[4-Amino-*N*-(pyrimidin-2-yl)benzene-sulfonamido-*κN*](triphenylphosphine-*κP*)gold(I)

Ernesto Schulz Lang,* Robert Alan Burrow and Lenice de Lourenço Marques

Departamento de Química, Universidade Federal de Santa Maria, Santa Maria RS, 97119-900, Brazil

Correspondence e-mail: eslang@quimica.ufsm.br

The title compound, $[Au(C_{10}H_9N_4O_2S)(C_{18}H_{15}P)]$, is nearly linear at Au^I, with Au—N = 2.0707 (18) Å, Au—P = 2.2310 (8) Å and N—Au—P 171.93 (5)°. The molecules are linked by intermolecular N—H···O bonds.

Comment

Metal complexes of 4-amino-*N*-(pyrimidin-2-yl)benzene-sulfonamide (sulfadiazine) are widely used to prevent bacterial infection in both humans and animals during the treatment of burns (Yuan *et al.*, 2001). The effectiveness of these complexes for burn treatment depends on the presence of both the metal ion and the free ligand (Baenziger *et al.*, 1983; Raso *et al.*, 1997). Gold(I) complexes have found use in medicine, with those containing sulfur ligands being used for the treatment of rheumatoid arthritis (Shaw, 1999; Ahmad *et al.*, 2002). Despite the varied structural chemistry of sulfadiazine and its derivatives (Baenziger & Struss, 1976; Gutiérrez *et al.*, 2001), gold(I) complexes with these ligands have not been reported to date. In this context, we report the preparation and structural characterization of, and some observations on, the title compound, (I), also known as (sulfadiazinato)(triphenylphosphine)gold(I).
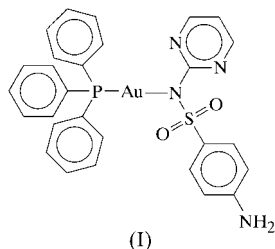
Single crystals of (I) were obtained by recrystallization from dichloromethane and petroleum ether of the crude product from the reaction of chloro(triphenylphosphine)gold(I), sulfadiazine and triethylamine in methanol. The asymmetric
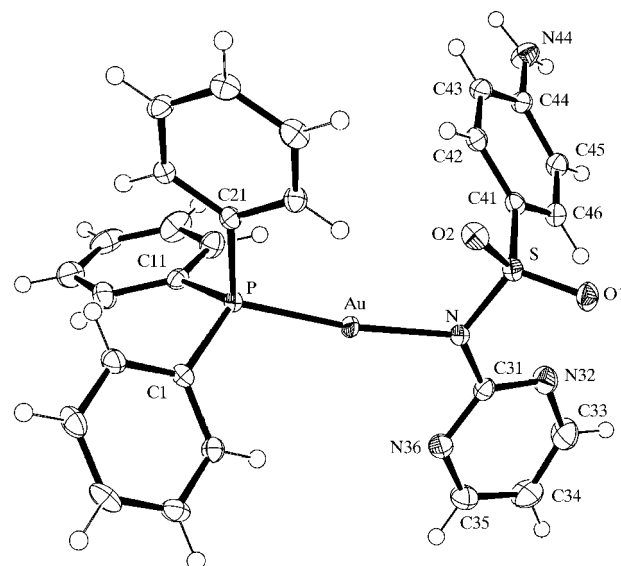
Figure 1
A view of the molecule of (I) with the atomic labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms have been omitted for clarity.

unit contains a complete molecule (Fig. 1) of the compound. Selected bond distances and angles are given in Table 1.

Compound (I) shows a nearly linear N—Au—P geometry with normal distances. The Au^I atom shows weak interactions with atoms O2 and N36 of the sulfadiazinate ligand. The sulfadiazinate N atom bonded to Au shows trigonal planar geometry, with the N atom lying 0.020 (2) Å out of the plane defined by atoms Au, S and C31. The pyrimidine ring is rotated slightly with respect to the plane of the N atom by 18.2 (11)°. The sulfonamide group is approximately tetrahedral, with the largest deviation being seen for the O1—S—O2 angle.

Atom O1 of the sulfonamide group participates in inter-molecular hydrogen bonding to the amino group (Table 2). The same pattern is observed in the structure of sulfadiazine (Shin *et al.*, 1975; Kokila *et al.*, 1995). This intermolecular hydrogen bond to the neighbouring molecule forms continuous chains along the *c* axis.

The two ring systems in the sulfadiazinate ligand of (I) can be considered as being in a *cisoid* conformation, since the C31—N—S—C41 torsion angle is less than 90°. The bond lengths and angles in the pyrimidine and phenyl rings are in good agreement with the values observed for such rings in both free sulfadiazine and the metal–sulfadiazinate complexes studied to date.

Experimental

To a solution of chloro(triphenylphosphine)gold(I) (0.2 mmol) in methanol (5 ml), a solution of sulfadiazine (0.1 mmol) in methanol (15 ml) and triethylamine (0.1 mmol) were added. The resulting mixture was stirred under reflux for 2 h and then cooled to room temperature, after which the precipitated solid was separated by

filtration (yield 85%, based on sulfadiazine). Recrystallization from dichloromethane and petroleum ether (1:1 v/v) afforded crystals of the pure product, (I), after two weeks. Elemental analysis, calculated (found): C 47.46 (47.08), H 3.42 (3.43), N 7.90 (7.66)%.

Crystal data

$[Au(C_{10}H_9N_4O_2S)(C_{18}H_{15}P)]$	$D_x = 1.838$ Mg m^{-3}
$M_r = 708.51$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 7802 reflections
$a = 11.878$ (5) Å	
$b = 13.329$ (5) Å	$\theta = 1.8$–30.8°
$c = 16.677$ (5) Å	$\mu = 5.92$ mm^{-1}
$\beta = 104.085$ (5)°	$T = 293$ (2) K
$V = 2561.0$ (16) Å^3	Block, colourless
$Z = 4$	$0.25 \times 0.19 \times 0.13$ mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	7802 independent reflections
φ and ω scans	6618 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.029$
	$\theta_{max} = 30.6°$
$T_{min} = 0.288$, $T_{max} = 0.463$	$h = -16 \rightarrow 16$
31 145 measured reflections	$k = -19 \rightarrow 19$
	$l = -23 \rightarrow 23$

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
$R(F) = 0.019$	
$wR(F^2) = 0.045$	
$S = 1.02$	$w = 1/[\sigma^2(F_o^2) + (0.0236P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
7802 reflections	
342 parameters	$(\Delta/\sigma)_{max} = 0.002$
	$\Delta\rho_{max} = 1.15$ e Å^{-3}
	$\Delta\rho_{min} = -0.54$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Au—N	2.0707 (18)	N—S	1.6320 (19)
Au—P	2.2310 (8)	S—O1	1.4405 (16)
Au—O2	2.9880 (19)	S—O2	1.4410 (17)
Au—N36	3.134 (2)	S—C41	1.759 (2)
N—Au—P	171.93 (5)	O1—S—O2	117.22 (10)
N—Au—O2	54.28 (6)	O1—S—N	110.19 (10)
P—Au—O2	118.18 (4)	O2—S—N	105.42 (10)
N—Au—N36	47.09 (6)	O1—S—C41	108.23 (10)
P—Au—N36	140.98 (4)	O2—S—C41	107.02 (10)
C31—N—S	122.60 (15)	N—S—C41	108.44 (10)
C31—N—Au	122.44 (14)	S—O2—Au	81.95 (7)
S—N—Au	114.92 (10)		
C31—N—S—C41	84.45 (19)		

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N44—H44$A\cdots$O1^i	0.93 (3)	2.00 (3)	2.909 (3)	165 (3)

Symmetry code: (i) $x, \frac{1}{2} - y, \frac{1}{2} + z$.

H atoms were constrained to riding positions, with C—H distances of 0.93 Å, except for the two H atoms on N44, which were allowed to refine freely.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97.

References

Ahmad, S., Isab, A. A., Perzanowski, H. P., Hussain, M. S. & Akhtar, M. N. (2002). *Transition Met. Chem.* **27**, 177–183.

Baenziger, N. C., Modak, S. L. & Fox, C. L. Jr (1983). *Acta Cryst.* C**39**, 1620–1623.

Baenziger, N. C. & Struss, A. W. (1976). *Inorg. Chem.* **15**, 1807–1809.

Bruker (1997). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

Gutiérrez, L., Alzuet, G., Borrás, J., Castiñeiras, A., Fortea, A. R. & Ruiz, E. (2001). *Inorg. Chem.* **40**, 3089–3096.

Kokila, M. K., Puttaraja, Kulkarni, M. V. & Thampi, S. (1995). *Acta Cryst.* C**51**, 333–336.

Raso, A. G., Fiol, J. J., Marmorell, G., López-Zafra, A. & Quirós, M. (1997). *Polyhedron*, **16**, 613–621.

Shaw, C. F. (1999). *Chem. Rev.* **99**, 2589–2600.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.

Shin, H. S., Ihn, G. S., Kim, H. S. & Koo, C. H. (1975). *J. Korean Chem. Soc.* **18**, 329–340.

Yuan, R.-X., Xiong, R.-G., Chen, Z.-F., Zhang, P., Ju, H.-X., Dai, Z., Guo, Z.-J., Fun, H.-K. & You, X.-Z. (2001). *J. Chem. Soc. Dalton Trans.* pp. 774–776.