

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

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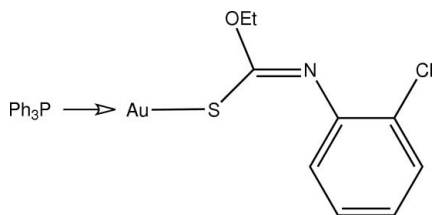
Received 18 November 2009; accepted 19 November 2009

Key indicators: single-crystal X-ray study;  $T = 223$  K; mean  $\sigma(\text{C}-\text{C}) = 0.008$  Å;  $R$  factor = 0.035;  $wR$  factor = 0.102; data-to-parameter ratio = 19.2.

The title compound,  $[\text{Au}(\text{C}_9\text{H}_9\text{ClNOS})(\text{C}_{18}\text{H}_{15}\text{P})]$ , features a linear  $S,P$ -donor set with a small deviation from the ideal linear geometry due to the proximity of the methoxy O atom to Au [ $\text{Au}\cdots\text{O} = 2.986$  (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

$[\text{Au}(\text{C}_9\text{H}_9\text{ClNOS})(\text{C}_{18}\text{H}_{15}\text{P})]$   
 $M_r = 673.92$   
 Monoclinic,  $P2_1/n$   
 $a = 8.8401$  (5) Å  
 $b = 26.0187$  (14) Å

$c = 10.8595$  (6) Å  
 $\beta = 94.850$  (1)°  
 $V = 2488.8$  (2) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation

$\mu = 6.19$  mm<sup>-1</sup>  
 $T = 223$  K

0.32 × 0.16 × 0.02 mm

### Data collection

Bruker SMART CCD diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2000)  
 $T_{\min} = 0.410$ ,  $T_{\max} = 1$

17516 measured reflections  
 5712 independent reflections  
 4803 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.049$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$   
 $wR(F^2) = 0.102$   
 $S = 1.03$   
 5712 reflections

298 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 1.69$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.98$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Au—S1	2.3131 (11)	Au—P1	2.2574 (11)
S1—Au—P1	177.45 (4)		

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SHELXTL (Sheldrick, 2008); 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: SJ2690).

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**supplementary materials**

*Acta Cryst.* (2009). E65, m1683 [ doi:10.1107/S1600536809049459 ]

**[(*Z*)-*N*-(2-Chlorophenyl)-*O*-ethylthiocarbamato- $\kappa$ S](triphenylphosphine- $\kappa$ 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, (C<sub>5</sub>H<sub>5</sub>)<sub>3</sub>PAu[SC(OEt)N(C<sub>6</sub>H<sub>4</sub>Cl-*o*)], was synthesized, (I). In (I), Fig. 1, the thiocarbamide functions as a thiolate ligand, a conclusion confirmed by the magnitudes of the C1—S1 and C1=N1 bond distances of 1.759 (5) and 1.265 (6) Å, respectively; the conformation about C1N1 is *Z*. A twist is evident between the central SC(O)N chromophore (maximum deviation = 0.021 (5) Å for the C1 atom) and the N-bound aryl ring as seen in the C1—N1—C2—C3 torsion angle of -133.7 (5)°. The thiocarbamato and phosphine ligands define an *S*, *P* donor set, Table 1. The deviation of the S1—Au—P1 angle [177.45 (4) °] from linearity is ascribed to the close approach of the O1 atom to Au [2.986 (4) Å].

**Experimental**

Compound (I) was prepared following the standard literature procedure from the reaction of Ph<sub>3</sub>AuCl and EtOC(S)N(H)(C<sub>6</sub>H<sub>4</sub>Cl-*o*) 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  $U_{iso}(H) = 1.2–1.5U_{eq}(C)$ . A rotating group model was used for the methyl groups. The maximum and minimum residual electron density peaks of 1.69 and 0.98 e Å<sup>-3</sup>, respectively, were located 0.83 Å and 1.47 Å from the Au atom.

**Figures**

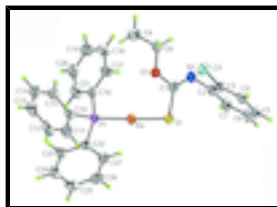


Fig. 1. Molecular structure of (I) showing atom-labelling scheme and displacement ellipsoids at the 50% probability level.

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

*Crystal data*

[Au(C<sub>9</sub>H<sub>9</sub>ClNOS)(C<sub>18</sub>H<sub>15</sub>P)]

$M_r = 673.92$

Monoclinic,  $P2_1/n$

Hall symbol: -P 2yn

$F(000) = 1312$

$D_x = 1.799 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71069 \text{ \AA}$

Cell parameters from 5468 reflections

# supplementary materials

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$a = 8.8401 (5) \text{ \AA}$	$\theta = 2.5\text{--}28.2^\circ$
$b = 26.0187 (14) \text{ \AA}$	$\mu = 6.19 \text{ mm}^{-1}$
$c = 10.8595 (6) \text{ \AA}$	$T = 223 \text{ K}$
$\beta = 94.850 (1)^\circ$	Plate, colourless
$V = 2488.8 (2) \text{ \AA}^3$	$0.32 \times 0.16 \times 0.02 \text{ mm}$
$Z = 4$	

## Data collection

Bruker SMART CCD diffractometer	5712 independent reflections
Radiation source: fine-focus sealed tube graphite	4803 reflections with $I > 2\sigma(I)$
$\omega$ scans	$R_{\text{int}} = 0.049$
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$\theta_{\text{max}} = 27.5^\circ$ , $\theta_{\text{min}} = 1.6^\circ$
$T_{\text{min}} = 0.410$ , $T_{\text{max}} = 1$	$h = -9 \rightarrow 11$
17516 measured reflections	$k = -33 \rightarrow 32$
	$l = -14 \rightarrow 13$

## Refinement

Refinement on $F^2$	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.035$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.102$	H-atom parameters constrained
$S = 1.03$	$w = 1/[\sigma^2(F_o^2) + (0.0543P)^2]$
5712 reflections	where $P = (F_o^2 + 2F_c^2)/3$
298 parameters	$(\Delta/\sigma)_{\text{max}} = 0.001$
0 restraints	$\Delta\rho_{\text{max}} = 1.69 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.98 \text{ e \AA}^{-3}$

## 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 ( $\text{\AA}^2$ )

$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
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Au	0.239069 (19)	0.104287 (7)	0.092536 (15)	0.03276 (8)
Cl1	0.91579 (15)	0.17981 (6)	-0.11081 (11)	0.0464 (3)
S1	0.36556 (14)	0.14702 (5)	-0.05484 (10)	0.0355 (3)
P1	0.12476 (13)	0.06311 (5)	0.24242 (10)	0.0306 (3)
O1	0.5141 (4)	0.16861 (14)	0.1570 (3)	0.0367 (8)
N1	0.6231 (5)	0.20353 (17)	-0.0042 (4)	0.0376 (9)
C1	0.5152 (5)	0.1776 (2)	0.0337 (4)	0.0344 (10)
C2	0.6273 (5)	0.2179 (2)	-0.1288 (4)	0.0351 (10)
C3	0.7614 (5)	0.21131 (19)	-0.1871 (4)	0.0337 (10)
C4	0.7746 (6)	0.2294 (2)	-0.3057 (4)	0.0405 (11)
H4	0.8658	0.2246	-0.3429	0.049*
C5	0.6550 (6)	0.2542 (2)	-0.3693 (5)	0.0429 (12)
H5	0.6635	0.2663	-0.4500	0.051*
C6	0.5227 (6)	0.2612 (2)	-0.3132 (5)	0.0440 (12)
H6	0.4403	0.2781	-0.3563	0.053*
C7	0.5093 (6)	0.2439 (2)	-0.1948 (5)	0.0418 (12)
H7	0.4184	0.2497	-0.1579	0.050*
C8	0.6417 (6)	0.1891 (2)	0.2348 (5)	0.0462 (13)
H8A	0.6378	0.2267	0.2348	0.055*
H8B	0.7373	0.1784	0.2029	0.055*
C9	0.6343 (8)	0.1697 (3)	0.3603 (5)	0.073 (2)
H9A	0.7201	0.1826	0.4128	0.110*
H9B	0.6371	0.1324	0.3595	0.110*
H9C	0.5406	0.1811	0.3921	0.110*
C10	0.2264 (5)	0.00525 (19)	0.2929 (4)	0.0328 (10)
C11	0.2483 (6)	-0.0325 (2)	0.2058 (5)	0.0456 (13)
H11	0.2094	-0.0276	0.1233	0.055*
C12	0.3266 (7)	-0.0772 (2)	0.2384 (6)	0.0520 (14)
H12	0.3398	-0.1025	0.1784	0.062*
C13	0.3852 (7)	-0.0848 (2)	0.3588 (7)	0.0558 (16)
H13	0.4391	-0.1150	0.3809	0.067*
C14	0.3644 (6)	-0.0479 (2)	0.4462 (6)	0.0526 (15)
H14	0.4027	-0.0532	0.5286	0.063*
C15	0.2867 (6)	-0.0026 (2)	0.4131 (5)	0.0442 (13)
H15	0.2752	0.0228	0.4732	0.053*
C16	0.1206 (6)	0.10257 (17)	0.3797 (4)	0.0319 (10)
C17	0.2334 (6)	0.1390 (2)	0.4037 (5)	0.0439 (12)
H17	0.3034	0.1450	0.3448	0.053*
C18	0.2451 (7)	0.1666 (2)	0.5129 (5)	0.0498 (14)
H18	0.3229	0.1910	0.5285	0.060*
C19	0.1414 (7)	0.1580 (2)	0.5989 (5)	0.0465 (13)
H19	0.1498	0.1760	0.6742	0.056*
C20	0.0255 (7)	0.1231 (2)	0.5749 (5)	0.0465 (13)
H20	-0.0474	0.1184	0.6320	0.056*
C21	0.0165 (7)	0.0948 (2)	0.4661 (5)	0.0443 (13)
H21	-0.0607	0.0702	0.4511	0.053*
C22	-0.0695 (5)	0.04190 (18)	0.2042 (4)	0.0311 (9)
C23	-0.1225 (6)	-0.0036 (2)	0.2526 (5)	0.0455 (13)
H23	-0.0565	-0.0245	0.3032	0.055*

## supplementary materials

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C24	-0.2714 (6)	-0.0178 (3)	0.2264 (5)	0.0538 (15)
H24	-0.3072	-0.0485	0.2595	0.065*
C25	-0.3683 (6)	0.0124 (3)	0.1522 (5)	0.0506 (14)
H25	-0.4700	0.0025	0.1346	0.061*
C26	-0.3165 (6)	0.0573 (2)	0.1034 (5)	0.0472 (13)
H26	-0.3831	0.0781	0.0531	0.057*
C27	-0.1665 (6)	0.0718 (2)	0.1284 (5)	0.0389 (11)
H27	-0.1307	0.1021	0.0937	0.047*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Au	0.03321 (12)	0.03459 (13)	0.03128 (12)	-0.00426 (7)	0.00752 (8)	0.00257 (7)
Cl1	0.0390 (6)	0.0635 (9)	0.0364 (6)	0.0048 (6)	0.0010 (5)	0.0004 (6)
S1	0.0370 (6)	0.0421 (7)	0.0278 (5)	-0.0071 (5)	0.0054 (4)	0.0029 (5)
P1	0.0301 (6)	0.0316 (6)	0.0307 (5)	-0.0039 (5)	0.0064 (5)	0.0022 (5)
O1	0.0388 (18)	0.043 (2)	0.0284 (15)	-0.0089 (15)	0.0051 (14)	0.0008 (14)
N1	0.038 (2)	0.041 (2)	0.0341 (19)	-0.0061 (18)	0.0068 (17)	0.0066 (18)
C1	0.036 (2)	0.040 (3)	0.028 (2)	-0.001 (2)	0.0068 (19)	-0.001 (2)
C2	0.036 (2)	0.038 (3)	0.032 (2)	-0.006 (2)	0.0055 (19)	0.006 (2)
C3	0.031 (2)	0.036 (3)	0.034 (2)	-0.0022 (19)	0.0021 (18)	-0.002 (2)
C4	0.043 (3)	0.042 (3)	0.039 (2)	-0.007 (2)	0.010 (2)	-0.001 (2)
C5	0.053 (3)	0.039 (3)	0.037 (2)	-0.005 (2)	0.004 (2)	0.008 (2)
C6	0.052 (3)	0.035 (3)	0.045 (3)	0.002 (2)	0.005 (2)	0.013 (2)
C7	0.040 (3)	0.037 (3)	0.050 (3)	0.000 (2)	0.011 (2)	0.011 (2)
C8	0.049 (3)	0.050 (3)	0.038 (3)	-0.011 (3)	-0.003 (2)	0.002 (2)
C9	0.070 (5)	0.110 (6)	0.040 (3)	-0.031 (4)	-0.003 (3)	0.007 (4)
C10	0.028 (2)	0.033 (3)	0.037 (2)	-0.0068 (18)	0.0070 (18)	0.001 (2)
C11	0.049 (3)	0.045 (3)	0.043 (3)	0.002 (2)	0.010 (2)	0.004 (2)
C12	0.056 (3)	0.029 (3)	0.074 (4)	0.000 (2)	0.025 (3)	-0.002 (3)
C13	0.040 (3)	0.041 (3)	0.087 (5)	0.004 (2)	0.008 (3)	0.016 (3)
C14	0.046 (3)	0.049 (4)	0.060 (3)	-0.003 (3)	-0.009 (3)	0.018 (3)
C15	0.047 (3)	0.040 (3)	0.045 (3)	-0.007 (2)	-0.002 (2)	0.002 (2)
C16	0.036 (2)	0.028 (2)	0.033 (2)	0.0018 (18)	0.0050 (19)	0.0028 (18)
C17	0.045 (3)	0.041 (3)	0.047 (3)	-0.012 (2)	0.010 (2)	-0.006 (2)
C18	0.051 (3)	0.046 (3)	0.053 (3)	-0.012 (3)	0.004 (3)	-0.015 (3)
C19	0.057 (3)	0.041 (3)	0.042 (3)	0.010 (3)	0.006 (2)	-0.008 (2)
C20	0.059 (3)	0.041 (3)	0.043 (3)	0.002 (3)	0.024 (3)	0.000 (2)
C21	0.048 (3)	0.042 (3)	0.045 (3)	-0.007 (2)	0.018 (2)	0.000 (2)
C22	0.030 (2)	0.031 (2)	0.033 (2)	-0.0043 (18)	0.0058 (18)	-0.0025 (19)
C23	0.039 (3)	0.045 (3)	0.052 (3)	-0.011 (2)	-0.002 (2)	0.011 (3)
C24	0.046 (3)	0.055 (4)	0.060 (3)	-0.020 (3)	0.001 (3)	0.011 (3)
C25	0.031 (3)	0.068 (4)	0.053 (3)	-0.008 (3)	0.003 (2)	-0.012 (3)
C26	0.040 (3)	0.052 (3)	0.048 (3)	0.011 (3)	-0.005 (2)	-0.002 (3)
C27	0.040 (3)	0.036 (3)	0.040 (2)	0.005 (2)	0.003 (2)	0.000 (2)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

Au—S1	2.3131 (11)	C11—H11	0.9400
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Au—P1	2.2574 (11)	C12—C13	1.379 (9)
Cl1—C3	1.740 (5)	C12—H12	0.9400
S1—C1	1.759 (5)	C13—C14	1.372 (9)
P1—C16	1.813 (5)	C13—H13	0.9400
P1—C10	1.814 (5)	C14—C15	1.396 (8)
P1—C22	1.818 (5)	C14—H14	0.9400
O1—C1	1.360 (5)	C15—H15	0.9400
O1—C8	1.453 (6)	C16—C17	1.384 (7)
N1—C1	1.265 (6)	C16—C21	1.384 (7)
N1—C2	1.407 (6)	C17—C18	1.383 (7)
C2—C7	1.391 (7)	C17—H17	0.9400
C2—C3	1.401 (6)	C18—C19	1.382 (8)
C3—C4	1.385 (7)	C18—H18	0.9400
C4—C5	1.375 (7)	C19—C20	1.377 (8)
C4—H4	0.9400	C19—H19	0.9400
C5—C6	1.376 (7)	C20—C21	1.388 (8)
C5—H5	0.9400	C20—H20	0.9400
C6—C7	1.377 (7)	C21—H21	0.9400
C6—H6	0.9400	C22—C27	1.378 (7)
C7—H7	0.9400	C22—C23	1.392 (7)
C8—C9	1.460 (7)	C23—C24	1.374 (7)
C8—H8A	0.9800	C23—H23	0.9400
C8—H8B	0.9800	C24—C25	1.374 (8)
C9—H9A	0.9700	C24—H24	0.9400
C9—H9B	0.9700	C25—C26	1.376 (9)
C9—H9C	0.9700	C25—H25	0.9400
C10—C15	1.383 (7)	C26—C27	1.384 (8)
C10—C11	1.389 (7)	C26—H26	0.9400
C11—C12	1.384 (8)	C27—H27	0.9400
S1—Au—P1	177.45 (4)	C13—C12—C11	120.1 (6)
C1—S1—Au	102.98 (16)	C13—C12—H12	120.0
C16—P1—C10	105.4 (2)	C11—C12—H12	120.0
C16—P1—C22	106.0 (2)	C14—C13—C12	119.7 (6)
C10—P1—C22	104.5 (2)	C14—C13—H13	120.2
C16—P1—Au	111.44 (16)	C12—C13—H13	120.2
C10—P1—Au	111.79 (15)	C13—C14—C15	120.3 (5)
C22—P1—Au	116.84 (15)	C13—C14—H14	119.9
C1—O1—C8	116.1 (4)	C15—C14—H14	119.9
C1—N1—C2	122.4 (4)	C10—C15—C14	120.6 (5)
N1—C1—O1	118.8 (4)	C10—C15—H15	119.7
N1—C1—S1	128.1 (4)	C14—C15—H15	119.7
O1—C1—S1	113.1 (3)	C17—C16—C21	118.8 (5)
C7—C2—C3	116.9 (4)	C17—C16—P1	118.6 (4)
C7—C2—N1	123.0 (4)	C21—C16—P1	122.4 (4)
C3—C2—N1	119.7 (4)	C18—C17—C16	121.2 (5)
C4—C3—C2	121.4 (5)	C18—C17—H17	119.4
C4—C3—Cl1	118.6 (4)	C16—C17—H17	119.4
C2—C3—Cl1	120.1 (4)	C19—C18—C17	119.3 (5)
C5—C4—C3	120.3 (5)	C19—C18—H18	120.4

## supplementary materials

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C5—C4—H4	119.8	C17—C18—H18	120.4
C3—C4—H4	119.8	C20—C19—C18	120.3 (5)
C4—C5—C6	119.1 (5)	C20—C19—H19	119.9
C4—C5—H5	120.4	C18—C19—H19	119.9
C6—C5—H5	120.4	C19—C20—C21	120.0 (5)
C5—C6—C7	120.9 (5)	C19—C20—H20	120.0
C5—C6—H6	119.6	C21—C20—H20	120.0
C7—C6—H6	119.6	C16—C21—C20	120.4 (5)
C6—C7—C2	121.4 (5)	C16—C21—H21	119.8
C6—C7—H7	119.3	C20—C21—H21	119.8
C2—C7—H7	119.3	C27—C22—C23	119.6 (4)
O1—C8—C9	108.8 (5)	C27—C22—P1	119.5 (4)
O1—C8—H8A	109.9	C23—C22—P1	120.9 (4)
C9—C8—H8A	109.9	C24—C23—C22	119.9 (5)
O1—C8—H8B	109.9	C24—C23—H23	120.1
C9—C8—H8B	109.9	C22—C23—H23	120.1
H8A—C8—H8B	108.3	C25—C24—C23	120.4 (5)
C8—C9—H9A	109.5	C25—C24—H24	119.8
C8—C9—H9B	109.5	C23—C24—H24	119.8
H9A—C9—H9B	109.5	C24—C25—C26	120.1 (5)
C8—C9—H9C	109.5	C24—C25—H25	120.0
H9A—C9—H9C	109.5	C26—C25—H25	120.0
H9B—C9—H9C	109.5	C25—C26—C27	120.0 (5)
C15—C10—C11	118.3 (5)	C25—C26—H26	120.0
C15—C10—P1	123.3 (4)	C27—C26—H26	120.0
C11—C10—P1	118.4 (4)	C22—C27—C26	120.0 (5)
C12—C11—C10	121.1 (5)	C22—C27—H27	120.0
C12—C11—H11	119.5	C26—C27—H27	120.0
C10—C11—H11	119.5		
C2—N1—C1—O1	-175.2 (4)	C11—C10—C15—C14	-1.4 (8)
C2—N1—C1—S1	9.1 (8)	P1—C10—C15—C14	-179.7 (4)
C8—O1—C1—N1	-1.4 (7)	C13—C14—C15—C10	1.6 (9)
C8—O1—C1—S1	174.9 (4)	C10—P1—C16—C17	93.6 (4)
Au—S1—C1—N1	175.3 (5)	C22—P1—C16—C17	-155.9 (4)
Au—S1—C1—O1	-0.6 (4)	Au—P1—C16—C17	-27.8 (5)
C1—N1—C2—C7	53.7 (8)	C10—P1—C16—C21	-81.0 (5)
C1—N1—C2—C3	-133.7 (5)	C22—P1—C16—C21	29.5 (5)
C7—C2—C3—C4	-0.8 (7)	Au—P1—C16—C21	157.6 (4)
N1—C2—C3—C4	-173.8 (5)	C21—C16—C17—C18	1.3 (8)
C7—C2—C3—C11	179.3 (4)	P1—C16—C17—C18	-173.5 (4)
N1—C2—C3—C11	6.4 (7)	C16—C17—C18—C19	-0.6 (9)
C2—C3—C4—C5	-0.1 (8)	C17—C18—C19—C20	-1.4 (9)
C11—C3—C4—C5	179.7 (4)	C18—C19—C20—C21	2.8 (9)
C3—C4—C5—C6	0.5 (8)	C17—C16—C21—C20	0.0 (8)
C4—C5—C6—C7	0.2 (8)	P1—C16—C21—C20	174.6 (4)
C5—C6—C7—C2	-1.2 (9)	C19—C20—C21—C16	-2.0 (9)
C3—C2—C7—C6	1.5 (8)	C16—P1—C22—C27	88.7 (4)
N1—C2—C7—C6	174.2 (5)	C10—P1—C22—C27	-160.2 (4)
C1—O1—C8—C9	-171.8 (5)	Au—P1—C22—C27	-36.1 (4)



## supplementary materials

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C16—P1—C10—C15	-1.3 (5)	C16—P1—C22—C23	-89.9 (4)
C22—P1—C10—C15	-112.8 (4)	C10—P1—C22—C23	21.1 (5)
Au—P1—C10—C15	119.9 (4)	Au—P1—C22—C23	145.3 (4)
C16—P1—C10—C11	-179.6 (4)	C27—C22—C23—C24	-1.2 (8)
C22—P1—C10—C11	68.9 (4)	P1—C22—C23—C24	177.4 (5)
Au—P1—C10—C11	-58.4 (4)	C22—C23—C24—C25	0.3 (9)
C15—C10—C11—C12	0.9 (8)	C23—C24—C25—C26	0.1 (9)
P1—C10—C11—C12	179.2 (4)	C24—C25—C26—C27	0.4 (9)
C10—C11—C12—C13	-0.4 (9)	C23—C22—C27—C26	1.7 (8)
C11—C12—C13—C14	0.5 (9)	P1—C22—C27—C26	-177.0 (4)
C12—C13—C14—C15	-1.1 (9)	C25—C26—C27—C22	-1.3 (8)

Fig. 1

