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[(Z)-N-(4-Chlorophenyl)-O-methylthio-carbamato-κS](triphenylphosphine-κP)-gold(I)

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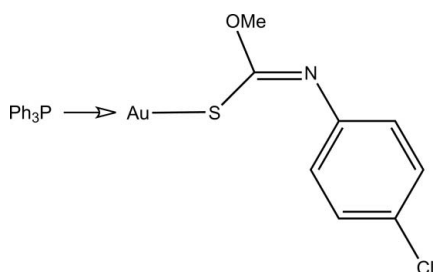
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Key indicators: single-crystal X-ray study; $T = 223$ K; mean $\sigma(\text{C}-\text{C}) = 0.008$ Å; R factor = 0.029; wR factor = 0.090; data-to-parameter ratio = 19.2.

The title compound, $[\text{Au}(\text{C}_8\text{H}_7\text{ClNOS})(\text{C}_{18}\text{H}_{15}\text{P})]$, is characterized by a linear S, P -donor set with a small deviation from the ideal linearity [$\text{S}-\text{Au}-\text{P} = 175.14$ (5°)] due to the close approach of the O atom to the Au atom [$\text{Au}\cdots\text{O} = 2.882$ (3) Å]. Loosely associated dimers are formed in the crystal structure through $\text{C}-\text{H}\cdots\text{O}$ interactions.

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

 $[\text{Au}(\text{C}_8\text{H}_7\text{ClNOS})(\text{C}_{18}\text{H}_{15}\text{P})]$ $M_r = 659.89$ Monoclinic, $P2_1/n$ $a = 9.1781$ (6) Å $b = 17.5679$ (12) Å $c = 15.5384$ (11) Å $\beta = 104.156$ (2°) $V = 2429.3$ (3) Å³ $Z = 4$ Mo $K\alpha$ radiation $\mu = 6.34$ mm⁻¹ $T = 223$ K $0.11 \times 0.10 \times 0.07$ mm

Data collection

Bruker SMART APEX CCD

diffractometer

Absorption correction: multi-scan

(SADABS; Bruker, 2001)

 $T_{\min} = 0.363$, $T_{\max} = 1.000$

17091 measured reflections

5570 independent reflections

4526 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.042$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.029$ $wR(F^2) = 0.090$ $S = 1.06$

5570 reflections

290 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 1.17$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.62$ e Å⁻³

Table 1

Selected bond lengths (Å).

Au—S1	2.3018 (12)	Au—P1	2.2473 (12)
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Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C3}-\text{H3}\cdots\text{O1}^i$	0.94	2.52	3.365 (6)	150

Symmetry code: (i) $-x, -y, -z + 1$.

Data collection: SMART (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); 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, 1999); software used to prepare material for publication: publCIF (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2256).

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supplementary materials

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[(*Z*)-*N*-(4-Chlorophenyl)-*O*-methylthiocarbamato- κ S](triphenylphosphine- κ P)gold(I)

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

Comment

As a part of systematic studies of phosphinegold(I) thiocarbamides (Ho *et al.* 2006; Ho & Tiekink, 2007; Kuan *et al.*, 2008), the title compound, [(C₅H₅)₃P]Au[SC(OMe)N(C₆H₄Cl-*p*)], was synthesized.

The thiocarbamide functions as a thiolate ligand as seen in the magnitudes of the C1—S1 and C1—N1 bond distances of 1.756 (5) and 1.271 (6) Å, respectively; the conformation about C1—N1 is *Z*. While the central SC(O)N chromophore is planar as seen in the S1—C1—N1—C2 and O1—C1—N1—C2 torsion angles of -0.8 (7) and -179.0 (4)°, respectively, the N-bound aryl ring is orthogonal to this plane as seen in the C1—N1—C2—C3 torsion angle of -76.6 (6)°. The thiocarbamide and phosphine ligands define an S, P donor set (Table 1 and Fig. 1). The deviation of the S1—Au—P1 angle [175.14 (5)°] from linearity is traced to the close approach of the O1 atom to the Au atom [2.882 (3) Å]. In the crystal structure, centrosymmetrically related molecules associate *via* C—H...O interactions (Table 2 and Fig. 2). The dimeric units formed are consolidated into the crystal structure by C—H... π interactions. The closest such contact occurs between C24—H24 and the ring centroid (Cg) of (C15—C20)ⁱ [C24...Cgⁱ = 3.552 (6), H24...Cgⁱ = 2.73 Å, C24—H24...Cgⁱ = 146°, symmetry code: (i) -1+x, y, z].

Experimental

The title compound was prepared following the standard literature procedure from the reaction of Ph₃AuCl and MeOC(S)N(H)(C₆H₄Cl-*p*) in the presence of base (Hall *et al.*, 1993).

Refinement

H atoms were geometrically placed (C—H = 0.94 and 0.97 Å) and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2(1.5$ for methyl) $U_{\text{eq}}(\text{C})$. The maximum and minimum residual electron density peaks of 1.17 and 0.62 e Å⁻³, respectively, were located 0.88 and 1.39 Å from the Au atom.

Figures

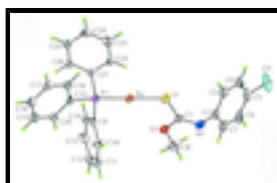


Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

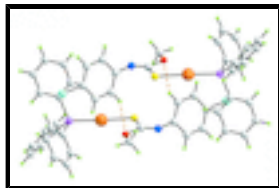


Fig. 2. Supramolecular dimer in the title compound, mediated by C—H...O contacts (orange dashed lines). [Colour codes: Au orange; Cl cyan; S yellow; P pink; O red; N blue; C grey; and H green.]

[(Z)-N-(4-Chlorophenyl)-O-methylthiocarbamato-κS](triphenylphosphine-κP)gold(I)

Crystal data

[Au(C₈H₇ClNOS)(C₁₈H₁₅P)]

$M_r = 659.89$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 9.1781$ (6) Å

$b = 17.5679$ (12) Å

$c = 15.5384$ (11) Å

$\beta = 104.156$ (2)°

$V = 2429.3$ (3) Å³

$Z = 4$

$F(000) = 1280$

$D_x = 1.804$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å

Cell parameters from 4456 reflections

$\theta = 2.3$ – 25.0 °

$\mu = 6.34$ mm⁻¹

$T = 223$ K

Block, colourless

$0.11 \times 0.10 \times 0.07$ mm

Data collection

Bruker SMART APEX CCD
diffractometer

Radiation source: fine-focus sealed tube
graphite

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2001)

$T_{\min} = 0.363$, $T_{\max} = 1.000$

17091 measured reflections

5570 independent reflections

4526 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.042$

$\theta_{\max} = 27.5$ °, $\theta_{\min} = 1.8$ °

$h = -11 \rightarrow 10$

$k = -22 \rightarrow 22$

$l = -20 \rightarrow 14$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.029$

$wR(F^2) = 0.090$

$S = 1.06$

5570 reflections

290 parameters

0 restraints

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

$w = 1/[\sigma^2(F_o^2) + (0.0462P)^2P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 1.17$ e Å⁻³

$\Delta\rho_{\min} = -0.62$ e Å⁻³

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Au	0.14582 (2)	0.203115 (10)	0.426452 (12)	0.02944 (8)
Cl1	0.2539 (2)	-0.28046 (9)	0.29800 (15)	0.0761 (6)
S1	0.19317 (16)	0.07649 (7)	0.40658 (8)	0.0372 (3)
P1	0.08624 (13)	0.32352 (7)	0.45280 (8)	0.0265 (3)
O1	0.2450 (4)	0.10253 (19)	0.5758 (2)	0.0342 (8)
N1	0.2656 (4)	-0.0229 (2)	0.5444 (3)	0.0352 (9)
C1	0.2379 (5)	0.0450 (3)	0.5172 (3)	0.0303 (10)
C2	0.2605 (5)	-0.0827 (3)	0.4832 (3)	0.0350 (11)
C3	0.1251 (5)	-0.1125 (3)	0.4349 (3)	0.0378 (12)
H3	0.0343	-0.0911	0.4410	0.045*
C4	0.1222 (6)	-0.1735 (3)	0.3779 (4)	0.0428 (13)
H4	0.0304	-0.1931	0.3443	0.051*
C5	0.2552 (7)	-0.2045 (3)	0.3715 (5)	0.0461 (14)
C6	0.3906 (7)	-0.1768 (3)	0.4203 (5)	0.0507 (16)
H6	0.4809	-0.1996	0.4153	0.061*
C7	0.3939 (6)	-0.1165 (3)	0.4754 (4)	0.0434 (13)
H7	0.4866	-0.0976	0.5084	0.052*
C8	0.2730 (7)	0.0813 (4)	0.6684 (3)	0.0519 (15)
H8A	0.1966	0.0456	0.6762	0.078*
H8B	0.2699	0.1263	0.7040	0.078*
H8C	0.3712	0.0576	0.6870	0.078*
C9	0.1409 (5)	0.3443 (3)	0.5711 (3)	0.0295 (10)
C10	0.2879 (6)	0.3272 (3)	0.6162 (4)	0.0466 (14)
H10	0.3539	0.3047	0.5859	0.056*
C11	0.3363 (7)	0.3434 (4)	0.7058 (4)	0.0535 (16)
H11	0.4351	0.3316	0.7368	0.064*
C12	0.2396 (7)	0.3768 (3)	0.7492 (4)	0.0471 (14)
H12	0.2730	0.3885	0.8099	0.057*
C13	0.0944 (6)	0.3936 (3)	0.7049 (4)	0.0436 (13)
H13	0.0283	0.4159	0.7352	0.052*
C14	0.0462 (6)	0.3773 (3)	0.6154 (3)	0.0326 (11)
H14	-0.0528	0.3892	0.5848	0.039*
C15	0.1717 (5)	0.3984 (2)	0.4012 (3)	0.0267 (9)
C16	0.1530 (5)	0.3965 (3)	0.3101 (3)	0.0323 (10)
H16	0.0989	0.3563	0.2770	0.039*
C17	0.2129 (6)	0.4530 (3)	0.2673 (3)	0.0358 (11)
H17	0.1990	0.4513	0.2053	0.043*
C18	0.2926 (6)	0.5118 (3)	0.3152 (4)	0.0382 (12)
H18	0.3328	0.5506	0.2862	0.046*
C19	0.3131 (6)	0.5133 (3)	0.4061 (4)	0.0382 (12)
H19	0.3684	0.5530	0.4393	0.046*
C20	0.2532 (5)	0.4570 (3)	0.4485 (3)	0.0344 (11)
H20	0.2681	0.4586	0.5105	0.041*
C21	-0.1136 (5)	0.3406 (3)	0.4161 (3)	0.0259 (9)
C22	-0.2118 (6)	0.2803 (3)	0.4140 (4)	0.0425 (13)

supplementary materials

H22	-0.1735	0.2315	0.4309	0.051*
C23	-0.3653 (6)	0.2911 (3)	0.3874 (5)	0.0500 (15)
H23	-0.4307	0.2499	0.3868	0.060*
C24	-0.4224 (6)	0.3617 (3)	0.3618 (4)	0.0421 (13)
H24	-0.5268	0.3689	0.3428	0.051*
C25	-0.3268 (6)	0.4219 (3)	0.3641 (3)	0.0361 (11)
H25	-0.3664	0.4705	0.3470	0.043*
C26	-0.1724 (5)	0.4122 (3)	0.3913 (3)	0.0312 (10)
H26	-0.1079	0.4540	0.3930	0.037*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au	0.03688 (12)	0.02458 (11)	0.02522 (11)	0.00819 (7)	0.00444 (8)	0.00001 (7)
Cl1	0.0969 (14)	0.0355 (8)	0.1131 (17)	-0.0060 (8)	0.0587 (13)	-0.0165 (9)
S1	0.0577 (8)	0.0266 (6)	0.0267 (6)	0.0125 (6)	0.0092 (6)	0.0013 (5)
P1	0.0296 (6)	0.0242 (6)	0.0250 (6)	0.0058 (5)	0.0050 (5)	-0.0002 (5)
O1	0.0384 (18)	0.0375 (19)	0.0250 (18)	0.0022 (15)	0.0045 (14)	0.0035 (15)
N1	0.032 (2)	0.037 (2)	0.037 (2)	0.0053 (17)	0.0106 (18)	0.0114 (19)
C1	0.028 (2)	0.036 (3)	0.027 (3)	0.0034 (19)	0.007 (2)	0.003 (2)
C2	0.035 (3)	0.028 (2)	0.043 (3)	0.003 (2)	0.013 (2)	0.012 (2)
C3	0.033 (3)	0.034 (3)	0.051 (3)	0.004 (2)	0.018 (2)	0.008 (2)
C4	0.038 (3)	0.035 (3)	0.058 (4)	-0.003 (2)	0.016 (3)	0.003 (3)
C5	0.056 (4)	0.026 (3)	0.065 (4)	0.001 (2)	0.030 (3)	0.006 (2)
C6	0.047 (3)	0.032 (3)	0.081 (5)	0.014 (2)	0.033 (3)	0.011 (3)
C7	0.032 (3)	0.040 (3)	0.061 (4)	0.006 (2)	0.019 (3)	0.015 (3)
C8	0.064 (4)	0.066 (4)	0.021 (3)	0.003 (3)	0.002 (3)	0.001 (3)
C9	0.038 (3)	0.024 (2)	0.025 (2)	0.0043 (19)	0.004 (2)	0.0020 (18)
C10	0.043 (3)	0.056 (4)	0.036 (3)	0.021 (3)	0.000 (2)	-0.006 (3)
C11	0.053 (4)	0.067 (4)	0.033 (3)	0.017 (3)	-0.005 (3)	-0.002 (3)
C12	0.067 (4)	0.043 (3)	0.025 (3)	0.001 (3)	-0.002 (3)	-0.003 (2)
C13	0.056 (3)	0.045 (3)	0.033 (3)	0.003 (3)	0.015 (3)	-0.005 (2)
C14	0.036 (3)	0.034 (3)	0.027 (3)	0.001 (2)	0.008 (2)	-0.001 (2)
C15	0.027 (2)	0.023 (2)	0.031 (2)	0.0050 (17)	0.0086 (19)	-0.0006 (19)
C16	0.036 (3)	0.029 (2)	0.030 (3)	0.003 (2)	0.004 (2)	-0.001 (2)
C17	0.040 (3)	0.039 (3)	0.029 (3)	0.006 (2)	0.011 (2)	0.003 (2)
C18	0.037 (3)	0.030 (3)	0.049 (3)	0.001 (2)	0.014 (2)	0.004 (2)
C19	0.038 (3)	0.033 (3)	0.043 (3)	-0.003 (2)	0.011 (2)	-0.003 (2)
C20	0.041 (3)	0.032 (3)	0.027 (3)	0.005 (2)	0.003 (2)	-0.003 (2)
C21	0.027 (2)	0.030 (2)	0.019 (2)	0.0047 (18)	0.0020 (18)	0.0013 (18)
C22	0.042 (3)	0.029 (3)	0.050 (3)	0.001 (2)	-0.003 (3)	0.011 (2)
C23	0.037 (3)	0.050 (4)	0.061 (4)	-0.008 (2)	0.008 (3)	0.011 (3)
C24	0.033 (3)	0.055 (4)	0.038 (3)	0.006 (2)	0.008 (2)	0.000 (3)
C25	0.041 (3)	0.032 (3)	0.033 (3)	0.012 (2)	0.004 (2)	-0.001 (2)
C26	0.033 (3)	0.030 (2)	0.029 (3)	0.0040 (19)	0.007 (2)	-0.002 (2)

Geometric parameters (\AA , $^\circ$)

Au—S1	2.3018 (12)	C11—H11	0.9400
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Au—P1	2.2473 (12)	C12—C13	1.374 (8)
C11—C5	1.755 (6)	C12—H12	0.9400
S1—C1	1.756 (5)	C13—C14	1.381 (7)
P1—C21	1.808 (4)	C13—H13	0.9400
P1—C15	1.815 (5)	C14—H14	0.9400
P1—C9	1.820 (5)	C15—C20	1.375 (6)
O1—C1	1.352 (6)	C15—C16	1.384 (6)
O1—C8	1.447 (6)	C16—C17	1.383 (7)
N1—C1	1.271 (6)	C16—H16	0.9400
N1—C2	1.409 (7)	C17—C18	1.375 (7)
C2—C3	1.387 (7)	C17—H17	0.9400
C2—C7	1.393 (7)	C18—C19	1.380 (7)
C3—C4	1.387 (8)	C18—H18	0.9400
C3—H3	0.9400	C19—C20	1.375 (7)
C4—C5	1.362 (8)	C19—H19	0.9400
C4—H4	0.9400	C20—H20	0.9400
C5—C6	1.377 (9)	C21—C22	1.385 (7)
C6—C7	1.357 (8)	C21—C26	1.386 (6)
C6—H6	0.9400	C22—C23	1.381 (8)
C7—H7	0.9400	C22—H22	0.9400
C8—H8A	0.9700	C23—C24	1.366 (7)
C8—H8B	0.9700	C23—H23	0.9400
C8—H8C	0.9700	C24—C25	1.369 (7)
C9—C14	1.363 (7)	C24—H24	0.9400
C9—C10	1.393 (7)	C25—C26	1.387 (7)
C10—C11	1.384 (8)	C25—H25	0.9400
C10—H10	0.9400	C26—H26	0.9400
C11—C12	1.370 (8)		
P1—Au—S1	175.14 (5)	C11—C12—C13	120.7 (5)
C1—S1—Au	100.35 (17)	C11—C12—H12	119.6
C21—P1—C15	104.8 (2)	C13—C12—H12	119.6
C21—P1—C9	107.1 (2)	C12—C13—C14	119.5 (5)
C15—P1—C9	105.0 (2)	C12—C13—H13	120.2
C21—P1—Au	111.82 (15)	C14—C13—H13	120.2
C15—P1—Au	116.79 (15)	C9—C14—C13	120.6 (5)
C9—P1—Au	110.73 (15)	C9—C14—H14	119.7
C1—O1—C8	116.4 (4)	C13—C14—H14	119.7
C1—N1—C2	120.3 (4)	C20—C15—C16	118.7 (4)
N1—C1—O1	120.3 (4)	C20—C15—P1	123.0 (4)
N1—C1—S1	126.9 (4)	C16—C15—P1	118.4 (3)
O1—C1—S1	112.7 (3)	C17—C16—C15	120.7 (5)
C3—C2—C7	118.8 (5)	C17—C16—H16	119.6
C3—C2—N1	121.6 (4)	C15—C16—H16	119.6
C7—C2—N1	119.4 (5)	C18—C17—C16	120.0 (5)
C4—C3—C2	120.8 (5)	C18—C17—H17	120.0
C4—C3—H3	119.6	C16—C17—H17	120.0
C2—C3—H3	119.6	C17—C18—C19	119.3 (5)
C5—C4—C3	118.5 (5)	C17—C18—H18	120.3
C5—C4—H4	120.7	C19—C18—H18	120.3

supplementary materials

C3—C4—H4	120.7	C20—C19—C18	120.4 (5)
C4—C5—C6	121.6 (6)	C20—C19—H19	119.8
C4—C5—C11	119.2 (5)	C18—C19—H19	119.8
C6—C5—C11	119.2 (4)	C15—C20—C19	120.8 (5)
C7—C6—C5	120.1 (5)	C15—C20—H20	119.6
C7—C6—H6	120.0	C19—C20—H20	119.6
C5—C6—H6	120.0	C22—C21—C26	118.7 (4)
C6—C7—C2	120.2 (5)	C22—C21—P1	119.0 (4)
C6—C7—H7	119.9	C26—C21—P1	122.3 (4)
C2—C7—H7	119.9	C23—C22—C21	120.8 (5)
O1—C8—H8A	109.5	C23—C22—H22	119.6
O1—C8—H8B	109.5	C21—C22—H22	119.6
H8A—C8—H8B	109.5	C24—C23—C22	120.1 (5)
O1—C8—H8C	109.5	C24—C23—H23	119.9
H8A—C8—H8C	109.5	C22—C23—H23	119.9
H8B—C8—H8C	109.5	C23—C24—C25	119.7 (5)
C14—C9—C10	119.8 (5)	C23—C24—H24	120.1
C14—C9—P1	122.9 (4)	C25—C24—H24	120.1
C10—C9—P1	117.3 (4)	C24—C25—C26	120.8 (5)
C11—C10—C9	119.6 (5)	C24—C25—H25	119.6
C11—C10—H10	120.2	C26—C25—H25	119.6
C9—C10—H10	120.2	C21—C26—C25	119.7 (5)
C12—C11—C10	119.7 (5)	C21—C26—H26	120.1
C12—C11—H11	120.1	C25—C26—H26	120.1
C10—C11—H11	120.1		
C2—N1—C1—O1	-179.0 (4)	P1—C9—C14—C13	-178.5 (4)
C2—N1—C1—S1	-0.8 (7)	C12—C13—C14—C9	0.6 (8)
C8—O1—C1—N1	-4.9 (6)	C21—P1—C15—C20	110.4 (4)
C8—O1—C1—S1	176.7 (4)	C9—P1—C15—C20	-2.2 (4)
Au—S1—C1—N1	175.8 (4)	Au—P1—C15—C20	-125.2 (4)
Au—S1—C1—O1	-6.0 (3)	C21—P1—C15—C16	-69.1 (4)
C1—N1—C2—C3	-76.6 (6)	C9—P1—C15—C16	178.3 (4)
C1—N1—C2—C7	108.0 (5)	Au—P1—C15—C16	55.2 (4)
C7—C2—C3—C4	-1.8 (8)	C20—C15—C16—C17	-1.0 (7)
N1—C2—C3—C4	-177.2 (5)	P1—C15—C16—C17	178.5 (4)
C2—C3—C4—C5	1.2 (8)	C15—C16—C17—C18	0.3 (7)
C3—C4—C5—C6	0.1 (9)	C16—C17—C18—C19	0.5 (8)
C3—C4—C5—C11	-178.7 (4)	C17—C18—C19—C20	-0.6 (8)
C4—C5—C6—C7	-0.9 (9)	C16—C15—C20—C19	0.9 (7)
C11—C5—C6—C7	178.0 (4)	P1—C15—C20—C19	-178.6 (4)
C5—C6—C7—C2	0.3 (9)	C18—C19—C20—C15	-0.1 (8)
C3—C2—C7—C6	1.0 (8)	C15—P1—C21—C22	155.3 (4)
N1—C2—C7—C6	176.5 (5)	C9—P1—C21—C22	-93.6 (4)
C21—P1—C9—C14	-8.7 (5)	Au—P1—C21—C22	27.9 (4)
C15—P1—C9—C14	102.3 (4)	C15—P1—C21—C26	-25.9 (4)
Au—P1—C9—C14	-130.9 (4)	C9—P1—C21—C26	85.3 (4)
C21—P1—C9—C10	173.1 (4)	Au—P1—C21—C26	-153.3 (3)
C15—P1—C9—C10	-75.9 (5)	C26—C21—C22—C23	0.3 (8)
Au—P1—C9—C10	51.0 (5)	P1—C21—C22—C23	179.2 (5)

C14—C9—C10—C11	0.4 (9)	C21—C22—C23—C24	0.6 (10)
P1—C9—C10—C11	178.6 (5)	C22—C23—C24—C25	-1.1 (10)
C9—C10—C11—C12	-0.6 (10)	C23—C24—C25—C26	0.5 (8)
C10—C11—C12—C13	0.8 (10)	C22—C21—C26—C25	-0.8 (7)
C11—C12—C13—C14	-0.8 (9)	P1—C21—C26—C25	-179.7 (4)
C10—C9—C14—C13	-0.4 (8)	C24—C25—C26—C21	0.4 (7)

Hydrogen-bond geometry (\AA , $^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C3—H3 \cdots O1 ⁱ	0.94	2.52	3.365 (6)	150

Symmetry codes: (i) $-x, -y, -z+1$.

Fig. 1

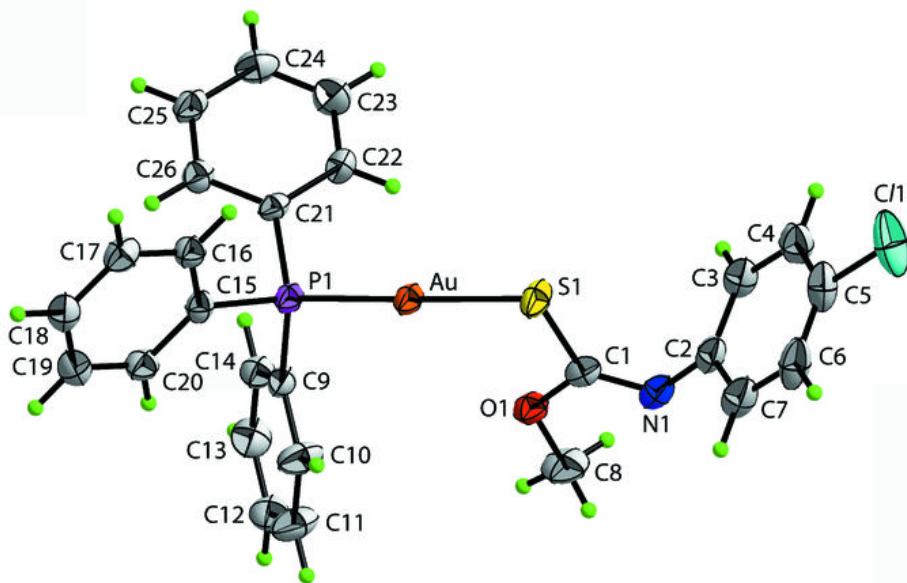


Fig. 2

