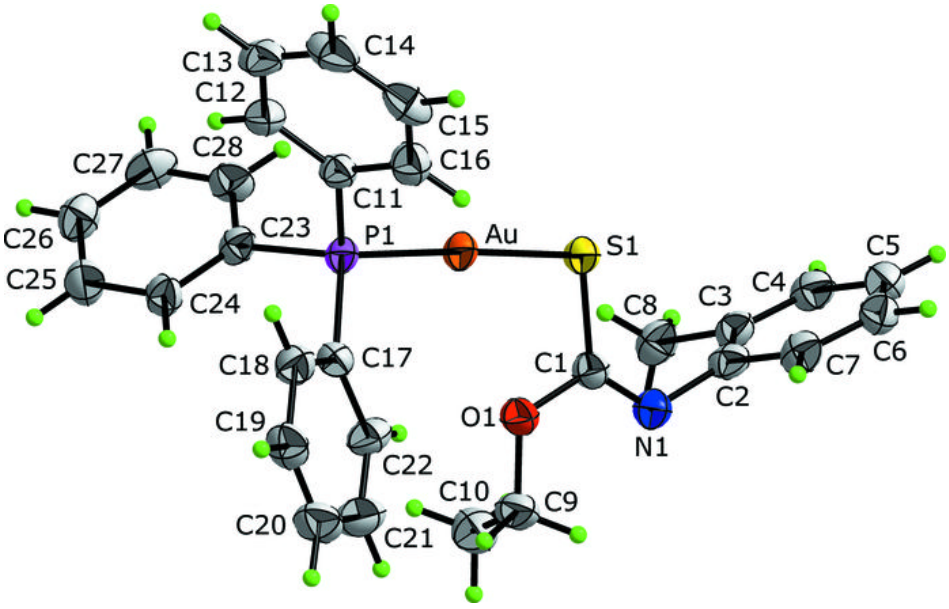

C14
C13
C12
C15
C28
C27
C16
C11
C23
P1
Au
S1
C26
C25
C24
C5
C4
C3
C8
C18
C17
C1
C6
C7
C2
C19
O1
N1
C22
C10
C9
C20
C21

Fig. 2