

[*Z*]-*O*-Methyl-*N*-propylthiocarbamato-*κS*](triphenylphosphine-*κP*)gold(I)

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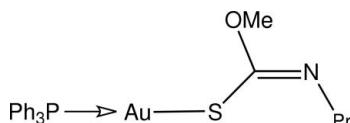
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Key indicators: single-crystal X-ray study; $T = 223\text{ K}$; mean $\sigma(\text{C}-\text{C}) = 0.010\text{ \AA}$; R factor = 0.045; wR factor = 0.106; data-to-parameter ratio = 20.3.

In the title compound, $[\text{Au}(\text{C}_5\text{H}_{10}\text{NOS})(\text{C}_{18}\text{H}_{15}\text{P})]$, the Au^{I} atom is linearly coordinated within an *S,P*-donor set with distortion from an ideal linear geometry [$\text{S}-\text{Au}-\text{P} = 176.71(6)\text{ }^\circ$] due to an intramolecular $\text{Au}\cdots\text{O}$ contact [2.943 (4) \AA]. In the crystal structure, centrosymmetrically related molecules associate via $\text{C}-\text{H}\cdots\text{O}$ interactions.

Related literature

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



Experimental

Crystal data

$[\text{Au}(\text{C}_5\text{H}_{10}\text{NOS})(\text{C}_{18}\text{H}_{15}\text{P})]$

$M_r = 591.44$

Monoclinic, $P2_1/n$

$a = 13.9852(16)\text{ \AA}$

$b = 11.1592(13)\text{ \AA}$

$c = 15.0975(17)\text{ \AA}$

$\beta = 107.605(2)\text{ }^\circ$

$V = 2245.8(4)\text{ \AA}^3$

$Z = 4$

Mo $K\alpha$ radiation

$\mu = 6.73\text{ mm}^{-1}$

$T = 223\text{ K}$

$0.26 \times 0.13 \times 0.01\text{ mm}$

Data collection

Bruker SMART CCD diffractometer

Absorption correction: multi-scan (*SADABS*; Bruker, 2000)

$T_{\min} = 0.376$, $T_{\max} = 1$

15397 measured reflections

5165 independent reflections

4702 reflections with $I > 2\sigma(I)$

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

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$

$wR(F^2) = 0.106$

$S = 1.20$

5165 reflections

254 parameters

H-atom parameters constrained

$\Delta\rho_{\max} = 1.41\text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -2.23\text{ e \AA}^{-3}$

Table 1
Selected bond lengths (\AA).

| Au—S1 | 2.3089 (16) | Au—P1 | 2.2557 (16) |
|-------|-------------|-------|-------------|
|-------|-------------|-------|-------------|

Table 2

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

| D—H \cdots A | D—H | H \cdots A | D \cdots A | D—H \cdots A |
|----------------------------------|------|--------------|--------------|----------------|
| C14—H14 \cdots O1 ⁱ | 0.94 | 2.51 | 3.314 (10) | 143 |

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

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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2583).

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supplementary materials

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[*(Z*)-*O*-Methyl-*N*-propylthiocarbamato- κ S](triphenylphosphine- κ P)gold(I)

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Comment

The structure of the title compound, (I), was determined as a part of an on-going study of the structural systematics, including luminescence properties, of molecules related to the general formula $R_3PAu[SC(OR')NR'']$ for R , R' and R'' = alkyl and aryl (Ho *et al.* 2006; Ho & Tiekink, 2007; Kuan *et al.*, 2008).

The Au atom exists within the expected linear geometry defined by the S and P donor atoms. The C1—S1 and C1=N1 bond distances of 1.775 (7) and 1.265 (8) Å, respectively, confirm that the carbonimidothioate ligand is functioning as a thiolate. The small deviation from linearity about the Au atom is ascribed to the close approach of the O1 atom, Au···O1 is 2.943 (4) Å. The most prominent intermolecular interaction occurring in the crystal structure is a C—H···O contact, Table 1, which occurs between centrosymmetrically related molecules leading to a dimeric aggregate, Fig. 2.

Experimental

Compound (I) was prepared following the standard literature procedure from the reaction of Ph_3PAuCl and $MeOC(S)N(H)Pr$ 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 1.41 and 2.23 e Å^{−3}, respectively, were located 0.82 Å and 1.59 Å from the Au and H2O atoms, respectively.

Figures

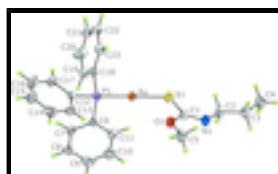


Fig. 1. Molecular structure of (I) showing atom-labelling scheme and displacement ellipsoids at the 50% probability level.

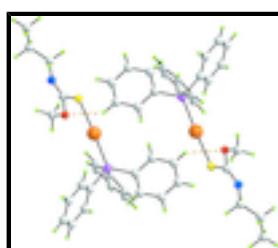


Fig. 2. Supramolecular dimer formation in (I) mediated by C—H···O contacts (orange dashed lines). Colour code: Au, orange; S, yellow; P, pink; O, red; N, blue; C, grey; and H, green.

supplementary materials

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Crystal data

| | |
|---|---|
| [Au(C ₅ H ₁₀ NOS)(C ₁₈ H ₁₅ P)] | $F_{000} = 1152$ |
| $M_r = 591.44$ | $D_x = 1.749 \text{ Mg m}^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation, $\lambda = 0.71069 \text{ \AA}$ |
| Hall symbol: -P 2yn | Cell parameters from 953 reflections |
| $a = 13.9852 (16) \text{ \AA}$ | $\theta = 2.3\text{--}29.6^\circ$ |
| $b = 11.1592 (13) \text{ \AA}$ | $\mu = 6.73 \text{ mm}^{-1}$ |
| $c = 15.0975 (17) \text{ \AA}$ | $T = 223 \text{ K}$ |
| $\beta = 107.605 (2)^\circ$ | Plate, colourless |
| $V = 2245.8 (4) \text{ \AA}^3$ | $0.26 \times 0.13 \times 0.01 \text{ mm}$ |
| $Z = 4$ | |

Data collection

| | |
|--|--|
| Bruker SMART CCD diffractometer | 5165 independent reflections |
| Radiation source: fine-focus sealed tube | 4702 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{\text{int}} = 0.047$ |
| $T = 223 \text{ K}$ | $\theta_{\text{max}} = 27.5^\circ$ |
| ω scans | $\theta_{\text{min}} = 1.7^\circ$ |
| Absorption correction: multi-scan (SADABS; Bruker, 2000) | $h = -18 \rightarrow 18$ |
| $T_{\text{min}} = 0.376$, $T_{\text{max}} = 1$ | $k = -14 \rightarrow 8$ |
| 15397 measured reflections | $l = -19 \rightarrow 17$ |

Refinement

| | |
|--|--|
| Refinement on F^2 | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.045$ | H-atom parameters constrained |
| $wR(F^2) = 0.106$ | $w = 1/[\sigma^2(F_o^2) + (0.0416P)^2 + 1.6273P]$ |
| $S = 1.20$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 5165 reflections | $(\Delta/\sigma)_{\text{max}} = 0.001$ |
| 254 parameters | $\Delta\rho_{\text{max}} = 1.41 \text{ e \AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{\text{min}} = -2.23 \text{ e \AA}^{-3}$ |
| | 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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|---------------|---------------|---------------|----------------------------------|
| Au | 0.260547 (17) | 0.07193 (2) | 0.417669 (15) | 0.03002 (9) |
| S1 | 0.15590 (13) | -0.09274 (15) | 0.39447 (11) | 0.0358 (4) |
| P1 | 0.35886 (12) | 0.23644 (14) | 0.44661 (10) | 0.0289 (3) |
| O1 | 0.1670 (3) | -0.0064 (4) | 0.5583 (3) | 0.0388 (10) |
| N1 | 0.0665 (4) | -0.1720 (5) | 0.5213 (4) | 0.0413 (13) |
| C1 | 0.1230 (5) | -0.0969 (6) | 0.4992 (5) | 0.0361 (14) |
| C2 | 0.0194 (6) | -0.2655 (7) | 0.4551 (6) | 0.0488 (18) |
| H2A | 0.0678 | -0.3301 | 0.4584 | 0.059* |
| H2B | 0.0002 | -0.2325 | 0.3920 | 0.059* |
| C3 | -0.0724 (6) | -0.3162 (7) | 0.4743 (6) | 0.0512 (19) |
| H3A | -0.1191 | -0.2508 | 0.4744 | 0.061* |
| H3B | -0.0526 | -0.3530 | 0.5361 | 0.061* |
| C4 | -0.1253 (7) | -0.4091 (8) | 0.4026 (7) | 0.065 (2) |
| H4A | -0.1845 | -0.4379 | 0.4167 | 0.097* |
| H4B | -0.0803 | -0.4756 | 0.4040 | 0.097* |
| H4C | -0.1449 | -0.3730 | 0.3412 | 0.097* |
| C5 | 0.1410 (6) | -0.0002 (8) | 0.6435 (5) | 0.0499 (19) |
| H5A | 0.0687 | -0.0055 | 0.6297 | 0.075* |
| H5B | 0.1644 | 0.0752 | 0.6745 | 0.075* |
| H5C | 0.1724 | -0.0661 | 0.6837 | 0.075* |
| C6 | 0.4147 (4) | 0.2585 (5) | 0.5707 (4) | 0.0285 (12) |
| C7 | 0.5023 (5) | 0.3241 (6) | 0.6067 (4) | 0.0360 (14) |
| H7 | 0.5353 | 0.3561 | 0.5662 | 0.043* |
| C8 | 0.5413 (5) | 0.3427 (6) | 0.7009 (5) | 0.0427 (16) |
| H8 | 0.6009 | 0.3867 | 0.7246 | 0.051* |
| C9 | 0.4926 (6) | 0.2962 (7) | 0.7608 (5) | 0.0470 (17) |
| H9 | 0.5187 | 0.3096 | 0.8251 | 0.056* |
| C10 | 0.4067 (6) | 0.2309 (7) | 0.7263 (5) | 0.0507 (19) |
| H10 | 0.3744 | 0.1991 | 0.7674 | 0.061* |
| C11 | 0.3664 (5) | 0.2108 (7) | 0.6318 (4) | 0.0412 (15) |
| H11 | 0.3073 | 0.1657 | 0.6088 | 0.049* |
| C12 | 0.4645 (4) | 0.2387 (5) | 0.4006 (4) | 0.0284 (12) |
| C13 | 0.5248 (5) | 0.1371 (7) | 0.4103 (5) | 0.0429 (16) |
| H13 | 0.5071 | 0.0665 | 0.4355 | 0.052* |
| C14 | 0.6109 (6) | 0.1398 (8) | 0.3828 (6) | 0.053 (2) |
| H14 | 0.6528 | 0.0722 | 0.3914 | 0.064* |
| C15 | 0.6347 (6) | 0.2424 (8) | 0.3428 (5) | 0.0516 (19) |
| H15 | 0.6925 | 0.2442 | 0.3234 | 0.062* |

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|-----|------------|------------|------------|-------------|
| C16 | 0.5748 (6) | 0.3410 (8) | 0.3311 (5) | 0.053 (2) |
| H16 | 0.5918 | 0.4102 | 0.3038 | 0.064* |
| C17 | 0.4894 (5) | 0.3408 (6) | 0.3590 (4) | 0.0371 (14) |
| H17 | 0.4483 | 0.4091 | 0.3500 | 0.045* |
| C18 | 0.2886 (5) | 0.3729 (6) | 0.4041 (4) | 0.0331 (13) |
| C19 | 0.3025 (5) | 0.4783 (7) | 0.4533 (4) | 0.0372 (15) |
| H19 | 0.3493 | 0.4819 | 0.5129 | 0.045* |
| C20 | 0.2475 (6) | 0.5802 (7) | 0.4153 (5) | 0.050 (2) |
| H20 | 0.2549 | 0.6512 | 0.4503 | 0.060* |
| C21 | 0.1823 (6) | 0.5762 (7) | 0.3265 (5) | 0.0487 (19) |
| H21 | 0.1466 | 0.6453 | 0.3001 | 0.058* |
| C22 | 0.1691 (6) | 0.4714 (7) | 0.2761 (5) | 0.0472 (18) |
| H22 | 0.1235 | 0.4688 | 0.2159 | 0.057* |
| C23 | 0.2227 (5) | 0.3702 (7) | 0.3139 (5) | 0.0432 (16) |
| H23 | 0.2148 | 0.2993 | 0.2789 | 0.052* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|---------------|-------------|-------------|
| Au | 0.03095 (14) | 0.02962 (14) | 0.02940 (14) | -0.00472 (10) | 0.00897 (9) | 0.00101 (9) |
| S1 | 0.0416 (9) | 0.0345 (8) | 0.0341 (8) | -0.0110 (7) | 0.0155 (7) | -0.0047 (7) |
| P1 | 0.0293 (8) | 0.0287 (8) | 0.0274 (7) | -0.0022 (6) | 0.0067 (6) | 0.0020 (6) |
| O1 | 0.039 (3) | 0.046 (3) | 0.036 (2) | -0.004 (2) | 0.019 (2) | -0.003 (2) |
| N1 | 0.041 (3) | 0.044 (3) | 0.043 (3) | -0.010 (3) | 0.018 (3) | 0.000 (3) |
| C1 | 0.036 (3) | 0.036 (3) | 0.036 (3) | -0.001 (3) | 0.011 (3) | 0.002 (3) |
| C2 | 0.052 (5) | 0.043 (4) | 0.060 (5) | -0.017 (3) | 0.030 (4) | -0.005 (4) |
| C3 | 0.040 (4) | 0.052 (5) | 0.066 (5) | -0.009 (3) | 0.022 (4) | 0.003 (4) |
| C4 | 0.062 (6) | 0.065 (6) | 0.068 (6) | -0.022 (5) | 0.021 (4) | -0.002 (5) |
| C5 | 0.054 (5) | 0.061 (5) | 0.042 (4) | -0.011 (4) | 0.027 (3) | -0.013 (4) |
| C6 | 0.029 (3) | 0.031 (3) | 0.025 (3) | 0.002 (2) | 0.007 (2) | 0.002 (2) |
| C7 | 0.036 (3) | 0.035 (3) | 0.037 (3) | -0.006 (3) | 0.012 (3) | 0.006 (3) |
| C8 | 0.044 (4) | 0.040 (4) | 0.035 (3) | -0.001 (3) | -0.001 (3) | -0.002 (3) |
| C9 | 0.050 (4) | 0.054 (5) | 0.034 (3) | 0.009 (4) | 0.008 (3) | -0.006 (3) |
| C10 | 0.055 (5) | 0.059 (5) | 0.042 (4) | 0.005 (4) | 0.021 (3) | 0.004 (4) |
| C11 | 0.039 (4) | 0.051 (4) | 0.036 (3) | 0.002 (3) | 0.015 (3) | 0.002 (3) |
| C12 | 0.026 (3) | 0.035 (3) | 0.025 (3) | -0.005 (2) | 0.008 (2) | -0.001 (2) |
| C13 | 0.044 (4) | 0.038 (4) | 0.050 (4) | 0.007 (3) | 0.019 (3) | 0.014 (3) |
| C14 | 0.043 (4) | 0.058 (5) | 0.060 (5) | 0.017 (4) | 0.017 (4) | 0.011 (4) |
| C15 | 0.049 (4) | 0.071 (6) | 0.041 (4) | 0.001 (4) | 0.023 (3) | -0.003 (4) |
| C16 | 0.064 (5) | 0.051 (5) | 0.058 (5) | -0.004 (4) | 0.038 (4) | 0.008 (4) |
| C17 | 0.047 (4) | 0.031 (3) | 0.039 (3) | 0.002 (3) | 0.021 (3) | 0.005 (3) |
| C18 | 0.037 (3) | 0.026 (3) | 0.033 (3) | 0.004 (3) | 0.005 (3) | -0.001 (3) |
| C19 | 0.025 (3) | 0.050 (4) | 0.034 (3) | 0.000 (3) | 0.004 (2) | 0.002 (3) |
| C20 | 0.065 (5) | 0.036 (4) | 0.049 (4) | 0.007 (3) | 0.016 (4) | -0.002 (3) |
| C21 | 0.050 (4) | 0.053 (5) | 0.046 (4) | 0.013 (4) | 0.019 (3) | 0.018 (4) |
| C22 | 0.042 (4) | 0.057 (5) | 0.039 (4) | 0.008 (4) | 0.007 (3) | 0.012 (3) |
| C23 | 0.044 (4) | 0.043 (4) | 0.039 (4) | -0.007 (3) | 0.007 (3) | 0.000 (3) |

Geometric parameters (Å, °)

| | | | |
|------------|-------------|-------------|------------|
| Au—S1 | 2.3089 (16) | C9—C10 | 1.367 (11) |
| Au—P1 | 2.2557 (16) | C9—H9 | 0.9400 |
| S1—C1 | 1.775 (7) | C10—C11 | 1.385 (10) |
| P1—C12 | 1.813 (6) | C10—H10 | 0.9400 |
| P1—C6 | 1.816 (6) | C11—H11 | 0.9400 |
| P1—C18 | 1.821 (6) | C12—C13 | 1.394 (9) |
| O1—C1 | 1.364 (8) | C12—C17 | 1.396 (8) |
| O1—C5 | 1.440 (7) | C13—C14 | 1.387 (10) |
| N1—C1 | 1.265 (8) | C13—H13 | 0.9400 |
| N1—C2 | 1.457 (9) | C14—C15 | 1.382 (11) |
| C2—C3 | 1.508 (9) | C14—H14 | 0.9400 |
| C2—H2A | 0.9800 | C15—C16 | 1.361 (11) |
| C2—H2B | 0.9800 | C15—H15 | 0.9400 |
| C3—C4 | 1.520 (11) | C16—C17 | 1.380 (10) |
| C3—H3A | 0.9800 | C16—H16 | 0.9400 |
| C3—H3B | 0.9800 | C17—H17 | 0.9400 |
| C4—H4A | 0.9700 | C18—C19 | 1.373 (9) |
| C4—H4B | 0.9700 | C18—C23 | 1.395 (9) |
| C4—H4C | 0.9700 | C19—C20 | 1.395 (10) |
| C5—H5A | 0.9700 | C19—H19 | 0.9400 |
| C5—H5B | 0.9700 | C20—C21 | 1.375 (10) |
| C5—H5C | 0.9700 | C20—H20 | 0.9400 |
| C6—C7 | 1.389 (8) | C21—C22 | 1.377 (11) |
| C6—C11 | 1.402 (9) | C21—H21 | 0.9400 |
| C7—C8 | 1.377 (9) | C22—C23 | 1.380 (10) |
| C7—H7 | 0.9400 | C22—H22 | 0.9400 |
| C8—C9 | 1.388 (10) | C23—H23 | 0.9400 |
| C8—H8 | 0.9400 | | |
| P1—Au—S1 | 176.71 (6) | C10—C9—C8 | 120.0 (6) |
| C1—S1—Au | 102.0 (2) | C10—C9—H9 | 120.0 |
| C12—P1—C6 | 104.3 (3) | C8—C9—H9 | 120.0 |
| C12—P1—C18 | 105.6 (3) | C9—C10—C11 | 121.1 (7) |
| C6—P1—C18 | 105.5 (3) | C9—C10—H10 | 119.5 |
| C12—P1—Au | 117.2 (2) | C11—C10—H10 | 119.5 |
| C6—P1—Au | 110.9 (2) | C10—C11—C6 | 119.3 (7) |
| C18—P1—Au | 112.3 (2) | C10—C11—H11 | 120.4 |
| C1—O1—C5 | 115.8 (5) | C6—C11—H11 | 120.4 |
| C1—N1—C2 | 118.9 (6) | C13—C12—C17 | 119.1 (6) |
| N1—C1—O1 | 120.8 (6) | C13—C12—P1 | 119.1 (5) |
| N1—C1—S1 | 127.1 (5) | C17—C12—P1 | 121.8 (5) |
| O1—C1—S1 | 112.1 (5) | C14—C13—C12 | 120.2 (7) |
| N1—C2—C3 | 111.8 (6) | C14—C13—H13 | 119.9 |
| N1—C2—H2A | 109.3 | C12—C13—H13 | 119.9 |
| C3—C2—H2A | 109.3 | C15—C14—C13 | 119.6 (7) |
| N1—C2—H2B | 109.3 | C15—C14—H14 | 120.2 |
| C3—C2—H2B | 109.3 | C13—C14—H14 | 120.2 |

supplementary materials

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|---------------|------------|-----------------|------------|
| H2A—C2—H2B | 107.9 | C16—C15—C14 | 120.4 (7) |
| C2—C3—C4 | 112.2 (7) | C16—C15—H15 | 119.8 |
| C2—C3—H3A | 109.2 | C14—C15—H15 | 119.8 |
| C4—C3—H3A | 109.2 | C15—C16—C17 | 121.0 (7) |
| C2—C3—H3B | 109.2 | C15—C16—H16 | 119.5 |
| C4—C3—H3B | 109.2 | C17—C16—H16 | 119.5 |
| H3A—C3—H3B | 107.9 | C16—C17—C12 | 119.6 (7) |
| C3—C4—H4A | 109.5 | C16—C17—H17 | 120.2 |
| C3—C4—H4B | 109.5 | C12—C17—H17 | 120.2 |
| H4A—C4—H4B | 109.5 | C19—C18—C23 | 119.4 (6) |
| C3—C4—H4C | 109.5 | C19—C18—P1 | 123.6 (5) |
| H4A—C4—H4C | 109.5 | C23—C18—P1 | 116.9 (5) |
| H4B—C4—H4C | 109.5 | C18—C19—C20 | 120.4 (6) |
| O1—C5—H5A | 109.5 | C18—C19—H19 | 119.8 |
| O1—C5—H5B | 109.5 | C20—C19—H19 | 119.8 |
| H5A—C5—H5B | 109.5 | C21—C20—C19 | 119.7 (7) |
| O1—C5—H5C | 109.5 | C21—C20—H20 | 120.2 |
| H5A—C5—H5C | 109.5 | C19—C20—H20 | 120.2 |
| H5B—C5—H5C | 109.5 | C20—C21—C22 | 120.3 (7) |
| C7—C6—C11 | 119.1 (6) | C20—C21—H21 | 119.8 |
| C7—C6—P1 | 121.8 (5) | C22—C21—H21 | 119.8 |
| C11—C6—P1 | 119.0 (5) | C23—C22—C21 | 120.0 (7) |
| C8—C7—C6 | 120.6 (6) | C23—C22—H22 | 120.0 |
| C8—C7—H7 | 119.7 | C21—C22—H22 | 120.0 |
| C6—C7—H7 | 119.7 | C22—C23—C18 | 120.1 (7) |
| C7—C8—C9 | 119.9 (7) | C22—C23—H23 | 119.9 |
| C7—C8—H8 | 120.0 | C18—C23—H23 | 119.9 |
| C9—C8—H8 | 120.0 | | |
| C2—N1—C1—O1 | 178.7 (6) | C6—P1—C12—C17 | -99.5 (5) |
| C2—N1—C1—S1 | -1.6 (10) | C18—P1—C12—C17 | 11.5 (6) |
| C5—O1—C1—N1 | -2.7 (9) | Au—P1—C12—C17 | 137.5 (5) |
| C5—O1—C1—S1 | 177.6 (5) | C17—C12—C13—C14 | 3.0 (10) |
| Au—S1—C1—N1 | -179.7 (6) | P1—C12—C13—C14 | -174.6 (6) |
| Au—S1—C1—O1 | 0.1 (5) | C12—C13—C14—C15 | -2.3 (12) |
| C1—N1—C2—C3 | -158.4 (7) | C13—C14—C15—C16 | 0.7 (13) |
| N1—C2—C3—C4 | 176.9 (7) | C14—C15—C16—C17 | 0.1 (13) |
| C12—P1—C6—C7 | 29.9 (6) | C15—C16—C17—C12 | 0.7 (12) |
| C18—P1—C6—C7 | -81.2 (6) | C13—C12—C17—C16 | -2.2 (10) |
| Au—P1—C6—C7 | 156.9 (5) | P1—C12—C17—C16 | 175.3 (6) |
| C12—P1—C6—C11 | -151.9 (5) | C12—P1—C18—C19 | -93.4 (6) |
| C18—P1—C6—C11 | 97.1 (6) | C6—P1—C18—C19 | 16.7 (7) |
| Au—P1—C6—C11 | -24.8 (6) | Au—P1—C18—C19 | 137.7 (5) |
| C11—C6—C7—C8 | -0.3 (10) | C12—P1—C18—C23 | 81.9 (6) |
| P1—C6—C7—C8 | 177.9 (5) | C6—P1—C18—C23 | -167.9 (5) |
| C6—C7—C8—C9 | -0.4 (11) | Au—P1—C18—C23 | -46.9 (6) |
| C7—C8—C9—C10 | 0.8 (11) | C23—C18—C19—C20 | 3.2 (10) |
| C8—C9—C10—C11 | -0.5 (12) | P1—C18—C19—C20 | 178.5 (6) |
| C9—C10—C11—C6 | -0.1 (12) | C18—C19—C20—C21 | -2.9 (11) |
| C7—C6—C11—C10 | 0.5 (10) | C19—C20—C21—C22 | 1.9 (12) |

supplementary materials

| | | | |
|----------------|------------|-----------------|------------|
| P1—C6—C11—C10 | −177.8 (6) | C20—C21—C22—C23 | −1.2 (12) |
| C6—P1—C12—C13 | 78.1 (6) | C21—C22—C23—C18 | 1.5 (11) |
| C18—P1—C12—C13 | −170.9 (5) | C19—C18—C23—C22 | −2.6 (11) |
| Au—P1—C12—C13 | −45.0 (6) | P1—C18—C23—C22 | −178.1 (6) |

Hydrogen-bond geometry (Å, °)

| | | | | |
|---------------------------|------|-------|------------|---------|
| D—H···A | D—H | H···A | D···A | D—H···A |
| C14—H14···O1 ⁱ | 0.94 | 2.51 | 3.314 (10) | 143 |

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

supplementary materials

Fig. 1

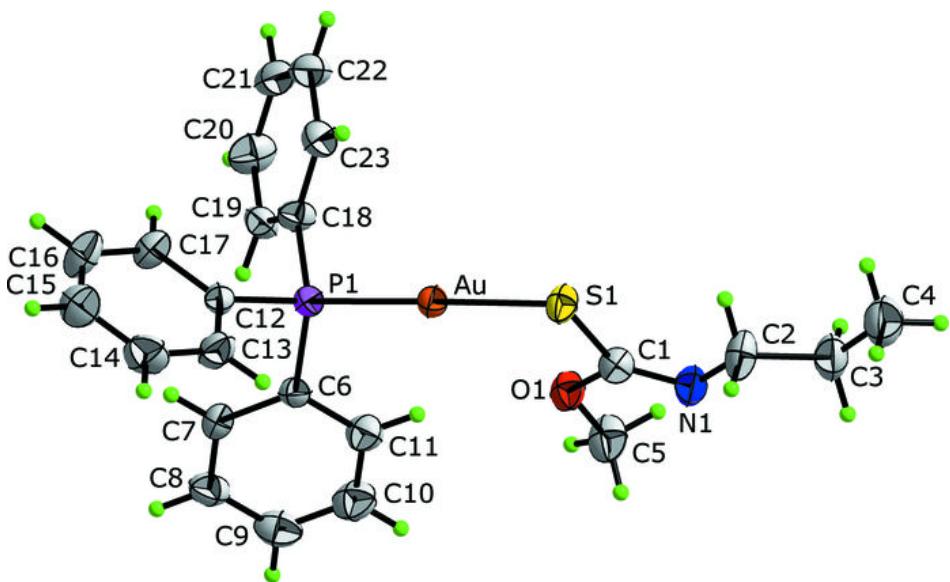


Fig. 2

