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{(*Z*)-*O*-Ethyl *N*-[4-(methoxycarbonyl)phenyl]-thiocarbamato-κ*S*}(tricyclohexylphosphine-κ*P*)-gold(**I**)

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A near-linear P—Au—S geometry is found for the Au atom in the title complex, $(C_6H_{11})_3PAu[SC(OCH_2CH_3){=}NC_6H_4\text{-}\{C({=}O\}OCH_3\text{-}4)]$ or $[Au(C_{11}H_{12}NO_3S)(C_{18}H_{33}P)]$.

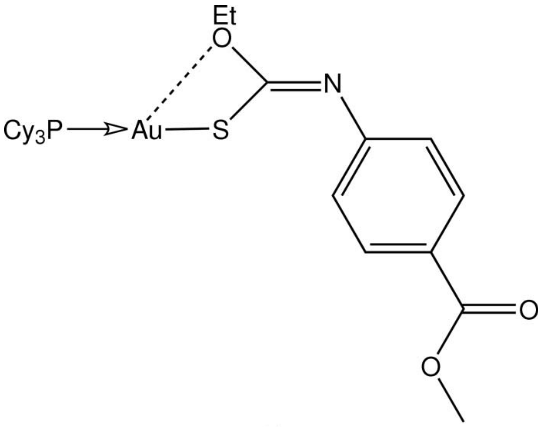
Key indicators

Single-crystal X-ray study
T = 223 K
Mean σ(C–C) = 0.006 Å
Disorder in main residue
R factor = 0.028
wR factor = 0.071
Data-to-parameter ratio = 17.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

The structural chemistry of mono- and dinuclear complexes related to the title complex, (I), sometimes reveals intra- or intermolecular aurophilic Au···Au interactions (Hall *et al.*, 1993; Ho *et al.*, 2006, 2007; Ho & Tiekink, 2007). In (I) (Fig. 1), the expected linear coordination geometry is found for Au, as defined by the S and P atoms (Table 1). An intramolecular Au···O interaction of 3.129 (2) Å is also present.



(I)

In the crystal structure of (I) (Fig. 2), the molecules are aligned so as to potentially form Au···Au interactions. Thus, centrosymmetrically related molecules approach each other so that Au···Au^{iii} is 5.9631 (2) Å [symmetry code: (iii) $1 - x$, $1 - y$, $1 - z$], a distance too great to represent a significant interaction, perhaps because the intervention of the bulky cyclohexyl groups precludes closer association. There are a number of C—H···O interactions in the crystal structure, involving both O atoms of the nitro group, which help to consolidate the packing (Fig. 2). The two most significant of these (involving the major disorder component) are summarized in Table 2.

Experimental

The title compound was prepared from the reaction of $(C_6H_{11})_3PAuCl$ and $S{=}C(OCH_2CH_3){=}N(H)C_6H_4\{C({=}O)OCH_3\text{-}4\}$ (Ho *et al.*, 2005) following a literature procedure (Ho *et al.*, 2006). Colourless crystals of (I) were obtained from the layering of ethanol on a dichloromethane solution (m.p. 416–417 K).

Crystal data

$[Au(C_{11}H_{12}NO_3S)(C_{18}H_{33}P)]$
$M_r = 715.66$
Monoclinic, $P2_1/n$
$a = 15.2963 (8)$ Å
$b = 9.1081 (4)$ Å
$c = 22.2657 (11)$ Å
$\beta = 96.837 (1)^\circ$
$V = 3080.0 (3)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 4.93$ mm^{-1}
$T = 223 (2)$ K
$0.29 \times 0.24 \times 0.10$ mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{\min} = 0.386$, $T_{\max} = 1$
(expected range = 0.236–0.611)
21294 measured reflections
7060 independent reflections
6020 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.039$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.071$
$S = 1.03$
7060 reflections
395 parameters
116 restraints
H-atom parameters constrained
$\Delta\rho_{\max} = 1.27$ e Å^{-3}
$\Delta\rho_{\min} = -0.59$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Au—S1	2.2954 (9)	Au—P1	2.2638 (8)
S1—Au—P1	174.39 (3)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C25—H25a···O1$^{\rm i}$	0.98	2.65	3.363 (14)	130
C16—H16a···O2$^{\rm ii}$	0.98	2.67	3.427 (10)	134

Symmetry codes: (i) $x + \frac{1}{2}, -y + \frac{3}{2}, z - \frac{1}{2}$; (ii) $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$.

Disorder in the aromatic ring, extending to include the nitro groups, was resolved into two components with occupancies (from refinement) of 0.63 (2) and 0.37 (2). In the disorder model, the aromatic rings were constrained as regular hexagons, with C—C = 1.39 Å. For the other atoms, pairs of related distances were restrained to lie within 0.01 Å of each other, and the U_{ij} values of the disordered atoms were restrained to approximate to isotropic displacement behaviour. The H atoms were positioned geometrically (C—H = 0.94–0.98 Å) and refined as riding, with $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C) or $1.5U_{\rm eq}$(methyl C). The maximum residual electron-density peak was located 0.90 Å from the Au atom.

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, 1997); molecular graphics: *ORTEPII* (Johnson, 1976) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXL97*.

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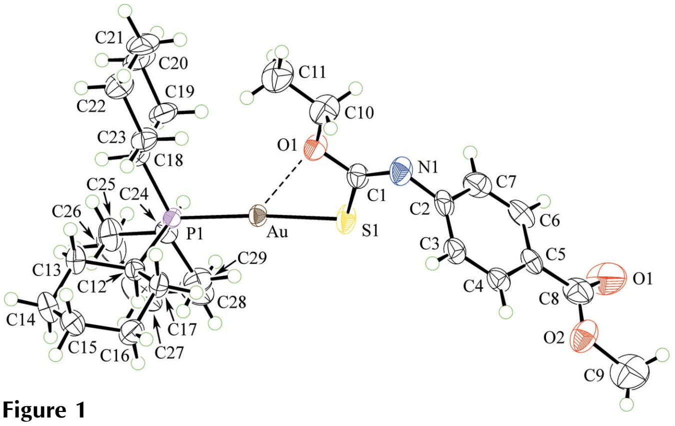

Figure 1
The molecular structure of (I), showing displacement ellipsoids at the 50% probability level (arbitrary spheres for the H atoms). For clarity, only the major component of the disordered atoms is shown.

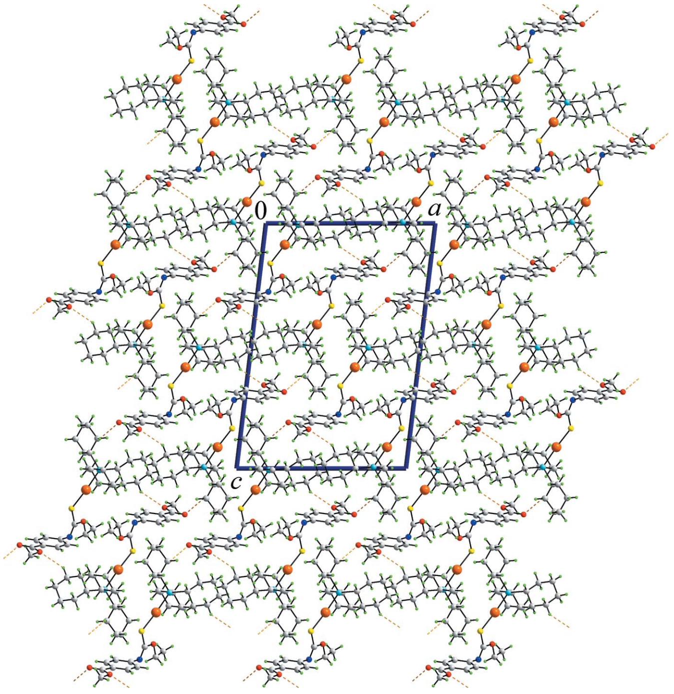

Figure 2
View of the crystal packing in (I). For clarity, only the major component of the disordered atoms is shown. The C—H···O interactions are shown as orange dashed lines. Colour code: Au orange, S yellow, P pink, O red, N blue, C grey and H green.

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