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μ-Sulfido-bis{[1,1′-bis(diphenylphosphanyl)ferrocene-κ^2P,P']gold} methanol monosolvate

Takuma Itai, Tatsuhiro Kojima* and Takumi Konno

Department of Chemistry, Graduate School of Science, Osaka University, Toyonaka, Osaka 560-0043, Japan. *Correspondence e-mail: kojimat15@chem.sci.osaka-u.ac.jp

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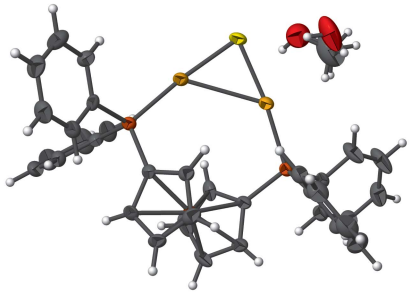
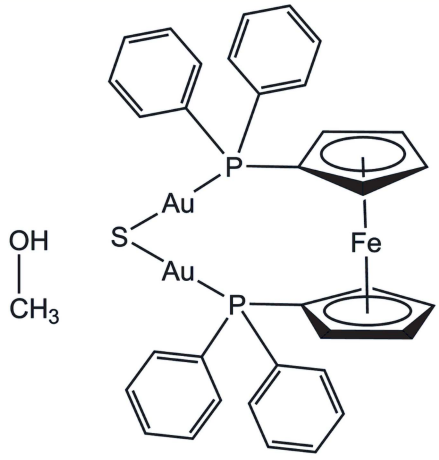
Structural data: full structural data are available from iucrdata.iucr.org

The gold complex in title compound, $[Au_2Fe(C_{17}H_{14}P)_2S]\cdot CH_3OH$, (I)·$CH_3OH$, is closely similar to the previously reported (I)·$2CHCl_3$, reported in the literature [Canales *et al.* (1996). *J. Am. Chem. Soc.* **118**, 4839–4845]. Both crystallize in the monoclinic crystal systems but the space groups differ, $P2_1/n$ for (I)·CH_3OH compared to $P2/n$ for (I)·$2CHCl_3$. The two structures can be considered as polymorphs due to solvation differences. In (I)·CH_3OH, all atoms of the methanol solvent molecule are disordered over two sets of sites with an occupancy ratio of 0.822 (12):0.178 (12). The crystal structure features O—H···S, C—H···S hydrogen bonds and C—H···π interactions that stack the complex molecules along the *a*-axis direction.

3D view



Chemical scheme



Structure description

The asymmetric unit in the title crystal structure contains one $[Au_2(dppf)(S)]$ complex molecule, (I)·CH_3OH, dppf = 1,1′-bis(diphenylphosphino)ferrocene) and a methanol solvate molecule, all atoms of which are disordered over two sets of sites with a 0.822 (12):0.178 (12) occupancy ratio, Fig. 1. Both Au^I cations adopt a slightly distorted linear coordination geometry, each binding separate P atoms from the dppf ligand and bridged by the sulfido anion, leading to a close intramolecular Au—Au contact of 2.8857 (3) Å, similar to that observed in the closely related (I)·$2CHCl_3$ (Canales *et al.*, 1996). The Au—S and Au—P distances, Table 1, are also similar to those in the earlier report. The space groups of these two structures differ, $P2_1/n$ for (I)·CH_3OH and $P2/n$ for (I)·$2CHCl_3$. The two structures can be considered as polymorphs due to solvation differences which will significantly affect the crystal packing. Apart from the polymorph, only two examples of digoldsufide systems similarly bridged by bidentate diphenylphosphino ligands, (μ_2-2,5-bis(diphenylphosphinomethyl)thiophene)(μ_2-sulfido)di-

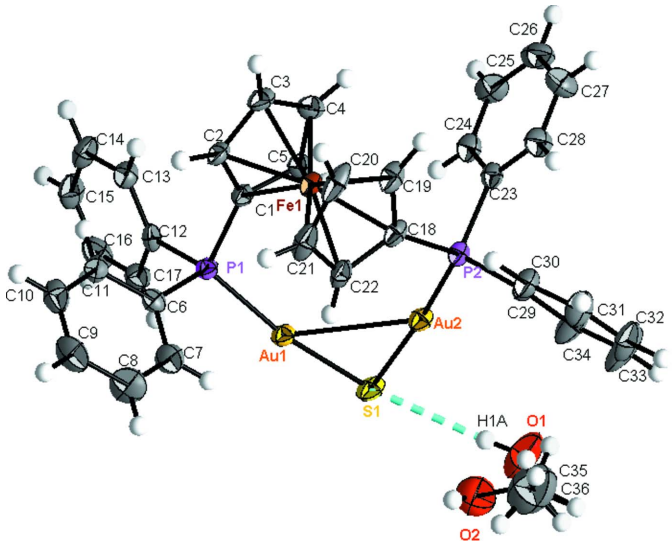


Figure 1
The molecular structure of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are drawn as spheres of arbitrary radii.

gold(I) (Chen *et al.*, 1998) and {μ_2-1,4-bis[(di-;phenylphosphino)methyl]benzene}(μ_2-sulfido)digold(I) chloroform solvate (Hofreiter *et al.*, 1995) are found in the Cambridge Structural Database (Groom & Allen, 2014).

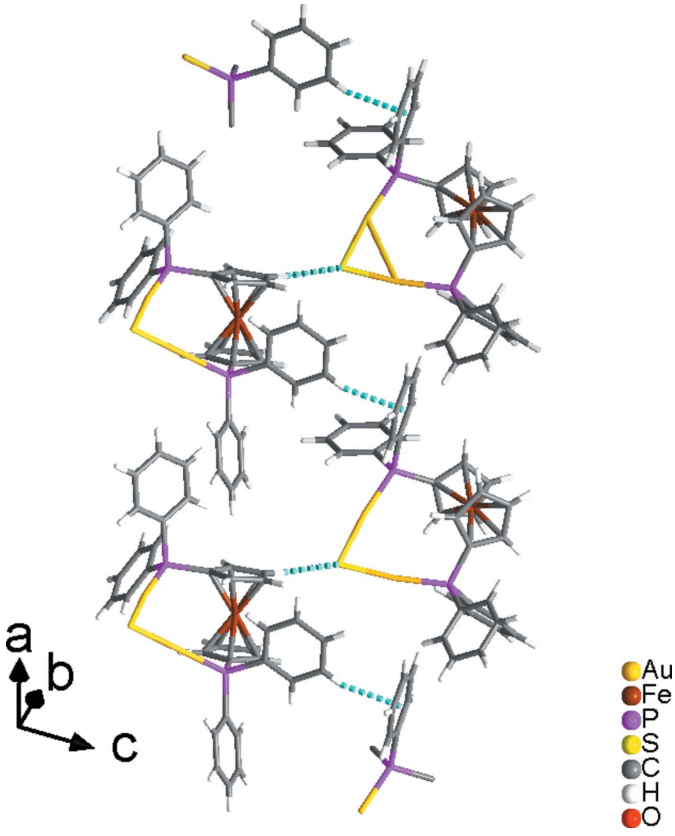


Figure 2
Overall packing for the title compound viewed approximately along the *b* axis.

Table 1
Selected geometric parameters (Å, °).

Au1—P1	2.2524 (12)	Au2—S1	2.2988 (12)
Au1—S1	2.3036 (12)	Au1—Au2	2.8857 (3)
Au2—P2	2.2452 (12)		
S1—Au1—Au2	51.10 (3)	P2—Au2—S1	172.59 (4)
S1—Au2—Au1	51.24 (3)	P1—Au1—Au2	122.96 (3)
P1—Au1—S1	171.06 (4)	P2—Au2—Au1	122.54 (3)

Table 2
Hydrogen-bond geometry (Å, °).

*Cg*1 and *Cg*2 are the centroids of the C7–C11 and C12–C16 phenyl rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···S1	0.84	2.63	3.465 (6)	170
C3—H3···S1^{i}	0.95	2.79	3.734 (5)	175
C27—H27···*Cg*(1)^{ii}	0.95	2.83	3.659 (6)	146
C32—H32···*Cg*(2)^{iii}	0.95	2.88	3.717 (6)	147

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

In the crystal structure, an O—H···S hydrogen bond links the major disorder component of the methanol molecule to the complex molecule in the asymmetric unit, Table 2. A C—H···S hydrogen bond and two edge-to-face C—H···π contacts link adjacent complex molecules, stacking them along the *a*-axis direction, Fig. 2. For the polymorphic structure,

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Au_2Fe(C_{17}H_{14}P)_2S]\cdot CH_4O$
M_r	1012.39
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	200
a, *b*, *c* (Å)	13.7434 (13), 12.6277 (13), 18.7630 (18)
β (°)	98.352 (7)
V (Å^3)	3221.7 (5)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	9.72
Crystal size (mm)	0.30 × 0.10 × 0.01
Data collection	
Diffractometer	Rigaku VariMax RAPID diffractometer
Absorption correction	Multi-scan (*ABSCOR*; Higashi, 1995)
T_{min}, T_{max}	0.572, 0.995
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	26469, 6105, 5445
R_{int}	0.045
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.610
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.031, 0.052, 1.13
No. of reflections	6105
No. of parameters	392
No. of restraints	8
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.03, −0.55

Computer programs: *PROCESS-AUTO* (Rigaku, 2000), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *DIAMOND* (Putz & Brandenburg, 2011), *WinGX* (Farrugia, 2012).

which lies about a twofold rotation axis, C—H···S and C—H···Cl hydrogen bonds, a weaker C—H···π contact and an intermolecular Cl···Cl halogen bond stabilize the structure.

Synthesis and crystallization

To a solution of [1,1′-bis(diphenylphosphino)ferrocene]bis(D-penicillaminato)digold (15.0 mg, 15.8 mmol) in 3 ml of methanol was added 20 µL (0.02 mmol) of an aqueous sodium hydrogen sulfide solution (1 *M*). The solution was allowed to stand at room temperature for 1 h when small quantities of yellow needle-like crystals of $[Au_2(C_{34}H_{28}FeP_2)(S)]\cdot CH_3OH$ were obtained.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All atoms of the methanol solvate molecules were disordered over two sets ofsites. Their occupancies were refined to sum to unity and converged at 0.822 (12) and 0.178 (12), respectively. Ten reflections below $\theta_{min} = 3.227$, with $F_o <<< F_c$ were omitted as they were likely to have been obscured by the beamstop.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x152492 [doi:10.1107/S241431461502492X]

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Crystal data

$[Au_2Fe(C_{17}H_{14}P)_2S]\cdot CH_4O$
M_r = 1012.39
Monoclinic, $P2_1/n$
a = 13.7434 (13) Å
b = 12.6277 (13) Å
c = 18.7630 (18) Å
β = 98.352 (7)°
V = 3221.7 (5) Å^3
Z = 4
$F(000)$ = 1920
D_x = 2.087 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71075 Å
Cell parameters from 8771 reflections
θ = 3.0–27.5°
μ = 9.72 mm^{-1}
T = 200 K
Needle, yellow
0.30 × 0.10 × 0.01 mm

Data collection

Rigaku VariMax RAPID diffractometer
Radiation source: fine-focus sealed tube
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.572, T_{max} = 0.995
26469 measured reflections
6105 independent reflections
5445 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 25.7°, θ_{min} = 3.2°
h = −16→16
k = −15→15
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.052
S = 1.13
6105 reflections
392 parameters
8 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0208P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.03 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Au1	0.39803 (2)	0.23503 (2)	0.09507 (2)	0.02544 (6)	
Au2	0.23078 (2)	0.20488 (2)	0.16975 (2)	0.02555 (6)	
Fe1	0.47576 (5)	0.32726 (5)	0.31861 (3)	0.02381 (15)	
P1	0.54820 (9)	0.27998 (9)	0.15170 (6)	0.0231 (3)	
P2	0.23049 (9)	0.25682 (9)	0.28416 (6)	0.0235 (3)	
S1	0.24432 (9)	0.17001 (10)	0.05135 (6)	0.0315 (3)	
C1	0.5572 (3)	0.2623 (3)	0.2479 (2)	0.0226 (10)	
C2	0.6197 (3)	0.3142 (4)	0.3044 (2)	0.0274 (10)	
H2	0.6635	0.3708	0.2989	0.033*	
C3	0.6049 (4)	0.2665 (4)	0.3704 (3)	0.0308 (11)	
H3	0.6367	0.2859	0.4170	0.037*	
C4	0.5348 (3)	0.1852 (4)	0.3546 (3)	0.0320 (11)	
H4	0.5112	0.1404	0.3890	0.038*	
C5	0.5054 (3)	0.1814 (3)	0.2799 (2)	0.0260 (10)	
H5	0.4592	0.1334	0.2550	0.031*	
C6	0.5925 (3)	0.4134 (3)	0.1388 (2)	0.0265 (10)	
C7	0.5275 (4)	0.4882 (4)	0.1072 (3)	0.0432 (14)	
H7	0.4600	0.4709	0.0944	0.052*	
C8	0.5609 (5)	0.5893 (4)	0.0940 (4)	0.0604 (18)	
H8	0.5159	0.6404	0.0713	0.073*	
C9	0.6571 (5)	0.6162 (4)	0.1131 (3)	0.0498 (15)	
H9	0.6789	0.6857	0.1043	0.060*	
C10	0.7220 (4)	0.5426 (4)	0.1448 (3)	0.0403 (13)	
H10	0.7891	0.5613	0.1586	0.048*	
C11	0.6908 (3)	0.4405 (4)	0.1572 (2)	0.0321 (11)	
H11	0.7368	0.3892	0.1783	0.038*	
C12	0.6439 (3)	0.1923 (3)	0.1277 (2)	0.0246 (10)	
C13	0.7252 (3)	0.1646 (4)	0.1775 (3)	0.0316 (11)	
H13	0.7322	0.1926	0.2249	0.038*	
C14	0.7960 (4)	0.0964 (4)	0.1582 (3)	0.0402 (13)	
H14	0.8520	0.0788	0.1921	0.048*	
C15	0.7848 (4)	0.0543 (4)	0.0900 (3)	0.0408 (13)	
H15	0.8333	0.0075	0.0767	0.049*	
C16	0.7043 (4)	0.0793 (4)	0.0407 (3)	0.0423 (14)	
H16	0.6968	0.0492	−0.0061	0.051*	
C17	0.6335 (4)	0.1488 (3)	0.0594 (2)	0.0311 (11)	
H17	0.5779	0.1664	0.0251	0.037*	
C18	0.3279 (3)	0.3494 (3)	0.3119 (2)	0.0254 (10)	
C19	0.3748 (3)	0.3704 (4)	0.3834 (3)	0.0334 (12)	
H19	0.3623	0.3349	0.4257	0.040*	
C20	0.4427 (3)	0.4529 (4)	0.3803 (3)	0.0439 (15)	
H20	0.4843	0.4826	0.4201	0.053*	
C21	0.4383 (4)	0.4837 (4)	0.3079 (3)	0.0419 (14)	
H21	0.4763	0.5384	0.2907	0.050*	
C22	0.3681 (3)	0.4201 (3)	0.2646 (3)	0.0320 (12)	

H22	0.3511	0.4239	0.2138	0.038*	
C23	0.2466 (3)	0.1536 (3)	0.3525 (2)	0.0254 (10)	
C24	0.2985 (3)	0.0625 (4)	0.3396 (3)	0.0324 (11)	
H24	0.3234	0.0548	0.2952	0.039*	
C25	0.3141 (4)	−0.0162 (4)	0.3903 (3)	0.0410 (13)	
H25	0.3494	−0.0781	0.3809	0.049*	
C26	0.2785 (4)	−0.0056 (4)	0.4547 (3)	0.0459 (14)	
H26	0.2897	−0.0602	0.4898	0.055*	
C27	0.2269 (4)	0.0834 (4)	0.4687 (3)	0.0483 (15)	
H27	0.2020	0.0904	0.5131	0.058*	
C28	0.2115 (4)	0.1625 (4)	0.4175 (3)	0.0363 (12)	
H28	0.1761	0.2242	0.4272	0.044*	
C29	0.1186 (3)	0.3250 (3)	0.2995 (2)	0.0241 (10)	
C30	0.1185 (4)	0.4138 (4)	0.3427 (3)	0.0321 (11)	
H30	0.1791	0.4446	0.3634	0.038*	
C31	0.0309 (4)	0.4580 (4)	0.3558 (3)	0.0408 (13)	
H31	0.0318	0.5182	0.3863	0.049*	
C32	−0.0563 (4)	0.4163 (4)	0.3254 (3)	0.0508 (16)	
H32	−0.1162	0.4474	0.3345	0.061*	
C33	−0.0578 (4)	0.3285 (4)	0.2812 (4)	0.065 (2)	
H33	−0.1189	0.2990	0.2602	0.077*	
C34	0.0291 (4)	0.2838 (4)	0.2676 (3)	0.0499 (16)	
H34	0.0278	0.2245	0.2364	0.060*	
O1	−0.0057 (4)	0.1917 (5)	0.0573 (5)	0.095 (3)	0.822 (12)
H1A	0.0554	0.1950	0.0574	0.143*	0.822 (12)
C35	−0.0431 (17)	0.2927 (15)	0.0602 (13)	0.113 (7)	0.822 (12)
H35A	−0.0284	0.3335	0.0187	0.170*	0.822 (12)
H35B	−0.0131	0.3273	0.1048	0.170*	0.822 (12)
H35C	−0.1145	0.2889	0.0593	0.170*	0.822 (12)
O2	0.025 (2)	0.292 (2)	0.0241 (16)	0.074 (11)*	0.178 (12)
H2B	0.0519	0.3513	0.0309	0.111*	0.178 (12)
C36	−0.042 (4)	0.284 (4)	0.063 (3)	0.024 (11)*	0.178 (12)
H36A	−0.0388	0.3442	0.0962	0.037*	0.178 (12)
H36B	−0.0333	0.2179	0.0908	0.037*	0.178 (12)
H36C	−0.1065	0.2830	0.0326	0.037*	0.178 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.02336 (10)	0.03084 (10)	0.02091 (10)	0.00051 (8)	−0.00083 (7)	−0.00180 (7)
Au2	0.02393 (10)	0.02795 (10)	0.02366 (10)	−0.00089 (8)	−0.00025 (7)	−0.00423 (7)
Fe1	0.0194 (3)	0.0265 (3)	0.0249 (4)	0.0004 (3)	0.0013 (3)	−0.0051 (3)
P1	0.0212 (6)	0.0264 (6)	0.0210 (6)	0.0000 (5)	0.0008 (5)	−0.0009 (5)
P2	0.0200 (6)	0.0252 (6)	0.0250 (6)	−0.0006 (5)	0.0024 (5)	−0.0031 (5)
S1	0.0268 (7)	0.0415 (7)	0.0235 (6)	−0.0007 (6)	−0.0051 (5)	−0.0083 (5)
C1	0.019 (2)	0.027 (2)	0.023 (2)	0.002 (2)	0.0030 (19)	−0.0018 (19)
C2	0.017 (2)	0.037 (3)	0.027 (3)	0.001 (2)	−0.002 (2)	−0.004 (2)
C3	0.025 (3)	0.044 (3)	0.021 (3)	0.007 (2)	−0.002 (2)	−0.005 (2)

C4	0.034 (3)	0.037 (3)	0.025 (3)	0.009 (2)	0.005 (2)	0.003 (2)
C5	0.026 (3)	0.026 (2)	0.025 (3)	0.002 (2)	0.004 (2)	−0.0005 (19)
C6	0.031 (3)	0.028 (2)	0.022 (3)	0.000 (2)	0.007 (2)	−0.0012 (19)
C7	0.040 (3)	0.037 (3)	0.052 (4)	−0.004 (3)	0.004 (3)	0.008 (3)
C8	0.062 (5)	0.033 (3)	0.085 (5)	−0.002 (3)	0.006 (4)	0.015 (3)
C9	0.066 (4)	0.026 (3)	0.059 (4)	−0.014 (3)	0.014 (3)	0.005 (3)
C10	0.041 (3)	0.045 (3)	0.035 (3)	−0.017 (3)	0.008 (3)	−0.008 (2)
C11	0.027 (3)	0.039 (3)	0.030 (3)	−0.003 (2)	0.005 (2)	−0.001 (2)
C12	0.022 (2)	0.026 (2)	0.029 (3)	−0.001 (2)	0.011 (2)	−0.0021 (19)
C13	0.026 (3)	0.035 (3)	0.033 (3)	−0.001 (2)	0.004 (2)	−0.003 (2)
C14	0.024 (3)	0.041 (3)	0.056 (4)	0.005 (2)	0.004 (3)	−0.001 (3)
C15	0.034 (3)	0.039 (3)	0.053 (4)	0.008 (3)	0.019 (3)	−0.004 (3)
C16	0.057 (4)	0.039 (3)	0.035 (3)	0.007 (3)	0.020 (3)	−0.001 (2)
C17	0.033 (3)	0.036 (3)	0.025 (3)	0.003 (2)	0.006 (2)	0.000 (2)
C18	0.019 (2)	0.029 (2)	0.028 (3)	0.004 (2)	0.002 (2)	−0.011 (2)
C19	0.025 (3)	0.045 (3)	0.031 (3)	0.003 (2)	0.006 (2)	−0.017 (2)
C20	0.020 (3)	0.046 (3)	0.065 (4)	−0.001 (2)	0.001 (3)	−0.035 (3)
C21	0.024 (3)	0.023 (2)	0.078 (5)	−0.001 (2)	0.006 (3)	−0.005 (3)
C22	0.017 (3)	0.027 (2)	0.052 (3)	0.004 (2)	0.006 (2)	0.005 (2)
C23	0.023 (2)	0.027 (2)	0.027 (3)	−0.004 (2)	0.004 (2)	−0.0046 (19)
C24	0.029 (3)	0.032 (3)	0.035 (3)	−0.002 (2)	0.005 (2)	−0.003 (2)
C25	0.043 (3)	0.026 (3)	0.052 (4)	0.002 (2)	0.000 (3)	0.001 (2)
C26	0.048 (4)	0.039 (3)	0.046 (4)	−0.004 (3)	−0.006 (3)	0.013 (3)
C27	0.054 (4)	0.058 (3)	0.034 (3)	−0.001 (3)	0.011 (3)	0.008 (3)
C28	0.039 (3)	0.038 (3)	0.033 (3)	0.007 (2)	0.011 (2)	−0.002 (2)
C29	0.019 (2)	0.026 (2)	0.026 (3)	−0.001 (2)	−0.0004 (19)	0.0022 (19)
C30	0.025 (3)	0.034 (3)	0.037 (3)	−0.001 (2)	0.003 (2)	−0.006 (2)
C31	0.034 (3)	0.032 (3)	0.057 (4)	0.004 (2)	0.011 (3)	−0.012 (2)
C32	0.027 (3)	0.040 (3)	0.087 (5)	0.008 (3)	0.013 (3)	−0.004 (3)
C33	0.023 (3)	0.047 (3)	0.117 (6)	0.002 (3)	−0.012 (3)	−0.024 (4)
C34	0.029 (3)	0.037 (3)	0.079 (5)	0.001 (3)	−0.008 (3)	−0.023 (3)
O1	0.038 (4)	0.083 (5)	0.159 (8)	−0.005 (3)	−0.009 (4)	0.015 (4)
C35	0.090 (10)	0.089 (9)	0.155 (16)	−0.001 (7)	0.001 (9)	0.010 (8)

Geometric parameters (Å, º)

Au1—P1	2.2524 (12)	C15—C16	1.372 (7)
Au1—S1	2.3036 (12)	C15—H15	0.9500
Au2—P2	2.2452 (12)	C16—C17	1.392 (6)
Au2—S1	2.2988 (12)	C16—H16	0.9500
Au1—Au2	2.8857 (3)	C17—H17	0.9500
Fe1—C1	2.029 (4)	C18—C19	1.425 (6)
Fe1—C18	2.037 (4)	C18—C22	1.426 (6)
Fe1—C22	2.038 (5)	C19—C20	1.406 (7)
Fe1—C2	2.041 (4)	C19—H19	0.9500
Fe1—C4	2.042 (5)	C20—C21	1.405 (7)
Fe1—C5	2.043 (4)	C20—H20	0.9500
Fe1—C21	2.044 (5)	C21—C22	1.416 (7)

Fe1—C3	2.046 (5)	C21—H21	0.9500
Fe1—C19	2.047 (4)	C22—H22	0.9500
Fe1—C20	2.053 (5)	C23—C28	1.379 (6)
P1—C1	1.805 (4)	C23—C24	1.393 (6)
P1—C6	1.819 (4)	C24—C25	1.371 (7)
P1—C12	1.825 (4)	C24—H24	0.9500
P2—C18	1.797 (4)	C25—C26	1.374 (7)
P2—C23	1.820 (5)	C25—H25	0.9500
P2—C29	1.822 (4)	C26—C27	1.375 (7)
C1—C2	1.423 (6)	C26—H26	0.9500
C1—C5	1.427 (6)	C27—C28	1.381 (7)
C2—C3	1.418 (6)	C27—H27	0.9500
C2—H2	0.9500	C28—H28	0.9500
C3—C4	1.410 (7)	C29—C30	1.383 (6)
C3—H3	0.9500	C29—C34	1.388 (7)
C4—C5	1.401 (6)	C30—C31	1.381 (6)
C4—H4	0.9500	C30—H30	0.9500
C5—H5	0.9500	C31—C32	1.356 (7)
C6—C7	1.373 (6)	C31—H31	0.9500
C6—C11	1.389 (6)	C32—C33	1.383 (7)
C7—C8	1.392 (7)	C32—H32	0.9500
C7—H7	0.9500	C33—C34	1.378 (7)
C8—C9	1.362 (8)	C33—H33	0.9500
C8—H8	0.9500	C34—H34	0.9500
C9—C10	1.364 (7)	O1—C35	1.378 (18)
C9—H9	0.9500	O1—H1A	0.8400
C10—C11	1.389 (6)	C35—H35A	0.9800
C10—H10	0.9500	C35—H35B	0.9800
C11—H11	0.9500	C35—H35C	0.9800
C12—C17	1.383 (6)	O2—C36	1.26 (6)
C12—C13	1.393 (6)	O2—H2B	0.8400
C13—C14	1.386 (6)	C36—H36A	0.9800
C13—H13	0.9500	C36—H36B	0.9800
C14—C15	1.375 (7)	C36—H36C	0.9800
C14—H14	0.9500		

S1—Au1—Au2	51.10 (3)	C10—C9—H9	120.2
S1—Au2—Au1	51.24 (3)	C9—C10—C11	120.5 (5)
P1—Au1—S1	171.06 (4)	C9—C10—H10	119.8
P2—Au2—S1	172.59 (4)	C11—C10—H10	119.8
P1—Au1—Au2	122.96 (3)	C10—C11—C6	120.0 (5)
P2—Au2—Au1	122.54 (3)	C10—C11—H11	120.0
C1—Fe1—C18	130.97 (18)	C6—C11—H11	120.0
C1—Fe1—C22	109.71 (19)	C17—C12—C13	119.1 (4)
C18—Fe1—C22	40.97 (17)	C17—C12—P1	119.2 (4)
C1—Fe1—C2	40.94 (17)	C13—C12—P1	121.6 (3)
C18—Fe1—C2	168.62 (18)	C14—C13—C12	120.5 (5)
C22—Fe1—C2	128.96 (18)	C14—C13—H13	119.8

C1—Fe1—C4	68.34 (17)	C12—C13—H13	119.8
C18—Fe1—C4	119.05 (18)	C15—C14—C13	119.7 (5)
C22—Fe1—C4	153.41 (19)	C15—C14—H14	120.2
C2—Fe1—C4	68.08 (18)	C13—C14—H14	120.2
C1—Fe1—C5	41.03 (16)	C16—C15—C14	120.6 (5)
C18—Fe1—C5	110.54 (18)	C16—C15—H15	119.7
C22—Fe1—C5	120.68 (19)	C14—C15—H15	119.7
C2—Fe1—C5	68.50 (18)	C15—C16—C17	120.1 (5)
C4—Fe1—C5	40.12 (18)	C15—C16—H16	119.9
C1—Fe1—C21	118.8 (2)	C17—C16—H16	119.9
C18—Fe1—C21	68.06 (18)	C12—C17—C16	120.0 (5)
C22—Fe1—C21	40.60 (19)	C12—C17—H17	120.0
C2—Fe1—C21	107.47 (19)	C16—C17—H17	120.0
C4—Fe1—C21	164.5 (2)	C19—C18—C22	107.8 (4)
C5—Fe1—C21	153.8 (2)	C19—C18—P2	127.6 (4)
C1—Fe1—C3	68.64 (18)	C22—C18—P2	124.5 (4)
C18—Fe1—C3	150.45 (19)	C19—C18—Fe1	69.9 (2)
C22—Fe1—C3	165.73 (18)	C22—C18—Fe1	69.5 (2)
C2—Fe1—C3	40.62 (18)	P2—C18—Fe1	128.5 (2)
C4—Fe1—C3	40.36 (19)	C20—C19—C18	108.1 (5)
C5—Fe1—C3	68.06 (19)	C20—C19—Fe1	70.2 (3)
C21—Fe1—C3	126.7 (2)	C18—C19—Fe1	69.2 (2)
C1—Fe1—C19	169.06 (18)	C20—C19—H19	125.9
C18—Fe1—C19	40.85 (18)	C18—C19—H19	125.9
C22—Fe1—C19	68.7 (2)	Fe1—C19—H19	126.3
C2—Fe1—C19	148.51 (19)	C21—C20—C19	108.0 (5)
C4—Fe1—C19	108.0 (2)	C21—C20—Fe1	69.6 (3)
C5—Fe1—C19	129.69 (19)	C19—C20—Fe1	69.7 (3)
C21—Fe1—C19	67.6 (2)	C21—C20—H20	126.0
C3—Fe1—C19	115.7 (2)	C19—C20—H20	126.0
C1—Fe1—C20	150.34 (19)	Fe1—C20—H20	126.3
C18—Fe1—C20	68.17 (18)	C20—C21—C22	109.1 (4)
C22—Fe1—C20	68.4 (2)	C20—C21—Fe1	70.3 (3)
C2—Fe1—C20	115.72 (19)	C22—C21—Fe1	69.5 (2)
C4—Fe1—C20	127.0 (2)	C20—C21—H21	125.4
C5—Fe1—C20	165.7 (2)	C22—C21—H21	125.4
C21—Fe1—C20	40.1 (2)	Fe1—C21—H21	126.4
C3—Fe1—C20	105.7 (2)	C21—C22—C18	106.9 (5)
C19—Fe1—C20	40.10 (18)	C21—C22—Fe1	69.9 (3)
C1—P1—C6	105.8 (2)	C18—C22—Fe1	69.5 (3)
C1—P1—C12	103.0 (2)	C21—C22—H22	126.5
C6—P1—C12	105.18 (19)	C18—C22—H22	126.5
C1—P1—Au1	111.46 (15)	Fe1—C22—H22	125.6
C6—P1—Au1	118.15 (16)	C28—C23—C24	118.4 (4)
C12—P1—Au1	112.01 (16)	C28—C23—P2	122.8 (3)
C18—P2—C23	104.6 (2)	C24—C23—P2	118.8 (3)
C18—P2—C29	104.90 (19)	C25—C24—C23	120.7 (4)
C23—P2—C29	104.3 (2)	C25—C24—H24	119.7

C18—P2—Au2	111.26 (15)	C23—C24—H24	119.7
C23—P2—Au2	116.60 (14)	C24—C25—C26	120.0 (5)
C29—P2—Au2	114.08 (15)	C24—C25—H25	120.0
Au2—S1—Au1	77.66 (4)	C26—C25—H25	120.0
C2—C1—C5	107.5 (4)	C25—C26—C27	120.4 (5)
C2—C1—P1	129.4 (3)	C25—C26—H26	119.8
C5—C1—P1	122.9 (3)	C27—C26—H26	119.8
C2—C1—Fe1	70.0 (2)	C26—C27—C28	119.3 (5)
C5—C1—Fe1	70.0 (2)	C26—C27—H27	120.3
P1—C1—Fe1	129.7 (2)	C28—C27—H27	120.3
C3—C2—C1	107.9 (4)	C23—C28—C27	121.2 (5)
C3—C2—Fe1	69.9 (3)	C23—C28—H28	119.4
C1—C2—Fe1	69.1 (2)	C27—C28—H28	119.4
C3—C2—H2	126.0	C30—C29—C34	118.7 (4)
C1—C2—H2	126.0	C30—C29—P2	123.2 (4)
Fe1—C2—H2	126.5	C34—C29—P2	118.0 (4)
C4—C3—C2	107.8 (4)	C31—C30—C29	120.5 (5)
C4—C3—Fe1	69.7 (3)	C31—C30—H30	119.8
C2—C3—Fe1	69.5 (3)	C29—C30—H30	119.8
C4—C3—H3	126.1	C32—C31—C30	120.5 (5)
C2—C3—H3	126.1	C32—C31—H31	119.7
Fe1—C3—H3	126.3	C30—C31—H31	119.7
C5—C4—C3	108.9 (4)	C31—C32—C33	119.9 (5)
C5—C4—Fe1	69.9 (3)	C31—C32—H32	120.1
C3—C4—Fe1	69.9 (3)	C33—C32—H32	120.1
C5—C4—H4	125.5	C34—C33—C32	120.1 (5)
C3—C4—H4	125.5	C34—C33—H33	119.9
Fe1—C4—H4	126.2	C32—C33—H33	119.9
C4—C5—C1	107.9 (4)	C33—C34—C29	120.3 (5)
C4—C5—Fe1	69.9 (3)	C33—C34—H34	119.9
C1—C5—Fe1	69.0 (2)	C29—C34—H34	119.9
C4—C5—H5	126.0	C35—O1—H1A	109.5
C1—C5—H5	126.0	O1—C35—H35A	109.5
Fe1—C5—H5	126.6	O1—C35—H35B	109.5
C7—C6—C11	119.1 (4)	H35A—C35—H35B	109.5
C7—C6—P1	119.0 (4)	O1—C35—H35C	109.5
C11—C6—P1	121.8 (4)	H35A—C35—H35C	109.5
C6—C7—C8	119.9 (5)	H35B—C35—H35C	109.5
C6—C7—H7	120.1	C36—O2—H2B	109.5
C8—C7—H7	120.1	O2—C36—H36A	109.5
C9—C8—C7	120.9 (6)	O2—C36—H36B	109.5
C9—C8—H8	119.5	H36A—C36—H36B	109.5
C7—C8—H8	119.5	O2—C36—H36C	109.5
C8—C9—C10	119.6 (5)	H36A—C36—H36C	109.5
C8—C9—H9	120.2	H36B—C36—H36C	109.5
C6—P1—C1—C2	−24.5 (5)	C23—P2—C18—C19	−28.2 (4)
C12—P1—C1—C2	85.6 (4)	C29—P2—C18—C19	81.2 (4)

Au1—P1—C1—C2	−154.1 (4)	Au2—P2—C18—C19	−154.9 (3)
C6—P1—C1—C5	162.0 (4)	C23—P2—C18—C22	155.5 (3)
C12—P1—C1—C5	−87.9 (4)	C29—P2—C18—C22	−95.0 (4)
Au1—P1—C1—C5	32.4 (4)	Au2—P2—C18—C22	28.8 (4)
C6—P1—C1—Fe1	71.6 (3)	C23—P2—C18—Fe1	65.2 (3)
C12—P1—C1—Fe1	−178.3 (3)	C29—P2—C18—Fe1	174.7 (3)
Au1—P1—C1—Fe1	−58.1 (3)	Au2—P2—C18—Fe1	−61.5 (3)
C5—C1—C2—C3	−0.9 (5)	C22—C18—C19—C20	0.1 (5)
P1—C1—C2—C3	−175.2 (3)	P2—C18—C19—C20	−176.6 (3)
Fe1—C1—C2—C3	59.3 (3)	Fe1—C18—C19—C20	59.6 (3)
C5—C1—C2—Fe1	−60.2 (3)	C22—C18—C19—Fe1	−59.5 (3)
P1—C1—C2—Fe1	125.5 (4)	P2—C18—C19—Fe1	123.8 (3)
C1—C2—C3—C4	0.6 (5)	C18—C19—C20—C21	0.3 (5)
Fe1—C2—C3—C4	59.4 (3)	Fe1—C19—C20—C21	59.3 (3)
C1—C2—C3—Fe1	−58.8 (3)	C18—C19—C20—Fe1	−59.0 (3)
C2—C3—C4—C5	0.0 (5)	C19—C20—C21—C22	−0.6 (5)
Fe1—C3—C4—C5	59.3 (3)	Fe1—C20—C21—C22	58.8 (3)
C2—C3—C4—Fe1	−59.3 (3)	C19—C20—C21—Fe1	−59.4 (3)
C3—C4—C5—C1	−0.5 (5)	C20—C21—C22—C18	0.6 (5)
Fe1—C4—C5—C1	58.7 (3)	Fe1—C21—C22—C18	59.9 (3)
C3—C4—C5—Fe1	−59.3 (3)	C20—C21—C22—Fe1	−59.3 (3)
C2—C1—C5—C4	0.9 (5)	C19—C18—C22—C21	−0.5 (5)
P1—C1—C5—C4	175.6 (3)	P2—C18—C22—C21	176.4 (3)
Fe1—C1—C5—C4	−59.3 (3)	Fe1—C18—C22—C21	−60.2 (3)
C2—C1—C5—Fe1	60.2 (3)	C19—C18—C22—Fe1	59.7 (3)
P1—C1—C5—Fe1	−125.1 (3)	P2—C18—C22—Fe1	−123.4 (3)
C1—P1—C6—C7	−113.1 (4)	C18—P2—C23—C28	82.6 (4)
C12—P1—C6—C7	138.3 (4)	C29—P2—C23—C28	−27.3 (5)
Au1—P1—C6—C7	12.5 (4)	Au2—P2—C23—C28	−154.0 (4)
C1—P1—C6—C11	69.6 (4)	C18—P2—C23—C24	−95.9 (4)
C12—P1—C6—C11	−38.9 (4)	C29—P2—C23—C24	154.2 (4)
Au1—P1—C6—C11	−164.8 (3)	Au2—P2—C23—C24	27.4 (4)
C11—C6—C7—C8	0.2 (8)	C28—C23—C24—C25	0.0 (7)
P1—C6—C7—C8	−177.2 (4)	P2—C23—C24—C25	178.7 (4)
C6—C7—C8—C9	−1.2 (9)	C23—C24—C25—C26	−0.1 (8)
C7—C8—C9—C10	0.8 (10)	C24—C25—C26—C27	0.3 (9)
C8—C9—C10—C11	0.5 (9)	C25—C26—C27—C28	−0.4 (9)
C9—C10—C11—C6	−1.5 (7)	C24—C23—C28—C27	−0.1 (8)
C7—C6—C11—C10	1.2 (7)	P2—C23—C28—C27	−178.7 (4)
P1—C6—C11—C10	178.4 (3)	C26—C27—C28—C23	0.3 (9)
C1—P1—C12—C17	152.1 (3)	C18—P2—C29—C30	−16.6 (4)
C6—P1—C12—C17	−97.4 (4)	C23—P2—C29—C30	93.1 (4)
Au1—P1—C12—C17	32.2 (4)	Au2—P2—C29—C30	−138.6 (4)
C1—P1—C12—C13	−25.2 (4)	C18—P2—C29—C34	165.1 (4)
C6—P1—C12—C13	85.4 (4)	C23—P2—C29—C34	−85.2 (4)
Au1—P1—C12—C13	−145.1 (3)	Au2—P2—C29—C34	43.1 (4)
C17—C12—C13—C14	1.6 (7)	C34—C29—C30—C31	2.3 (7)
P1—C12—C13—C14	178.9 (4)	P2—C29—C30—C31	−176.0 (4)

C12—C13—C14—C15	−1.3 (7)	C29—C30—C31—C32	−1.3 (8)
C13—C14—C15—C16	0.1 (8)	C30—C31—C32—C33	0.3 (9)
C14—C15—C16—C17	0.7 (8)	C31—C32—C33—C34	−0.4 (10)
C13—C12—C17—C16	−0.8 (7)	C32—C33—C34—C29	1.5 (10)
P1—C12—C17—C16	−178.1 (3)	C30—C29—C34—C33	−2.4 (8)
C15—C16—C17—C12	−0.4 (7)	P2—C29—C34—C33	175.9 (5)

Hydrogen-bond geometry (Å, º)

Cg1 and Cg2 are the centroids of the C7–C11 and C12–C16 phenyl rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···S1	0.84	2.63	3.465 (6)	170
C3—H3···S1^{i}	0.95	2.79	3.734 (5)	175
C27—H27···*Cg*(1)^{ii}	0.95	2.83	3.659 (6)	146
C32—H32···*Cg*(2)^{iii}	0.95	2.88	3.717 (6)	147

Symmetry codes: (i) *x*+1/2, −*y*+1/2, *z*+1/2; (ii) *x*−1/2, −*y*+1/2, *z*+1/2; (iii) −*x*+1/2, *y*+1/2, −*z*+1/2.