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Key indicators

Single-crystal X-ray study

 $T = 295\text{ K}$ Mean $\sigma(\text{C}-\text{C}) = 0.008\text{ \AA}$ R factor = 0.030 wR factor = 0.079

Data-to-parameter ratio = 20.2

For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Bromo[(diphenylphosphino- κP)(diphenyl-
phosphinoyl)methane]gold(I) acetonitrile
solvate

In the title compound, $[\text{AuBr}(\text{dppmO})] \cdot \text{CH}_3\text{CN}$ [$\text{dppmO} = \text{Ph}_2\text{P}(\text{CH}_2)\text{P}(\text{O})\text{Ph}_2$], the dppmO ligand coordinates through the P donor to give a linear two-coordinate $\text{P}-\text{Au}-\text{Br}$ gold(I) complex. The $\text{Au}-\text{Br}$ and $\text{Au}-\text{P}$ bond lengths are $2.241(2)$ and $2.4069(19)\text{ \AA}$, respectively. The $\text{P}-\text{Au}-\text{Br}$ and $\text{P}=\text{O}$ groups lie almost parallel to each other [$\text{O}-\text{P} \cdots \text{P}-\text{Au} = 8.3(2)^\circ$], while the intramolecular $\text{Au} \cdots \text{O}$ distance is $3.274(4)\text{ \AA}$.

Comment

Mixed bidentate phosphine-phosphine oxide ligands of general formula $\text{R}_2\text{P}-\text{Y}-\text{P}(\text{O})\text{R}_2$, where Y is an organic spacer group, represent an important class of bidentate chelating ligands incorporating both soft (P) and hard (O) donor atoms (Grushin, 2001). Transition metal complexes of these ligands show a variety of structural forms (*e.g.* Coyle *et al.*, 1998; Saravanabharathi *et al.*, 2002; Faller & Parr, 2000) with evidence for both bidentate and monodentate coordination of the ligand to the metal atom.

We report here the structure of the acetonitrile solvate of the 1:1 complex of $\text{Ph}_2\text{P}(\text{CH}_2)\text{P}(\text{O})\text{Ph}_2$ with gold(I) bromide, $[(\text{dppmO})\text{AuBr}] \cdot \text{CH}_3\text{CN}$, (I). The structure comprises discrete molecules of $[(\text{dppmO})\text{AuBr}]$ and acetonitrile separated by normal van der Waals distances (Fig. 1). The dppmO ligand coordinates to the gold through the P atom to yield a linear two-coordinate $\text{P}-\text{Au}-\text{Br}$ geometry, with $\text{Au}-\text{P} = 2.241(2)\text{ \AA}$, $\text{Au}-\text{Br} = 2.4069(19)\text{ \AA}$ and $\text{P}-\text{Au}-\text{Br} = 178.53(4)^\circ$. These parameters are similar to those recorded for other two-coordinate R_3PAuBr complexes (Bott *et al.*, 2000). The $\text{P}=\text{O}$ bond length of $1.490(3)\text{ \AA}$ is also in accord with values recorded for other phosphine oxides (See *et al.*, 1998).

The $\text{P}-\text{Au}-\text{Br}$ and $\text{P}=\text{O}$ groups lie almost parallel, with the torsion angle $\text{O}-\text{P} \cdots \text{P}-\text{Au}$ $8.3(2)^\circ$. For comparison, in the structure of the benzene solvate of the dioxide, dppmO_2 (Antipin *et al.*, 1980), the $\text{P}=\text{O}$ bonds are almost antiparallel, whereas in the structures of adducts of dppmO_2 with sodium halides (Hewertson *et al.*, 1970; Ding *et al.*, 2000) coordination of the O atoms to the sodium cation results in parallel $\text{P}=\text{O}$ bonds and an $\text{Na} \cdots \text{O}$ distance of $2.457(1)\text{ \AA}$. An intermediate situation is observed for the structure of the 2:1 gold chloride

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