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# [4-Amino-*N*-(pyrimidin-2-yl)benzenesulfonamido-*κN*](triphenylarsine-*κ*As)gold(**I**)

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**Key indicators**

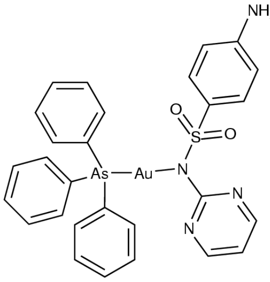
Single-crystal X-ray study
*T* = 173 K
Mean σ(C–C) = 0.003 Å
*R* factor = 0.018
*wR* factor = 0.043
Data-to-parameter ratio = 28.4

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

The title compound, [Au($C_{10}H_9N_4O_2S$)($C_{18}H_{15}As$)], is isostructural with the triphenylphosphine analog [Lang *et al.* (2003). *Acta Cryst.* C**59**, m95–m96]. The geometry is nearly linear at the Au$^I$ center, with Au—N = 2.0552 (15) Å, Au—As = 2.3266 (6) Å and N—Au—As = 171.56 (4)°. The molecules are joined by intermolecular N—H···O bonds between the amine and sulfonyl groups of the sulfadiazine ligand. The slightly shorter Au—N distance in the title compound compared to its triphenylphosphine analog is due to packing effects.

## Comment

Recently, we reported the preparation and structural characterization of [4-amino-*N*-(pyrimidin-2-yl)benzenesulfonamido-*κN*](tripheylphosphine-*κP*)gold(I), also known as (sulfadiazinato)(triphenylphosphine)gold(I) (Lang *et al.*, 2003). In this paper, we report the isostructural title compound, (I), also called (sulfadizinato)(triphenylarsine)gold(I). Compound (I) was obtained by the reaction of chloro(triphenylarsine)gold(I), sulfadiazine and triethylamine in methanol; recrystallization from dichloromethane and petroleum ether afforded single crystals. The asymmetric unit contains a complete molecule (Fig. 1) of the compound. Selected bond distances and angles are given in Table 1.



(I)

Compound (I) is almost identical to its triphenylphosphine isostructural counterpart. The Au atom shows weak interactions with atoms O1 and N16 of the sulfadiazinate ligand [distances 2.9926 (13) and 3.0863 (17) Å respectively]. The sulfadiazinate N atom bonded to Au shows trigonal planar geometry; the sum of the angles about atom N1 is 360. The sulfonamide group is approximately tetrahedral. The two ring systems in the sulfadiazinate ligand of (I) can be considered as being in a *cisoid* conformation, since the C1—S—N1—C11 torsion angle is approximately 90°. Atom O2 of the sulfonamide group participates in intermolecular hydrogen bonding to the amino group of a neighboring molecule, forming continuous chains along the *c* axis (Table 2 and Fig. 2).

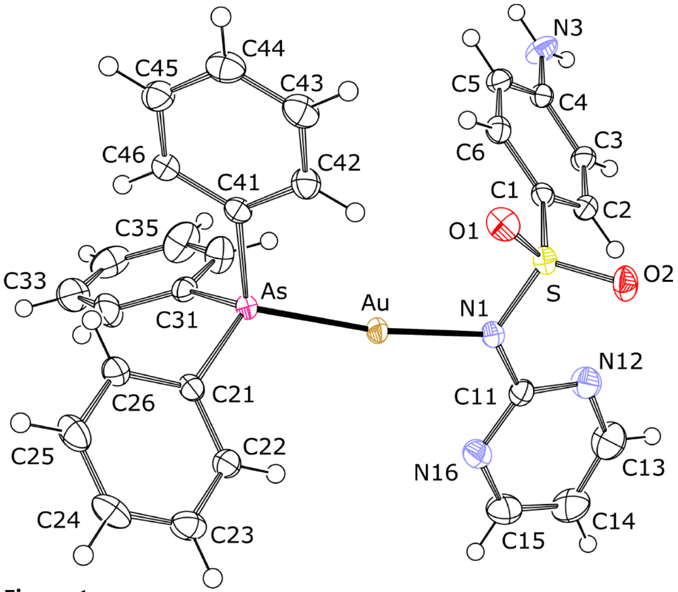


**Figure 1**
A view of the molecule of (I), with the atomic labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

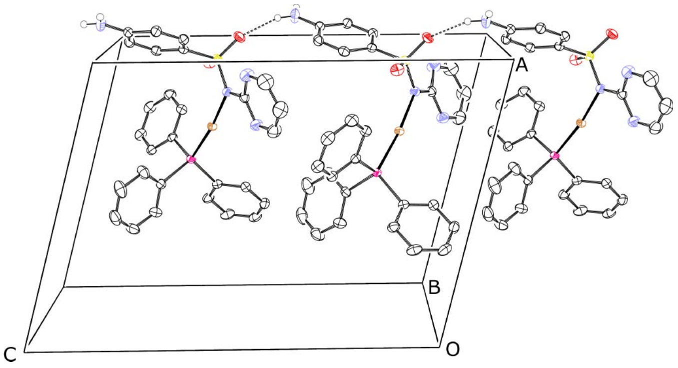


**Figure 2**
Packing diagram of (I), showing the hydrogen bonding with dashed lines. Colour codes: gold Au, pink As, yellow S, red O, blue N, black C and gray H.

The compound (I) has a slightly shorter N—Au distance than that seen in (sulfadiazinato)(triphenylphosphine)gold(I), which has an N—Au distance of 2.0707 (18) Å. As the triphenylarsine ligand is slightly more Lewis basic than the triphenylphosphine ligand (Aroney *et al.*, 1994), the *trans* influence predicts a longer Au—N bond length for the former compared to the latter (Jones & Williams, 1977). The shorter distance in this case is likely caused by the packing forces due to the slightly larger triphenylarsine ligand. This is also shown by the closer intermolecular hydrogen bond interaction between an H atom of the amine group and an O atom of the nitro group in the sufadiazinate ligand in (I). The H···O distance is 0.10 Å shorter in (I) than in the triphenylphosphine analog. The bond distances within the sulfadiazinate ligands of the two complexes are equivalent.

## Experimental

To a solution of chloro(triphenylarsine)gold(I) (0.1 mmol) in methanol (5 ml), a solution of sulfadiazine (0.1 mmol) in methanol (5 ml) and triethylamine (0.1 mmol) were added. The resulting mixture was stirred under reflux for 2 h and them cooled to room temperature, after which the precipitated solid was separated by filtration (yield 80%, 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 44.69/43.75, H 3.21/3.22, N 7.45/7.16%.

*Crystal data*

$[\mathrm{Au(C_{10}H_9N_4O_2S)(C_{18}H_{15}As)}]$
$M_r = 752.46$
Monoclinic, $P2_1/c$
$a = 12.0550$ (18) Å
$b = 13.360$ (2) Å
$c = 16.774$ (3) Å
$\beta = 104.46$ (3)°
$V = 2616.0$ (8) Å$^3$
$Z = 4$
$D_x = 1.911$ Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 1705 reflections
$\theta = 2.7$–26.9°
$\mu = 6.99$ mm$^{-1}$
$T = 173$ (2) K
Block, colorless
0.30 × 0.20 × 0.15 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.221$, $T_{\max} = 0.350$
35747 measured reflections
9482 independent reflections
8101 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.025$
$\theta_{\max} = 33.0$°
$h = -18 \rightarrow 17$
$k = -20 \rightarrow 20$
$l = -23 \rightarrow 25$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.018$
$wR(F^2) = 0.043$
$S = 1.00$
9482 reflections
334 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0236P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.004$
$\Delta\rho_{\max} = 1.03$ e Å$^{-3}$
$\Delta\rho_{\min} = -0.59$ e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Au—N1 | 2.0552 (15) | Au···O2 | 4.3238 (15) |
| Au—As | 2.3266 (6) | S—O1 | 1.4384 (13) |
| Au···N16 | 3.0863 (19) | S—O2 | 1.4417 (14) |
| Au—O1 | 2.9926 (16) | S—N1 | 1.6309 (16) |
| | | | |
| N1—Au—As | 171.56 (4) | O1—S—O2 | 117.35 (9) |
| N1—Au—O1 | 54.00 (5) | O1—S—N1 | 105.08 (8) |
| As—Au—O2 | 151.31 (2) | O2—S—N1 | 110.28 (8) |
| N16—Au—O2 | 66.83 (5) | | |
| C1—S—N1—C11 | −84.01 (16) | | |

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3*B*···O2$^{\rm i}$ | 0.88 | 2.08 | 2.931 (2) | 162 |

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

All H atoms were placed in calculated positions, with C—H distances of 0.95 Å and N—H distances of 0.88 Å. They were included in the refinement in the riding-model approximation, with $U_{\rm iso} = 1.2U_{\rm eq}$ of the carrier atom. The largest peak in the final difference Fourier map is located 0.75 Å from the Au atom.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve

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structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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