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Bis[μ-bis(diphenylphosphino)methane-κ^2P:P']digold(I)(*Au*—*Au*) dinitrate perdeuteromethanol solvate

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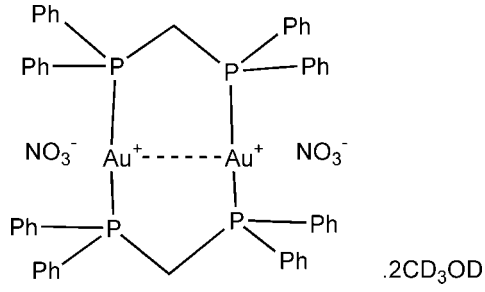
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.005 Å; R factor = 0.022; wR factor = 0.052; data-to-parameter ratio = 16.2.

In the centrosymmetric dicationic cyclic title compound $[Au_2(C_{25}H_{22}P_2)_2](NO_3)_2{\cdot}2CD_3OD$, an aurophilic interaction with a distance of 3.0245 (3) Å is found between the linear-dicoordinated Au^I centres. The perdeuteromethanol solvent molecules are linked to the nitrate anions *via* hydrogen bonds.

Related literature

For related literature, see: Angermaier & Schmidbaur (1995); Bauer & Schmidbaur (1997); Cooper *et al.* (1984); Jaw *et al.* (1989); Khan *et al.* (1989); King *et al.* (1989); Liou *et al.* (1994); Malatesta *et al.* (1966); Perreault *et al.* (1992); Porter *et al.* (1989); Schmidbaur *et al.* (2005); Uson *et al.* (1986); Wang & Liu (1994).



Experimental

Crystal data

$[Au_2(C_{25}H_{22}P_2)_2](NO_3)_2{\cdot}2CD_4O$
M_r = 1358.71
Monoclinic, $P2_1/n$
a = 11.6214 (8) Å
b = 13.6313 (9) Å
c = 16.4319 (12) Å
β = 109.048 (1)°
V = 2460.5 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 6.14 mm^{-1}
T = 100 (2) K
0.27 × 0.19 × 0.13 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.256, T_{max} = 0.450
14182 measured reflections
5019 independent reflections
4626 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.052
S = 1.06
5019 reflections
309 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Au1—P1	2.3116 (8)	P1—C1	1.821 (3)
Au1—P2^i	2.3175 (8)	P2—C31	1.805 (3)
Au1—Au1^i	3.0245 (3)	P2—C41	1.818 (3)
P1—C21	1.811 (3)	P2—C1	1.832 (3)
P1—C11	1.814 (3)		
P1—Au1—P2^i	177.76 (3)	P2^i—Au1—Au1^i	91.70 (2)
P1—Au1—Au1^i	89.62 (2)		

Symmetry code: (i) $-x+1, -y+1, -z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—D4···O3	0.84	2.10	2.908 (4)	161

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *X-SEED*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2244).

References

Angermaier, K. A. & Schmidbaur, H. (1995). *J. Chem. Soc. Dalton Trans.* pp. 559–564.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bauer, A. & Schmidbaur, H. (1997). *J. Chem. Soc. Dalton Trans.* pp. 1115–1116.
Bruker (2002). *SADABS* (Version 2.05) and *SMART* (Version 5.628). Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2003). *SAINT*. Version 6.45. Bruker AXS Inc., Madison, Wisconsin, USA.
Cooper, M. K., Mitchell, L. E., Hendrick, K., McPartlin, M. & Scott, A. (1984). *Inorg. Chim. Acta*, **84**, L9–L10.
Jaw, H. R. C., Savas, M. M., Rogers, R. D. & Mason, W. R. (1989). *Inorg. Chem.* **28**, 1028–1037.
Khan, Md. N. I., King, C., Heinrich, D. D., Fackler, J. P. Jr & Poter, L. C. (1989). *Inorg. Chem.* **28**, 2150–2154.
King, C., Wang, J. C., Khan, Md. N. I. & Fackler, J. P. Jr (1989). *Inorg. Chem.* **28**, 2145–2149.

Liou, L.-S., Liu, C.-P. & Wang, J.-C. (1994). *Acta Cryst.* C**50**, 538–540.
Malatesta, L., Naldini, L., Simonetta, G. & Cariati, F. (1966). *Coord. Chem. Rev.* **1**, 255–262.
Perreault, D., Drouin, M., Michel, A., Miskowski, V. M., Schaefer, W. P. & Harvey, P. D. (1992). *Inorg. Chem.* **31**, 685–702.
Porter, L. C., Khan, Md. N. I., King, C. & Fackler, J. P. (1989). *Acta Cryst.* C**45**, 947–949.
Schmidbaur, H., Cronje, S., Djordjevic, B. & Schuster, O. (2005). *Chem. Phys.* **311**, 151–161.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Uson, R., Laguna, A., Laguna, M., Gimeno, M. C., Jones, G. J., Fittschen, C. & Sheldrick, G. M. (1986). *J. Chem. Soc. Chem. Commun.* pp. 509–510.
Wang, J.-C. & Liu, L.-K. (1994). *Acta Cryst.* C**50**, 704–706.

supplementary materials

Acta Cryst. (2007). E**63**, m2137-m2138 [**doi:10.1107/S1600536807030887**]

Bis[μ-bis(diphenylphosphino)methane-κ^2P:P']digold(I)(*Au*-*Au*) dinitrate perdeuteromethanol solvate

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Comment

Binuclear gold complexes with bridging bidentate ligands and various counter-ions have been the subject of several studies due to their rich luminescence and bonding properties (King *et al.*, 1989) and have been structurally characterized (Jaw *et al.*, 1989; Khan *et al.*, 1989; Porter *et al.*, 1989; Liou *et al.*, 1994; Wang & Liu, 1994; Bauer & Schmidbaur, 1997). The bridging methylene carbon can be exploited as a coordination and reactive centre. Neutral homo- or heterometallic tetranuclear derivatives have been reported (Uson *et al.*, 1986). It is assumed that Au···Au distances are determined by electronic effects of the substituents *L* and *X* at gold but it has become more obvious that steric effects play a decisive role. The weak forces associated with Au···Au contacts can be overruled by steric repulsion and other factors like packing forces (Angermaier & Schmidbaur, 1995). Here we report another crystal and molecular structure containing this dication. Each nitrate counter anion engages in a hydrogen bond to one perdeuteromethanol lattice solvent.

The asymmetric unit of (A) consists of one half of the dication, $[(\mu\text{-dppm})_2Au_2]^{2+}$, containing one nitrate anion and one deuterated methanol molecule. The rest of the molecule is related by a centre of symmetry between the gold atoms of each dimer. The Au···Au separation is 3.0245 (3) Å. This agrees with a weak Au···Au interaction (Schmidbaur *et al.*, 2005). In this instance the steric constraints of the dppm ligand assist the aurophillic interaction in the $Au_2P_4C_2$ ring which has a chair conformation (Perreault *et al.*, 1992; Bauer & Schmidbaur, 1997). The Au centres adopt a normal linear two-coordinate geometry of 177.76 (3) Å, slightly distorted from ideality by the aurophilic bonding. Channels of anions are observed running parallel to the *a* axis. Two oxygen atoms of the nitrate are aligned towards the gold atom in the cation with distances of 3.470 (2) Å for O2–Au1^{i} [symmetry code: (i) = $-x + 1, -y + 1, -z$] and 3.357 (2) Å for O1—Au1.

Experimental

The title compound was prepared using $(\mu\text{-dppm})_2AuCl_2$ (Cooper *et al.*, 1984) and literature methods (Malatesa *et al.*, 1966). Colourless crystals that were suitable for X-Ray diffraction were obtained at 251 K in deuterated methanol.

Refinement

Hydrogen atoms were positioned geometrically and constrained to ride on their parent atoms with distances for aromatic C—H = 0.95 Å, methyl C—D = 0.98 Å and methanol O—D = 0.84 Å. U_{iso} values were set at 1.2 times U_{eq}(C,*O*) for all H/D atoms except for methyl D at 1.5 U_{eq}(C). A residual electron density peak of 1.64 e Å^{-3} was located 1.188 Å next to O2.

Figures

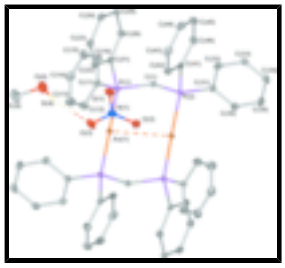


Fig. 1. The molecular structure of (A), showing atom labels and 50% probability displacement ellipsoids for non-H atoms.

Bis[μ-bis(diphenylphosphino)methane-κ^2*P*:*P*']digold(I)(Au—Au) dinitrate perdeuteromethanol solvate

Crystal data

$[Au_2(C_{25}H_{22}P_2)_2](NO_3)_2{\cdot}2CD_4O$	F_{000} = 1320
M_r = 1358.71	D_x = 1.834 Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point: 414.8 K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 11.6214 (8) Å	Cell parameters from 6683 reflections
b = 13.6313 (9) Å	θ = 2.4–26.4°
c = 16.4319 (12) Å	μ = 6.14 mm^{-1}
β = 109.0480 (10)°	T = 100 (2) K
V = 2460.5 (3) Å^3	Prism, colourless
Z = 2	0.27 × 0.19 × 0.13 mm

Data collection

Bruker APEX CCD area-detector diffractometer	5019 independent reflections
Radiation source: fine-focus sealed tube	4626 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.025
T = 100(2) K	θ_{max} = 26.4°
ω scans	θ_{min} = 1.9°
Absorption correction: multi-scan (SADABS; Bruker, 2002)	h = −14→14
T_{min} = 0.256, T_{max} = 0.450	k = −17→12
14182 measured reflections	l = −20→18

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.022	H-atom parameters constrained
$wR(F^2)$ = 0.052	$w = 1/[\sigma^2(F_o^2) + (0.0256P)^2 + 0.7357P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.001$
5019 reflections	$\Delta\rho_{max} = 1.64$ e Å^{-3}
309 parameters	$\Delta\rho_{min} = -0.46$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	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	0.408600 (9)	0.485644 (8)	0.046685 (7)	0.01107 (5)
P1	0.26529 (6)	0.57042 (6)	−0.06166 (5)	0.01064 (16)
P2	0.45307 (7)	0.60437 (6)	−0.15453 (5)	0.01081 (16)
O1	0.6025 (2)	0.78397 (16)	0.18981 (15)	0.0216 (5)
O2	0.6738 (2)	0.66210 (17)	0.13524 (14)	0.0230 (5)
O3	0.5548 (2)	0.63412 (17)	0.21084 (15)	0.0248 (5)
O4	0.3636 (2)	0.7250 (2)	0.26312 (16)	0.0338 (6)
D4	0.4274	0.6978	0.2610	0.051*
N1	0.6106 (2)	0.6935 (2)	0.17854 (17)	0.0182 (6)
C1	0.2969 (3)	0.5708 (2)	−0.16312 (19)	0.0122 (6)
H1A	0.2404	0.6173	−0.2029	0.015*
H1B	0.2796	0.5046	−0.1891	0.015*
C4	0.3516 (4)	0.7089 (3)	0.3450 (3)	0.0389 (10)
D4A	0.4209	0.7384	0.3894	0.058*
D4B	0.3496	0.6383	0.3554	0.058*
D4C	0.2759	0.7390	0.3468	0.058*
C11	0.1141 (3)	0.5171 (2)	−0.0928 (2)	0.0132 (6)
C12	0.0970 (3)	0.4237 (3)	−0.0638 (2)	0.0220 (7)
H12	0.1636	0.3896	−0.0247	0.026*
C13	−0.0175 (3)	0.3809 (2)	−0.0922 (2)	0.0264 (8)
H13	−0.0291	0.3173	−0.0727	0.032*
C14	−0.1141 (3)	0.4298 (3)	−0.1485 (2)	0.0224 (7)
H14	−0.1922	0.3999	−0.1678	0.027*
C15	−0.0980 (3)	0.5223 (3)	−0.1770 (2)	0.0226 (8)
H15	−0.1654	0.5562	−0.2155	0.027*
C16	0.0151 (3)	0.5660 (2)	−0.1499 (2)	0.0187 (7)

H16	0.0257	0.6296	−0.1701	0.022*
C21	0.2552 (2)	0.6982 (2)	−0.03458 (19)	0.0115 (6)
C22	0.3051 (3)	0.7273 (2)	0.0513 (2)	0.0150 (6)
H22	0.3408	0.6798	0.0945	0.018*
C23	0.3027 (3)	0.8244 (2)	0.0735 (2)	0.0171 (7)
H23	0.3366	0.8438	0.1320	0.021*
C24	0.2508 (3)	0.8942 (2)	0.0104 (2)	0.0170 (7)
H24	0.2498	0.9613	0.0259	0.020*
C25	0.2008 (3)	0.8660 (2)	−0.0748 (2)	0.0154 (6)
H25	0.1648	0.9137	−0.1177	0.019*
C26	0.2031 (3)	0.7684 (2)	−0.0975 (2)	0.0154 (6)
H26	0.1692	0.7493	−0.1561	0.018*
C31	0.4599 (3)	0.5910 (2)	−0.2622 (2)	0.0132 (6)
C32	0.3662 (3)	0.6220 (2)	−0.3352 (2)	0.0150 (6)
H32	0.2903	0.6422	−0.3306	0.018*
C33	0.3844 (3)	0.6232 (2)	−0.4144 (2)	0.0160 (7)
H33	0.3211	0.6454	−0.4638	0.019*
C34	0.4930 (3)	0.5925 (2)	−0.4223 (2)	0.0199 (7)
H34	0.5052	0.5946	−0.4767	0.024*
C35	0.5846 (3)	0.5587 (3)	−0.3505 (2)	0.0214 (7)
H35	0.6590	0.5363	−0.3562	0.026*
C36	0.5691 (3)	0.5571 (2)	−0.2710 (2)	0.0187 (7)
H36	0.6322	0.5331	−0.2223	0.022*
C41	0.4729 (3)	0.7353 (2)	−0.1336 (2)	0.0128 (6)
C42	0.5348 (3)	0.7659 (2)	−0.0495 (2)	0.0163 (7)
H42	0.5652	0.7187	−0.0052	0.020*
C43	0.5520 (3)	0.8650 (3)	−0.0308 (2)	0.0216 (7)
H43	0.5931	0.8856	0.0266	0.026*
C44	0.5096 (3)	0.9340 (2)	−0.0954 (2)	0.0208 (7)
H44	0.5222	1.0019	−0.0827	0.025*
C45	0.4485 (3)	0.9034 (2)	−0.1791 (2)	0.0207 (7)
H45	0.4191	0.9508	−0.2234	0.025*
C46	0.4301 (3)	0.8047 (2)	−0.1984 (2)	0.0176 (7)
H46	0.3884	0.7844	−0.2558	0.021*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.00955 (7)	0.01244 (7)	0.01065 (7)	0.00124 (4)	0.00248 (5)	0.00256 (4)
P1	0.0095 (3)	0.0108 (4)	0.0113 (4)	0.0002 (3)	0.0029 (3)	0.0006 (3)
P2	0.0099 (4)	0.0119 (4)	0.0102 (4)	0.0001 (3)	0.0027 (3)	0.0013 (3)
O1	0.0273 (13)	0.0147 (12)	0.0199 (13)	−0.0031 (10)	0.0036 (10)	−0.0014 (9)
O2	0.0262 (12)	0.0255 (13)	0.0175 (13)	0.0054 (10)	0.0075 (10)	0.0000 (10)
O3	0.0308 (13)	0.0208 (13)	0.0224 (14)	−0.0106 (10)	0.0083 (11)	0.0022 (10)
O4	0.0357 (15)	0.0440 (17)	0.0221 (14)	−0.0021 (13)	0.0098 (12)	0.0010 (12)
N1	0.0187 (14)	0.0206 (15)	0.0105 (14)	−0.0001 (12)	−0.0018 (11)	−0.0004 (11)
C1	0.0114 (14)	0.0128 (15)	0.0114 (15)	0.0015 (12)	0.0025 (12)	0.0015 (12)
C4	0.055 (3)	0.037 (2)	0.032 (2)	−0.012 (2)	0.022 (2)	−0.0014 (18)

C11	0.0118 (15)	0.0148 (16)	0.0138 (16)	−0.0007 (12)	0.0052 (13)	−0.0006 (12)
C12	0.0181 (16)	0.0187 (18)	0.029 (2)	0.0009 (13)	0.0073 (15)	0.0064 (14)
C13	0.0214 (17)	0.0187 (18)	0.040 (2)	−0.0025 (14)	0.0110 (16)	0.0043 (15)
C14	0.0141 (16)	0.0269 (19)	0.026 (2)	−0.0064 (14)	0.0065 (14)	−0.0047 (15)
C15	0.0140 (16)	0.033 (2)	0.0194 (19)	0.0003 (14)	0.0033 (14)	0.0046 (14)
C16	0.0156 (15)	0.0171 (17)	0.0229 (18)	−0.0003 (13)	0.0056 (14)	0.0034 (13)
C21	0.0098 (14)	0.0117 (15)	0.0143 (16)	0.0001 (11)	0.0057 (12)	−0.0002 (12)
C22	0.0134 (15)	0.0178 (17)	0.0131 (16)	0.0005 (12)	0.0035 (13)	0.0026 (12)
C23	0.0187 (16)	0.0208 (17)	0.0121 (16)	0.0006 (13)	0.0054 (13)	−0.0043 (13)
C24	0.0171 (16)	0.0135 (16)	0.0227 (18)	−0.0001 (12)	0.0098 (14)	−0.0024 (13)
C25	0.0170 (15)	0.0129 (16)	0.0178 (17)	0.0049 (12)	0.0076 (13)	0.0049 (12)
C26	0.0157 (15)	0.0173 (16)	0.0124 (16)	0.0005 (13)	0.0036 (13)	0.0007 (12)
C31	0.0138 (14)	0.0118 (15)	0.0155 (16)	−0.0019 (12)	0.0068 (13)	−0.0010 (12)
C32	0.0123 (15)	0.0135 (16)	0.0173 (17)	−0.0010 (12)	0.0023 (13)	−0.0023 (12)
C33	0.0201 (16)	0.0145 (16)	0.0111 (16)	−0.0012 (13)	0.0022 (13)	0.0001 (12)
C34	0.0246 (17)	0.0228 (18)	0.0144 (17)	−0.0033 (14)	0.0091 (14)	−0.0004 (13)
C35	0.0161 (16)	0.029 (2)	0.0218 (18)	0.0018 (14)	0.0101 (14)	0.0017 (15)
C36	0.0155 (15)	0.0219 (18)	0.0195 (18)	0.0026 (13)	0.0069 (13)	0.0032 (14)
C41	0.0111 (14)	0.0130 (15)	0.0153 (16)	−0.0007 (12)	0.0058 (13)	−0.0008 (12)
C42	0.0143 (15)	0.0191 (17)	0.0140 (17)	0.0040 (13)	0.0028 (13)	0.0023 (13)
C43	0.0162 (16)	0.0253 (19)	0.0199 (18)	−0.0008 (14)	0.0013 (14)	−0.0087 (14)
C44	0.0197 (16)	0.0141 (17)	0.029 (2)	0.0004 (13)	0.0080 (15)	−0.0046 (14)
C45	0.0248 (17)	0.0139 (17)	0.0243 (19)	0.0015 (14)	0.0092 (15)	0.0055 (13)
C46	0.0184 (16)	0.0195 (17)	0.0134 (17)	−0.0012 (13)	0.0033 (13)	0.0007 (13)

Geometric parameters (Å, °)

Au1—P1	2.3116 (8)	C21—C26	1.393 (4)
Au1—P2^{i}	2.3175 (8)	C21—C22	1.397 (4)
Au1—Au1^{i}	3.0245 (3)	C22—C23	1.375 (4)
Au1—O3	3.357 (2)	C22—H22	0.9500
P1—C21	1.811 (3)	C23—C24	1.391 (4)
P1—C11	1.814 (3)	C23—H23	0.9500
P1—C1	1.821 (3)	C24—C25	1.384 (4)
P2—C31	1.805 (3)	C24—H24	0.9500
P2—C41	1.818 (3)	C25—C26	1.384 (4)
P2—C1	1.832 (3)	C25—H25	0.9500
P2—Au1^{i}	2.3175 (8)	C26—H26	0.9500
O1—N1	1.256 (3)	C31—C32	1.397 (4)
O2—N1	1.253 (3)	C31—C36	1.402 (4)
O2—Au1^{i}	3.470 (2)	C32—C33	1.385 (4)
O3—N1	1.257 (3)	C32—H32	0.9500
O4—C4	1.414 (4)	C33—C34	1.376 (4)
O4—D4	0.8400	C33—H33	0.9500
C1—H1A	0.9900	C34—C35	1.384 (5)
C1—H1B	0.9900	C34—H34	0.9500
C4—D4A	0.9800	C35—C36	1.376 (4)
C4—D4B	0.9800	C35—H35	0.9500

C4—D4C	0.9800	C36—H36	0.9500
C11—C16	1.394 (4)	C41—C46	1.389 (4)
C11—C12	1.396 (4)	C41—C42	1.397 (4)
C12—C13	1.387 (4)	C42—C43	1.385 (4)
C12—H12	0.9500	C42—H42	0.9500
C13—C14	1.372 (5)	C43—C44	1.384 (5)
C13—H13	0.9500	C43—H43	0.9500
C14—C15	1.378 (5)	C44—C45	1.389 (5)
C14—H14	0.9500	C44—H44	0.9500
C15—C16	1.379 (4)	C45—C46	1.383 (4)
C15—H15	0.9500	C45—H45	0.9500
C16—H16	0.9500	C46—H46	0.9500
P1—Au1—P2^{i}	177.76 (3)	C26—C21—C22	119.4 (3)
P1—Au1—Au1^{i}	89.62 (2)	C26—C21—P1	121.7 (2)
P2^{i}—Au1—Au1^{i}	91.70 (2)	C22—C21—P1	118.8 (2)
P1—Au1—O3	111.47 (4)	C23—C22—C21	120.2 (3)
P2^{i}—Au1—O3	70.24 (4)	C23—C22—H22	119.9
Au1^{i}—Au1—O3	94.27 (4)	C21—C22—H22	119.9
C21—P1—C11	108.68 (13)	C22—C23—C24	120.1 (3)
C21—P1—C1	105.71 (14)	C22—C23—H23	119.9
C11—P1—C1	102.07 (14)	C24—C23—H23	119.9
C21—P1—Au1	112.32 (10)	C25—C24—C23	120.1 (3)
C11—P1—Au1	113.89 (10)	C25—C24—H24	120.0
C1—P1—Au1	113.37 (10)	C23—C24—H24	120.0
C31—P2—C41	103.94 (14)	C24—C25—C26	120.1 (3)
C31—P2—C1	104.97 (14)	C24—C25—H25	120.0
C41—P2—C1	108.72 (13)	C26—C25—H25	120.0
C31—P2—Au1^{i}	117.03 (10)	C25—C26—C21	120.1 (3)
C41—P2—Au1^{i}	111.21 (10)	C25—C26—H26	120.0
C1—P2—Au1^{i}	110.44 (10)	C21—C26—H26	120.0
N1—O2—Au1^{i}	129.75 (18)	C32—C31—C36	119.3 (3)
N1—O3—Au1	104.14 (18)	C32—C31—P2	122.7 (2)
C4—O4—D4	109.5	C36—C31—P2	117.7 (2)
O2—N1—O1	120.3 (3)	C33—C32—C31	119.7 (3)
O2—N1—O3	119.9 (3)	C33—C32—H32	120.2
O1—N1—O3	119.7 (3)	C31—C32—H32	120.2
P1—C1—P2	114.91 (16)	C34—C33—C32	120.8 (3)
P1—C1—H1A	108.5	C34—C33—H33	119.6
P2—C1—H1A	108.5	C32—C33—H33	119.6
P1—C1—H1B	108.5	C33—C34—C35	119.6 (3)
P2—C1—H1B	108.5	C33—C34—H34	120.2
H1A—C1—H1B	107.5	C35—C34—H34	120.2
O4—C4—D4A	109.5	C36—C35—C34	120.8 (3)
O4—C4—D4B	109.5	C36—C35—H35	119.6
D4A—C4—D4B	109.5	C34—C35—H35	119.6
O4—C4—D4C	109.5	C35—C36—C31	119.8 (3)
D4A—C4—D4C	109.5	C35—C36—H36	120.1

D4B—C4—D4C	109.5	C31—C36—H36	120.1
C16—C11—C12	119.2 (3)	C46—C41—C42	119.7 (3)
C16—C11—P1	120.6 (2)	C46—C41—P2	122.1 (2)
C12—C11—P1	120.1 (2)	C42—C41—P2	118.2 (2)
C13—C12—C11	119.8 (3)	C43—C42—C41	120.1 (3)
C13—C12—H12	120.1	C43—C42—H42	119.9
C11—C12—H12	120.1	C41—C42—H42	119.9
C14—C13—C12	120.4 (3)	C44—C43—C42	120.2 (3)
C14—C13—H13	119.8	C44—C43—H43	119.9
C12—C13—H13	119.8	C42—C43—H43	119.9
C13—C14—C15	120.1 (3)	C43—C44—C45	119.6 (3)
C13—C14—H14	119.9	C43—C44—H44	120.2
C15—C14—H14	119.9	C45—C44—H44	120.2
C14—C15—C16	120.4 (3)	C46—C45—C44	120.7 (3)
C14—C15—H15	119.8	C46—C45—H45	119.7
C16—C15—H15	119.8	C44—C45—H45	119.7
C15—C16—C11	120.1 (3)	C45—C46—C41	119.8 (3)
C15—C16—H16	120.0	C45—C46—H46	120.1
C11—C16—H16	120.0	C41—C46—H46	120.1
$P2^{i}$—Au1—P1—C21	136.7 (7)	C11—P1—C21—C22	110.4 (2)
$Au1^{i}$—Au1—P1—C21	−97.16 (10)	C1—P1—C21—C22	−140.7 (2)
O3—Au1—P1—C21	−2.72 (11)	Au1—P1—C21—C22	−16.6 (3)
$P2^{i}$—Au1—P1—C11	12.6 (7)	C26—C21—C22—C23	0.1 (4)
$Au1^{i}$—Au1—P1—C11	138.74 (11)	P1—C21—C22—C23	177.7 (2)
O3—Au1—P1—C11	−126.82 (12)	C21—C22—C23—C24	−0.2 (5)
$P2^{i}$—Au1—P1—C1	−103.6 (7)	C22—C23—C24—C25	0.4 (5)
$Au1^{i}$—Au1—P1—C1	22.60 (11)	C23—C24—C25—C26	−0.5 (5)
O3—Au1—P1—C1	117.04 (11)	C24—C25—C26—C21	0.4 (5)
P1—Au1—O3—N1	−64.04 (18)	C22—C21—C26—C25	−0.2 (4)
$P2^{i}$—Au1—O3—N1	117.50 (18)	P1—C21—C26—C25	−177.7 (2)
$Au1^{i}$—Au1—O3—N1	27.23 (18)	C41—P2—C31—C32	−72.2 (3)
$Au1^{i}$—O2—N1—O1	−123.0 (2)	C1—P2—C31—C32	41.9 (3)
$Au1^{i}$—O2—N1—O3	56.9 (3)	$Au1^{i}$—P2—C31—C32	164.8 (2)
Au1—O3—N1—O2	−49.4 (3)	C41—P2—C31—C36	101.2 (3)
Au1—O3—N1—O1	130.5 (2)	C1—P2—C31—C36	−144.6 (2)
C21—P1—C1—P2	74.66 (18)	$Au1^{i}$—P2—C31—C36	−21.8 (3)
C11—P1—C1—P2	−171.74 (16)	C36—C31—C32—C33	−3.0 (4)
Au1—P1—C1—P2	−48.81 (18)	P2—C31—C32—C33	170.4 (2)
C31—P2—C1—P1	176.49 (16)	C31—C32—C33—C34	1.1 (5)
C41—P2—C1—P1	−72.8 (2)	C32—C33—C34—C35	1.0 (5)
$Au1^{i}$—P2—C1—P1	49.50 (18)	C33—C34—C35—C36	−1.3 (5)
C21—P1—C11—C16	46.3 (3)	C34—C35—C36—C31	−0.6 (5)
C1—P1—C11—C16	−65.1 (3)	C32—C31—C36—C35	2.7 (5)
Au1—P1—C11—C16	172.3 (2)	P2—C31—C36—C35	−171.0 (3)
C21—P1—C11—C12	−137.5 (3)	C31—P2—C41—C46	32.8 (3)
C1—P1—C11—C12	111.1 (3)	C1—P2—C41—C46	−78.7 (3)

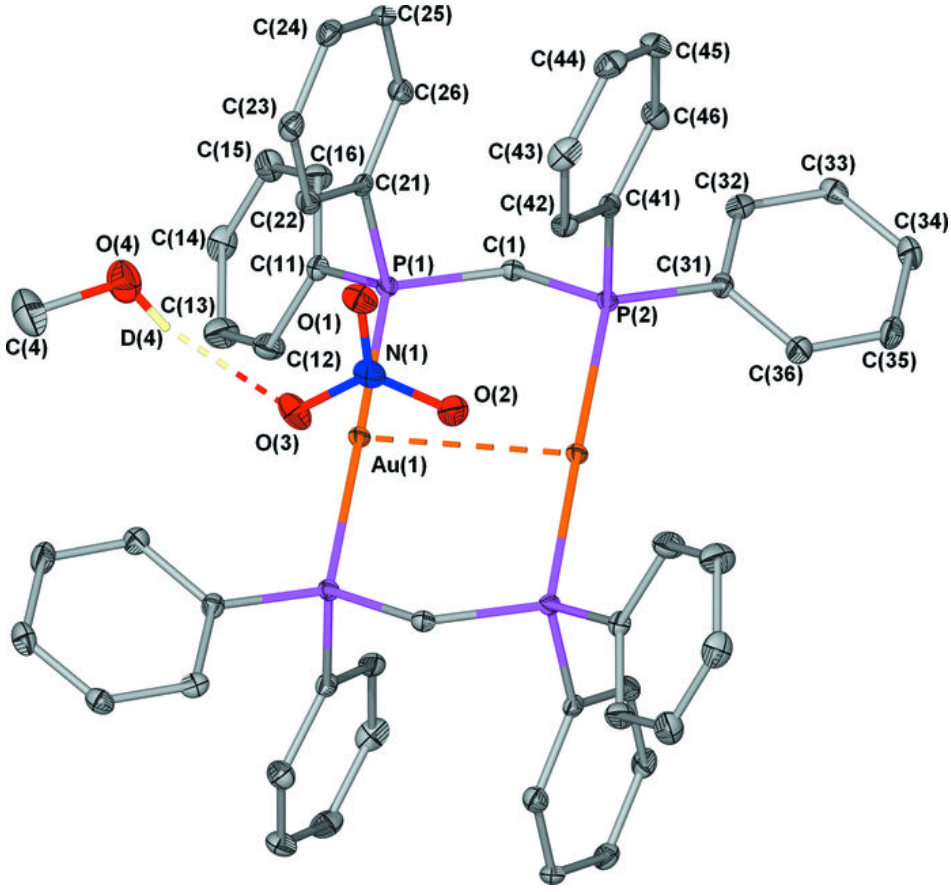
Au1—P1—C11—C12	−11.5 (3)	Au1^{i}—P2—C41—C46	159.5 (2)
C16—C11—C12—C13	0.3 (5)	C31—P2—C41—C42	−146.4 (2)
P1—C11—C12—C13	−175.9 (3)	C1—P2—C41—C42	102.2 (3)
C11—C12—C13—C14	−0.2 (5)	Au1^{i}—P2—C41—C42	−19.6 (3)
C12—C13—C14—C15	−0.2 (6)	C46—C41—C42—C43	0.8 (5)
C13—C14—C15—C16	0.6 (6)	P2—C41—C42—C43	180.0 (2)
C14—C15—C16—C11	−0.5 (5)	C41—C42—C43—C44	−1.0 (5)
C12—C11—C16—C15	0.1 (5)	C42—C43—C44—C45	0.7 (5)
P1—C11—C16—C15	176.3 (3)	C43—C44—C45—C46	−0.3 (5)
C11—P1—C21—C26	−72.1 (3)	C44—C45—C46—C41	0.1 (5)
C1—P1—C21—C26	36.9 (3)	C42—C41—C46—C45	−0.4 (5)
Au1—P1—C21—C26	161.0 (2)	P2—C41—C46—C45	−179.5 (2)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—D4···O3	0.84	2.10	2.908 (4)	161

Fig. 1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