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(*R*)-(+)-[μ-2,2′-Bis(diphenylphosphino)-1,1′-binaphthalene-κ^2*P*:*P*′]bis[chlorido-gold(I)] dichloromethane solvate

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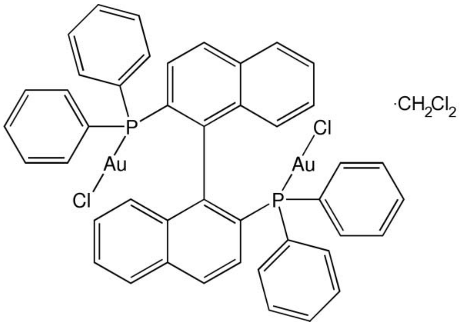
Key indicators: single-crystal X-ray study; *T* = 165 K; mean σ(C–C) = 0.014 Å; *R* factor = 0.038; *wR* factor = 0.077; data-to-parameter ratio = 19.8.

In the crystal structure of the title compound, $[Au_2Cl_2(C_{44}H_{32}P_2)]\cdot CH_2Cl_2$, the molecule is located on a twofold axis. The naphthyl group is slightly bent; the angle between the planes of the two six-membered rings is 3.5 (5)°. The angle between the mean planes of the two symmetry-related naphthyl groups is 84.4 (1)°. The P—Au—Cl group is almost linear, with an angle of 175.5 (1)°. The dichloromethane solvent molecule lies on a twofold axis and connects the AuCl groups of two symmetry-related molecules *via* intermolecular C—H···Cl hydrogen bonding.

Related literature

Gold catalysis is becoming increasingly important (Hashmi & Hutchings, 2006) and the use of chiral gold complexes for enantioselective catalysis is one of the latest hot topics (Hashmi, 2005). In this context detailed structural information about these gold complexes is of great importance. Thus we conducted a crystal structure analysis of the title compound, which was prepared by analogy to related compounds (King & Eisch, 1986). The structure of a closely related molecule has been reported by Muñoz *et al.* (2005).



Experimental

Crystal data

$[Au_2Cl_2(C_{44}H_{32}P_2)]\cdot CH_2Cl_2$
M_r = 1172.40
Monoclinic, *C*2
a = 19.480 (3) Å
b = 8.6889 (13) Å
c = 14.085 (2) Å
β = 122.361 (15)°
V = 2013.8 (6) Å^3
Z = 2
Mo *K*α radiation
μ = 7.65 mm^{-1}
T = 165 (2) K
0.55 × 0.08 × 0.06 mm

Data collection

Siemens SMART 1K CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
T_{min} = 0.459, T_{max} = 0.632
15554 measured reflections
4750 independent reflections
3716 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.077
S = 1.01
4750 reflections
240 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.40 e Å^{-3}
$\Delta\rho_{min}$ = −1.33 e Å^{-3}
Absolute structure: Flack (1983), 2122 Friedel pairs
Flack parameter: 0.003 (9)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C23—H23*A*···Cl1	0.99	2.62	3.611 (11)	174

Data collection: *SMART* (Siemens, 1995); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1996); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2053).

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supplementary materials

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(*R*)-(+)-[μ-2,2'-Bis(diphenylphosphino)-1,1'-binaphthalene-κ^2P:P']bis[chloridogold(I)] dichloromethane solvate

J. W. Bats, M. Hamzic and A. S. K. Hashmi

Comment

The molecule has twofold symmetry and there is a crystallographic twofold axis passing through the midpoint of the C10—C10 bond. The naphthyl group is slightly bend: the angle between the planes of the two six-membered rings is 3.5 (5)°. Moreover atom C10 deviates 0.064 (5)Å from the plane through C1/C2/C3/C4/C9. The angle between the best planes of the two symmetry-related naphthyl groups is 84.4 (1)°. Both phenyl groups attached to P1 are essentially planar. The P—Au—Cl bond is almost linear with a bond angle of 175.5 (1)°. The dichloromethane solvate group also lies on a twofold axis. Its H atoms donate weak hydrogen bonds to Cl atoms of two symmetry-related Au—Cl groups (see Table). The crystal packing also shows a number of additional intermolecular C—H···Cl contacts with H···Cl distances between 3.00 and 3.15Å and a number of weak intermolecular C—H···π(benzene) interactions (*Cg*1, *Cg*2 and *Cg*3 are the centroids of the benzene rings labeled C1/C2/C3/C4/C9/C10, C4/C5/C6/C7/C8/C9 and C11/C12/C13/C14/C15/C16 respectively). The crystal structure of the corresponding bis(ditolylphosphino) compound has been reported by Muñoz *et al.* (2005). The conformation of that molecule, however, differs considerably from the conformation of the title compound.

Experimental

The title compound was prepared in analogy to related compounds in the literature (King & Eisch, 1986). Single crystals were obtained by recrystallization from dichloromethane.

Refinement

H atoms were geometrically positioned using fixed distances: C(sp^2)-H = 0.95 Å, $C_{secondary}$—H = 0.99 Å and U_{iso}(H) = 1.2U_{eq}(C). The absolute configuration of the molecule was determined from the value of the Flack *x* parameter (Flack, 1983) using 2122 Friedel pairs. The maximum and minimum difference peaks are within 1Å from the Au atom.

Figures

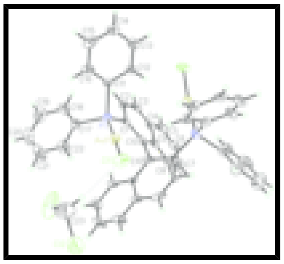

Fig. 1. Molecular structure of (I) with atomic numbering scheme and displacement ellipsoids are drawn at the 50% probability level. The H atoms are drawn as small spheres of arbitrary radius and the C—H···Cl hydrogen bonding is shown as a dotted lines. Symmetry codes: i = −*x*, *y*, −*z*,

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Crystal data

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M_r = 1172.40

Monoclinic, *C*2

Hall symbol: C 2y

a = 19.480 (3) Å

b = 8.6889 (13) Å

c = 14.085 (2) Å

β = 122.361 (15)°

V = 2013.8 (6) Å^3

Z = 2

F_{000} = 1120

D_x = 1.933 Mg m^{-3}

Mo *K*α radiation
λ = 0.71073 Å

Cell parameters from 124 reflections

θ = 3–23°

μ = 7.65 mm^{-1}

T = 165 (2) K

Rod, colourless

0.55 × 0.08 × 0.06 mm

Data collection

Siemens SMART 1K CCD diffractometer

Radiation source: normal-focus sealed tube

Monochromator: graphite

T = 165(2) K

ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 2000)

T_{min} = 0.459, T_{max} = 0.632

15554 measured reflections

4750 independent reflections

3716 reflections with $I > 2\sigma(I)$

R_{int} = 0.051

θ_{max} = 28.6°

θ_{min} = 1.7°

h = −26→25

k = −11→11

l = −18→18

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.077$

S = 1.01

4750 reflections

240 parameters

1 restraint

Primary atom site location: heavy-atom method

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.03P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001

$\Delta\rho_{max}$ = 1.40 e Å^{-3}

$\Delta\rho_{min}$ = −1.33 e Å^{-3}

Extinction correction: none

Absolute structure: Flack (1983)

Flack parameter: 0.003 (9)

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	0.030660 (16)	0.00085 (4)	0.21397 (2)	0.03045 (9)
Cl1	−0.06153 (14)	−0.0668 (3)	0.2601 (2)	0.0431 (6)
Cl2	−0.0766 (2)	0.2910 (6)	0.4864 (3)	0.1173 (16)
P1	0.12613 (12)	0.0508 (2)	0.17702 (16)	0.0231 (5)
C1	0.1051 (5)	0.1638 (9)	0.0544 (7)	0.0165 (18)
C2	0.1626 (5)	0.1598 (9)	0.0248 (7)	0.0254 (18)
H2A	0.2095	0.0973	0.0670	0.030*
C3	0.1532 (5)	0.2451 (9)	−0.0654 (7)	0.030 (2)
H3A	0.1933	0.2392	−0.0841	0.036*
C4	0.0855 (5)	0.3389 (8)	−0.1280 (6)	0.0230 (17)
C5	0.0773 (6)	0.4282 (9)	−0.2159 (7)	0.034 (2)
H5A	0.1161	0.4195	−0.2369	0.041*
C6	0.0126 (6)	0.5296 (11)	−0.2726 (7)	0.038 (3)
H6A	0.0080	0.5922	−0.3310	0.046*
C7	−0.0463 (5)	0.5400 (8)	−0.2439 (7)	0.034 (2)
H7A	−0.0908	0.6087	−0.2838	0.041*
C8	−0.0399 (5)	0.4501 (8)	−0.1575 (6)	0.0238 (18)
H8A	−0.0796	0.4586	−0.1382	0.029*
C9	0.0256 (4)	0.3467 (8)	−0.0985 (6)	0.0205 (16)
C10	0.0334 (4)	0.2521 (8)	−0.0094 (6)	0.0188 (16)
C11	0.1655 (5)	−0.1328 (8)	0.1610 (7)	0.0244 (17)
C12	0.1319 (5)	−0.1978 (10)	0.0548 (8)	0.028 (2)
H12A	0.0926	−0.1418	−0.0096	0.033*
C13	0.1546 (5)	−0.3407 (9)	0.0421 (7)	0.034 (2)
H13A	0.1310	−0.3831	−0.0311	0.041*
C14	0.2102 (5)	−0.4225 (9)	0.1318 (7)	0.032 (2)
H14A	0.2257	−0.5219	0.1219	0.039*
C15	0.2445 (5)	−0.3616 (10)	0.2380 (8)	0.039 (2)
H15A	0.2840	−0.4186	0.3017	0.047*
C16	0.2207 (5)	−0.2143 (9)	0.2517 (7)	0.033 (2)
H16A	0.2436	−0.1724	0.3249	0.040*
C17	0.2116 (5)	0.1490 (9)	0.2941 (6)	0.0265 (19)
C18	0.2862 (6)	0.1502 (11)	0.3116 (8)	0.045 (2)

H18A	0.2958	0.0933	0.2622	0.053*
C19	0.3532 (7)	0.2352 (12)	0.4034 (9)	0.058 (3)
H19A	0.4056	0.2341	0.4139	0.069*
C20	0.3388 (6)	0.3176 (12)	0.4750 (8)	0.052 (3)
H20A	0.3814	0.3743	0.5357	0.063*
C21	0.2618 (8)	0.3168 (12)	0.4574 (8)	0.059 (3)
H21A	0.2517	0.3740	0.5063	0.071*
C22	0.1985 (6)	0.2331 (10)	0.3689 (7)	0.039 (2)
H22A	0.1462	0.2328	0.3589	0.047*
C23	0.0000	0.178 (2)	0.5000	0.073 (5)
H23A	−0.0212	0.1107	0.4330	0.088*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.03470 (15)	0.02825 (14)	0.03155 (14)	0.0041 (2)	0.01983 (12)	0.0057 (3)
Cl1	0.0461 (13)	0.0405 (12)	0.0593 (15)	0.0033 (10)	0.0393 (12)	0.0099 (11)
Cl2	0.061 (2)	0.208 (5)	0.073 (2)	0.008 (3)	0.029 (2)	−0.049 (3)
P1	0.0270 (11)	0.0210 (11)	0.0246 (10)	0.0053 (7)	0.0160 (9)	0.0023 (7)
C1	0.025 (5)	0.011 (4)	0.019 (4)	−0.010 (3)	0.016 (4)	−0.005 (3)
C2	0.015 (4)	0.027 (4)	0.032 (5)	0.004 (3)	0.011 (4)	−0.006 (4)
C3	0.035 (5)	0.026 (4)	0.050 (5)	−0.015 (4)	0.037 (5)	−0.022 (4)
C4	0.031 (5)	0.013 (4)	0.030 (4)	−0.008 (3)	0.020 (4)	−0.006 (3)
C5	0.055 (6)	0.027 (4)	0.039 (5)	−0.009 (4)	0.038 (5)	−0.007 (4)
C6	0.079 (6)	0.021 (8)	0.035 (4)	−0.007 (5)	0.045 (5)	−0.001 (4)
C7	0.049 (5)	0.014 (6)	0.035 (5)	0.001 (3)	0.020 (4)	0.002 (3)
C8	0.029 (4)	0.021 (4)	0.030 (4)	−0.003 (3)	0.022 (4)	0.000 (3)
C9	0.024 (4)	0.017 (4)	0.021 (4)	−0.013 (3)	0.013 (3)	−0.008 (3)
C10	0.024 (4)	0.018 (4)	0.014 (4)	−0.003 (3)	0.010 (3)	−0.002 (3)
C11	0.023 (4)	0.018 (4)	0.037 (5)	0.001 (3)	0.019 (4)	−0.004 (3)
C12	0.029 (6)	0.016 (5)	0.037 (5)	−0.001 (4)	0.017 (5)	−0.005 (4)
C13	0.036 (5)	0.023 (4)	0.043 (5)	−0.010 (4)	0.020 (5)	−0.007 (4)
C14	0.032 (5)	0.019 (4)	0.053 (6)	−0.007 (4)	0.028 (5)	−0.004 (4)
C15	0.042 (5)	0.034 (5)	0.048 (6)	0.009 (4)	0.029 (5)	0.020 (4)
C16	0.046 (6)	0.024 (5)	0.038 (5)	0.009 (4)	0.028 (5)	0.007 (4)
C17	0.034 (5)	0.021 (4)	0.021 (4)	0.003 (3)	0.013 (4)	0.003 (3)
C18	0.042 (6)	0.047 (6)	0.041 (6)	−0.004 (5)	0.020 (5)	−0.020 (4)
C19	0.052 (7)	0.058 (7)	0.048 (7)	0.001 (5)	0.017 (6)	0.010 (5)
C20	0.053 (7)	0.064 (7)	0.028 (5)	−0.023 (5)	0.014 (5)	−0.003 (5)
C21	0.099 (9)	0.051 (7)	0.033 (6)	−0.010 (6)	0.039 (6)	−0.005 (5)
C22	0.039 (5)	0.056 (6)	0.026 (5)	0.000 (4)	0.021 (4)	0.006 (4)
C23	0.072 (12)	0.076 (11)	0.102 (14)	0.000	0.067 (11)	0.000

Geometric parameters (Å, °)

Au1—P1	2.226 (2)	C11—C12	1.392 (12)
Au1—Cl1	2.290 (2)	C12—C13	1.362 (11)
Cl2—C23	1.712 (10)	C12—H12A	0.9500
P1—C17	1.811 (8)	C13—C14	1.345 (11)

P1—C1	1.833 (8)	C13—H13A	0.9500
P1—C11	1.835 (7)	C14—C15	1.376 (12)
C1—C2	1.388 (11)	C14—H14A	0.9500
C1—C10	1.416 (11)	C15—C16	1.409 (11)
C2—C3	1.395 (12)	C15—H15A	0.9500
C2—H2A	0.9500	C16—H16A	0.9500
C3—C4	1.393 (11)	C17—C18	1.338 (12)
C3—H3A	0.9500	C17—C22	1.413 (11)
C4—C5	1.396 (11)	C18—C19	1.454 (13)
C4—C9	1.434 (10)	C18—H18A	0.9500
C5—C6	1.386 (12)	C19—C20	1.383 (14)
C5—H5A	0.9500	C19—H19A	0.9500
C6—C7	1.409 (12)	C20—C21	1.384 (14)
C6—H6A	0.9500	C20—H20A	0.9500
C7—C8	1.394 (10)	C21—C22	1.400 (13)
C7—H7A	0.9500	C21—H21A	0.9500
C8—C9	1.410 (10)	C22—H22A	0.9500
C8—H8A	0.9500	C23—Cl2^{ii}	1.712 (10)
C9—C10	1.439 (10)	C23—H23A	0.9900
C10—C10^{i}	1.459 (14)	C23—H23A^{ii}	0.9900
C11—C16	1.349 (11)		

P1—Au1—Cl1	175.47 (8)	C13—C12—C11	120.8 (8)
C17—P1—C1	103.8 (4)	C13—C12—H12A	119.6
C17—P1—C11	106.3 (4)	C11—C12—H12A	119.6
C1—P1—C11	104.3 (4)	C14—C13—C12	120.9 (8)
C17—P1—Au1	110.8 (3)	C14—C13—H13A	119.6
C1—P1—Au1	122.1 (3)	C12—C13—H13A	119.6
C11—P1—Au1	108.4 (2)	C13—C14—C15	119.8 (8)
C2—C1—C10	120.3 (7)	C13—C14—H14A	120.1
C2—C1—P1	117.4 (6)	C15—C14—H14A	120.1
C10—C1—P1	122.3 (6)	C14—C15—C16	119.6 (8)
C1—C2—C3	121.8 (7)	C14—C15—H15A	120.2
C1—C2—H2A	119.1	C16—C15—H15A	120.2
C3—C2—H2A	119.1	C11—C16—C15	120.1 (8)
C4—C3—C2	120.3 (7)	C11—C16—H16A	119.9
C4—C3—H3A	119.8	C15—C16—H16A	119.9
C2—C3—H3A	119.8	C18—C17—C22	118.1 (8)
C3—C4—C5	120.4 (8)	C18—C17—P1	123.3 (7)
C3—C4—C9	119.1 (7)	C22—C17—P1	118.5 (7)
C5—C4—C9	120.4 (7)	C17—C18—C19	122.5 (9)
C6—C5—C4	120.1 (8)	C17—C18—H18A	118.8
C6—C5—H5A	120.0	C19—C18—H18A	118.8
C4—C5—H5A	120.0	C20—C19—C18	118.5 (10)
C5—C6—C7	120.2 (8)	C20—C19—H19A	120.8
C5—C6—H6A	119.9	C18—C19—H19A	120.8
C7—C6—H6A	119.9	C19—C20—C21	119.4 (10)
C8—C7—C6	120.6 (8)	C19—C20—H20A	120.3
C8—C7—H7A	119.7	C21—C20—H20A	120.3

C6—C7—H7A	119.7	C20—C21—C22	121.0 (10)
C7—C8—C9	120.1 (7)	C20—C21—H21A	119.5
C7—C8—H8A	120.0	C22—C21—H21A	119.5
C9—C8—H8A	120.0	C21—C22—C17	120.6 (9)
C8—C9—C4	118.6 (7)	C21—C22—H22A	119.7
C8—C9—C10	121.2 (7)	C17—C22—H22A	119.7
C4—C9—C10	120.2 (7)	Cl2—C23—Cl2^{ii}	109.7 (10)
C1—C10—C9	118.1 (7)	Cl2—C23—H23A	109.7
C1—C10—C10^{i}	123.9 (7)	Cl2^{ii}—C23—H23A	109.7
C9—C10—C10^{i}	118.0 (7)	Cl2—C23—H23A^{ii}	109.7
C16—C11—C12	118.9 (7)	Cl2^{ii}—C23—H23A^{ii}	109.7
C16—C11—P1	120.9 (6)	H23A—C23—H23A^{ii}	108.2
C12—C11—P1	119.8 (6)		

C17—P1—C1—C2	68.2 (6)	C4—C9—C10—C10^{i}	−173.6 (6)
C11—P1—C1—C2	−43.0 (6)	C17—P1—C11—C16	39.3 (8)
Au1—P1—C1—C2	−166.0 (5)	C1—P1—C11—C16	148.6 (7)
C17—P1—C1—C10	−112.1 (6)	Au1—P1—C11—C16	−79.9 (7)
C11—P1—C1—C10	136.7 (6)	C17—P1—C11—C12	−147.8 (7)
Au1—P1—C1—C10	13.7 (7)	C1—P1—C11—C12	−38.5 (7)
C10—C1—C2—C3	2.1 (11)	Au1—P1—C11—C12	93.1 (7)
P1—C1—C2—C3	−178.3 (6)	C16—C11—C12—C13	−0.6 (13)
C1—C2—C3—C4	0.6 (11)	P1—C11—C12—C13	−173.6 (7)
C2—C3—C4—C5	177.9 (7)	C11—C12—C13—C14	0.0 (14)
C2—C3—C4—C9	0.1 (10)	C12—C13—C14—C15	0.1 (13)
C3—C4—C5—C6	−175.4 (7)	C13—C14—C15—C16	0.4 (12)
C9—C4—C5—C6	2.4 (11)	C12—C11—C16—C15	1.1 (12)
C4—C5—C6—C7	−1.7 (12)	P1—C11—C16—C15	174.1 (6)
C5—C6—C7—C8	0.8 (12)	C14—C15—C16—C11	−1.0 (13)
C6—C7—C8—C9	−0.6 (11)	C1—P1—C17—C18	−69.1 (8)
C7—C8—C9—C4	1.3 (10)	C11—P1—C17—C18	40.6 (9)
C7—C8—C9—C10	−179.6 (6)	Au1—P1—C17—C18	158.1 (7)
C3—C4—C9—C8	175.6 (6)	C1—P1—C17—C22	108.7 (7)
C5—C4—C9—C8	−2.2 (10)	C11—P1—C17—C22	−141.6 (6)
C3—C4—C9—C10	−3.5 (10)	Au1—P1—C17—C22	−24.0 (7)
C5—C4—C9—C10	178.7 (7)	C22—C17—C18—C19	−0.5 (14)
C2—C1—C10—C9	−5.3 (10)	P1—C17—C18—C19	177.3 (7)
P1—C1—C10—C9	175.0 (5)	C17—C18—C19—C20	0.0 (15)
C2—C1—C10—C10^{i}	174.3 (6)	C18—C19—C20—C21	0.0 (15)
P1—C1—C10—C10^{i}	−5.4 (9)	C19—C20—C21—C22	0.4 (15)
C8—C9—C10—C1	−173.0 (6)	C20—C21—C22—C17	−0.9 (14)
C4—C9—C10—C1	6.0 (10)	C18—C17—C22—C21	1.0 (13)
C8—C9—C10—C10^{i}	7.4 (9)	P1—C17—C22—C21	−177.0 (7)

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

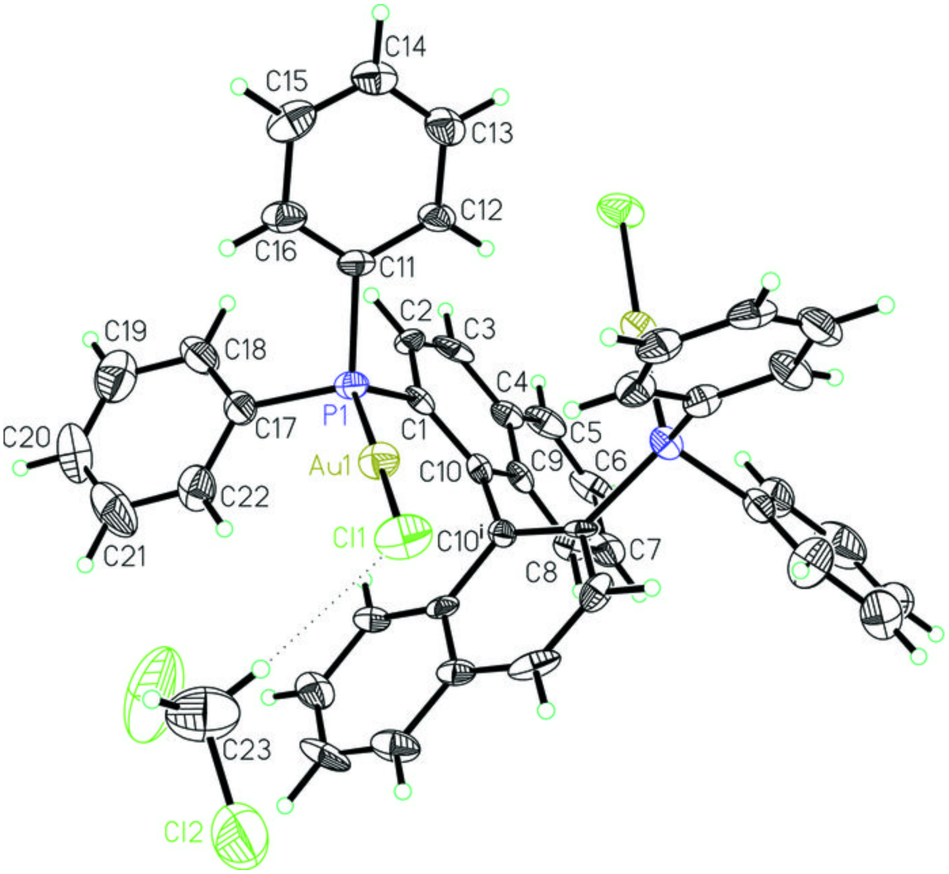
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

C6—H6A···Cl1^{iii}	0.95	3.12	3.614 (10)	114
C15—H15A···Cl2^{iv}	0.95	3.15	3.618 (11)	113
C16—H16A···Cl2^{iv}	0.95	3.00	3.542 (10)	118
C19—H19A···Cl1^{v}	0.95	3.10	3.658 (14)	120
C23—H23A···Cl1	0.99	2.62	3.611 (11)	174
C3—H3A···Cg3^{vi}	0.95	2.89	3.837	179
C8—H8A···Cg3^{iii}	0.95	3.07	3.792	134
C13—H13A···Cg2^{vii}	0.95	2.61	3.447	147
C14—H14A···Cg1^{vii}	0.95	3.05	3.612	119

Symmetry codes: (iii) $-x, y+1, -z$; (iv) $x+1/2, y-1/2, z$; (v) $x+1/2, y+1/2, z$; (vi) $-x+1/2, y+1/2, -z$; (vii) $x, y-1, z$.

Fig. 1


C14
C15
C13
C12
C16
C11
C2
C3
C19
C18
C4
P1
C5
C20
C17
C1
C6
C9
Au1
C10
C22
Cl1
C10ⁱ
C7
C21
C8
C23
Cl2