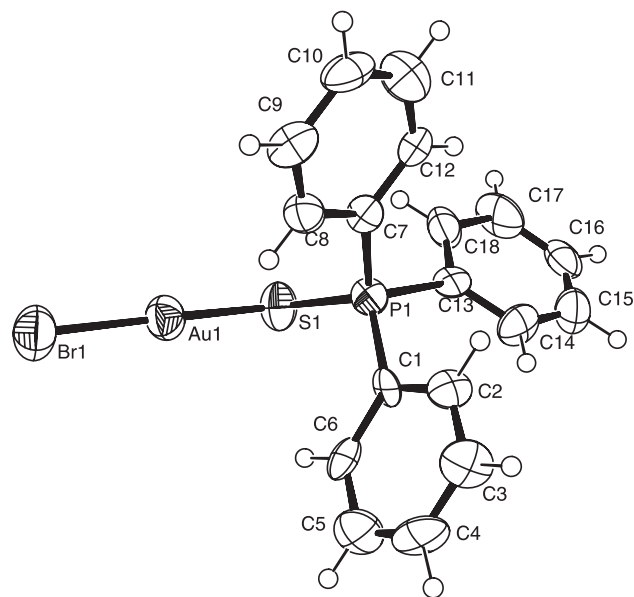


Crystal structure of bromotri(phenyl)phosphinesulphidegold(I), $(C_6H_5)_3PSAuBr$

M. S. Hussain*, A. A. Isab*, A. Saeed and A. R. Al-Arfaj

King Fahd University of Petroleum and Minerals, Department of Chemistry, Dhahran, 31261, Saudi Arabia

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Abstract

$C_{18}H_{15}AuBrPS$, monoclinic, $P12_1/n1$ (No. 14), $a = 12.420(5)$ Å, $b = 9.469(4)$ Å, $c = 15.080(7)$ Å, $\beta = 95.57(4)^\circ$, $V = 1765.1$ Å³, $Z = 4$, $R_{gt}(F) = 0.047$, $wR_{ref}(F^2) = 0.124$, $T = 302$ K.

Source of material

The title compound was prepared by mixing equimolar amounts of acetone solution of triphenylphosphinesulphide and aqueous solution of AuBr. The complex immediately precipitated upon mixing of the two solutions. Acetone was evaporated at room temperature and the complex was filtered and recrystallized from acetone to obtain light yellow crystals (mp 428 K – 429 K; yield 49%). The compound was characterized by elemental analysis, FTIR and ¹H- and ¹³C-NMR spectra.

Experimental details

A crystal of the complex was mounted on a glass fiber at room temperature with epoxy glue. Carbon-bound H atoms were placed at idealized positions with $d(C-H) = 0.96$ Å, $U(H) = 0.08$ Å² (riding). The H atom parameters were not refined.

Discussion

We recently reported the synthesis, X-ray structures and solution equilibria of cyanogold complexes of a series of phosphines $[R_3P]$ with $R =$ phenyl, cyclohexyl, and 2-cyanoethyl [1–3]. All trialkyl/arylphosphines studied so far form linear monomeric complexes with cyanogold except the ligand, tri(2-cyanoethyl)phosphine (CEP), which forms an ionic complex $[(CEP)_2Au][Au(CN)_2]$ [4]. When AuCN is replaced by AuBr [5] or by AuCl [6] even CEP forms linear species. A large formation constant [7] of $[Au(CN)_2]^-$, in addition to the unique electronic characteristics of CEP, are believed to cause ligand disproportionation of initially formed monomer $[(CEP)AuCN]$ which ultimately forms an ionic species. The coordination and crystallographic studies of gold complexes of different phosphine were undertaken because of their resemblance to several anti-arthritis drugs [8].

The figure shows the complex bromotri(phenyl)phosphinesulphidegold(I), $(phenyl)_3PSAuBr$, with labeling of the non-H atoms (displacement ellipsoids at 50% probability level; H atoms are drawn as circles of arbitrary radius).

In the title complex, the gold atom has linear coordination with $S1-Au1-Br1$ angle of $175.8(2)^\circ$, and $d(Au1-Br1) = 2.379(3)$ Å, $d(Au1-S1) = 2.285$ Å. In the corresponding selenide complex [9], the $Se1-Au1-Br1$ angle is $177.97(4)^\circ$ and $d(Au1-Br1) = 2.3843(9)$ Å, $d(Au1-Se1) = 2.3776(9)$ Å. In the corresponding $(phenyl)_3PSeAuCl$ [10], the Au—Se and Au—Cl bond distances are $2.371(2)$ Å and $2.277(6)$ Å, respectively. The P(1) atom in the title complex has the usual tetrahedral environment, as is the case with other phosphinogold complexes. The $P1-S1-Au1$ angle is $105.6(3)^\circ$.

Table 1. Data collection and handling.

Crystal:	light yellow rectangle, size $0.02 \times 0.08 \times 0.42$ mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ :	108.00 cm ⁻¹
Diffractometer, scan mode:	Siemens R3M, $\omega/2\theta$
$2\theta_{max}$:	50°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	3259, 3108
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 1774
$N(param)_{refined}$:	200
Programs:	SHELXS-86 [11], SHELXL-93 [12], DIFABS [13]

* Correspondence authors

(e-mail: sakhawat@kfupm.edu.sa and aisab@kfupm.edu.sa)