

Ahmed A. Mohamed,<sup>a</sup>  
Daniel Rabinovich<sup>b</sup> and  
John P. Fackler<sup>a\*</sup><sup>a</sup>Laboratory for Molecular Structure and Bonding, Department of Chemistry, Texas A & M University, PO Box 30012, College Station, Texas 77842-3012, USA, and <sup>b</sup>University of North Carolina at Charlotte, 9201 University City Boulevard, Charlotte, NC 28223-0001, USACorrespondence e-mail:  
fackler@mail.chem.tamu.edu

## Key indicators

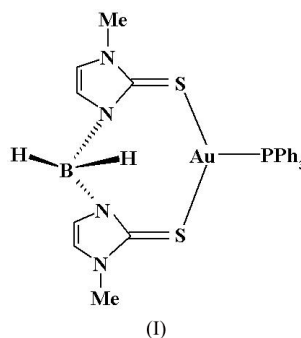
Single-crystal X-ray study  
T = 110 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.009 \text{ \AA}$   
R factor = 0.041  
wR factor = 0.110  
Data-to-parameter ratio = 20.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## [Bis(2-mercapto-1-methylimidazol-3-yl)-borato](triphenylphosphine)gold(I)

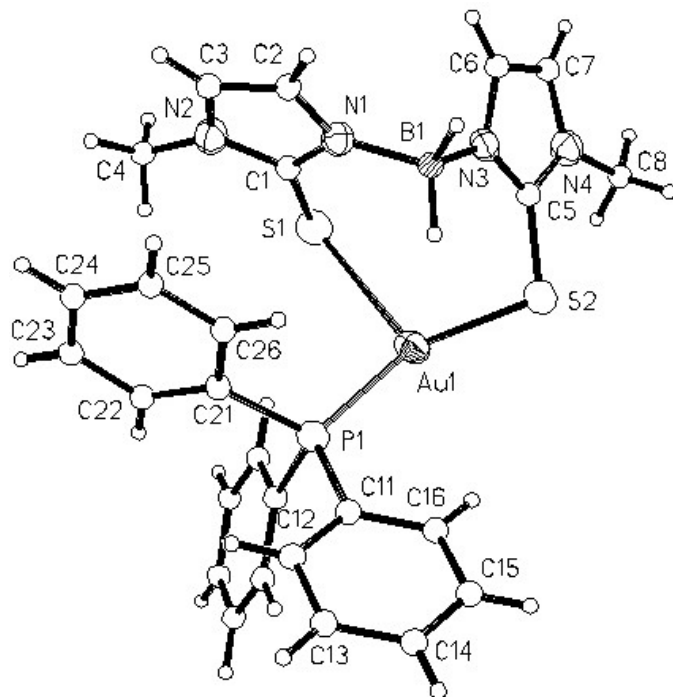
The Au atom in the title complex,  $[\text{Au}(\text{C}_8\text{H}_{12}\text{BN}_4\text{S}_2)(\text{C}_{18}\text{H}_{15}\text{P})]$ , is coordinated by two S (thione) atoms and one phosphine ligand in a distorted trigonal environment. The gold center is displaced by 0.048 (1) Å from the coordination mean plane. The Au–S<sub>thione</sub> distances are 2.3511 (8) and 2.8155 (12) Å, and the Au–P distance is 2.2557 (12) Å.

## Comment

The coordination chemistry of the nitrogen-donor poly(pyrazol-1-yl)borate ligands has been extensively investigated with various metals (Trofimenko, 1999; Parkin, 1995). Recently, the coordination of these ligands has been studied with coinage (group 11) metals (Santini *et al.*, 1998; Effendy *et al.*, 2000). Softer (sulfur) donor ligands were synthesized by the reaction of molten 2-thiol-1-methylimidazole (methimazole) with borohydride salts, to produce the hydrobis-(methimazolyl)borate anion (abbreviated Bm) (Kimblin *et al.*, 1997) or hydrotris(methimazolyl)borate anion (abbreviated Tm) (Garner *et al.*, 1996). Poly(methimazolyl)borate complexes were suggested to be models of enzymes (Kimblin *et al.*, 1997). Silver(I) complexes of Tm have been characterized, such as  $\text{Cy}_3\text{PAg}(\text{Tm})$  (Santini *et al.*, 1999). We report here the first gold complex, (I), of a poly(methimazolyl)borate ligand, bis(2-mercapto-1-methylimidazolyl)borate ( $\text{Bm}^{\text{Me}}$ ).



The unit cell of  $\text{Ph}_3\text{PAu}(\text{Bm}^{\text{Me}})$  contains four discrete symmetry-related molecules. The Au atom is coordinated in a distorted trigonal environment. The molecular structure is shown in Fig. 1, and selected bond distances and angles are given in Table 1. The P–Au–S angles are somewhat compressed [ $\text{S1}-\text{Au1}-\text{P1} = 98.78 (4)^\circ$ ] and somewhat enlarged [ $\text{P1}-\text{Au1}-\text{S2} = 159.74 (4)^\circ$ ]; the chelate angle at the Au atom,  $\text{S1}-\text{Au1}-\text{S2}$ , is  $101.15 (4)^\circ$ . The slight deviation of the sum of angles about the gold center from  $360^\circ$  is due to the displacement of Au1 by 0.048 (1) Å from the  $\text{AuS}_2\text{P}$  mean plane. The angles in the highly asymmetric eight-membered ring range from  $101.15 (4)^\circ$ , for  $\text{S1}-\text{Au1}-\text{S2}$ , to  $130.0 (4)^\circ$ , for  $\text{S2}-\text{C5}-\text{N3}$ .



**Figure 1**  
The molecular structure of (I). Displacement ellipsoids are shown at the 50% probability level for non-H atoms.

The Au—S<sub>thione</sub> distances are Au1—S1 = 2.8155 (12) Å and Au1—S2 = 2.3511 (12) Å. The C—S bond lengths of 1.707 (5) and 1.725 (5) Å are intermediate between single- and double-bond values. The Au—P distance, 2.2557 (12) Å, lies in the range observed for phosphine–gold complexes. The B atom is tetrahedrally coordinated. The thioimazolyl rings are approximately perpendicular to each other.

## Experimental

To a solution of bis(2-mercaptoimidazolyl)borate, Na[Bm<sup>Me</sup>], in dichloromethane (10 ml) was added Ph<sub>3</sub>PAuNO<sub>3</sub> (1:1 stoichiometric ratio), dissolved in dichloromethane (10 ml). The resulting mixture was stirred for 3 h and filtered to remove NaNO<sub>3</sub>. The solution was evaporated to 5 ml and ether was added to give an off-white precipitate. Block crystals were obtained by slow diffusion of ether into a dichloromethane solution of the title compound.

### Crystal data

[Au(C<sub>8</sub>H<sub>12</sub>BN<sub>4</sub>S<sub>2</sub>)(C<sub>18</sub>H<sub>15</sub>P)]  
*M<sub>r</sub>* = 698.38  
 Monoclinic, *P*<sub>2</sub><sub>1</sub>/*c*  
*a* = 20.7037 (12) Å  
*b* = 8.6870 (5) Å  
*c* = 15.2487 (9) Å  
 $\beta$  = 95.643 (1)°  
*V* = 2729.2 (3) Å<sup>3</sup>  
*Z* = 4

*D<sub>x</sub>* = 1.700 Mg m<sup>-3</sup>  
 Mo *K* $\alpha$  radiation  
 Cell parameters from 8187 reflections  
 $\theta$  = 2.0–28.3°  
 $\mu$  = 5.62 mm<sup>-1</sup>  
*T* = 110 (2) K  
 Block, colorless  
 0.29 × 0.13 × 0.13 mm

### Data collection

Bruker SMART area-detector diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Blessing, 1995)  
 $T_{\min}$  = 0.351,  $T_{\max}$  = 0.495  
 17546 measured reflections

6619 independent reflections  
 5410 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}}$  = 0.087  
 $\theta_{\text{max}}$  = 28.3°  
 $h$  = -26 → 26  
 $k$  = -11 → 11  
 $l$  = -20 → 20

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)]$  = 0.041  
 $wR(F^2)$  = 0.110  
 $S$  = 1.04  
 6619 reflections  
 319 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0604P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}}$  = 0.001  
 $\Delta\rho_{\text{max}}$  = 1.86 e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}}$  = -2.35 e Å<sup>-3</sup>  
 Extinction correction: SHELXL97  
 Extinction coefficient: 0.00132 (17)

**Table 1**

Selected geometric parameters (Å, °).

Au1—P1	2.2557 (12)	S2—C5	1.725 (5)
Au1—S2	2.3511 (12)	N1—B1	1.561 (6)
Au1—S1	2.8155 (13)	N3—B1	1.559 (7)
S1—C1	1.707 (5)		
P1—Au1—S2	159.74 (4)	S2—Au1—S1	101.15 (4)
P1—Au1—S1	98.78 (4)	N3—B1—N1	110.6 (4)

The maximum and minimum residual electron-density peaks in the final difference Fourier map were located at distances of 0.89 and 0.88 Å, respectively, from Au1.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1990); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Siemens, 1996); software used to prepare material for publication: SHELXL97.

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