Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

A third polymorph of (2-thiazolidinethionato)-(triphenylphosphine)gold(I)

Ulrike E. I. Horvath* and Helgard G. Raubenheimer

Department of Chemistry and Polymer Science, University of Stellenbosch, Private Bag X1, Matieland 7602, South Africa

Correspondence e-mail: uhorvath@sun.ac.za

Received 15 June 2006
Accepted 17 June 2006.

The title compound, $[Au(C_3H_4NS_2)(C_{18}H_{15}P)]$, is a third polymorphic form of a compound previously reported by Grant, Forward & Fackler Jr [*Z. Kristallogr.* (1996). **211**, 483–484]. At 100 K, the present polymorph shows triclinic symmetry, as do the other two polymorphs.

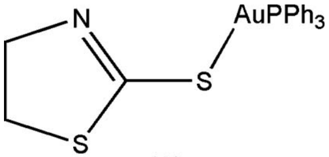
Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.011 Å
R factor = 0.041
wR factor = 0.088
Data-to-parameter ratio = 17.6

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

Comment

In the preceding paper (Horvath *et al.*, 2006), we reported a polymorph, (I), of a known compound (Grant *et al.*, 1996). The molecular structure of the title compound is shown in Fig. 1. The C1—S2 separation [1.693 (8) Å] in the thione ligand of (II) is somewhat less than in the other two polymorphic forms [1.733 (7) Å for (I) and 1.765 Å for the form reported by Grant *et al.* (1996)]. All the other bond lengths within the thione unit of the three structures are essentially identical. The influence of the Au atom and the non-rigid five-membered thione ring explains the rather larger thermal motion of atom S2, and also of C2 and C3. The most significant difference among the three polymorphs occurs in the distorted tetrahedral arrangement of the phenyl rings, with large differences in their respective torsion angles. This leads to a different packing mode of the present structure compared with those in the other polymorphs.



(II)

In contrast to polymorph (I), where the crystal structure is dominated by N···H and S···H contacts, leading towards a rather inefficient packing of the molecules, the packing along the *a* axis of (II) is now characterized by perpendicularly arranged molecules with N1···H17^{i} [symmetry code: (i) x, $y-1$, z] contacts of about 2.58 Å with molecules of the neighbouring layer in the crystal structure (Fig. 2). The P1—Au1—S1 bond angle [176.06 (7)°] is nearly linear, as expected, and does not differ from reported values in similar structures (Macalindong *et al.*, 2006).

Experimental

The preparation of the compound followed a similar procedure as described for polymorph (I) (Horvath *et al.*, 2006). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of a CH_2Cl_2 solution at 243 K.

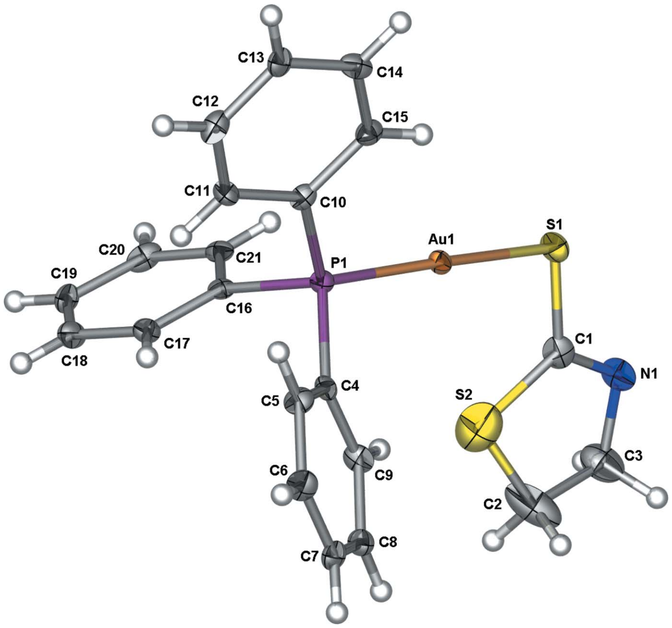


Figure 1
The molecular structure of (II), showing atom labels and 50% probability ellipsoids for non-H atoms.

Crystal data

$[Au(C_3H_4NS_2)(C_{18}H_{15}P)]$
$M_r = 577.43$
Triclinic, $P\bar{1}$
$a = 8.2258$ (11) Å
$b = 11.0179$ (15) Å
$c = 12.1641$ (17) Å
$\alpha = 71.411$ (2)°
$\beta = 75.984$ (2)°
$\gamma = 68.848$ (2)°
$V = 964.4$ (2) Å^3
$Z = 2$
$D_x = 1.988$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 7.93$ mm^{-1}
$T = 100$ (2) K
Block, colourless
0.14 × 0.12 × 0.12 mm

Data collection

Bruker APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Blessing, 1995)
$T_{\rm min} = 0.305$, $T_{\rm max} = 0.386$
10322 measured reflections
3924 independent reflections
3596 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.041$
$\theta_{\rm max} = 26.4°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.088$
$S = 1.11$
3924 reflections
223 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0333P)^2 + 4.2376P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 1.77$ e Å^{-3}
$\Delta\rho_{\rm min} = -2.15$ e Å^{-3}

All H atoms were positioned geometrically (C—H = 0.95 and 0.99 Å for aromatic CH and CH$_2$, respectively) and constrained to ride on their parent atoms; $U_{\rm iso}$(H) values were set at 1.2 times $U_{\rm eq}$(C) for CH$_2$ and CH groups. Due to a unexpected high electron density around C19 the anisotropic displacement of the atoms in *para* positions were constrained to be the same as C7 using the EADP routine in *SHELXL*97. The highest peak is 0.52 Å from Au1 and the deepest hole is 0.51 Å also from Au1.

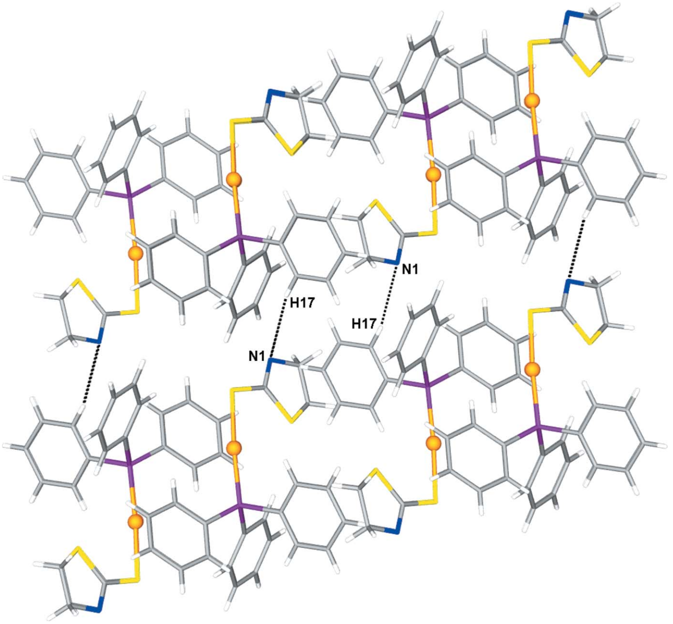


Figure 2
The packing, viewed along the *a* axis. The closest N···H contacts are shown as dashed lines. The symmetry code for atom H17 is (x, $y - 1$, z).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Atwood & Barbour, 2003; Barbour, 2001); software used to prepare material for publication: *X-SEED*.

We thank the Claude Harris Leon Foundation for financial support, and Mintek and Harmony Gold for their generous loan of gold.

References

Atwood, J. L. & Barbour, L. J. (2003). *Cryst. Growth Des.* **3**, 3–8.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Bruker (2001). *SMART*. Version 5.625. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2002). *SAINT*. Version 6.36a. Bruker AXS Inc., Madison, Wisconsin, USA.
Grant, T. A., Forward, J. M. & Fackler, J. P. Jr (1996). *Z. Kristallogr.* **211**, 483–484.
Horvath, U. E. I., Cronje, S., Nogai, S. D. & Raubenheimer, H. G. (2006). *Acta Cryst.* E**62**, m1641—m1643.
Macalindong, J. S., Fronczek, F. R., Schuerman, J. A., Selbin, J. & Watkins, S. F. (2006). *Acta Cryst.* E**62**, m889–m890.
Sheldrick, G. M. (1997). *SHELXS97*, *SHELXL97* and *SADABS* (Version 2.05). University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.