

$[\mu\text{-}1,2\text{-Bis(diphenylphosphanyl)benzene-}\kappa^2\text{P:P}']\text{bis[chloridogold(I)]}$

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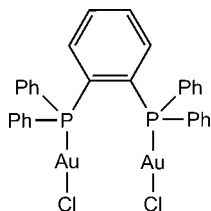
Received 13 December 2010; accepted 16 December 2010

Key indicators: single-crystal X-ray study; $T = 200$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.023; wR factor = 0.041; data-to-parameter ratio = 19.8.

In the crystal structure of the non-solvate form of the title compound, $[\text{Au}_2\text{Cl}_2(\text{C}_{30}\text{H}_{24}\text{P}_2)]$, two almost linear $\text{P}-\text{Au}^{\text{I}}-\text{Cl}$ units [175.87 (3) and 171.48 (3) $^\circ$] are in a skewed arrangement with a $\text{Cl}-\text{Au}\cdots\text{Au}-\text{Cl}$ torsion angle of -65.29 (3) $^\circ$ so as to form an intramolecular $\text{Au}\cdots\text{Au}$ interaction [3.0563 (2) Å]. The complex molecules are connected each other through intermolecular $\text{C}-\text{H}\cdots\pi$ interactions, giving a sheet structure parallel to the bc plane.

Related literature

For the crystal structure of the diethylether solvate form of the title compound, $[(\text{AuCl})_2(\text{C}_{30}\text{H}_{24}\text{P}_2)]\cdot(\text{C}_2\text{H}_5)_2\text{O}$, see: Mohamed *et al.* (2003). For closely related structures, see: Hashimoto *et al.* (2010).



Experimental

Crystal data

$[\text{Au}_2\text{Cl}_2(\text{C}_{30}\text{H}_{24}\text{P}_2)]$

$M_r = 911.27$

Monoclinic, $P2_1/c$

$a = 13.0733$ (2) Å

$b = 12.4206$ (2) Å

$c = 17.4630$ (3) Å

$\beta = 96.795$ (7) $^\circ$

$V = 2815.69$ (8) Å³

$Z = 4$

Mo $K\alpha$ radiation

$\mu = 10.73$ mm⁻¹

$T = 200$ K

$0.15 \times 0.10 \times 0.10$ mm

Data collection

Rigaku R-AXIS VII diffractometer

Absorption correction: multi-scan

(*ABSCOR*; Higashi, 1995)

$T_{\text{min}} = 0.189$, $T_{\text{max}} = 0.341$

31710 measured reflections

6438 independent reflections

5897 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.030$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.023$

$wR(F^2) = 0.041$

$S = 1.16$

6438 reflections

325 parameters

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.54$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.80$ e Å⁻³

Table 1

Selected bond lengths (Å).

| | | | |
|---------|------------|---------|------------|
| Au1—P1 | 2.2256 (8) | Au2—P2 | 2.2279 (7) |
| Au1—Cl1 | 2.2739 (8) | Au2—Cl2 | 2.2792 (8) |

Table 2

Hydrogen-bond geometry (Å, $^\circ$).

C_g is the centroid of the $\text{C}25\text{--C}30$ ring.

| $D\text{--}H\cdots A$ | $D\text{--}H$ | $H\cdots A$ | $D\cdots A$ | $D\text{--}H\cdots A$ |
|---|---------------|-------------|-------------|-----------------------|
| $\text{C}15\text{--}H15\cdots C_g^i$ | 0.95 | 2.82 | 3.569 (4) | 137 |
| $\text{C}21\text{--}H21\cdots C_g^{ii}$ | 0.95 | 2.84 | 3.559 (4) | 134 |

Symmetry codes: (i) $x, -y + \frac{3}{2}, z - \frac{1}{2}$; (ii) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *Yadokari-XG 2009* (Kabuto *et al.*, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2006) and *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *Yadokari-XG 2009* and *pubCIF* (Westrip, 2010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2645).

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supplementary materials

Acta Cryst. (2011). E67, m121 [doi:10.1107/S1600536810052803]

[μ -1,2-Bis(diphenylphosphanyl)benzene- $\kappa^2 P:P'$]bis[chloridogold(I)]

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Comment

[(AuCl)₂(diphosphine)]-type digold(I) complexes have been known as a good starting material to produce [(AuL)₂(diphosphine)]-type digold(I) metallounits. Recently, we found that a digold(I) complex, [{Au(D-Hpen)}₂(dppm)] (D-pen = D-penicillamate, dppm = 1,2-bis(diphenylphosphino)methane), which was prepared from [(AuCl)₂(dppm)] and D-pen, can act as a hexadentate-S₂N₂O₂ metalloligand toward a Ni^{II} center to give a unique trinuclear Ni^{II}Au^I₂ complex with a nine-membered metalloring, [NiAu₂(D-pen)₂(dppm)] (Hashimoto *et al.*, 2010). In the course of our study on a digold(I) metalloligand system having both D-pen and diphosphines, we started to use [(AuCl)₂(dppbz)] (dppbz = *o*-phenylenebis(diphenylphosphine)) instead of [(AuCl)₂(dppm)]. Herein, we report the crystal structure of the non-solvate form of [(AuCl)₂(dppbz)] (I). The crystal structure of the diethylether solvate form of the title compound, [(AuCl)₂(dppbz)].Et₂O (II), has been reported by Mohamed *et al.* (2003).

The asymmetric unit of (I) contains only a complex molecule without a significant solvent accessible space, which is distinct from the solvated structure of (II) (Mohamed *et al.*, 2003). The complex molecule is composed of two [Au^ICl] units that are linked by a dppbz ligand through Au—P bonds, forming a digold(I) structure in [(AuCl)₂(dppbz)] (Fig. 1). In (I), two approximately linear P—Au^I—Cl units are skewed each other so as to form an intramolecular Au^I⋯Au^I interaction. This conformational feature is the same as that in (II). In the crystal (I), the Au^I⋯Au^I distance [3.05634 (17) Å] is longer than that in (II) [2.966 (1) Å], and the Cl—Au^I⋯Au^I—Cl torsion angle [−65.29 (3)°] is larger than that in (II) [−63.92 (7)°]. The other bond distances and angles in (I) are similar to those in (II).

The crystal structure of (I) is stabilized by several intermolecular C—H⋯ π interactions. Each complex molecule is connected with four adjacent molecules through a C—H⋯ π interaction [H15⋯Cgⁱ = 2.82 Å and H21⋯Cgⁱⁱ = 2.84 Å; symmetry codes: (i) *x*, 3/2−*y*, −1/2 + *z*, (ii) 1−*x*, −1/2 + *y*, 1/2−*z*]; Cg is the centroid of the C25–C30 ring] to construct a two-dimensional sheet structure (Fig. 2). Such an intermolecular C—H⋯ π interaction has not been observed in (II).

Experimental

To a solution containing tetrahydrothiophenechlorogold(I) (100 mg, 0.32 mmol) in 10 ml of CH₂Cl₂ was added *o*-phenylenebis(diphenylphosphine) (140 mg, 0.31 mmol). After stirring for 20 minutes, 100 ml of diethylether was added to the reaction solution. The resulting white powder was recrystallized from CH₂Cl₂ by diffusing diethylether, which afforded colorless block crystals of (I).

Refinement

H atoms were placed at calculated positions and refined with isotropic displacement parameters [*U*_{iso}(H) = 1.2*U*_{eq}(C)] and a riding model (C—H = 0.95 Å).

Figures

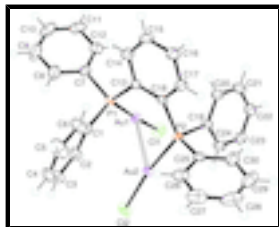


Fig. 1. A view of molecular structure of the title compound, showing the atom-numbering scheme and 50% probability displacement ellipsoids.

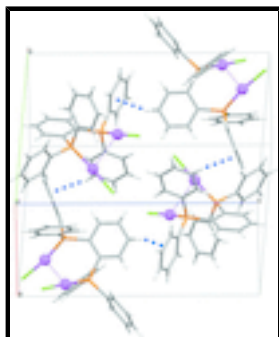


Fig. 2. A crystal packing drawing of the title compound. The blue lines indicate C—H... π interactions.

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Crystal data

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Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 13.0733$ (2) Å

$b = 12.4206$ (2) Å

$c = 17.4630$ (3) Å

$\beta = 96.795$ (7)°

$V = 2815.69$ (8) Å³

$Z = 4$

$F(000) = 1704$

$D_x = 2.150$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å

Cell parameters from 24394 reflections

$\theta = 3.1$ – 27.5 °

$\mu = 10.73$ mm⁻¹

$T = 200$ K

Block, white

$0.15 \times 0.10 \times 0.10$ mm

Data collection

Rigaku R-Axis VII
diffractometer

Radiation source: fine-focus sealed tube
graphite

Detector resolution: 10.000 pixels mm⁻¹

ω scans

Absorption correction: multi-scan
(*ABSCOR*; Higashi, 1995)

$T_{\min} = 0.189$, $T_{\max} = 0.341$

31710 measured reflections

6438 independent reflections

5897 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.030$

$\theta_{\max} = 27.5$ °, $\theta_{\min} = 3.1$ °

$h = -16 \rightarrow 16$

$k = -15 \rightarrow 16$

$l = -22 \rightarrow 22$

Refinement

| | |
|---------------------------------|--|
| Refinement on F^2 | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.023$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.041$ | H-atom parameters constrained |
| $S = 1.16$ | $w = 1/[\sigma^2(F_o^2) + (0.0112P)^2 + 2.7453P]$ |
| 6438 reflections | where $P = (F_o^2 + 2F_c^2)/3$ |
| 325 parameters | $(\Delta/\sigma)_{\max} = 0.002$ |
| 0 restraints | $\Delta\rho_{\max} = 0.54 \text{ e } \text{\AA}^{-3}$ |
| | $\Delta\rho_{\min} = -0.80 \text{ e } \text{\AA}^{-3}$ |

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|--------------|----------------------------------|
| Au1 | 0.283249 (9) | 0.406709 (9) | 0.296038 (6) | 0.02169 (4) |
| Au2 | 0.229077 (9) | 0.602225 (9) | 0.389584 (6) | 0.02065 (4) |
| Cl1 | 0.38861 (7) | 0.31036 (7) | 0.38364 (5) | 0.0385 (2) |
| Cl2 | 0.13663 (7) | 0.53399 (7) | 0.48118 (5) | 0.0371 (2) |
| P1 | 0.18427 (6) | 0.49382 (6) | 0.20367 (4) | 0.01918 (16) |
| P2 | 0.33234 (6) | 0.68257 (6) | 0.31436 (4) | 0.01836 (16) |
| C1 | 0.0679 (2) | 0.5541 (2) | 0.23080 (17) | 0.0234 (7) |
| C2 | 0.0205 (3) | 0.5115 (3) | 0.29040 (19) | 0.0340 (8) |
| H2 | 0.0486 | 0.4490 | 0.3164 | 0.041* |
| C3 | -0.0664 (3) | 0.5576 (3) | 0.3129 (2) | 0.0444 (10) |
| H3 | -0.0972 | 0.5282 | 0.3548 | 0.053* |
| C4 | -0.1088 (3) | 0.6462 (3) | 0.2748 (2) | 0.0444 (10) |
| H4 | -0.1690 | 0.6783 | 0.2904 | 0.053* |
| C5 | -0.0643 (3) | 0.6886 (3) | 0.2142 (3) | 0.0523 (11) |
| H5 | -0.0945 | 0.7492 | 0.1872 | 0.063* |
| C6 | 0.0241 (3) | 0.6436 (3) | 0.1923 (2) | 0.0379 (9) |
| H6 | 0.0550 | 0.6738 | 0.1507 | 0.045* |
| C7 | 0.1435 (2) | 0.4040 (2) | 0.12379 (17) | 0.0236 (7) |

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| | | | | |
|-----|------------|------------|--------------|-------------|
| C8 | 0.0401 (3) | 0.3877 (3) | 0.0987 (2) | 0.0380 (9) |
| H8 | -0.0107 | 0.4299 | 0.1194 | 0.046* |
| C9 | 0.0104 (3) | 0.3101 (3) | 0.0436 (2) | 0.0502 (10) |
| H9 | -0.0606 | 0.2972 | 0.0279 | 0.060* |
| C10 | 0.0833 (3) | 0.2523 (3) | 0.0118 (2) | 0.0463 (10) |
| H10 | 0.0626 | 0.2002 | -0.0267 | 0.056* |
| C11 | 0.1864 (3) | 0.2685 (3) | 0.03467 (19) | 0.0402 (9) |
| H11 | 0.2365 | 0.2285 | 0.0115 | 0.048* |
| C12 | 0.2168 (3) | 0.3431 (3) | 0.09162 (19) | 0.0328 (8) |
| H12 | 0.2879 | 0.3527 | 0.1088 | 0.039* |
| C13 | 0.2511 (2) | 0.6058 (2) | 0.16336 (17) | 0.0197 (6) |
| C14 | 0.2447 (3) | 0.6146 (2) | 0.08372 (18) | 0.0280 (7) |
| H14 | 0.2084 | 0.5613 | 0.0523 | 0.034* |
| C15 | 0.2902 (3) | 0.6993 (3) | 0.04926 (17) | 0.0306 (7) |
| H15 | 0.2860 | 0.7031 | -0.0053 | 0.037* |
| C16 | 0.3408 (3) | 0.7769 (3) | 0.09325 (17) | 0.0311 (8) |
| H16 | 0.3711 | 0.8358 | 0.0695 | 0.037* |
| C17 | 0.3483 (2) | 0.7703 (2) | 0.17310 (17) | 0.0269 (7) |
| H17 | 0.3840 | 0.8250 | 0.2035 | 0.032* |
| C18 | 0.3046 (2) | 0.6855 (2) | 0.20917 (16) | 0.0202 (6) |
| C19 | 0.4619 (2) | 0.6301 (2) | 0.33296 (16) | 0.0209 (6) |
| C20 | 0.5251 (3) | 0.6146 (3) | 0.27570 (18) | 0.0305 (7) |
| H20 | 0.5006 | 0.6304 | 0.2235 | 0.037* |
| C21 | 0.6239 (3) | 0.5762 (3) | 0.2947 (2) | 0.0399 (9) |
| H21 | 0.6671 | 0.5651 | 0.2553 | 0.048* |
| C22 | 0.6606 (3) | 0.5538 (3) | 0.37001 (19) | 0.0325 (8) |
| H22 | 0.7287 | 0.5276 | 0.3826 | 0.039* |
| C23 | 0.5983 (3) | 0.5693 (3) | 0.42694 (19) | 0.0298 (7) |
| H23 | 0.6237 | 0.5544 | 0.4791 | 0.036* |
| C24 | 0.4994 (2) | 0.6062 (2) | 0.40878 (18) | 0.0271 (7) |
| H24 | 0.4563 | 0.6156 | 0.4484 | 0.032* |
| C25 | 0.3414 (2) | 0.8233 (2) | 0.34357 (16) | 0.0216 (6) |
| C26 | 0.2503 (3) | 0.8795 (3) | 0.34737 (19) | 0.0321 (8) |
| H26 | 0.1862 | 0.8474 | 0.3287 | 0.039* |
| C27 | 0.2528 (3) | 0.9822 (3) | 0.3782 (2) | 0.0422 (9) |
| H27 | 0.1904 | 1.0207 | 0.3805 | 0.051* |
| C28 | 0.3447 (4) | 1.0283 (3) | 0.4055 (2) | 0.0490 (11) |
| H28 | 0.3458 | 1.0983 | 0.4275 | 0.059* |
| C29 | 0.4353 (4) | 0.9744 (3) | 0.4013 (2) | 0.0462 (10) |
| H29 | 0.4990 | 1.0076 | 0.4195 | 0.055* |
| C30 | 0.4338 (3) | 0.8710 (3) | 0.37043 (19) | 0.0339 (8) |
| H30 | 0.4965 | 0.8334 | 0.3679 | 0.041* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|-------------|-------------|
| Au1 | 0.02405 (7) | 0.02000 (6) | 0.02113 (6) | -0.00025 (5) | 0.00320 (5) | 0.00152 (4) |
| Au2 | 0.02083 (7) | 0.02433 (7) | 0.01768 (6) | -0.00245 (5) | 0.00596 (5) | 0.00182 (4) |

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C11 | 0.0439 (5) | 0.0344 (5) | 0.0352 (5) | 0.0106 (4) | -0.0034 (4) | 0.0077 (4) |
| C12 | 0.0305 (4) | 0.0520 (5) | 0.0309 (4) | -0.0058 (4) | 0.0116 (4) | 0.0160 (4) |
| P1 | 0.0189 (4) | 0.0204 (4) | 0.0184 (4) | -0.0017 (3) | 0.0030 (3) | -0.0002 (3) |
| P2 | 0.0203 (4) | 0.0216 (4) | 0.0138 (4) | -0.0025 (3) | 0.0045 (3) | -0.0004 (3) |
| C1 | 0.0204 (16) | 0.0254 (16) | 0.0246 (16) | -0.0056 (13) | 0.0039 (13) | -0.0075 (12) |
| C2 | 0.0252 (18) | 0.046 (2) | 0.0313 (19) | -0.0061 (16) | 0.0074 (15) | 0.0009 (15) |
| C3 | 0.030 (2) | 0.069 (3) | 0.038 (2) | -0.0064 (19) | 0.0160 (17) | -0.0050 (19) |
| C4 | 0.028 (2) | 0.048 (2) | 0.061 (3) | -0.0017 (18) | 0.0181 (19) | -0.025 (2) |
| C5 | 0.041 (2) | 0.029 (2) | 0.090 (3) | 0.0116 (18) | 0.022 (2) | -0.004 (2) |
| C6 | 0.036 (2) | 0.0316 (19) | 0.048 (2) | 0.0066 (16) | 0.0167 (18) | 0.0031 (16) |
| C7 | 0.0255 (17) | 0.0236 (16) | 0.0214 (16) | -0.0004 (13) | 0.0015 (13) | 0.0007 (12) |
| C8 | 0.0298 (19) | 0.037 (2) | 0.046 (2) | 0.0058 (16) | -0.0034 (17) | -0.0149 (16) |
| C9 | 0.041 (2) | 0.052 (2) | 0.053 (3) | -0.003 (2) | -0.0140 (19) | -0.019 (2) |
| C10 | 0.067 (3) | 0.034 (2) | 0.035 (2) | 0.0033 (19) | -0.010 (2) | -0.0139 (16) |
| C11 | 0.058 (3) | 0.0335 (19) | 0.0293 (19) | 0.0136 (18) | 0.0077 (18) | -0.0084 (15) |
| C12 | 0.032 (2) | 0.0336 (18) | 0.0331 (19) | 0.0030 (15) | 0.0070 (15) | -0.0048 (14) |
| C13 | 0.0181 (15) | 0.0222 (15) | 0.0190 (15) | 0.0019 (12) | 0.0030 (12) | 0.0018 (11) |
| C14 | 0.0326 (18) | 0.0284 (17) | 0.0222 (16) | -0.0012 (14) | 0.0000 (14) | 0.0000 (13) |
| C15 | 0.042 (2) | 0.0367 (18) | 0.0139 (15) | -0.0024 (16) | 0.0064 (14) | 0.0026 (13) |
| C16 | 0.041 (2) | 0.0308 (18) | 0.0217 (16) | -0.0092 (15) | 0.0065 (15) | 0.0051 (13) |
| C17 | 0.0331 (19) | 0.0278 (17) | 0.0198 (15) | -0.0072 (14) | 0.0028 (14) | -0.0021 (12) |
| C18 | 0.0191 (15) | 0.0271 (16) | 0.0148 (14) | -0.0009 (12) | 0.0032 (12) | 0.0011 (11) |
| C19 | 0.0217 (16) | 0.0222 (15) | 0.0194 (15) | -0.0022 (12) | 0.0050 (12) | -0.0005 (11) |
| C20 | 0.0272 (18) | 0.046 (2) | 0.0187 (16) | 0.0034 (15) | 0.0047 (14) | -0.0029 (14) |
| C21 | 0.0284 (19) | 0.065 (2) | 0.0280 (19) | 0.0073 (18) | 0.0101 (16) | -0.0085 (17) |
| C22 | 0.0213 (17) | 0.0395 (19) | 0.036 (2) | 0.0058 (15) | 0.0017 (15) | -0.0024 (15) |
| C23 | 0.0304 (19) | 0.0355 (18) | 0.0228 (17) | 0.0012 (15) | 0.0004 (14) | 0.0043 (13) |
| C24 | 0.0256 (17) | 0.0354 (18) | 0.0212 (16) | 0.0027 (14) | 0.0072 (13) | 0.0015 (13) |
| C25 | 0.0299 (17) | 0.0228 (15) | 0.0131 (14) | -0.0030 (13) | 0.0068 (13) | 0.0013 (11) |
| C26 | 0.043 (2) | 0.0284 (17) | 0.0262 (17) | 0.0031 (16) | 0.0101 (16) | 0.0053 (13) |
| C27 | 0.066 (3) | 0.0287 (19) | 0.035 (2) | 0.0113 (19) | 0.0192 (19) | 0.0077 (15) |
| C28 | 0.097 (4) | 0.0248 (18) | 0.0281 (19) | -0.001 (2) | 0.019 (2) | -0.0004 (15) |
| C29 | 0.074 (3) | 0.033 (2) | 0.030 (2) | -0.021 (2) | 0.0001 (19) | -0.0035 (15) |
| C30 | 0.041 (2) | 0.0309 (18) | 0.0297 (18) | -0.0079 (16) | 0.0021 (16) | -0.0017 (14) |

Geometric parameters (Å, °)

| | | | |
|---------|--------------|---------|-----------|
| Au1—P1 | 2.2256 (8) | C13—C14 | 1.388 (4) |
| Au1—C11 | 2.2739 (8) | C13—C18 | 1.407 (4) |
| Au1—Au2 | 3.05634 (17) | C14—C15 | 1.381 (4) |
| Au2—P2 | 2.2279 (7) | C14—H14 | 0.9500 |
| Au2—C12 | 2.2792 (8) | C15—C16 | 1.355 (4) |
| P1—C1 | 1.808 (3) | C15—H15 | 0.9500 |
| P1—C7 | 1.816 (3) | C16—C17 | 1.389 (4) |
| P1—C13 | 1.827 (3) | C16—H16 | 0.9500 |
| P2—C19 | 1.809 (3) | C17—C18 | 1.384 (4) |
| P2—C25 | 1.821 (3) | C17—H17 | 0.9500 |
| P2—C18 | 1.830 (3) | C19—C20 | 1.384 (4) |
| C1—C2 | 1.378 (4) | C19—C24 | 1.388 (4) |

supplementary materials

| | | | |
|-------------|-------------|-------------|-----------|
| C1—C6 | 1.387 (5) | C20—C21 | 1.381 (5) |
| C2—C3 | 1.372 (5) | C20—H20 | 0.9500 |
| C2—H2 | 0.9500 | C21—C22 | 1.373 (5) |
| C3—C4 | 1.368 (6) | C21—H21 | 0.9500 |
| C3—H3 | 0.9500 | C22—C23 | 1.371 (5) |
| C4—C5 | 1.373 (6) | C22—H22 | 0.9500 |
| C4—H4 | 0.9500 | C23—C24 | 1.373 (5) |
| C5—C6 | 1.377 (5) | C23—H23 | 0.9500 |
| C5—H5 | 0.9500 | C24—H24 | 0.9500 |
| C6—H6 | 0.9500 | C25—C30 | 1.377 (4) |
| C7—C8 | 1.385 (5) | C25—C26 | 1.388 (4) |
| C7—C12 | 1.391 (4) | C26—C27 | 1.383 (5) |
| C8—C9 | 1.385 (5) | C26—H26 | 0.9500 |
| C8—H8 | 0.9500 | C27—C28 | 1.364 (6) |
| C9—C10 | 1.362 (5) | C27—H27 | 0.9500 |
| C9—H9 | 0.9500 | C28—C29 | 1.370 (6) |
| C10—C11 | 1.374 (5) | C28—H28 | 0.9500 |
| C10—H10 | 0.9500 | C29—C30 | 1.392 (5) |
| C11—C12 | 1.383 (5) | C29—H29 | 0.9500 |
| C11—H11 | 0.9500 | C30—H30 | 0.9500 |
| C12—H12 | 0.9500 | | |
| P1—Au1—Cl1 | 175.87 (3) | C14—C13—C18 | 118.8 (3) |
| P1—Au1—Au2 | 81.343 (19) | C14—C13—P1 | 118.1 (2) |
| Cl1—Au1—Au2 | 102.64 (2) | C18—C13—P1 | 123.1 (2) |
| P2—Au2—Cl2 | 171.48 (3) | C15—C14—C13 | 121.3 (3) |
| P2—Au2—Au1 | 81.132 (19) | C15—C14—H14 | 119.4 |
| Cl2—Au2—Au1 | 104.79 (2) | C13—C14—H14 | 119.4 |
| C1—P1—C7 | 106.00 (14) | C16—C15—C14 | 120.1 (3) |
| C1—P1—C13 | 103.96 (14) | C16—C15—H15 | 120.0 |
| C7—P1—C13 | 106.38 (14) | C14—C15—H15 | 120.0 |
| C1—P1—Au1 | 116.51 (10) | C15—C16—C17 | 119.9 (3) |
| C7—P1—Au1 | 110.53 (10) | C15—C16—H16 | 120.0 |
| C13—P1—Au1 | 112.70 (10) | C17—C16—H16 | 120.0 |
| C19—P2—C25 | 105.53 (14) | C18—C17—C16 | 121.2 (3) |
| C19—P2—C18 | 104.91 (13) | C18—C17—H17 | 119.4 |
| C25—P2—C18 | 105.09 (13) | C16—C17—H17 | 119.4 |
| C19—P2—Au2 | 110.65 (10) | C17—C18—C13 | 118.8 (3) |
| C25—P2—Au2 | 106.77 (9) | C17—C18—P2 | 115.4 (2) |
| C18—P2—Au2 | 122.62 (10) | C13—C18—P2 | 125.6 (2) |
| C2—C1—C6 | 118.5 (3) | C20—C19—C24 | 119.1 (3) |
| C2—C1—P1 | 120.4 (3) | C20—C19—P2 | 123.1 (2) |
| C6—C1—P1 | 121.1 (2) | C24—C19—P2 | 117.7 (2) |
| C3—C2—C1 | 121.1 (3) | C21—C20—C19 | 119.7 (3) |
| C3—C2—H2 | 119.4 | C21—C20—H20 | 120.1 |
| C1—C2—H2 | 119.4 | C19—C20—H20 | 120.1 |
| C4—C3—C2 | 119.9 (3) | C22—C21—C20 | 120.7 (3) |
| C4—C3—H3 | 120.0 | C22—C21—H21 | 119.6 |
| C2—C3—H3 | 120.0 | C20—C21—H21 | 119.6 |
| C3—C4—C5 | 119.9 (3) | C23—C22—C21 | 119.7 (3) |

| | | | |
|-----------------|--------------|-----------------|------------|
| C3—C4—H4 | 120.0 | C23—C22—H22 | 120.1 |
| C5—C4—H4 | 120.0 | C21—C22—H22 | 120.1 |
| C4—C5—C6 | 120.3 (4) | C22—C23—C24 | 120.2 (3) |
| C4—C5—H5 | 119.8 | C22—C23—H23 | 119.9 |
| C6—C5—H5 | 119.8 | C24—C23—H23 | 119.9 |
| C5—C6—C1 | 120.1 (3) | C23—C24—C19 | 120.5 (3) |
| C5—C6—H6 | 119.9 | C23—C24—H24 | 119.7 |
| C1—C6—H6 | 119.9 | C19—C24—H24 | 119.7 |
| C8—C7—C12 | 119.1 (3) | C30—C25—C26 | 119.3 (3) |
| C8—C7—P1 | 121.3 (2) | C30—C25—P2 | 122.2 (2) |
| C12—C7—P1 | 119.4 (3) | C26—C25—P2 | 117.9 (2) |
| C9—C8—C7 | 120.3 (3) | C27—C26—C25 | 120.1 (3) |
| C9—C8—H8 | 119.9 | C27—C26—H26 | 119.9 |
| C7—C8—H8 | 119.9 | C25—C26—H26 | 119.9 |
| C10—C9—C8 | 119.8 (4) | C28—C27—C26 | 120.1 (4) |
| C10—C9—H9 | 120.1 | C28—C27—H27 | 120.0 |
| C8—C9—H9 | 120.1 | C26—C27—H27 | 120.0 |
| C9—C10—C11 | 120.9 (3) | C27—C28—C29 | 120.5 (3) |
| C9—C10—H10 | 119.5 | C27—C28—H28 | 119.8 |
| C11—C10—H10 | 119.5 | C29—C28—H28 | 119.7 |
| C10—C11—C12 | 119.7 (3) | C28—C29—C30 | 119.9 (4) |
| C10—C11—H11 | 120.2 | C28—C29—H29 | 120.0 |
| C12—C11—H11 | 120.2 | C30—C29—H29 | 120.0 |
| C11—C12—C7 | 120.1 (3) | C25—C30—C29 | 120.0 (4) |
| C11—C12—H12 | 119.9 | C25—C30—H30 | 120.0 |
| C7—C12—H12 | 119.9 | C29—C30—H30 | 120.0 |
| P1—Au1—Au2—P2 | -70.42 (3) | P1—C13—C14—C15 | 177.7 (3) |
| Cl1—Au1—Au2—P2 | 108.45 (3) | C13—C14—C15—C16 | -1.1 (5) |
| P1—Au1—Au2—Cl2 | 115.85 (3) | C14—C15—C16—C17 | 1.0 (5) |
| Cl1—Au1—Au2—Cl2 | -65.29 (3) | C15—C16—C17—C18 | -0.1 (5) |
| Au2—Au1—P1—C1 | -42.04 (11) | C16—C17—C18—C13 | -0.7 (5) |
| Au2—Au1—P1—C7 | -163.09 (11) | C16—C17—C18—P2 | 174.4 (3) |
| Au2—Au1—P1—C13 | 78.02 (10) | C14—C13—C18—C17 | 0.6 (4) |
| Au1—Au2—P2—C19 | -63.84 (10) | P1—C13—C18—C17 | -176.6 (2) |
| Au1—Au2—P2—C25 | -178.20 (11) | C14—C13—C18—P2 | -173.9 (2) |
| Au1—Au2—P2—C18 | 60.75 (11) | P1—C13—C18—P2 | 8.9 (4) |
| C7—P1—C1—C2 | 96.0 (3) | C19—P2—C18—C17 | -78.0 (3) |
| C13—P1—C1—C2 | -152.0 (3) | C25—P2—C18—C17 | 33.0 (3) |
| Au1—P1—C1—C2 | -27.4 (3) | Au2—P2—C18—C17 | 154.9 (2) |
| C7—P1—C1—C6 | -83.8 (3) | C19—P2—C18—C13 | 96.7 (3) |
| C13—P1—C1—C6 | 28.2 (3) | C25—P2—C18—C13 | -152.3 (3) |
| Au1—P1—C1—C6 | 152.8 (2) | Au2—P2—C18—C13 | -30.5 (3) |
| C6—C1—C2—C3 | -1.7 (5) | C25—P2—C19—C20 | -101.8 (3) |
| P1—C1—C2—C3 | 178.5 (3) | C18—P2—C19—C20 | 9.0 (3) |
| C1—C2—C3—C4 | 1.4 (6) | Au2—P2—C19—C20 | 143.1 (2) |
| C2—C3—C4—C5 | 0.1 (6) | C25—P2—C19—C24 | 77.1 (3) |
| C3—C4—C5—C6 | -1.2 (6) | C18—P2—C19—C24 | -172.2 (2) |
| C4—C5—C6—C1 | 0.8 (6) | Au2—P2—C19—C24 | -38.1 (3) |
| C2—C1—C6—C5 | 0.6 (5) | C24—C19—C20—C21 | -0.1 (5) |

supplementary materials

| | | | |
|-----------------|------------|-----------------|------------|
| P1—C1—C6—C5 | -179.6 (3) | P2—C19—C20—C21 | 178.7 (3) |
| C1—P1—C7—C8 | -3.9 (3) | C19—C20—C21—C22 | -0.5 (6) |
| C13—P1—C7—C8 | -114.2 (3) | C20—C21—C22—C23 | 0.2 (6) |
| Au1—P1—C7—C8 | 123.2 (3) | C21—C22—C23—C24 | 0.6 (5) |
| C1—P1—C7—C12 | -178.1 (2) | C22—C23—C24—C19 | -1.1 (5) |
| C13—P1—C7—C12 | 71.6 (3) | C20—C19—C24—C23 | 0.9 (5) |
| Au1—P1—C7—C12 | -51.0 (3) | P2—C19—C24—C23 | -178.0 (2) |
| C12—C7—C8—C9 | 1.4 (5) | C19—P2—C25—C30 | 2.3 (3) |
| P1—C7—C8—C9 | -172.8 (3) | C18—P2—C25—C30 | -108.3 (3) |
| C7—C8—C9—C10 | -2.4 (6) | Au2—P2—C25—C30 | 120.1 (2) |
| C8—C9—C10—C11 | 1.2 (6) | C19—P2—C25—C26 | -169.8 (2) |
| C9—C10—C11—C12 | 1.1 (6) | C18—P2—C25—C26 | 79.7 (3) |
| C10—C11—C12—C7 | -2.1 (5) | Au2—P2—C25—C26 | -52.0 (2) |
| C8—C7—C12—C11 | 0.9 (5) | C30—C25—C26—C27 | -0.3 (5) |
| P1—C7—C12—C11 | 175.2 (3) | P2—C25—C26—C27 | 172.0 (2) |
| C1—P1—C13—C14 | -101.0 (3) | C25—C26—C27—C28 | -0.4 (5) |
| C7—P1—C13—C14 | 10.6 (3) | C26—C27—C28—C29 | 1.2 (5) |
| Au1—P1—C13—C14 | 131.9 (2) | C27—C28—C29—C30 | -1.2 (5) |
| C1—P1—C13—C18 | 76.2 (3) | C26—C25—C30—C29 | 0.3 (5) |
| C7—P1—C13—C18 | -172.1 (2) | P2—C25—C30—C29 | -171.7 (3) |
| Au1—P1—C13—C18 | -50.9 (3) | C28—C29—C30—C25 | 0.5 (5) |
| C18—C13—C14—C15 | 0.3 (5) | | |

Hydrogen-bond geometry (\AA , $^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-----------------------------------|-------|-------------|-------------|---------------|
| C15—H15 \cdots Cg ⁱ | 0.95 | 2.82 | 3.569 (4) | 137 |
| C21—H21 \cdots Cg ⁱⁱ | 0.95 | 2.84 | 3.559 (4) | 134 |

Symmetry codes: (i) $x, -y+3/2, z-1/2$; (ii) $-x+1, y-1/2, -z+1/2$.

Fig. 1

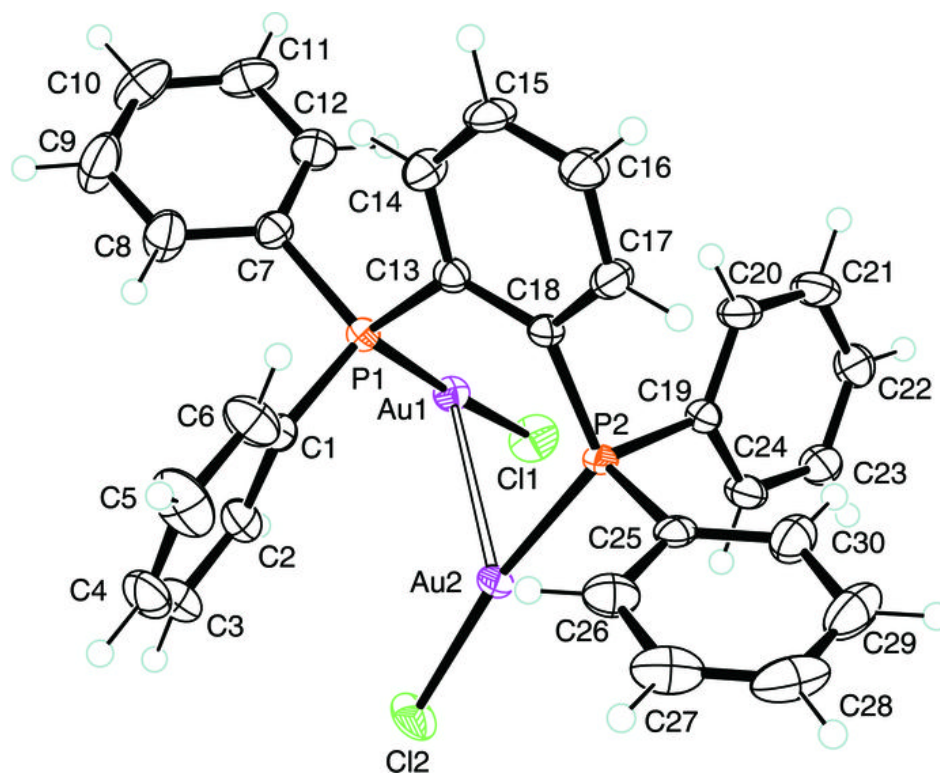


Fig. 2

