

Dichlorobis[(diphenylphosphinoethyl- $\kappa$ P)diphenylphosphine oxide]digold(I)(Au—Au) monohydrateZai-Lai Xie<sup>a,b</sup> and Zhong-Ning Chen<sup>a\*</sup><sup>a</sup>State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Fuzhou, Fujian 350002, People's Republic of China, and <sup>b</sup>Graduate School of the Chinese Academy of Sciences, Beijing 100039, People's Republic of ChinaCorrespondence e-mail:  
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## Key indicators

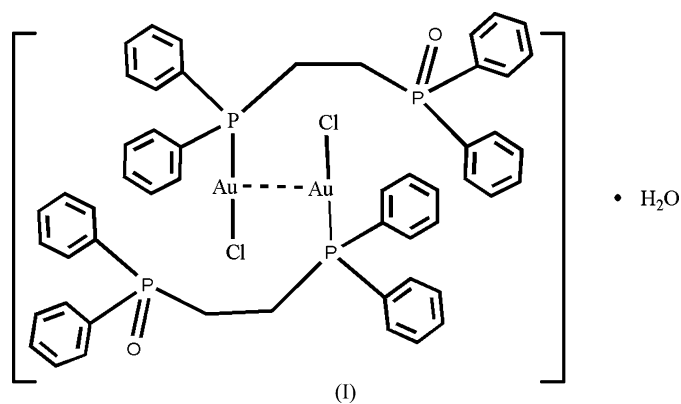
Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.011$  Å  
 $R$  factor = 0.043  
 $wR$  factor = 0.114  
Data-to-parameter ratio = 18.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the title compound,  $[\text{Au}_2\text{Cl}_2(\text{dppeo})_2] \cdot \text{H}_2\text{O}$ , where dppeo is (diphenylphosphinoethyl)diphenylphosphine oxide ( $\text{C}_{26}\text{H}_{24}\text{OP}_2$ ), each  $\text{Au}^{\text{I}}$  center is two-coordinated by Cl and P donors and exhibits an approximately linear arrangement. The dppeo ligand adopts a monodentate bonding mode.

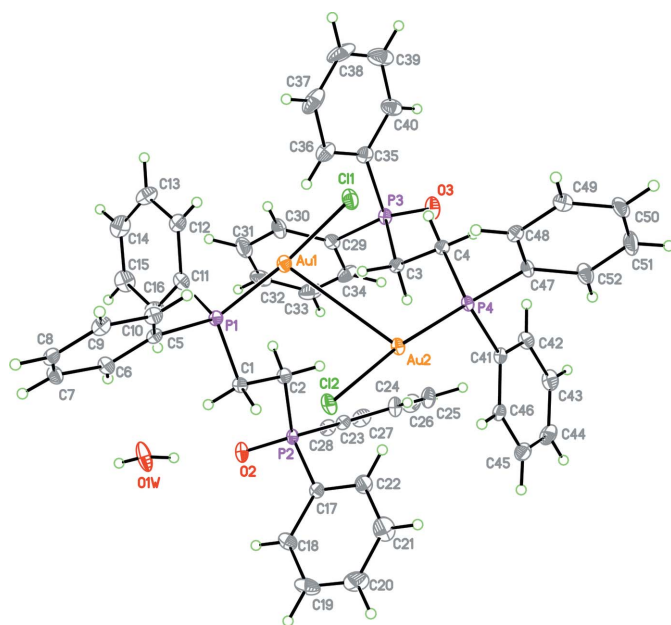
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## Comment

Binuclear complexes of gold with certain bidentate ligands are of great interest due to their rich luminescence and bonding properties. Several compounds of binuclear  $[\text{Au}_2(\mu\text{-dppm})_2]^{2+}$  dications [dppm is (diphenylphosphino)methane], counterbalanced by various anionic species, have been reported previously (Eggleston *et al.*, 1985; Bates & Wates, 1985). We report here the crystal structure of the title compound, (I), a binuclear complex of gold with the (diphenylphosphinoethyl)diphenylphosphine oxide (dppeo) ligand exhibiting a monodentate bonding mode.



The asymmetric unit of (I) consists of a  $[(\text{AuCl})_2(\text{dppeo})_2]$  complex and a water molecule. The structure of (I) with atomic numbering scheme is shown in Fig. 1. Selected bond lengths and angles are given in Table 1. The binuclear gold(I) array is ligand-unsupported. The two Au atoms are connected by an Au—Au interaction. The intramolecular Au—Au distance is 3.2170 (4) Å, which is longer than that observed in the gold complex  $[\text{Au}_2(\text{dppdiene})\text{Cl}_2]$  (dppdiene is 2,3-bis(bisphenylphosphino)-1,3-butadiene) [3.023 (1) Å; Schmidbaur *et al.*, 1989]. Each  $\text{Au}^{\text{I}}$  center is two-coordinated with Cl and P donors to exhibit an approximately linear geometry, the P—Au—Cl angles being 174.50 (5) and 172.65 (5)°. The Au—P distances are in agreement with those observed in  $[\text{Au}_2(\mu\text{-dppe})_2(\text{Cl})_2]$ , where dppe is (diphenylphosphino)ethane [2.231 (3) Å; Eggleston *et al.*, 1985]. The dppeo ligand adopts a monodentate bonding mode instead of the bridging or



**Figure 1**  
A drawing of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

bidentate chelating mode found for dppe.

The crystal packing is stabilized by O—H...O, C—H...O and C—H...Cl hydrogen bonds (Table 2) and C—H... $\pi$  interactions involving the C29—C34 phenyl ring (centroid Cg1).

## Experimental

Compound (I) was synthesized by modification of procedures reported by Schmidbaur *et al.* (1989) and Dziwok *et al.* (1990). It was unexpectedly obtained by the reaction of (diphenylphosphino)ethane with  $(\text{AuC}\equiv\text{CCH}_2)_4\text{C}_8\text{H}_{16}\text{N}_4$  [a gold complex with *N,N,N',N''*-tetra-(4-prop-1-yne)-1,4,7,10-tetraazacyclononane] in a 1:2 ratio in dichloromethane (30 ml) for 30 min. Prism-shaped white crystals suitable for X-ray diffraction measurements were grown by the slow diffusion of hexane into a dichloromethane solution at room temperature.

### Crystal data

$[\text{Au}_2\text{Cl}_2(\text{C}_{26}\text{H}_{24}\text{OP}_2)_2]\cdot\text{H}_2\text{O}$   
 $M_r = 1311.63$   
 Triclinic,  $P\bar{1}$   
 $a = 11.4510$  (3) Å  
 $b = 12.9718$  (4) Å  
 $c = 18.6903$  (5) Å  
 $\alpha = 86.052$  (7)°  
 $\beta = 77.064$  (6)°  
 $\gamma = 65.352$  (4)°

$V = 2458.33$  (16) Å<sup>3</sup>  
 $Z = 2$   
 $D_x = 1.772$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 6.24$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Prism, white  
 0.20 × 0.20 × 0.10 mm

### Data collection

Rigaku Mercury70 diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2000)  
 $T_{\min} = 0.368$ ,  $T_{\max} = 0.574$   
 (expected range = 0.344–0.536)

18239 measured reflections  
 10548 independent reflections  
 8728 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.043$   
 $\theta_{\text{max}} = 27.0^\circ$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.043$   
 $wR(F^2) = 0.114$   
 $S = 1.00$   
 10548 reflections  
 568 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0625P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 2.94 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -4.46 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters (Å, °).

|             |             |             |             |
|-------------|-------------|-------------|-------------|
| Au1—P1      | 2.2475 (14) | Au2—P4      | 2.2416 (13) |
| Au1—Cl1     | 2.3018 (14) | Au2—Cl2     | 2.3030 (13) |
| Au1—Au2     | 3.2170 (4)  |             |             |
| P1—Au1—Cl1  | 174.50 (5)  | P4—Au2—Cl2  | 172.65 (5)  |
| P1—Au1—Au2  | 106.71 (4)  | P4—Au2—Au1  | 107.54 (4)  |
| Cl1—Au1—Au2 | 78.61 (4)   | Cl2—Au2—Au1 | 79.13 (4)   |

**Table 2**

Hydrogen-bond geometry (Å, °).

| <i>D</i> —H... <i>A</i>    | <i>D</i> —H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> —H... <i>A</i> |
|----------------------------|-------------|---------------|-----------------------|-------------------------|
| O1W—H1WA...O3 <sup>i</sup> | 0.82        | 1.90          | 2.683 (6)             | 160                     |
| O1W—H1WB...O2              | 0.82        | 1.88          | 2.694 (6)             | 173                     |
| C1—H1B...O1W               | 0.97        | 2.33          | 3.292 (7)             | 171                     |
| C4—H4B...O1W <sup>ii</sup> | 0.97        | 2.32          | 3.272 (7)             | 169                     |
| C9—H9...Cl2 <sup>iii</sup> | 0.93        | 2.83          | 3.580 (6)             | 139                     |
| C26—H26...O3 <sup>iv</sup> | 0.93        | 2.38          | 3.251 (8)             | 155                     |
| C13—H13...Cg1 <sup>v</sup> | 0.93        | 2.83          | 3.561 (9)             | 137                     |

Symmetry codes: (i)  $x - 1, y, z$ ; (ii)  $x + 1, y, z$ ; (iii)  $-x, -y + 1, -z + 1$ ; (iv)  $-x + 2, -y, -z$ ; (v)  $-x + 1, -y + 1, -z$ .

H atoms were positioned geometrically, with C—H = 0.93 and 0.97 Å for aromatic and methylene H atoms, respectively, and O—H = 0.82 Å, and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  and  $1.2U_{\text{eq}}(\text{O})$ . The highest residual density peak is located 0.86 Å from atom Au2 and the deepest hole is located 0.87 Å from atom Au1.

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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