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[(*Z*)-*O*-Ethyl *N*-(4-nitrophenyl)thiocarbamato-κ*S*](triphenylphosphine-κ*P*)gold(I) dichloromethane solvate

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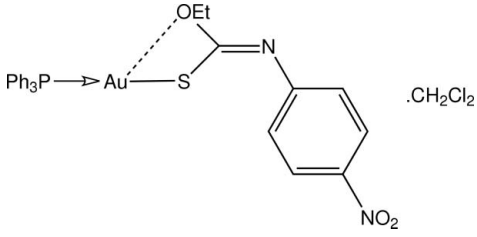
Key indicators: single-crystal X-ray study; T = 238 K; mean σ(C–C) = 0.013 Å; R factor = 0.055; wR factor = 0.128; data-to-parameter ratio = 19.0.

An *S*,*P*-donor set in the title solvate, $[Au(C_9H_9N_2O_3S)(C_{18}H_{15}P)]\cdot CH_2Cl_2$, defines a linear geometry for the Au^I atom [S—Au—P = 177.75 (7)°], with the minor distortion ascribed to the influence of an intramolecular Au···O contact [3.019 (6) Å]. In the crystal, the packing is stabilized by a network of C—H···S, C—H···N and C—H···O contacts.

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

$[Au(C_9H_9N_2O_3S)(C_{18}H_{15}P)]\cdot CH_2Cl_2$
M_r = 769.40
Triclinic, $P\overline{1}$
a = 8.7525 (7) Å
b = 11.1373 (9) Å
c = 15.8981 (13) Å
α = 104.311 (2)°
β = 105.559 (2)°
γ = 91.775 (2)°
V = 1438.7 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 5.46 mm^{-1}
T = 238 K
0.39 × 0.34 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.561, T_{max} = 1
10007 measured reflections
6534 independent reflections
5162 reflections with $I > 2\sigma(I)$
R_{int} = 0.064

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.128
S = 0.94
6534 reflections
343 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.69 e Å^{-3}
$\Delta\rho_{min}$ = −1.19 e Å^{-3}

Table 1
Selected bond lengths (Å).

Au—S1	2.3019 (19)	Au—P1	2.2545 (18)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C23—H23···N1^{i}	0.94	2.55	3.318 (11)	139
C14—H14···O3^{ii}	0.94	2.47	3.366 (12)	160
C28—H28a···O1^{iii}	0.98	2.52	3.330 (13)	140
C28—H28b···S1^{iv}	0.98	2.86	3.617 (11)	134

Symmetry codes: (i) $-x, -y+1, -z$; (ii) $-x+1, -y, -z$; (iii) $x+1, y, z+1$; (iv) $-x+1, -y, -z+1$.

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: *ORTEP-3* (Farrugia, 1997) and *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: HB5169).

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supporting information

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[(*Z*)-*O*-Ethyl *N*-(4-nitrophenyl)thiocarbamato-κS](triphenylphosphine-κP)gold(I) dichloromethane solvate

Soo Yei Ho and Edward R. T. Tiekink

S1. Comment

As a continuation of studies into the structural systematics of molecules with 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 title dichloromethane solvate, (I), was characterized. The Au atom in (I) exists in the expected linear geometry defined by S and P atoms, Table 1 and Fig. 1, with the deviation from the ideal 180° angle being related to the close approach of the O1 atom, 3.019 (6) Å. The structure follows closely literature precedents.

The crystal structure of (I) is stabilized by a series of large rings mediated by C—H···S, O and N contacts, Table 2 and Fig. 2. Thus, C_{phenyl}—*H*···O_{nitro} contacts link centrosymmetrically related molecules *via* 30-membered {···$ONC_4NCSAuPC_3H$}$_2$ synthons. Smaller centrosymmetric rings are formed through the agency of C_{phenyl}—*H*···N_{imine} contacts that lead to 16-membered {···$NCSAuPC_2H$}$_2$ synthons. Centrosymmetrically related dichloromethane molecules bridge a pair of complex molecules, forming C—H···O1, S1 contacts, leading to the formation of 12-membered {···OCS···HCH}$_2$ synthons.

S2. Experimental

The unsolvated compound was prepared following the standard literature procedure from the reaction of Ph_3PAuCl and $EtOC(S)N(H)C_6H_4NO_2$-4 in the presence of base (Hall *et al.*, 1993); m. pt. 423–425 K. Analysis for $C_{27}H_{24}AuN_2O_3PS$: found (calculated): C: 47.25 (47.38); H: 3.39 (3.53); N: 4.33 (4.09); S: 4.50 (4.68). IR (cm^{-1}): *ν*(C—S) 1102 s, 849*m*; *ν*(C—N) 1582 s; *ν*(C—O) 1145*m*. $^{31}P\{^1H\}$ NMR: *δ* 37.7 p.p.m. Yellow crystals of the dichloromethane solvate (I) were obtained from the layering of ethanol on a dichloromethane solution of the characterized product.

S3. 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 2.69 and 1.19 e Å^{-3}, respectively, were located 0.99 Å and 0.97 Å from the Au atom.

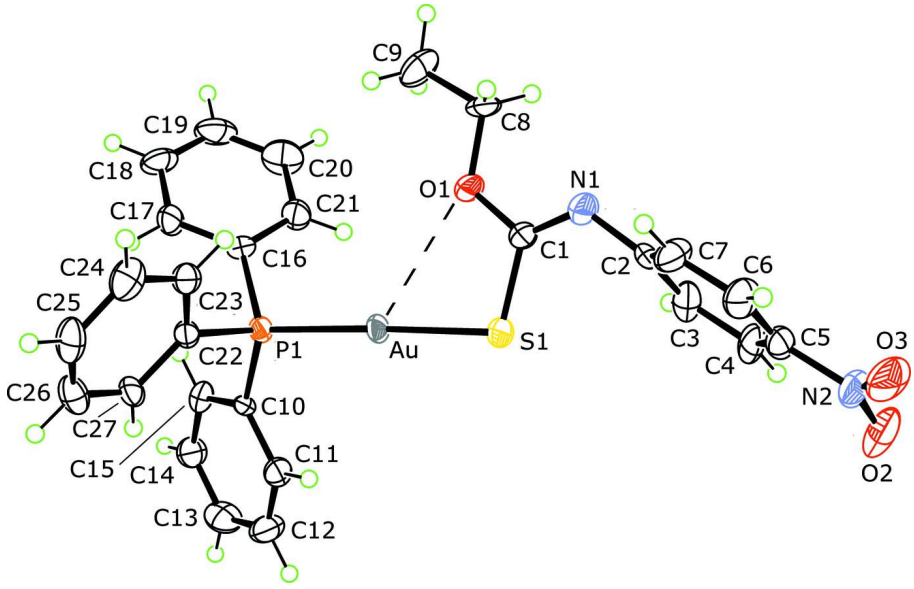

Figure 1

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

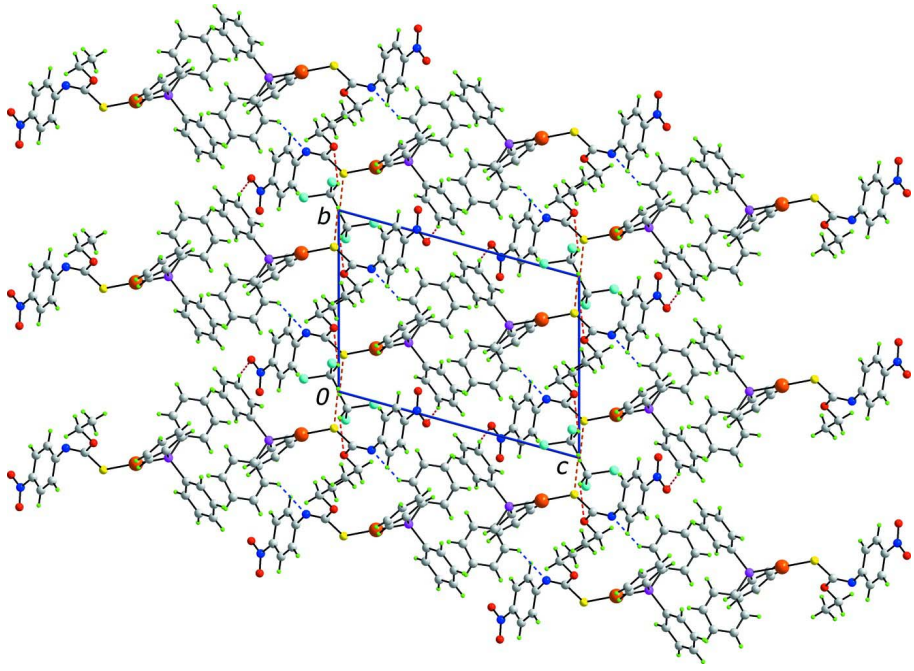

Figure 2

Unit-cell contents for (I) viewed in projection down the *a* axis. Colour code: Au, orange; Cl, cyan; S, yellow; P, pink; O, red; N, blue; C, grey; and H, green.

[(*Z*)-*O*-Ethyl *N*-(4-nitrophenyl)thiocarbamato-κS](triphenylphosphine- κP)gold(I) dichloromethane solvate

Crystal data

$[Au(C_9H_9N_2O_3S)(C_{18}H_{15}P)]\cdot CH_2Cl_2$
$M_r = 769.40$

Triclinic, $P\overline{1}$
Hall symbol: -P 1

a = 8.7525 (7) Å
b = 11.1373 (9) Å
c = 15.8981 (13) Å
α = 104.311 (2)°
β = 105.559 (2)°
γ = 91.775 (2)°
V = 1438.7 (2) Å^3
Z = 2
F(000) = 752

D_x = 1.776 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71069 Å
Cell parameters from 3380 reflections
θ = 2.7–25.5°
μ = 5.46 mm^{-1}
T = 238 K
Block, yellow
0.39 × 0.34 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.561, T_{max} = 1

10007 measured reflections
6534 independent reflections
5162 reflections with $I > 2\sigma(I)$
R_{int} = 0.064
θ_{max} = 27.5°, θ_{min} = 1.4°
h = −11→11
k = −12→14
l = −20→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.128
S = 0.94
6534 reflections
343 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
$w = 1/[\sigma^2(F_o^2) + (0.0474P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 2.69 e Å^{-3}
$\Delta\rho_{min}$ = −1.19 e 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^2)

	x	y	z	U_{iso}*/U_{eq}
Au	0.08336 (3)	0.29401 (3)	0.155405 (19)	0.02476 (11)
S1	0.1369 (2)	0.2101 (2)	0.02002 (14)	0.0337 (5)
P1	0.0409 (2)	0.37531 (18)	0.29087 (13)	0.0227 (4)
O1	−0.0966 (6)	0.3429 (5)	−0.0214 (4)	0.0304 (12)
O2	0.3929 (8)	−0.1228 (7)	−0.3297 (5)	0.061 (2)
O3	0.4680 (9)	0.0425 (7)	−0.3643 (5)	0.066 (2)
N1	0.0125 (8)	0.2734 (6)	−0.1360 (5)	0.0347 (16)
N2	0.3922 (9)	−0.0126 (8)	−0.3252 (5)	0.048 (2)

C1	0.0107 (9)	0.2789 (7)	−0.0565 (5)	0.0289 (17)
C2	0.1120 (9)	0.2009 (7)	−0.1789 (5)	0.0281 (17)
C3	0.1034 (10)	0.0715 (8)	−0.1934 (6)	0.038 (2)
H3	0.0336	0.0315	−0.1707	0.046*
C4	0.1951 (9)	0.0029 (8)	−0.2401 (6)	0.037 (2)
H4	0.1889	−0.0840	−0.2493	0.044*
C5	0.2968 (9)	0.0618 (8)	−0.2736 (6)	0.0337 (19)
C6	0.3108 (11)	0.1898 (9)	−0.2601 (6)	0.044 (2)
H6	0.3810	0.2292	−0.2830	0.053*
C7	0.2176 (11)	0.2575 (8)	−0.2117 (6)	0.038 (2)
H7	0.2264	0.3446	−0.2008	0.046*
C8	−0.2083 (10)	0.4005 (8)	−0.0801 (6)	0.035 (2)
H8A	−0.2696	0.3377	−0.1349	0.042*
H8B	−0.1517	0.4629	−0.0979	0.042*
C9	−0.3173 (11)	0.4610 (9)	−0.0275 (7)	0.047 (2)
H9A	−0.3948	0.5008	−0.0648	0.070*
H9B	−0.2552	0.5230	0.0264	0.070*
H9C	−0.3722	0.3983	−0.0101	0.070*
C10	0.0794 (8)	0.2722 (6)	0.3657 (5)	0.0175 (14)
C11	−0.0100 (9)	0.2683 (7)	0.4250 (5)	0.0289 (17)
H11	−0.0928	0.3197	0.4274	0.035*
C12	0.0222 (10)	0.1895 (8)	0.4802 (6)	0.0348 (19)
H12	−0.0391	0.1861	0.5200	0.042*
C13	0.1461 (11)	0.1148 (8)	0.4770 (6)	0.043 (2)
H13	0.1698	0.0627	0.5162	0.051*
C14	0.2344 (10)	0.1157 (8)	0.4174 (6)	0.040 (2)
H14	0.3160	0.0633	0.4144	0.048*
C15	0.2008 (9)	0.1957 (8)	0.3617 (6)	0.0328 (19)
H15	0.2607	0.1979	0.3210	0.039*
C16	−0.1630 (8)	0.4119 (7)	0.2803 (5)	0.0244 (16)
C17	−0.1997 (10)	0.5095 (8)	0.3435 (5)	0.0346 (19)
H17	−0.1180	0.5601	0.3917	0.042*
C18	−0.4767 (11)	0.4562 (10)	0.2640 (7)	0.049 (3)
H18	−0.5836	0.4713	0.2583	0.059*
C19	−0.3572 (11)	0.5311 (9)	0.3346 (6)	0.043 (2)
H19	−0.3830	0.5969	0.3767	0.052*
C20	−0.4417 (10)	0.3609 (10)	0.2025 (8)	0.054 (3)
H20	−0.5240	0.3094	0.1553	0.065*
C21	−0.2840 (9)	0.3400 (8)	0.2099 (6)	0.037 (2)
H21	−0.2596	0.2759	0.1661	0.045*
C22	0.1646 (8)	0.5220 (7)	0.3530 (5)	0.0241 (16)
C23	0.1571 (9)	0.6150 (7)	0.3100 (5)	0.0281 (17)
H23	0.0886	0.6027	0.2512	0.034*
C24	0.2522 (11)	0.7291 (8)	0.3543 (6)	0.042 (2)
H24	0.2473	0.7942	0.3260	0.051*
C25	0.3540 (11)	0.7435 (8)	0.4411 (6)	0.041 (2)
H25	0.4198	0.8186	0.4710	0.049*
C26	0.3595 (9)	0.6500 (8)	0.4834 (6)	0.0351 (19)

H26	0.4270	0.6619	0.5424	0.042*
C27	0.2666 (9)	0.5388 (8)	0.4397 (5)	0.0293 (17)
H27	0.2719	0.4740	0.4685	0.035*
C28	0.6962 (11)	0.0796 (10)	0.9653 (7)	0.052 (3)
H28A	0.7867	0.1437	0.9962	0.063*
H28B	0.7087	0.0138	0.9970	0.063*
Cl1	0.5199 (3)	0.1453 (2)	0.9715 (2)	0.0559 (7)
Cl2	0.6994 (4)	0.0171 (4)	0.8542 (2)	0.0823 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au	0.02296 (16)	0.03345 (18)	0.01681 (16)	0.00492 (11)	0.00790 (11)	0.00206 (11)
S1	0.0337 (11)	0.0484 (12)	0.0218 (10)	0.0176 (10)	0.0134 (9)	0.0068 (9)
P1	0.0173 (9)	0.0305 (10)	0.0186 (10)	0.0038 (8)	0.0062 (7)	0.0019 (8)
O1	0.029 (3)	0.038 (3)	0.029 (3)	0.015 (2)	0.014 (2)	0.010 (2)
O2	0.057 (5)	0.050 (4)	0.070 (5)	0.012 (4)	0.034 (4)	−0.011 (4)
O3	0.071 (5)	0.092 (6)	0.065 (5)	0.044 (5)	0.051 (4)	0.036 (4)
N1	0.039 (4)	0.040 (4)	0.031 (4)	0.016 (3)	0.018 (3)	0.011 (3)
N2	0.034 (4)	0.065 (6)	0.036 (5)	0.020 (4)	0.012 (4)	−0.003 (4)
C1	0.024 (4)	0.038 (5)	0.026 (4)	0.013 (3)	0.010 (3)	0.007 (3)
C2	0.031 (4)	0.039 (5)	0.011 (4)	0.015 (4)	0.002 (3)	0.004 (3)
C3	0.035 (5)	0.042 (5)	0.032 (5)	−0.004 (4)	0.013 (4)	−0.004 (4)
C4	0.031 (4)	0.033 (4)	0.034 (5)	−0.002 (4)	0.008 (4)	−0.014 (4)
C5	0.022 (4)	0.049 (5)	0.027 (4)	0.008 (4)	0.008 (3)	0.003 (4)
C6	0.045 (5)	0.057 (6)	0.044 (6)	0.017 (5)	0.028 (5)	0.021 (5)
C7	0.051 (5)	0.038 (5)	0.042 (5)	0.022 (4)	0.028 (5)	0.022 (4)
C8	0.034 (4)	0.044 (5)	0.034 (5)	0.025 (4)	0.012 (4)	0.018 (4)
C9	0.045 (5)	0.047 (5)	0.062 (7)	0.021 (5)	0.036 (5)	0.014 (5)
C10	0.016 (3)	0.019 (3)	0.014 (3)	0.003 (3)	−0.001 (3)	0.004 (3)
C11	0.031 (4)	0.027 (4)	0.030 (4)	0.003 (3)	0.014 (4)	0.001 (3)
C12	0.037 (5)	0.042 (5)	0.030 (5)	0.007 (4)	0.014 (4)	0.012 (4)
C13	0.050 (5)	0.037 (5)	0.044 (6)	0.003 (4)	0.005 (5)	0.024 (4)
C14	0.038 (5)	0.034 (5)	0.049 (6)	0.014 (4)	0.010 (4)	0.012 (4)
C15	0.022 (4)	0.048 (5)	0.027 (4)	0.010 (4)	0.010 (3)	0.003 (4)
C16	0.022 (4)	0.024 (4)	0.028 (4)	0.006 (3)	0.006 (3)	0.010 (3)
C17	0.031 (4)	0.049 (5)	0.023 (4)	0.012 (4)	0.011 (4)	0.004 (4)
C18	0.029 (5)	0.073 (7)	0.055 (7)	0.023 (5)	0.011 (5)	0.031 (6)
C19	0.040 (5)	0.058 (6)	0.044 (6)	0.031 (5)	0.023 (5)	0.022 (5)
C20	0.017 (4)	0.073 (7)	0.064 (7)	0.004 (4)	0.003 (4)	0.011 (6)
C21	0.024 (4)	0.047 (5)	0.031 (5)	0.007 (4)	0.002 (4)	−0.001 (4)
C22	0.019 (3)	0.030 (4)	0.020 (4)	0.004 (3)	0.006 (3)	0.001 (3)
C23	0.030 (4)	0.031 (4)	0.026 (4)	0.005 (3)	0.012 (3)	0.007 (3)
C24	0.052 (6)	0.039 (5)	0.045 (6)	0.006 (4)	0.030 (5)	0.010 (4)
C25	0.042 (5)	0.032 (5)	0.039 (5)	−0.011 (4)	0.012 (4)	−0.008 (4)
C26	0.024 (4)	0.046 (5)	0.028 (5)	−0.009 (4)	0.006 (3)	0.002 (4)
C27	0.030 (4)	0.040 (5)	0.016 (4)	0.006 (4)	0.007 (3)	0.003 (3)
C28	0.031 (5)	0.058 (6)	0.065 (7)	0.006 (5)	0.009 (5)	0.015 (5)

Cl1	0.0490 (14)	0.0489 (14)	0.0709 (19)	0.0094 (12)	0.0188 (13)	0.0154 (13)
Cl2	0.0596 (18)	0.116 (3)	0.064 (2)	0.0261 (18)	0.0179 (16)	0.0083 (18)

Geometric parameters (Å, º)

Au—S1	2.3019 (19)	C12—C13	1.391 (12)
Au—P1	2.2545 (18)	C12—H12	0.9400
S1—C1	1.755 (8)	C13—C14	1.376 (13)
P1—C16	1.816 (7)	C13—H13	0.9400
P1—C10	1.825 (7)	C14—C15	1.389 (12)
P1—C22	1.826 (8)	C14—H14	0.9400
O1—C1	1.352 (8)	C15—H15	0.9400
O1—C8	1.444 (9)	C16—C21	1.373 (11)
O2—N2	1.212 (10)	C16—C17	1.396 (10)
O3—N2	1.260 (11)	C17—C19	1.383 (11)
N1—C1	1.255 (10)	C17—H17	0.9400
N1—C2	1.401 (9)	C18—C20	1.356 (13)
N2—C5	1.460 (10)	C18—C19	1.380 (13)
C2—C7	1.382 (11)	C18—H18	0.9400
C2—C3	1.397 (12)	C19—H19	0.9400
C3—C4	1.362 (11)	C20—C21	1.386 (11)
C3—H3	0.9400	C20—H20	0.9400
C4—C5	1.377 (12)	C21—H21	0.9400
C4—H4	0.9400	C22—C23	1.370 (11)
C5—C6	1.385 (12)	C22—C27	1.390 (10)
C6—C7	1.383 (11)	C23—C24	1.408 (12)
C6—H6	0.9400	C23—H23	0.9400
C7—H7	0.9400	C24—C25	1.395 (13)
C8—C9	1.500 (10)	C24—H24	0.9400
C8—H8A	0.9800	C25—C26	1.367 (13)
C8—H8B	0.9800	C25—H25	0.9400
C9—H9A	0.9700	C26—C27	1.374 (11)
C9—H9B	0.9700	C26—H26	0.9400
C9—H9C	0.9700	C27—H27	0.9400
C10—C11	1.385 (10)	C28—Cl2	1.740 (11)
C10—C15	1.387 (9)	C28—Cl1	1.743 (9)
C11—C12	1.373 (11)	C28—H28A	0.9800
C11—H11	0.9400	C28—H28B	0.9800
P1—Au—S1	177.75 (7)	C11—C12—H12	120.1
C1—S1—Au	104.1 (2)	C13—C12—H12	120.1
C16—P1—C10	106.1 (3)	C14—C13—C12	121.1 (8)
C16—P1—C22	105.1 (3)	C14—C13—H13	119.5
C10—P1—C22	106.5 (3)	C12—C13—H13	119.5
C16—P1—Au	112.4 (3)	C13—C14—C15	118.8 (8)
C10—P1—Au	113.5 (2)	C13—C14—H14	120.6
C22—P1—Au	112.5 (2)	C15—C14—H14	120.6
C1—O1—C8	116.9 (6)	C10—C15—C14	120.5 (8)

C1—N1—C2	123.2 (7)	C10—C15—H15	119.7
O2—N2—O3	123.5 (7)	C14—C15—H15	119.7
O2—N2—C5	119.3 (8)	C21—C16—C17	119.3 (7)
O3—N2—C5	117.1 (8)	C21—C16—P1	119.2 (6)
N1—C1—O1	120.4 (7)	C17—C16—P1	121.4 (6)
N1—C1—S1	126.9 (6)	C19—C17—C16	119.4 (8)
O1—C1—S1	112.7 (6)	C19—C17—H17	120.3
C7—C2—C3	118.4 (7)	C16—C17—H17	120.3
C7—C2—N1	119.4 (7)	C20—C18—C19	120.8 (8)
C3—C2—N1	122.2 (8)	C20—C18—H18	119.6
C4—C3—C2	120.7 (8)	C19—C18—H18	119.6
C4—C3—H3	119.6	C18—C19—C17	120.0 (8)
C2—C3—H3	119.6	C18—C19—H19	120.0
C3—C4—C5	119.5 (8)	C17—C19—H19	120.0
C3—C4—H4	120.2	C18—C20—C21	119.6 (9)
C5—C4—H4	120.2	C18—C20—H20	120.2
C4—C5—C6	121.9 (7)	C21—C20—H20	120.2
C4—C5—N2	119.2 (8)	C16—C21—C20	120.8 (8)
C6—C5—N2	118.9 (8)	C16—C21—H21	119.6
C7—C6—C5	117.4 (8)	C20—C21—H21	119.6
C7—C6—H6	121.3	C23—C22—C27	120.6 (7)
C5—C6—H6	121.3	C23—C22—P1	117.4 (6)
C2—C7—C6	122.0 (8)	C27—C22—P1	122.0 (6)
C2—C7—H7	119.0	C22—C23—C24	119.7 (8)
C6—C7—H7	119.0	C22—C23—H23	120.2
O1—C8—C9	106.9 (7)	C24—C23—H23	120.2
O1—C8—H8A	110.3	C25—C24—C23	118.7 (8)
C9—C8—H8A	110.3	C25—C24—H24	120.7
O1—C8—H8B	110.3	C23—C24—H24	120.7
C9—C8—H8B	110.3	C26—C25—C24	121.0 (8)
H8A—C8—H8B	108.6	C26—C25—H25	119.5
C8—C9—H9A	109.5	C24—C25—H25	119.5
C8—C9—H9B	109.5	C25—C26—C27	120.1 (8)
H9A—C9—H9B	109.5	C25—C26—H26	119.9
C8—C9—H9C	109.5	C27—C26—H26	119.9
H9A—C9—H9C	109.5	C26—C27—C22	120.0 (8)
H9B—C9—H9C	109.5	C26—C27—H27	120.0
C11—C10—C15	119.9 (7)	C22—C27—H27	120.0
C11—C10—P1	121.6 (5)	Cl2—C28—Cl1	112.4 (6)
C15—C10—P1	118.5 (6)	Cl2—C28—H28A	109.1
C12—C11—C10	120.0 (7)	Cl1—C28—H28A	109.1
C12—C11—H11	120.0	Cl2—C28—H28B	109.1
C10—C11—H11	120.0	Cl1—C28—H28B	109.1
C11—C12—C13	119.7 (8)	H28A—C28—H28B	107.9

C2—N1—C1—O1	−174.9 (7)	C12—C13—C14—C15	1.8 (14)
C2—N1—C1—S1	5.0 (13)	C11—C10—C15—C14	−0.6 (12)
C8—O1—C1—N1	1.3 (11)	P1—C10—C15—C14	180.0 (6)

C8—O1—C1—S1	−178.6 (6)	C13—C14—C15—C10	−0.6 (13)
Au—S1—C1—N1	170.3 (8)	C10—P1—C16—C21	−92.8 (7)
Au—S1—C1—O1	−9.8 (6)	C22—P1—C16—C21	154.5 (7)
C1—N1—C2—C7	−122.3 (9)	Au—P1—C16—C21	31.8 (7)
C1—N1—C2—C3	60.6 (12)	C10—P1—C16—C17	85.6 (7)
C7—C2—C3—C4	−1.1 (13)	C22—P1—C16—C17	−27.1 (8)
N1—C2—C3—C4	176.0 (8)	Au—P1—C16—C17	−149.8 (6)
C2—C3—C4—C5	−0.3 (13)	C21—C16—C17—C19	0.7 (13)
C3—C4—C5—C6	1.0 (13)	P1—C16—C17—C19	−177.6 (7)
C3—C4—C5—N2	−178.7 (8)	C20—C18—C19—C17	0.0 (15)
O2—N2—C5—C4	−7.6 (12)	C16—C17—C19—C18	0.3 (14)
O3—N2—C5—C4	171.2 (8)	C19—C18—C20—C21	−1.2 (17)
O2—N2—C5—C6	172.6 (8)	C17—C16—C21—C20	−2.0 (14)
O3—N2—C5—C6	−8.5 (12)	P1—C16—C21—C20	176.4 (8)
C4—C5—C6—C7	−0.4 (14)	C18—C20—C21—C16	2.3 (16)
N2—C5—C6—C7	179.4 (8)	C16—P1—C22—C23	−68.1 (6)
C3—C2—C7—C6	1.8 (13)	C10—P1—C22—C23	179.5 (5)
N1—C2—C7—C6	−175.4 (8)	Au—P1—C22—C23	54.5 (6)
C5—C6—C7—C2	−1.1 (14)	C16—P1—C22—C27	113.7 (6)
C1—O1—C8—C9	178.0 (7)	C10—P1—C22—C27	1.3 (7)
C16—P1—C10—C11	−21.5 (7)	Au—P1—C22—C27	−123.7 (6)
C22—P1—C10—C11	90.1 (6)	C27—C22—C23—C24	−0.6 (11)
Au—P1—C10—C11	−145.5 (5)	P1—C22—C23—C24	−178.9 (6)
C16—P1—C10—C15	157.9 (6)	C22—C23—C24—C25	0.9 (11)
C22—P1—C10—C15	−90.4 (6)	C23—C24—C25—C26	−1.3 (13)
Au—P1—C10—C15	34.0 (6)	C24—C25—C26—C27	1.4 (13)
C15—C10—C11—C12	0.5 (11)	C25—C26—C27—C22	−1.2 (12)
P1—C10—C11—C12	179.9 (6)	C23—C22—C27—C26	0.8 (11)
C10—C11—C12—C13	0.7 (12)	P1—C22—C27—C26	178.9 (6)
C11—C12—C13—C14	−1.9 (14)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C23—H23···N1^{i}	0.94	2.55	3.318 (11)	139
C14—H14···O3^{ii}	0.94	2.47	3.366 (12)	160
C28—H28a···O1^{iii}	0.98	2.52	3.330 (13)	140
C28—H28b···S1^{iv}	0.98	2.86	3.617 (11)	134

Symmetry codes: (i) −*x*, −*y*+1, −*z*; (ii) −*x*+1, −*y*, −*z*; (iii) *x*+1, *y*, *z*+1; (iv) −*x*+1, −*y*, −*z*+1.