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## Structure Reports

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# [(Z)-N-(2-Chlorophenyl)-O-methylthio-carbamato- $\kappa$ S](triphenylphosphine- $\kappa$ P)-gold(I)

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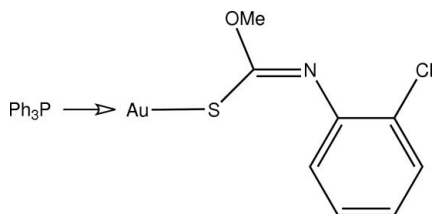
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Key indicators: single-crystal X-ray study;  $T = 223$  K; mean  $\sigma(\text{C}-\text{C}) = 0.008$  Å;  $R$  factor = 0.032;  $wR$  factor = 0.085; data-to-parameter ratio = 19.1.

In the title compound,  $[\text{Au}(\text{C}_8\text{H}_7\text{ClNOS})(\text{C}_{18}\text{H}_{15}\text{P})]$ , the Au<sup>I</sup> atom has a near-linear geometry, defined by an  $S, P$ -donor set [ $\text{S}-\text{Au}-\text{P} = 175.09(5)^\circ$ ]. The proximity of the methoxy O atom to Au may be responsible for the deviation from linearity [ $\text{Au}\cdots\text{O} = 2.959(4)$  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

 $[\text{Au}(\text{C}_8\text{H}_7\text{ClNOS})(\text{C}_{18}\text{H}_{15}\text{P})]$ 
 $M_r = 659.89$ Monoclinic,  $P2_1/n$  $a = 8.9388(5)$  Å $b = 26.2804(15)$  Å $c = 10.3233(6)$  Å $\beta = 96.599(1)^\circ$  $V = 2409.0(2)$  Å<sup>3</sup> $Z = 4$ Mo  $K\alpha$  radiation $\mu = 6.39$  mm<sup>-1</sup> $T = 223$  K $0.13 \times 0.10 \times 0.07$  mm

### Data collection

Bruker SMART CCD

diffractometer

Absorption correction: multi-scan

(SADABS; Bruker, 2000)

 $T_{\min} = 0.521$ ,  $T_{\max} = 1$ 

17015 measured reflections

5537 independent reflections

4400 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.047$ 

### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.032$  $wR(F^2) = 0.085$  $S = 1.04$ 

5537 reflections

290 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 1.17$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.54$  e Å<sup>-3</sup>
**Table 1**

Selected bond lengths (Å).

Au—S1	2.3086 (12)	Au—P1	2.2508 (12)
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Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SHELXTL (Bruker, 2000); 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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5235).

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## supporting information

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**[(Z)-N-(2-Chlorophenyl)-O-methylthiocarbamato- $\kappa$ S](triphenylphosphine- $\kappa$ P)gold(I)****Primjira P. Tadbuppa and Edward R. T. Tiekink****S1. Comment**

The motivation for systematic studies of phosphinegold(I) thiocarbamides, *e.g.* ( $R_3P$ )PAu[SC(OR')NR''], relates to the delineation of crystal packing characteristics, *e.g.* the propensity to form aurophilic (Au $\cdots$ Au) interactions (Ho & Tiekink, 2007; Kuan *et al.*, 2008), as well as the examination of their luminescence characteristics (Ho *et al.* 2006). The title compound, (C<sub>5</sub>H<sub>5</sub>)<sub>3</sub>PAu[SC(OMe)N(C<sub>6</sub>H<sub>4</sub>Cl-*o*)], (I), was synthesized during the course of these studies.

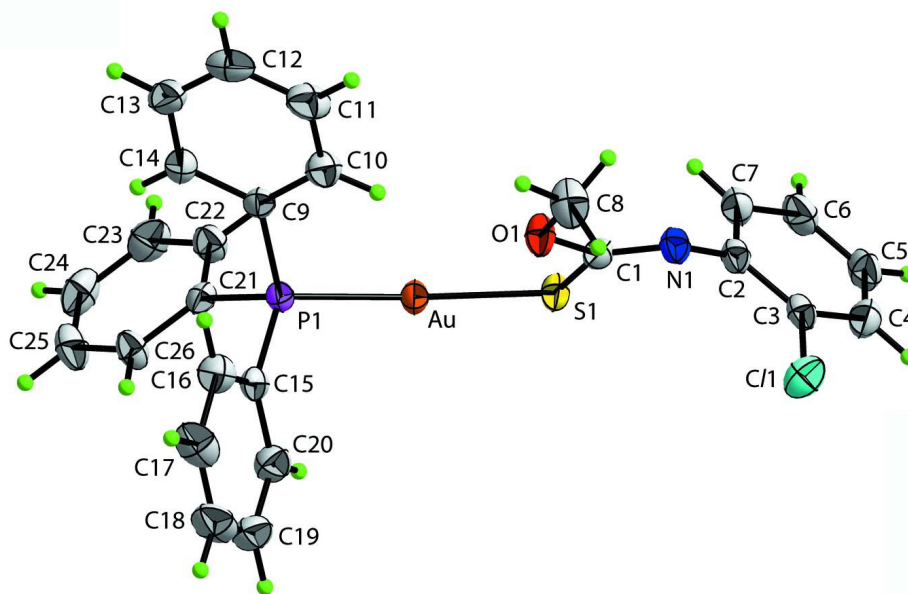
The thiocarbamato anion functions as a thiolate ligand in (I), Fig. 1, as seen in the magnitudes of the C1—S1 and C1=N1 bond distances of 1.762 (5) and 1.269 (6) Å, respectively; the conformation about C1=N1 is *Z*. The central SC(O)N chromophore has small but significant twists from planarity as seen in the S1—C1—N1—C2 and O1—C1—N1—C2 torsion angles of 10.0 (7) and -173.1 (4) °, respectively. The N-bound aryl ring is twisted out of this plane: the C1—N1—C2—C3 torsion angle is -126.3 (5) °. The thiocarbamato and phosphine ligands define an approximately linear *S, P* donor set, Table. The deviation of the S1—Au—P1 angle [175.09 (5) °] from the ideal linear geometry is ascribed to the close approach of the O1 atom [2.959 (4) Å] to Au.

**S2. Experimental**

Compound (I) was prepared following the standard literature procedure from the reaction of Ph<sub>3</sub>AuCl and MeOC(S)N(H) (C<sub>6</sub>H<sub>4</sub>Cl-*o*) in the presence of base (Hall *et al.*, 1993).

**S3. Refinement**

The H atoms were geometrically placed (C—H = 0.94–0.97 Å) and refined as riding with  $U_{iso}(H) = 1.2\text{--}1.5U_{eq}(C)$ . A rotating group model was used for the methyl group. The maximum and minimum residual electron density peaks of 1.17 and 0.54 e Å<sup>-3</sup>, respectively, are located 0.86 Å and 0.38 Å from the Au and H20 atoms, respectively.

**Figure 1**

Molecular structure of (I) showing displacement ellipsoids at the 50% probability level.

**[(Z)-N-(2-Chlorophenyl)-O-methylthiocarbamato- $\kappa$ S](triphenylphosphine- $\kappa$ P)gold(I)**

*Crystal data*

[Au(C<sub>8</sub>H<sub>7</sub>ClNOS)(C<sub>18</sub>H<sub>15</sub>P)]

$M_r = 659.89$

Monoclinic,  $P2_1/n$

Hall symbol: -P 2yn

$a = 8.9388$  (5) Å

$b = 26.2804$  (15) Å

$c = 10.3233$  (6) Å

$\beta = 96.599$  (1)°

$V = 2409.0$  (2) Å<sup>3</sup>

$Z = 4$

$F(000) = 1280$

$D_x = 1.819$  Mg m<sup>-3</sup>

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

Cell parameters from 3828 reflections

$\theta = 2.4$ – $24.2$ °

$\mu = 6.39$  mm<sup>-1</sup>

$T = 223$  K

Block, colourless

$0.13 \times 0.10 \times 0.07$  mm

*Data collection*

Bruker SMART CCD  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\omega$  scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2000)

$T_{\min} = 0.521$ ,  $T_{\max} = 1$

17015 measured reflections

5537 independent reflections

4400 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.047$

$\theta_{\max} = 27.5$ °,  $\theta_{\min} = 1.6$ °

$h = -11 \rightarrow 10$

$k = -34 \rightarrow 33$

$l = -13 \rightarrow 12$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.032$

$wR(F^2) = 0.085$

$S = 1.04$

5537 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

$$w = 1/[\sigma^2(F_o^2) + (0.0379P)^2]$$

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

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

$$\Delta\rho_{\max} = 1.17 \text{ e } \text{Å}^{-3}$$

$$\Delta\rho_{\min} = -0.54 \text{ e } \text{Å}^{-3}$$

*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<sup>2</sup>)*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Au	0.24654 (2)	0.102793 (8)	0.096786 (18)	0.02961 (8)
Cl1	0.89614 (16)	0.17339 (6)	-0.09989 (13)	0.0446 (3)
S1	0.37239 (14)	0.14902 (5)	-0.04703 (12)	0.0313 (3)
P1	0.13681 (14)	0.06089 (5)	0.25093 (12)	0.0267 (3)
O1	0.5076 (4)	0.16834 (14)	0.1853 (3)	0.0349 (9)
N1	0.6237 (5)	0.20523 (16)	0.0254 (4)	0.0320 (10)
C1	0.5160 (5)	0.17848 (19)	0.0581 (5)	0.0283 (11)
C2	0.6239 (6)	0.22061 (19)	-0.1058 (5)	0.0299 (11)
C3	0.7475 (5)	0.21050 (19)	-0.1725 (5)	0.0301 (11)
C4	0.7550 (6)	0.2287 (2)	-0.2976 (5)	0.0390 (13)
H4	0.8395	0.2213	-0.3407	0.047*
C5	0.6403 (7)	0.2573 (2)	-0.3584 (5)	0.0405 (13)
H5	0.6450	0.2697	-0.4432	0.049*
C6	0.5180 (6)	0.2676 (2)	-0.2937 (6)	0.0428 (14)
H6	0.4379	0.2869	-0.3356	0.051*
C7	0.5101 (6)	0.2503 (2)	-0.1685 (5)	0.0384 (13)
H7	0.4265	0.2589	-0.1253	0.046*
C8	0.6204 (7)	0.1907 (3)	0.2779 (5)	0.0468 (15)
H8A	0.7169	0.1748	0.2702	0.070*
H8B	0.5936	0.1855	0.3653	0.070*
H8C	0.6271	0.2268	0.2608	0.070*
C9	0.1331 (5)	0.10132 (18)	0.3935 (5)	0.0273 (10)
C10	0.2482 (6)	0.1366 (2)	0.4224 (5)	0.0366 (13)
H10	0.3225	0.1407	0.3658	0.044*
C11	0.2530 (6)	0.1655 (2)	0.5335 (6)	0.0444 (14)
H11	0.3326	0.1885	0.5538	0.053*
C12	0.1430 (7)	0.1611 (2)	0.6157 (6)	0.0441 (15)
H12	0.1479	0.1806	0.6923	0.053*
C13	0.0248 (7)	0.1275 (2)	0.5843 (6)	0.0454 (15)
H13	-0.0527	0.1253	0.6384	0.055*

C14	0.0199 (6)	0.0975 (2)	0.4747 (5)	0.0379 (13)
H14	-0.0599	0.0745	0.4547	0.045*
C15	0.2397 (5)	0.00408 (19)	0.3076 (5)	0.0301 (11)
C16	0.2844 (6)	-0.0052 (2)	0.4394 (5)	0.0386 (13)
H16	0.2640	0.0185	0.5031	0.046*
C17	0.3602 (7)	-0.0506 (2)	0.4751 (7)	0.0510 (16)
H17	0.3904	-0.0572	0.5637	0.061*
C18	0.3912 (7)	-0.0857 (2)	0.3836 (8)	0.0551 (18)
H18	0.4414	-0.1161	0.4095	0.066*
C19	0.3488 (7)	-0.0762 (2)	0.2546 (7)	0.0526 (17)
H19	0.3709	-0.1001	0.1917	0.063*
C20	0.2728 (6)	-0.0314 (2)	0.2154 (6)	0.0422 (14)
H20	0.2440	-0.0253	0.1263	0.051*
C21	-0.0550 (5)	0.03955 (19)	0.2088 (4)	0.0262 (10)
C22	-0.1585 (6)	0.0739 (2)	0.1473 (5)	0.0367 (13)
H22	-0.1274	0.1065	0.1245	0.044*
C23	-0.3071 (6)	0.0596 (3)	0.1200 (6)	0.0470 (15)
H23	-0.3778	0.0830	0.0807	0.056*
C24	-0.3536 (6)	0.0114 (3)	0.1495 (6)	0.0462 (15)
H24	-0.4551	0.0020	0.1294	0.055*
C25	-0.2516 (6)	-0.0228 (2)	0.2083 (6)	0.0449 (14)
H25	-0.2829	-0.0558	0.2283	0.054*
C26	-0.1020 (6)	-0.0087 (2)	0.2384 (5)	0.0332 (12)
H26	-0.0322	-0.0321	0.2791	0.040*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Au	0.02941 (12)	0.03086 (12)	0.02991 (12)	-0.00652 (9)	0.00915 (8)	0.00018 (9)
Cl1	0.0407 (8)	0.0589 (10)	0.0340 (7)	0.0071 (7)	0.0033 (6)	-0.0004 (7)
S1	0.0317 (7)	0.0374 (8)	0.0257 (6)	-0.0082 (6)	0.0074 (5)	0.0005 (5)
P1	0.0265 (7)	0.0255 (7)	0.0290 (7)	-0.0051 (5)	0.0073 (5)	-0.0014 (5)
O1	0.035 (2)	0.045 (2)	0.0252 (19)	-0.0108 (17)	0.0040 (15)	0.0024 (16)
N1	0.030 (2)	0.032 (3)	0.035 (2)	-0.0076 (19)	0.0042 (19)	-0.0003 (19)
C1	0.026 (2)	0.032 (3)	0.028 (3)	-0.001 (2)	0.006 (2)	-0.004 (2)
C2	0.032 (3)	0.029 (3)	0.029 (3)	-0.009 (2)	0.004 (2)	-0.001 (2)
C3	0.032 (3)	0.027 (3)	0.030 (3)	-0.009 (2)	0.001 (2)	0.000 (2)
C4	0.038 (3)	0.045 (3)	0.036 (3)	-0.008 (3)	0.012 (2)	-0.004 (3)
C5	0.054 (4)	0.037 (3)	0.031 (3)	-0.006 (3)	0.008 (3)	0.008 (2)
C6	0.045 (3)	0.034 (3)	0.049 (4)	-0.001 (3)	0.003 (3)	0.013 (3)
C7	0.036 (3)	0.034 (3)	0.046 (3)	-0.003 (2)	0.010 (3)	0.008 (3)
C8	0.050 (4)	0.060 (4)	0.029 (3)	-0.018 (3)	-0.003 (3)	0.001 (3)
C9	0.026 (3)	0.025 (3)	0.031 (3)	0.002 (2)	0.004 (2)	0.002 (2)
C10	0.031 (3)	0.036 (3)	0.043 (3)	-0.003 (2)	0.003 (2)	-0.005 (2)
C11	0.040 (3)	0.039 (3)	0.052 (4)	-0.006 (3)	-0.004 (3)	-0.014 (3)
C12	0.060 (4)	0.034 (3)	0.036 (3)	0.012 (3)	-0.002 (3)	-0.006 (3)
C13	0.062 (4)	0.037 (3)	0.040 (3)	0.007 (3)	0.020 (3)	0.000 (3)
C14	0.042 (3)	0.035 (3)	0.039 (3)	-0.007 (3)	0.015 (3)	-0.003 (2)

C15	0.020 (2)	0.029 (3)	0.041 (3)	-0.006 (2)	0.006 (2)	-0.003 (2)
C16	0.033 (3)	0.040 (3)	0.042 (3)	0.000 (2)	-0.001 (2)	-0.002 (3)
C17	0.040 (3)	0.044 (4)	0.065 (4)	0.000 (3)	-0.009 (3)	0.013 (3)
C18	0.037 (4)	0.035 (3)	0.093 (6)	0.011 (3)	0.004 (3)	0.009 (4)
C19	0.043 (4)	0.041 (4)	0.078 (5)	0.004 (3)	0.023 (3)	-0.009 (3)
C20	0.037 (3)	0.041 (3)	0.050 (4)	-0.001 (3)	0.010 (3)	-0.006 (3)
C21	0.022 (2)	0.033 (3)	0.024 (2)	-0.003 (2)	0.0043 (19)	-0.004 (2)
C22	0.037 (3)	0.033 (3)	0.039 (3)	0.000 (2)	0.003 (2)	0.005 (2)
C23	0.033 (3)	0.058 (4)	0.050 (4)	0.009 (3)	0.001 (3)	0.004 (3)
C24	0.024 (3)	0.071 (5)	0.043 (3)	-0.007 (3)	0.001 (2)	-0.009 (3)
C25	0.044 (3)	0.043 (3)	0.047 (4)	-0.020 (3)	0.001 (3)	0.000 (3)
C26	0.028 (3)	0.031 (3)	0.039 (3)	-0.005 (2)	-0.004 (2)	0.006 (2)

*Geometric parameters (Å, °)*

Au—S1	2.3086 (12)	C11—H11	0.9400
Au—P1	2.2508 (12)	C12—C13	1.386 (8)
Cl1—C3	1.746 (5)	C12—H12	0.9400
S1—C1	1.762 (5)	C13—C14	1.376 (8)
P1—C21	1.809 (5)	C13—H13	0.9400
P1—C15	1.815 (5)	C14—H14	0.9400
P1—C9	1.819 (5)	C15—C20	1.389 (7)
O1—C1	1.350 (6)	C15—C16	1.395 (7)
O1—C8	1.433 (6)	C16—C17	1.400 (8)
N1—C1	1.269 (6)	C16—H16	0.9400
N1—C2	1.414 (6)	C17—C18	1.371 (9)
C2—C7	1.383 (7)	C17—H17	0.9400
C2—C3	1.393 (7)	C18—C19	1.365 (9)
C3—C4	1.385 (7)	C18—H18	0.9400
C4—C5	1.365 (8)	C19—C20	1.396 (8)
C4—H4	0.9400	C19—H19	0.9400
C5—C6	1.372 (8)	C20—H20	0.9400
C5—H5	0.9400	C21—C26	1.380 (7)
C6—C7	1.380 (7)	C21—C22	1.393 (7)
C6—H6	0.9400	C22—C23	1.378 (8)
C7—H7	0.9400	C22—H22	0.9400
C8—H8A	0.9700	C23—C24	1.378 (9)
C8—H8B	0.9700	C23—H23	0.9400
C8—H8C	0.9700	C24—C25	1.372 (8)
C9—C14	1.390 (7)	C24—H24	0.9400
C9—C10	1.391 (7)	C25—C26	1.388 (7)
C10—C11	1.372 (7)	C25—H25	0.9400
C10—H10	0.9400	C26—H26	0.9400
C11—C12	1.376 (8)		
P1—Au—S1	175.09 (5)	C11—C12—C13	119.3 (5)
C1—S1—Au	102.08 (17)	C11—C12—H12	120.4
C21—P1—C15	104.7 (2)	C13—C12—H12	120.4

C21—P1—C9	105.7 (2)	C14—C13—C12	120.5 (5)
C15—P1—C9	106.0 (2)	C14—C13—H13	119.7
C21—P1—Au	117.37 (16)	C12—C13—H13	119.7
C15—P1—Au	112.61 (16)	C13—C14—C9	119.9 (5)
C9—P1—Au	109.65 (16)	C13—C14—H14	120.1
C1—O1—C8	117.1 (4)	C9—C14—H14	120.1
C1—N1—C2	119.9 (4)	C20—C15—C16	119.4 (5)
N1—C1—O1	119.8 (4)	C20—C15—P1	118.1 (4)
N1—C1—S1	126.9 (4)	C16—C15—P1	122.5 (4)
O1—C1—S1	113.2 (3)	C15—C16—C17	118.8 (5)
C7—C2—C3	117.3 (5)	C15—C16—H16	120.6
C7—C2—N1	121.8 (5)	C17—C16—H16	120.6
C3—C2—N1	120.5 (5)	C18—C17—C16	121.4 (6)
C4—C3—C2	121.4 (5)	C18—C17—H17	119.3
C4—C3—C11	118.5 (4)	C16—C17—H17	119.3
C2—C3—C11	120.1 (4)	C19—C18—C17	119.6 (6)
C5—C4—C3	120.3 (5)	C19—C18—H18	120.2
C5—C4—H4	119.9	C17—C18—H18	120.2
C3—C4—H4	119.9	C18—C19—C20	120.6 (6)
C4—C5—C6	119.0 (5)	C18—C19—H19	119.7
C4—C5—H5	120.5	C20—C19—H19	119.7
C6—C5—H5	120.5	C15—C20—C19	120.2 (6)
C5—C6—C7	121.3 (5)	C15—C20—H20	119.9
C5—C6—H6	119.3	C19—C20—H20	119.9
C7—C6—H6	119.3	C26—C21—C22	119.6 (5)
C6—C7—C2	120.7 (5)	C26—C21—P1	122.4 (4)
C6—C7—H7	119.7	C22—C21—P1	118.1 (4)
C2—C7—H7	119.7	C23—C22—C21	119.4 (5)
O1—C8—H8A	109.5	C23—C22—H22	120.3
O1—C8—H8B	109.5	C21—C22—H22	120.3
H8A—C8—H8B	109.5	C22—C23—C24	120.9 (6)
O1—C8—H8C	109.5	C22—C23—H23	119.5
H8A—C8—H8C	109.5	C24—C23—H23	119.5
H8B—C8—H8C	109.5	C25—C24—C23	119.9 (5)
C14—C9—C10	119.4 (5)	C25—C24—H24	120.1
C14—C9—P1	121.9 (4)	C23—C24—H24	120.1
C10—C9—P1	118.7 (4)	C24—C25—C26	119.9 (5)
C11—C10—C9	119.9 (5)	C24—C25—H25	120.1
C11—C10—H10	120.1	C26—C25—H25	120.1
C9—C10—H10	120.1	C21—C26—C25	120.4 (5)
C10—C11—C12	120.9 (5)	C21—C26—H26	119.8
C10—C11—H11	119.5	C25—C26—H26	119.8
C12—C11—H11	119.5		
C2—N1—C1—O1	-173.1 (4)	C10—C9—C14—C13	-1.8 (8)
C2—N1—C1—S1	10.0 (7)	P1—C9—C14—C13	177.5 (4)
C8—O1—C1—N1	2.5 (7)	C21—P1—C15—C20	74.9 (4)
C8—O1—C1—S1	179.8 (4)	C9—P1—C15—C20	-173.6 (4)

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Au—S1—C1—N1	174.2 (4)	Au—P1—C15—C20	-53.7 (4)
Au—S1—C1—O1	-2.9 (4)	C21—P1—C15—C16	-104.3 (4)
C1—N1—C2—C7	60.3 (7)	C9—P1—C15—C16	7.2 (5)
C1—N1—C2—C3	-126.3 (5)	Au—P1—C15—C16	127.1 (4)
C7—C2—C3—C4	-1.1 (7)	C20—C15—C16—C17	-0.7 (8)
N1—C2—C3—C4	-174.9 (5)	P1—C15—C16—C17	178.4 (4)
C7—C2—C3—C11	179.8 (4)	C15—C16—C17—C18	0.1 (9)
N1—C2—C3—C11	6.1 (7)	C16—C17—C18—C19	0.6 (10)
C2—C3—C4—C5	0.1 (8)	C17—C18—C19—C20	-0.7 (10)
C11—C3—C4—C5	179.2 (4)	C16—C15—C20—C19	0.6 (8)
C3—C4—C5—C6	0.0 (9)	P1—C15—C20—C19	-178.6 (4)
C4—C5—C6—C7	1.0 (9)	C18—C19—C20—C15	0.1 (9)
C5—C6—C7—C2	-2.0 (9)	C15—P1—C21—C26	9.0 (5)
C3—C2—C7—C6	2.1 (8)	C9—P1—C21—C26	-102.7 (4)
N1—C2—C7—C6	175.7 (5)	Au—P1—C21—C26	134.7 (4)
C21—P1—C9—C14	22.3 (5)	C15—P1—C21—C22	-172.6 (4)
C15—P1—C9—C14	-88.5 (5)	C9—P1—C21—C22	75.7 (4)
Au—P1—C9—C14	149.7 (4)	Au—P1—C21—C22	-46.9 (4)
C21—P1—C9—C10	-158.4 (4)	C26—C21—C22—C23	1.7 (8)
C15—P1—C9—C10	90.8 (4)	P1—C21—C22—C23	-176.7 (4)
Au—P1—C9—C10	-31.0 (5)	C21—C22—C23—C24	-1.8 (9)
C14—C9—C10—C11	3.2 (8)	C22—C23—C24—C25	0.8 (9)
P1—C9—C10—C11	-176.1 (4)	C23—C24—C25—C26	0.3 (9)
C9—C10—C11—C12	-1.8 (9)	C22—C21—C26—C25	-0.6 (8)
C10—C11—C12—C13	-0.9 (9)	P1—C21—C26—C25	177.7 (4)
C11—C12—C13—C14	2.3 (9)	C24—C25—C26—C21	-0.3 (8)
C12—C13—C14—C9	-0.9 (9)		

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