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(μ-Diphenylphosphanido-κ^2P:P')bis[2,2′-(pyridine-2,6-diyl)diphenyl-$\kappa^3C^1,N,C^{1'}$)-gold(III)] perchlorate acetonitrile solvate

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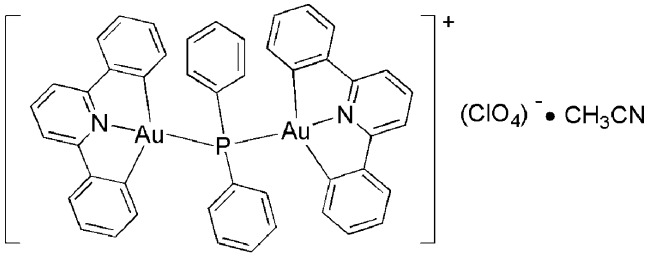
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.005 Å; R factor = 0.029; wR factor = 0.058; data-to-parameter ratio = 19.1.

The title complex, $[Au_2(C_{17}H_{11}N)_2(C_{12}H_{10}P)]ClO_4\cdot C_2H_3N$, contains two Au^{III} atoms bridged by a diphenylphosphanide ligand. Each Au atom is in a square-planar environment coordinated by diphenylphosphanide and 2,6-diphenylpyridine ligands. There are weak π–π stacking interactions between neighbouring molecules (the interplanar separations between two neighbouring dpp units are 3.40 and 3.57 Å). The intramolecular Au···Au separation is 3.788 (5) Å. The crystal structure shows weak intermolecular C—H···O and C—H···N hydrogen bonds involving an O atom of the perchlorate counter-ion and the N atom of the acetonitrile solvent molecule, respectively.

Related literature

For related literature, see: Goshe *et al.* (2003); Kui *et al.* (2006); Li *et al.* (2006); Lu *et al.* (2004); Wong *et al.* (1998); Yam *et al.* (2002).



Experimental

Crystal data

$[Au_2(C_{17}H_{11}N)_2(C_{12}H_{10}P)]ClO_4\cdot C_2H_3N$
M_r = 1178.14
Monoclinic, $P2_1/c$
a = 10.0612 (16) Å
b = 13.526 (2) Å
c = 29.640 (5) Å
β = 98.828 (4)°
V = 3985.9 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 7.51 mm^{-1}
T = 113 (2) K
0.32 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.147, T_{max} = 0.221
38570 measured reflections
10221 independent reflections
8923 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.057
S = 1.04
10221 reflections
534 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.52 e Å^{-3}
$\Delta\rho_{min}$ = −1.55 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Au1—N1	2.027 (3)	Au2—N2	2.041 (3)
Au1—C17	2.105 (3)	Au2—C18	2.091 (3)
Au1—C1	2.111 (3)	Au2—C34	2.113 (3)
Au1—P1	2.3121 (9)	Au2—P1	2.3180 (8)
N1—Au1—C17	79.97 (12)	N2—Au2—C18	80.19 (12)
N1—Au1—C1	80.18 (12)	N2—Au2—C34	80.02 (12)
C17—Au1—C1	160.10 (13)	C18—Au2—C34	160.15 (13)
N1—Au1—P1	172.84 (8)	N2—Au2—P1	173.99 (8)
C17—Au1—P1	95.15 (9)	C18—Au2—P1	93.98 (9)
C1—Au1—P1	104.75 (10)	C34—Au2—P1	105.84 (9)

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

D—H···A	D—H	H···A	D···A	D—H···A
C21—H21···O3^{i}	0.95	2.46	3.311 (7)	149
C36—H36···O2	0.95	2.57	3.372 (8)	143
C38—H38···O2^{ii}	0.95	2.59	3.540 (5)	175
C43—H43···O1^{iii}	0.95	2.59	3.517 (3)	165
C46—H46···N3^{iv}	0.95	2.62	3.417 (4)	142
C48—H48*C*···O1^{v}	0.98	2.54	3.423 (8)	150

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *XP* in *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2152).

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supplementary materials

Acta Cryst. (2008). E**64**, m1126-m1127 [**doi:10.1107/S1600536808024537**]

(μ-Diphenylphosphanido-κ^2P:P')bis[2,2'-(pyridine-2,6-diyl)diphenyl-κ^3C^1,N,$C^{1'}$)gold(III)] perchlorate acetonitrile solvate

X.-S. Li, J. Mo, S.-M. Zhang, L. Yuan and J.-H. Liu

Comment

Recently, extensive investigations on the biological properties of gold(III) have been reported (Kui *et al.*, 2006; Wong *et al.*, 1998). The stability of metal compounds is usually enhanced by multidentate chelating ligands. Li and his co-workers have reported multinuclear gold complex of 2,6-diphenyl-Pyridine ligand (dpp) to generate a planar gold(III) moiety (Li *et al.*, 2006). In this context, the title complex, (I), has been prepared and its crystal structure is reported here.

The title compound show gold(III) atoms bridged by diphenylphosphanide. Each Au atom is surrounded by one P atom from diphenylphosphanide ligand and two C atoms, one N atom from dpp in a square-planar geometry, the least-squares plane through Au^{III} and dpp has a mean deviation of 0.04 (3) Å. The intramolecular Au···Au contact of 3.788Å is beyond a normal range of metal-metal interactions for d^8 metal ions (3.09–3.50 Å) (Yam *et al.*, 2002; Goshe *et al.*, 2003; Lu *et al.*, 2004). The Au–N(pyridyl) distances (2.027 (3), 2.041 (3) Å) are comparable to the related distances found in $[Au(dpp)L]^{n+}$ analogues (1.94–2.06 Å), The Au–*C*(phenyl) distances (2.091 (3)–2.113 (3) Å) are comparable to the related distances found in $[Au(dpp)L]^{n+}$ analogues (2.06–2.13 Å) (Li *et al.*, 2006). The interplanar separation between two neighbouring dpp molecules are 3.40 and 3.57Å (Fig. 2). The crystal packing shows weak intermolecular C-H..O and C-H···N hydrogen bonds with O atoms of perchlorate counter-ion and N atom of acetonitrile molecule respectively. (Fig. 3, Table 2).

Experimental

A mixture of Au(dpp)Cl (0.092 g, 0.2 mmol) and diphenylphosphine (0.018 g, 0.1 mmol) in acetonitrile (30 ml) was stirred for 2 h. Excess $LiClO_4$ was then added to yield a yellow precipitate, which was filtered, washed with diethyl ether. The precipitate was redissolve in acetonitrile. Yellow crystals suitable for X-ray diffraction were formed by vapour diffusion of diethyl ethyl ether into acetonitrile solution.

Refinement

All hydrogen atoms were generated geometrically (C—H bond lengths of methyl group fixed at 0.98 Å, C—H bond lengths of pyridyl and phenyl fixed at 0.95 Å), assigned appropriated isotropic thermal parameters, $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

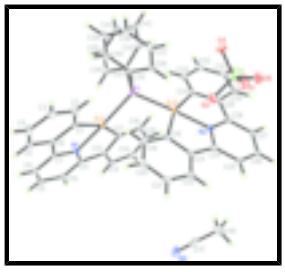


Fig. 1. Molecular structure of the title compound showing the atom-numbering scheme and displacement ellipsoids drawn at the 40% probability level.

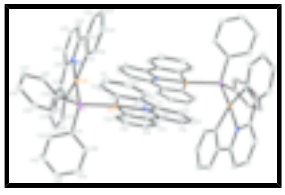


Fig. 2. There is π-π interaction between between neighbouring molecules. The anions and solvent molecules are not shown, and H atoms have been omitted. Displacement ellipsoids are at the 40% probability level and Atoms without label are generated by the symmetry operation (1 - *x*, 1 - *y*, -*z*).

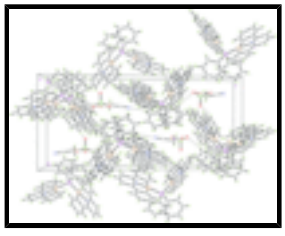


Fig. 3. The crystal packing of the complex, viewed down the *a* axis, showing hydrogen bonds as dashed lines.

[μ-Diphenylphosphanido-$\kappa^2P:P^1$]bis[(2,6-diphenylpyridine- $\kappa^3C^2,N,C^{2'}$)gold(III)] perchlorate acetonitrile solvate

Crystal data

$[Au_2(C_{17}H_{11}N)_2(C_{12}H_{10}P)]ClO_4\cdot C_2H_3N$	F_{000} = 2264
M_r = 1178.14	D_x = 1.963 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71070 Å
Hall symbol: -P 2ybc	Cell parameters from 13552 reflections
a = 10.0612 (16) Å	θ = 1.4–28.7º
b = 13.526 (2) Å	μ = 7.51 mm^{-1}
c = 29.640 (5) Å	*T* = 113 (2) K
β = 98.828 (4)º	Block, yellow
V = 3985.9 (11) Å^3	0.32 × 0.22 × 0.20 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	10221 independent reflections
Radiation source: fine-focus sealed tube	8923 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.039
Detector resolution: 7.31 pixels mm^{-1}	θ_{max} = 28.7º

T = 113(2) K

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

T_{min} = 0.147, T_{max} = 0.221

38570 measured reflections

θ_{min} = 1.4°

h = −13→13

k = −18→17

l = −39→39

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.028

$wR(F^2)$ = 0.057

S = 1.04

10221 reflections

534 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0278P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.002

$\Delta\rho_{max}$ = 1.52 e Å^{-3}

$\Delta\rho_{min}$ = −1.55 e Å^{-3}

Extinction correction: none

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Au1	0.638497 (12)	0.281287 (9)	0.032930 (4)	0.01055 (4)
Au2	0.566168 (12)	0.331694 (9)	0.152497 (4)	0.00993 (4)
Cl1	0.78527 (10)	0.29051 (6)	0.29597 (3)	0.01996 (19)
P1	0.60967 (9)	0.21001 (6)	0.10167 (3)	0.01063 (17)
O1	0.6459 (3)	0.3221 (3)	0.29088 (12)	0.0507 (9)
O2	0.8447 (3)	0.3313 (2)	0.25911 (10)	0.0406 (8)
O3	0.7868 (3)	0.18429 (18)	0.29417 (10)	0.0324 (7)
O5	0.8547 (3)	0.3239 (2)	0.33921 (10)	0.0333 (7)
N1	0.6406 (3)	0.33719 (18)	−0.03039 (9)	0.0119 (6)
N2	0.5487 (3)	0.44270 (18)	0.19785 (9)	0.0125 (6)
N3	0.6293 (4)	0.8322 (2)	0.06888 (13)	0.0353 (9)
C1	0.8332 (3)	0.2378 (2)	0.02273 (12)	0.0134 (7)

C2	0.9377 (4)	0.1917 (3)	0.05082 (13)	0.0196 (8)
H2	0.9268	0.1750	0.0812	0.024*
C3	1.0580 (4)	0.1693 (3)	0.03557 (14)	0.0234 (8)
H3	1.1276	0.1372	0.0556	0.028*
C4	1.0781 (4)	0.1929 (3)	−0.00813 (14)	0.0227 (8)
H4	1.1602	0.1759	−0.0183	0.027*
C5	0.9785 (4)	0.2413 (3)	−0.03691 (13)	0.0187 (8)
H5	0.9924	0.2590	−0.0669	0.022*
C6	0.8559 (3)	0.2646 (2)	−0.02188 (12)	0.0134 (7)
C7	0.7489 (3)	0.3170 (2)	−0.05110 (12)	0.0131 (7)
C8	0.7447 (4)	0.3461 (2)	−0.09612 (13)	0.0189 (8)
H8	0.8185	0.3328	−0.1117	0.023*
C9	0.6330 (4)	0.3944 (3)	−0.11806 (13)	0.0248 (9)
H9	0.6298	0.4134	−0.1491	0.030*
C10	0.5247 (4)	0.4158 (3)	−0.09585 (13)	0.0214 (8)
H10	0.4492	0.4511	−0.1110	0.026*
C11	0.5288 (3)	0.3846 (2)	−0.05116 (12)	0.0142 (7)
C12	0.4238 (3)	0.3933 (2)	−0.02224 (11)	0.0127 (7)
C13	0.3035 (4)	0.4442 (2)	−0.03724 (12)	0.0184 (7)
H13	0.2895	0.4741	−0.0666	0.022*
C14	0.2057 (4)	0.4508 (3)	−0.00958 (13)	0.0205 (8)
H14	0.1246	0.4858	−0.0195	0.025*
C15	0.2268 (4)	0.4059 (3)	0.03288 (13)	0.0207 (8)
H15	0.1593	0.4100	0.0520	0.025*
C16	0.3458 (4)	0.3546 (2)	0.04811 (12)	0.0173 (7)
H16	0.3577	0.3238	0.0773	0.021*
C17	0.4473 (3)	0.3480 (2)	0.02116 (12)	0.0134 (7)
C18	0.7480 (3)	0.4054 (2)	0.15075 (11)	0.0134 (7)
C19	0.8548 (3)	0.3858 (3)	0.12706 (12)	0.0159 (7)
H19	0.8515	0.3290	0.1080	0.019*
C20	0.9665 (4)	0.4483 (3)	0.13097 (13)	0.0233 (8)
H20	1.0380	0.4332	0.1146	0.028*
C21	0.9750 (4)	0.5317 (3)	0.15812 (14)	0.0232 (8)
H21	1.0506	0.5743	0.1599	0.028*
C22	0.8716 (4)	0.5523 (3)	0.18275 (12)	0.0211 (8)
H22	0.8770	0.6089	0.2019	0.025*
C23	0.7597 (3)	0.4903 (2)	0.17957 (12)	0.0158 (7)
C24	0.6487 (4)	0.5093 (2)	0.20564 (12)	0.0154 (7)
C25	0.6358 (4)	0.5876 (2)	0.23508 (12)	0.0205 (8)
H25	0.7051	0.6355	0.2416	0.025*
C26	0.5196 (4)	0.5942 (2)	0.25476 (12)	0.0215 (8)
H26	0.5077	0.6487	0.2739	0.026*
C27	0.4211 (4)	0.5227 (2)	0.24684 (12)	0.0188 (8)
H27	0.3433	0.5269	0.2613	0.023*
C28	0.4362 (3)	0.4449 (2)	0.21773 (11)	0.0135 (7)
C29	0.3418 (3)	0.3654 (2)	0.20285 (12)	0.0145 (7)
C30	0.2188 (4)	0.3568 (3)	0.22005 (13)	0.0190 (8)
H30	0.1987	0.4011	0.2429	0.023*
C31	0.1278 (4)	0.2837 (3)	0.20352 (13)	0.0207 (8)

H31	0.0463	0.2762	0.2157	0.025*
C32	0.1563 (4)	0.2214 (3)	0.16901 (13)	0.0202 (8)
H32	0.0926	0.1727	0.1569	0.024*
C33	0.2777 (3)	0.2295 (2)	0.15193 (12)	0.0171 (7)
H33	0.2949	0.1864	0.1282	0.021*
C34	0.3738 (3)	0.2993 (2)	0.16887 (11)	0.0124 (7)
C35	0.7453 (3)	0.1350 (2)	0.13295 (11)	0.0128 (7)
C36	0.7981 (3)	0.1545 (2)	0.17805 (12)	0.0139 (7)
H36	0.7716	0.2125	0.1924	0.017*
C37	0.8898 (3)	0.0893 (2)	0.20256 (12)	0.0172 (7)
H37	0.9238	0.1024	0.2337	0.021*
C38	0.9313 (3)	0.0060 (3)	0.18167 (13)	0.0184 (8)
H38	0.9949	−0.0376	0.1982	0.022*
C39	0.8799 (4)	−0.0139 (3)	0.13654 (13)	0.0208 (8)
H39	0.9095	−0.0707	0.1220	0.025*
C40	0.7854 (4)	0.0489 (3)	0.11244 (13)	0.0204 (8)
H40	0.7476	0.0334	0.0819	0.024*
C41	0.4844 (3)	0.1125 (2)	0.08729 (11)	0.0122 (7)
C42	0.4565 (4)	0.0507 (2)	0.12251 (13)	0.0215 (8)
H42	0.5013	0.0611	0.1528	0.026*
C43	0.3644 (4)	−0.0252 (3)	0.11367 (15)	0.0268 (9)
H43	0.3430	−0.0650	0.1380	0.032*
C44	0.3032 (4)	−0.0431 (3)	0.06923 (16)	0.0282 (10)
H44	0.2401	−0.0954	0.0631	0.034*
C45	0.3338 (4)	0.0151 (3)	0.03385 (14)	0.0242 (8)
H45	0.2940	0.0011	0.0034	0.029*
C46	0.4236 (3)	0.0948 (2)	0.04281 (12)	0.0155 (7)
H46	0.4424	0.1361	0.0186	0.019*
C47	0.6302 (4)	0.8197 (3)	0.10658 (16)	0.0301 (10)
C48	0.6321 (5)	0.8047 (4)	0.15590 (16)	0.0448 (12)
H48A	0.6670	0.8642	0.1725	0.067*
H48B	0.6899	0.7482	0.1662	0.067*
H48C	0.5405	0.7916	0.1618	0.067*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.01160 (7)	0.01217 (6)	0.00809 (6)	0.00003 (5)	0.00215 (5)	0.00087 (4)
Au2	0.01163 (7)	0.00982 (6)	0.00834 (6)	−0.00009 (5)	0.00155 (5)	−0.00021 (4)
Cl1	0.0299 (5)	0.0169 (4)	0.0141 (4)	−0.0020 (4)	0.0064 (4)	−0.0008 (3)
P1	0.0135 (4)	0.0105 (4)	0.0080 (4)	0.0006 (3)	0.0019 (3)	−0.0002 (3)
O1	0.036 (2)	0.065 (2)	0.050 (2)	0.0258 (17)	0.0025 (17)	−0.0007 (18)
O2	0.068 (2)	0.0353 (17)	0.0223 (17)	−0.0232 (16)	0.0181 (17)	−0.0033 (13)
O3	0.052 (2)	0.0138 (13)	0.0306 (18)	−0.0011 (13)	0.0035 (15)	−0.0016 (11)
O5	0.0417 (19)	0.0377 (17)	0.0206 (16)	−0.0132 (14)	0.0046 (14)	−0.0053 (13)
N1	0.0158 (15)	0.0110 (13)	0.0094 (14)	−0.0019 (11)	0.0036 (12)	0.0016 (10)
N2	0.0196 (15)	0.0096 (12)	0.0082 (14)	0.0016 (12)	0.0016 (12)	−0.0013 (10)
N3	0.052 (3)	0.0319 (19)	0.023 (2)	−0.0020 (18)	0.0084 (19)	−0.0059 (15)

C1	0.0123 (17)	0.0161 (16)	0.0127 (17)	−0.0003 (13)	0.0049 (14)	−0.0046 (13)
C2	0.0166 (19)	0.0259 (19)	0.0154 (19)	0.0015 (15)	−0.0007 (15)	0.0031 (15)
C3	0.018 (2)	0.030 (2)	0.021 (2)	0.0035 (16)	−0.0010 (16)	−0.0006 (16)
C4	0.0126 (19)	0.032 (2)	0.024 (2)	0.0026 (16)	0.0060 (16)	−0.0055 (16)
C5	0.0176 (19)	0.0222 (18)	0.0174 (19)	−0.0019 (15)	0.0063 (15)	−0.0009 (14)
C6	0.0142 (18)	0.0123 (15)	0.0136 (18)	−0.0023 (13)	0.0022 (14)	−0.0010 (12)
C7	0.0164 (18)	0.0111 (15)	0.0122 (17)	−0.0015 (13)	0.0035 (14)	−0.0016 (12)
C8	0.026 (2)	0.0181 (17)	0.0140 (19)	0.0015 (15)	0.0083 (16)	0.0009 (14)
C9	0.032 (2)	0.030 (2)	0.014 (2)	0.0038 (18)	0.0091 (17)	0.0079 (16)
C10	0.029 (2)	0.0221 (18)	0.0139 (19)	0.0071 (16)	0.0040 (16)	0.0076 (14)
C11	0.0203 (18)	0.0089 (15)	0.0127 (18)	−0.0018 (13)	0.0004 (14)	0.0021 (12)
C12	0.0162 (18)	0.0103 (15)	0.0111 (17)	−0.0010 (13)	0.0003 (14)	0.0001 (12)
C13	0.0211 (19)	0.0169 (16)	0.0164 (19)	−0.0007 (15)	0.0002 (15)	0.0039 (14)
C14	0.0180 (19)	0.0204 (18)	0.023 (2)	0.0064 (15)	0.0015 (16)	0.0034 (15)
C15	0.0155 (19)	0.0259 (19)	0.022 (2)	0.0023 (15)	0.0072 (16)	−0.0017 (15)
C16	0.0186 (19)	0.0216 (17)	0.0112 (18)	0.0016 (15)	0.0008 (14)	0.0029 (13)
C17	0.0134 (17)	0.0121 (15)	0.0151 (18)	0.0019 (13)	0.0034 (14)	0.0002 (13)
C18	0.0132 (17)	0.0153 (16)	0.0103 (17)	−0.0020 (13)	−0.0026 (13)	0.0045 (13)
C19	0.0131 (17)	0.0194 (17)	0.0147 (18)	0.0002 (14)	0.0001 (14)	0.0009 (14)
C20	0.018 (2)	0.032 (2)	0.020 (2)	−0.0012 (17)	0.0048 (16)	0.0053 (16)
C21	0.0145 (19)	0.027 (2)	0.027 (2)	−0.0088 (16)	−0.0008 (16)	0.0053 (16)
C22	0.028 (2)	0.0164 (17)	0.017 (2)	−0.0059 (16)	−0.0027 (16)	0.0020 (14)
C23	0.0172 (18)	0.0145 (16)	0.0145 (18)	−0.0003 (14)	−0.0013 (14)	0.0035 (13)
C24	0.0219 (19)	0.0123 (15)	0.0098 (17)	−0.0021 (14)	−0.0045 (14)	0.0009 (12)
C25	0.031 (2)	0.0137 (16)	0.0152 (19)	−0.0057 (15)	−0.0004 (16)	−0.0037 (13)
C26	0.039 (2)	0.0150 (17)	0.0103 (18)	0.0040 (16)	0.0026 (17)	−0.0039 (13)
C27	0.026 (2)	0.0168 (17)	0.0143 (19)	0.0075 (15)	0.0049 (16)	−0.0001 (13)
C28	0.0166 (18)	0.0138 (15)	0.0100 (17)	0.0046 (14)	0.0016 (14)	0.0006 (13)
C29	0.0154 (18)	0.0160 (16)	0.0116 (17)	0.0027 (14)	0.0008 (14)	0.0036 (13)
C30	0.0187 (19)	0.0213 (18)	0.019 (2)	0.0076 (15)	0.0076 (16)	0.0000 (14)
C31	0.0130 (18)	0.029 (2)	0.021 (2)	0.0020 (15)	0.0049 (15)	0.0052 (16)
C32	0.0130 (18)	0.0248 (19)	0.022 (2)	−0.0003 (15)	0.0016 (15)	0.0050 (15)
C33	0.0154 (18)	0.0188 (17)	0.0165 (19)	0.0022 (14)	0.0001 (15)	−0.0004 (14)
C34	0.0146 (17)	0.0144 (15)	0.0081 (16)	0.0001 (13)	0.0019 (13)	0.0029 (12)
C35	0.0154 (17)	0.0130 (15)	0.0104 (17)	0.0010 (13)	0.0033 (14)	0.0030 (12)
C36	0.0113 (17)	0.0159 (16)	0.0151 (18)	−0.0001 (13)	0.0034 (14)	0.0010 (13)
C37	0.0122 (17)	0.0244 (18)	0.0143 (19)	−0.0003 (14)	−0.0001 (14)	0.0054 (14)
C38	0.0141 (18)	0.0191 (17)	0.023 (2)	0.0032 (14)	0.0062 (15)	0.0063 (14)
C39	0.025 (2)	0.0153 (17)	0.024 (2)	0.0075 (15)	0.0075 (17)	−0.0007 (14)
C40	0.023 (2)	0.0201 (18)	0.017 (2)	0.0035 (15)	−0.0011 (15)	−0.0027 (14)
C41	0.0136 (17)	0.0104 (15)	0.0131 (17)	−0.0016 (13)	0.0034 (14)	−0.0030 (12)
C42	0.029 (2)	0.0169 (17)	0.020 (2)	−0.0023 (16)	0.0071 (17)	0.0006 (15)
C43	0.031 (2)	0.0155 (18)	0.037 (3)	−0.0063 (16)	0.015 (2)	0.0023 (16)
C44	0.022 (2)	0.0159 (18)	0.048 (3)	−0.0069 (16)	0.009 (2)	−0.0033 (17)
C45	0.020 (2)	0.0223 (19)	0.028 (2)	−0.0004 (16)	−0.0060 (16)	−0.0089 (16)
C46	0.0137 (18)	0.0177 (16)	0.0149 (18)	0.0008 (14)	0.0019 (14)	−0.0018 (13)
C47	0.040 (3)	0.0199 (19)	0.031 (3)	0.0015 (18)	0.006 (2)	−0.0050 (17)
C48	0.062 (3)	0.046 (3)	0.027 (3)	−0.001 (3)	0.008 (2)	0.008 (2)

Geometric parameters (Å, °)

Au1—N1	2.027 (3)	C20—C21	1.380 (5)
Au1—C17	2.105 (3)	C20—H20	0.9500
Au1—C1	2.111 (3)	C21—C22	1.388 (5)
Au1—P1	2.3121 (9)	C21—H21	0.9500
Au2—N2	2.041 (3)	C22—C23	1.395 (5)
Au2—C18	2.091 (3)	C22—H22	0.9500
Au2—C34	2.113 (3)	C23—C24	1.474 (5)
Au2—P1	2.3180 (8)	C24—C25	1.391 (4)
Cl1—O2	1.434 (3)	C25—C26	1.387 (5)
Cl1—O5	1.436 (3)	C25—H25	0.9500
Cl1—O3	1.438 (3)	C26—C27	1.378 (5)
Cl1—O1	1.451 (3)	C26—H26	0.9500
P1—C41	1.829 (3)	C27—C28	1.384 (4)
P1—C35	1.833 (3)	C27—H27	0.9500
N1—C11	1.357 (4)	C28—C29	1.458 (5)
N1—C7	1.358 (4)	C29—C30	1.413 (4)
N2—C24	1.344 (4)	C29—C34	1.421 (4)
N2—C28	1.354 (4)	C30—C31	1.386 (5)
N3—C47	1.129 (5)	C30—H30	0.9500
C1—C2	1.385 (5)	C31—C32	1.389 (5)
C1—C6	1.423 (5)	C31—H31	0.9500
C2—C3	1.389 (5)	C32—C33	1.396 (5)
C2—H2	0.9500	C32—H32	0.9500
C3—C4	1.379 (5)	C33—C34	1.389 (5)
C3—H3	0.9500	C33—H33	0.9500
C4—C5	1.379 (5)	C35—C36	1.386 (5)
C4—H4	0.9500	C35—C40	1.402 (4)
C5—C6	1.409 (4)	C36—C37	1.397 (5)
C5—H5	0.9500	C36—H36	0.9500
C6—C7	1.457 (5)	C37—C38	1.382 (5)
C7—C8	1.386 (5)	C37—H37	0.9500
C8—C9	1.374 (5)	C38—C39	1.385 (5)
C8—H8	0.9500	C38—H38	0.9500
C9—C10	1.387 (5)	C39—C40	1.389 (5)
C9—H9	0.9500	C39—H39	0.9500
C10—C11	1.384 (5)	C40—H40	0.9500
C10—H10	0.9500	C41—C46	1.387 (5)
C11—C12	1.464 (4)	C41—C42	1.399 (4)
C12—C13	1.404 (5)	C42—C43	1.382 (5)
C12—C17	1.412 (4)	C42—H42	0.9500
C13—C14	1.377 (5)	C43—C44	1.387 (6)
C13—H13	0.9500	C43—H43	0.9500
C14—C15	1.384 (5)	C44—C45	1.383 (5)
C14—H14	0.9500	C44—H44	0.9500
C15—C16	1.397 (5)	C45—C46	1.405 (5)
C15—H15	0.9500	C45—H45	0.9500

C16—C17	1.392 (4)	C46—H46	0.9500
C16—H16	0.9500	C47—C48	1.473 (6)
C18—C19	1.397 (4)	C48—H48A	0.9800
C18—C23	1.425 (5)	C48—H48B	0.9800
C19—C20	1.397 (5)	C48—H48C	0.9800
C19—H19	0.9500		
N1—Au1—C17	79.97 (12)	C21—C20—H20	119.3
N1—Au1—C1	80.18 (12)	C19—C20—H20	119.3
C17—Au1—C1	160.10 (13)	C20—C21—C22	119.1 (3)
N1—Au1—P1	172.84 (8)	C20—C21—H21	120.5
C17—Au1—P1	95.15 (9)	C22—C21—H21	120.5
C1—Au1—P1	104.75 (10)	C21—C22—C23	120.4 (3)
N2—Au2—C18	80.19 (12)	C21—C22—H22	119.8
N2—Au2—C34	80.02 (12)	C23—C22—H22	119.8
C18—Au2—C34	160.15 (13)	C22—C23—C18	121.1 (3)
N2—Au2—P1	173.99 (8)	C22—C23—C24	121.9 (3)
C18—Au2—P1	93.98 (9)	C18—C23—C24	117.1 (3)
C34—Au2—P1	105.84 (9)	N2—C24—C25	118.6 (3)
O2—Cl1—O5	110.88 (18)	N2—C24—C23	113.6 (3)
O2—Cl1—O3	110.39 (17)	C25—C24—C23	127.8 (3)
O5—Cl1—O3	109.96 (18)	C26—C25—C24	118.6 (3)
O2—Cl1—O1	108.4 (2)	C26—C25—H25	120.7
O5—Cl1—O1	109.28 (19)	C24—C25—H25	120.7
O3—Cl1—O1	107.8 (2)	C27—C26—C25	120.9 (3)
C41—P1—C35	98.71 (15)	C27—C26—H26	119.6
C41—P1—Au1	105.69 (11)	C25—C26—H26	119.6
C35—P1—Au1	119.48 (10)	C26—C27—C28	119.7 (3)
C41—P1—Au2	118.14 (10)	C26—C27—H27	120.2
C35—P1—Au2	105.32 (11)	C28—C27—H27	120.2
Au1—P1—Au2	109.78 (3)	N2—C28—C27	117.8 (3)
C11—N1—C7	123.8 (3)	N2—C28—C29	113.7 (3)
C11—N1—Au1	118.1 (2)	C27—C28—C29	128.4 (3)
C7—N1—Au1	117.8 (2)	C30—C29—C34	120.7 (3)
C24—N2—C28	124.4 (3)	C30—C29—C28	121.2 (3)
C24—N2—Au2	117.9 (2)	C34—C29—C28	118.1 (3)
C28—N2—Au2	117.7 (2)	C31—C30—C29	119.9 (3)
C2—C1—C6	117.3 (3)	C31—C30—H30	120.0
C2—C1—Au1	132.4 (3)	C29—C30—H30	120.0
C6—C1—Au1	110.3 (2)	C30—C31—C32	119.6 (3)
C1—C2—C3	121.4 (3)	C30—C31—H31	120.2
C1—C2—H2	119.3	C32—C31—H31	120.2
C3—C2—H2	119.3	C31—C32—C33	120.7 (3)
C4—C3—C2	121.1 (4)	C31—C32—H32	119.7
C4—C3—H3	119.5	C33—C32—H32	119.7
C2—C3—H3	119.5	C34—C33—C32	121.5 (3)
C5—C4—C3	119.6 (3)	C34—C33—H33	119.3
C5—C4—H4	120.2	C32—C33—H33	119.3
C3—C4—H4	120.2	C33—C34—C29	117.6 (3)
C4—C5—C6	120.0 (3)	C33—C34—Au2	132.0 (2)

C4—C5—H5	120.0	C29—C34—Au2	110.3 (2)
C6—C5—H5	120.0	C36—C35—C40	118.9 (3)
C5—C6—C1	120.6 (3)	C36—C35—P1	121.9 (2)
C5—C6—C7	121.5 (3)	C40—C35—P1	118.8 (3)
C1—C6—C7	117.8 (3)	C35—C36—C37	120.5 (3)
N1—C7—C8	118.0 (3)	C35—C36—H36	119.8
N1—C7—C6	113.6 (3)	C37—C36—H36	119.8
C8—C7—C6	128.4 (3)	C38—C37—C36	120.2 (3)
C9—C8—C7	119.5 (3)	C38—C37—H37	119.9
C9—C8—H8	120.2	C36—C37—H37	119.9
C7—C8—H8	120.2	C37—C38—C39	119.9 (3)
C8—C9—C10	121.3 (3)	C37—C38—H38	120.1
C8—C9—H9	119.3	C39—C38—H38	120.1
C10—C9—H9	119.3	C38—C39—C40	120.2 (3)
C11—C10—C9	118.7 (3)	C38—C39—H39	119.9
C11—C10—H10	120.7	C40—C39—H39	119.9
C9—C10—H10	120.7	C39—C40—C35	120.4 (3)
N1—C11—C10	118.6 (3)	C39—C40—H40	119.8
N1—C11—C12	113.2 (3)	C35—C40—H40	119.8
C10—C11—C12	128.1 (3)	C46—C41—C42	119.8 (3)
C13—C12—C17	121.2 (3)	C46—C41—P1	122.3 (3)
C13—C12—C11	121.2 (3)	C42—C41—P1	117.8 (3)
C17—C12—C11	117.6 (3)	C43—C42—C41	120.6 (4)
C14—C13—C12	120.2 (3)	C43—C42—H42	119.7
C14—C13—H13	119.9	C41—C42—H42	119.7
C12—C13—H13	119.9	C42—C43—C44	119.8 (4)
C13—C14—C15	119.2 (3)	C42—C43—H43	120.1
C13—C14—H14	120.4	C44—C43—H43	120.1
C15—C14—H14	120.4	C45—C44—C43	120.2 (3)
C14—C15—C16	121.1 (3)	C45—C44—H44	119.9
C14—C15—H15	119.5	C43—C44—H44	119.9
C16—C15—H15	119.5	C44—C45—C46	120.3 (4)
C17—C16—C15	120.9 (3)	C44—C45—H45	119.8
C17—C16—H16	119.5	C46—C45—H45	119.8
C15—C16—H16	119.5	C41—C46—C45	119.3 (3)
C16—C17—C12	117.4 (3)	C41—C46—H46	120.3
C16—C17—Au1	131.6 (3)	C45—C46—H46	120.3
C12—C17—Au1	111.0 (2)	N3—C47—C48	179.2 (5)
C19—C18—C23	117.1 (3)	C47—C48—H48A	109.5
C19—C18—Au2	131.7 (3)	C47—C48—H48B	109.5
C23—C18—Au2	111.2 (2)	H48A—C48—H48B	109.5
C18—C19—C20	120.9 (3)	C47—C48—H48C	109.5
C18—C19—H19	119.5	H48A—C48—H48C	109.5
C20—C19—H19	119.5	H48B—C48—H48C	109.5
C21—C20—C19	121.4 (3)		
C17—Au1—P1—C41	69.65 (14)	C34—Au2—C18—C23	3.3 (5)
C1—Au1—P1—C41	−109.99 (14)	P1—Au2—C18—C23	179.9 (2)
C17—Au1—P1—C35	179.50 (16)	C23—C18—C19—C20	−1.3 (5)
C1—Au1—P1—C35	−0.14 (16)	Au2—C18—C19—C20	178.8 (3)

C17—Au1—P1—Au2	−58.78 (10)	C18—C19—C20—C21	−0.2 (6)
C1—Au1—P1—Au2	121.58 (10)	C19—C20—C21—C22	1.4 (6)
C18—Au2—P1—C41	179.02 (15)	C20—C21—C22—C23	−0.9 (6)
C34—Au2—P1—C41	−2.15 (16)	C21—C22—C23—C18	−0.7 (5)
C18—Au2—P1—C35	70.08 (14)	C21—C22—C23—C24	179.3 (3)
C34—Au2—P1—C35	−111.09 (14)	C19—C18—C23—C22	1.8 (5)
C18—Au2—P1—Au1	−59.77 (9)	Au2—C18—C23—C22	−178.3 (3)
C34—Au2—P1—Au1	119.07 (10)	C19—C18—C23—C24	−178.2 (3)
C17—Au1—N1—C11	−2.2 (2)	Au2—C18—C23—C24	1.7 (4)
C1—Au1—N1—C11	179.3 (3)	C28—N2—C24—C25	−1.7 (5)
C17—Au1—N1—C7	−176.2 (3)	Au2—N2—C24—C25	177.5 (2)
C1—Au1—N1—C7	5.3 (2)	C28—N2—C24—C23	−179.8 (3)
C18—Au2—N2—C24	1.2 (2)	Au2—N2—C24—C23	−0.6 (4)
C34—Au2—N2—C24	−177.2 (3)	C22—C23—C24—N2	179.2 (3)
C18—Au2—N2—C28	−179.5 (3)	C18—C23—C24—N2	−0.8 (4)
C34—Au2—N2—C28	2.1 (2)	C22—C23—C24—C25	1.3 (6)
N1—Au1—C1—C2	175.4 (4)	C18—C23—C24—C25	−178.7 (3)
C17—Au1—C1—C2	171.1 (3)	N2—C24—C25—C26	−0.7 (5)
P1—Au1—C1—C2	−9.9 (4)	C23—C24—C25—C26	177.0 (3)
N1—Au1—C1—C6	−3.4 (2)	C24—C25—C26—C27	2.6 (5)
C17—Au1—C1—C6	−7.7 (5)	C25—C26—C27—C28	−2.1 (5)
P1—Au1—C1—C6	171.3 (2)	C24—N2—C28—C27	2.2 (5)
C6—C1—C2—C3	−2.3 (5)	Au2—N2—C28—C27	−177.0 (2)
Au1—C1—C2—C3	179.0 (3)	C24—N2—C28—C29	178.8 (3)
C1—C2—C3—C4	0.5 (6)	Au2—N2—C28—C29	−0.4 (4)
C2—C3—C4—C5	1.3 (6)	C26—C27—C28—N2	−0.2 (5)
C3—C4—C5—C6	−1.3 (6)	C26—C27—C28—C29	−176.3 (3)
C4—C5—C6—C1	−0.6 (5)	N2—C28—C29—C30	−179.8 (3)
C4—C5—C6—C7	179.2 (3)	C27—C28—C29—C30	−3.6 (6)
C2—C1—C6—C5	2.3 (5)	N2—C28—C29—C34	−2.7 (4)
Au1—C1—C6—C5	−178.7 (3)	C27—C28—C29—C34	173.5 (3)
C2—C1—C6—C7	−177.5 (3)	C34—C29—C30—C31	−0.5 (5)
Au1—C1—C6—C7	1.5 (4)	C28—C29—C30—C31	176.6 (3)
C11—N1—C7—C8	−0.3 (5)	C29—C30—C31—C32	−2.1 (6)
Au1—N1—C7—C8	173.4 (2)	C30—C31—C32—C33	2.2 (6)
C11—N1—C7—C6	−179.5 (3)	C31—C32—C33—C34	0.4 (6)
Au1—N1—C7—C6	−5.8 (4)	C32—C33—C34—C29	−2.9 (5)
C5—C6—C7—N1	−177.2 (3)	C32—C33—C34—Au2	179.1 (3)
C1—C6—C7—N1	2.6 (4)	C30—C29—C34—C33	2.9 (5)
C5—C6—C7—C8	3.8 (5)	C28—C29—C34—C33	−174.2 (3)
C1—C6—C7—C8	−176.5 (3)	C30—C29—C34—Au2	−178.7 (3)
N1—C7—C8—C9	0.3 (5)	C28—C29—C34—Au2	4.2 (4)
C6—C7—C8—C9	179.4 (3)	N2—Au2—C34—C33	174.9 (3)
C7—C8—C9—C10	0.9 (6)	C18—Au2—C34—C33	170.1 (3)
C8—C9—C10—C11	−2.2 (6)	P1—Au2—C34—C33	−6.5 (3)
C7—N1—C11—C10	−1.0 (5)	N2—Au2—C34—C29	−3.3 (2)
Au1—N1—C11—C10	−174.6 (2)	C18—Au2—C34—C29	−8.1 (5)
C7—N1—C11—C12	177.3 (3)	P1—Au2—C34—C29	175.4 (2)
Au1—N1—C11—C12	3.7 (4)	C41—P1—C35—C36	−120.8 (3)

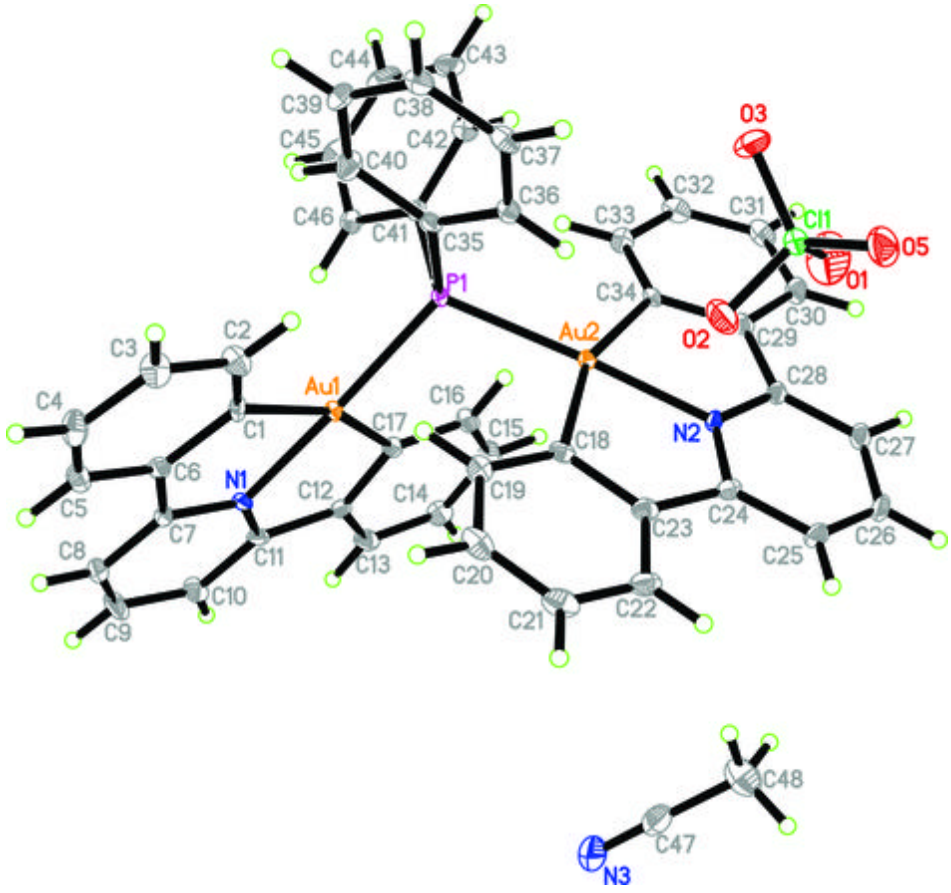
C9—C10—C11—N1	2.2 (5)	Au1—P1—C35—C36	125.5 (2)
C9—C10—C11—C12	−175.8 (3)	Au2—P1—C35—C36	1.6 (3)
N1—C11—C12—C13	177.0 (3)	C41—P1—C35—C40	51.5 (3)
C10—C11—C12—C13	−4.9 (6)	Au1—P1—C35—C40	−62.2 (3)
N1—C11—C12—C17	−3.5 (4)	Au2—P1—C35—C40	173.9 (2)
C10—C11—C12—C17	174.6 (3)	C40—C35—C36—C37	0.1 (5)
C17—C12—C13—C14	0.1 (5)	P1—C35—C36—C37	172.4 (2)
C11—C12—C13—C14	179.6 (3)	C35—C36—C37—C38	1.5 (5)
C12—C13—C14—C15	−0.7 (5)	C36—C37—C38—C39	−1.1 (5)
C13—C14—C15—C16	0.4 (6)	C37—C38—C39—C40	−1.0 (5)
C14—C15—C16—C17	0.6 (6)	C38—C39—C40—C35	2.7 (5)
C15—C16—C17—C12	−1.2 (5)	C36—C35—C40—C39	−2.2 (5)
C15—C16—C17—Au1	178.4 (3)	P1—C35—C40—C39	−174.7 (3)
C13—C12—C17—C16	0.9 (5)	C35—P1—C41—C46	−125.9 (3)
C11—C12—C17—C16	−178.6 (3)	Au1—P1—C41—C46	−1.8 (3)
C13—C12—C17—Au1	−178.8 (3)	Au2—P1—C41—C46	121.4 (3)
C11—C12—C17—Au1	1.7 (4)	C35—P1—C41—C42	50.2 (3)
N1—Au1—C17—C16	−179.4 (3)	Au1—P1—C41—C42	174.3 (2)
C1—Au1—C17—C16	−175.2 (3)	Au2—P1—C41—C42	−62.4 (3)
P1—Au1—C17—C16	5.8 (3)	C46—C41—C42—C43	−2.8 (5)
N1—Au1—C17—C12	0.2 (2)	P1—C41—C42—C43	−179.0 (3)
C1—Au1—C17—C12	4.4 (5)	C41—C42—C43—C44	2.8 (5)
P1—Au1—C17—C12	−174.6 (2)	C42—C43—C44—C45	−0.3 (6)
N2—Au2—C18—C19	178.4 (3)	C43—C44—C45—C46	−2.2 (6)
C34—Au2—C18—C19	−176.8 (3)	C42—C41—C46—C45	0.4 (5)
P1—Au2—C18—C19	−0.1 (3)	P1—C41—C46—C45	176.4 (2)
N2—Au2—C18—C23	−1.5 (2)	C44—C45—C46—C41	2.1 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C21—H21···O3^{i}	0.95	2.46	3.311 (7)	149
C36—H36···O2	0.95	2.57	3.372 (8)	143
C38—H38···O2^{ii}	0.95	2.59	3.540 (5)	175
C43—H43···O1^{iii}	0.95	2.59	3.517 (3)	165
C46—H46···N3^{iv}	0.95	2.62	3.417 (4)	142
C48—H48C···O1^{v}	0.98	2.54	3.423 (8)	150

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

Fig. 1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C38
C45
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C37
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C36
C46
C41
C35
P1
C34
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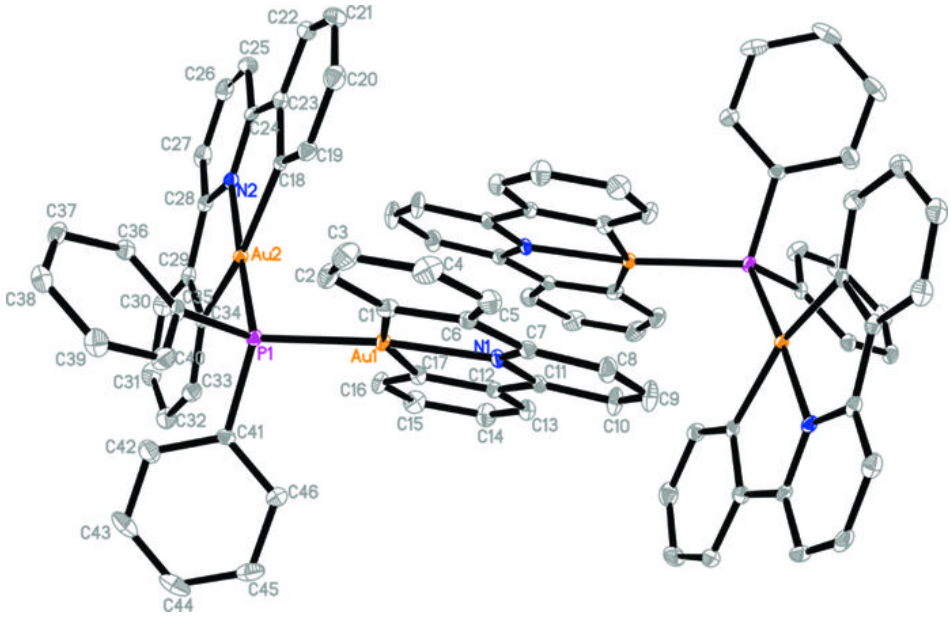
C2
Au1
C16
C4
C1
C17
C15
C18
N2
C27
C6
N1
C12
C14
C19
C23
C24
C5
C7
C11
C13
C20
C25
C26
C8
C10
C21
C22
C9
C48
C47
N3
O3
C32
C31
Cl1
O5
C33
O1
C30
O2
C29
C28

Fig. 2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C3
C2
C4
C38
C30
C35
C34
C1
C5
C6
C7
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C40
C31
C33
C17
C12
C11
C8
C16
C9
C32
C15
C14
C13
C10
C41
C42
C46
C43
C45
C44

Fig. 3