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trans-Dichloridobis[tris(4-methoxyphenyl)phosphane- κ P]platinum(II) acetone disolvate

Alfred Muller

Research Centre for Synthesis and Catalysis, Department of Chemistry, University of Johannesburg (APK Campus), PO Box 524, Auckland Park, Johannesburg, 2006, South Africa

Correspondence e-mail: mullera@uj.ac.za

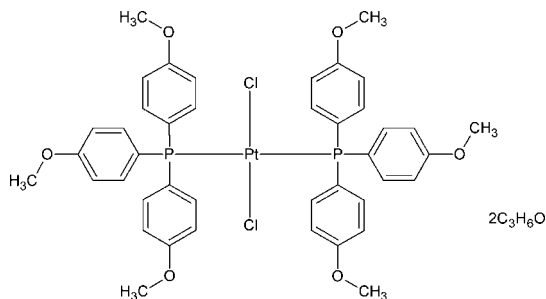
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 Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.019; wR factor = 0.040; data-to-parameter ratio = 20.6.

In the title compound, $[\text{PtCl}_2(\text{C}_{21}\text{H}_{21}\text{O}_3\text{P})_2] \cdot 2\text{C}_3\text{H}_6\text{O}$, the asymmetric unit contains a Pt^{II} ion situated on an inversion center, one chloride anion, one tris(4-methoxyphenyl)phosphane (L) ligand and one acetone solvent molecule. The Pt^{II} ion is coordinated by two P atoms [$\text{Pt}-\text{P} = 2.3196$ (5) Å] from two L ligands and two chloride anions [$\text{Pt}-\text{Cl} = 2.3075$ (5) Å] in a distorted square-planar geometry with $\text{P}-\text{Pt}-\text{Cl}$ angles of 88.016 (16) and 91.984 (16)°. The effective cone angle of the phosphane ligand was calculated to be 156° . Weak $\text{C}-\text{H} \cdots \text{O}$ and $\text{C}-\text{H} \cdots \text{Cl}$ hydrogen bonds hold molecules together.

Related literature

For related compounds, see: Spessard & Miessler (1996); van Blerk & Holzapfel (2009); Muller & Meijboom (2010). For background to cone angles, see: Tolman (1977); Otto (2001).



Experimental

Crystal data

 $[\text{PtCl}_2(\text{C}_{21}\text{H}_{21}\text{O}_3\text{P})_2] \cdot 2\text{C}_3\text{H}_6\text{O}$
 $M_r = 1086.84$

 Triclinic, $P\bar{1}$
 $a = 10.486$ (1) Å
 $b = 11.0360$ (11) Å
 $c = 11.3630$ (11) Å
 $\alpha = 85.787$ (2)°
 $\beta = 63.924$ (2)°
 $\gamma = 78.370$ (2)°

 $V = 1156.70$ (19) Å³
 $Z = 1$
 Mo $K\alpha$ radiation
 $\mu = 3.27$ mm⁻¹
 $T = 100$ K
 $0.19 \times 0.13 \times 0.11$ mm

Data collection

 Bruker APEX DUO 4K CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2008)
 $T_{\text{min}} = 0.679$, $T_{\text{max}} = 0.746$

 31470 measured reflections
 5799 independent reflections
 5763 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.042$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.019$
 $wR(F^2) = 0.040$
 $S = 1.04$
 5799 reflections

 282 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.68$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.51$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{C6}-\text{H6} \cdots \text{Cl1}$	0.95	2.7	3.493 (2)	142
$\text{C10}-\text{H10} \cdots \text{O1S}^{\text{I}}$	0.95	2.57	3.235 (3)	127
$\text{C12}-\text{H12} \cdots \text{O2}^{\text{II}}$	0.95	2.53	3.357 (2)	146

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

Data collection: APEX2 (Bruker, 2011); cell refinement: SAINT (Bruker, 2008); data reduction: SAINT and XPREP (Bruker, 2008); program(s) used to solve structure: SIR97 (Altomare *et al.*, 1999); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg & Putz, 2005); software used to prepare material for publication: publCIF (Westrip, 2010) and WinGX (Farrugia, 2012).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5352).

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Acta Cryst. (2012). E68, m1475 [doi:10.1107/S1600536812045643]

***trans*-Dichloridobis[tris(4-methoxyphenyl)phosphane- κ P]platinum(II) acetone disolvate**

Alfred Muller

S1. Comment

Transition metal complexes containing phosphane, arsine and stibine ligands are widely being investigated in various fields of organometallic chemistry (Spessard & Miessler, 1996). As part of a systematic investigation (Muller & Meijboom, 2010; van Blerk & Holzapfel, 2009) involving complexes with the general formula *trans/cis*-[MX₂(L)₂] (*M* = Pt or Pd; *X* = halogen, Me, Ph; *L* = Group 15 donor ligand), crystals of the title compound were obtained by the substitution of 1,5-cyclooctadiene (COD) with the tris(4-methoxyphenyl)phosphane from *cis*-[PtCl₂(COD)].

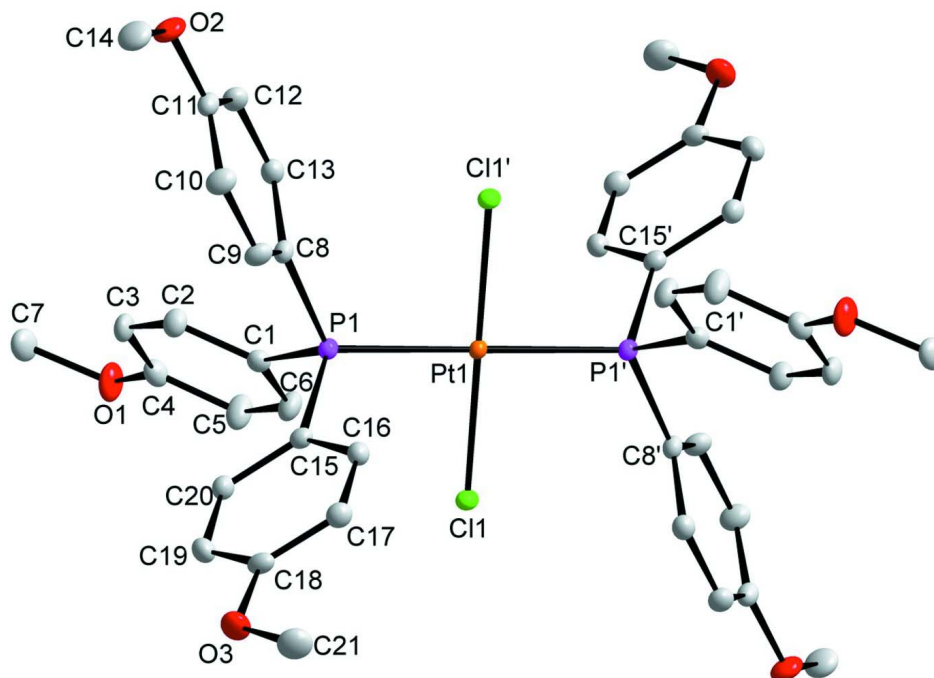
Molecules of the title compound (Fig. 1) crystallizes in the $P\bar{1}$ ($Z = 1$) space group with the Pt atom on an inversion center and two acetone solvate molecules accompanying it. Each pair of equivalent ligands is in a *trans* orientation with only slight distortion observed in the P—Pt—Cl angles from the ideal square-planar geometry. The orientation of the phosphanes is such that there is one 4-methoxyphenyl substituent close to the coordination plane, *i.e.* Cl1—Pt1—P1—C8 = -14.92 (7)°. The steric demand of phosphane ligand can be described by using an adaptation of the Tolman cone angle model (Tolman, 1977). By adjusting the Pt—P bond distance to 2.28 Å, and using the geometry from the title compound, an effective cone angle value (Otto, 2001) of 156° was obtained. The packing of the title compound shows weak C—H...Cl/O interactions (Table 1).

S2. Experimental

trans-Dichloridobis[tris(4-methoxyphenyl)phosphane]platinum(II) was prepared from reaction of *cis*-[PtCl₂(1,5-cyclooctadiene)] (10.8 mg, 0.0289 mmol) and tris(4-methoxyphenyl)phosphane (10 mg, 0.0259 mmol) in acetone. The mixture was refluxed for 4hrs, then filtered and crystals suitable for a single-crystal X-ray diffraction study was obtained by recrystallization from acetone. Analytical data: ³¹P {H} NMR (CDCl₃, 161.99 MHz): $\delta = 16.4$ (t, ¹J(³¹P-¹⁹⁵Pt) = 2586 Hz).

S3. Refinement

The aromatic and methyl H atoms were placed in geometrically idealized positions (C—H = 0.95–0.98) and allowed to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for aromatic and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms respectively. Methyl torsion angles were refined from electron density. Residual electron density values (< 1 Å⁻³) are within 1 Å from Pt and represent no physical meaning.

**Figure 1**

A view of the title complex, showing the atom-numbering scheme and 50% probability displacement ellipsoids [symmetry code: (') $1 - x, 1 - y, 1 - z$]. Hydrogen atoms and solvent molecules were omitted for clarity.

trans-Dichloridobis[tris(4-methoxyphenyl)phosphane- κP]platinum(II) acetone disolvate

Crystal data

$[\text{PtCl}_2(\text{C}_{21}\text{H}_{21}\text{O}_3\text{P})_2] \cdot 2\text{C}_3\text{H}_6\text{O}$

$M_r = 1086.84$

Triclinic, $P\bar{1}$

$a = 10.486$ (1) Å

$b = 11.0360$ (11) Å

$c = 11.3630$ (11) Å

$\alpha = 85.787$ (2)°

$\beta = 63.924$ (2)°

$\gamma = 78.370$ (2)°

$V = 1156.70$ (19) Å³

$Z = 1$

$F(000) = 548$

$D_x = 1.56$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å

Cell parameters from 9903 reflections

$\theta = 2.2\text{--}32.7^\circ$

$\mu = 3.27$ mm⁻¹

$T = 100$ K

Rectangle, colourless

$0.19 \times 0.13 \times 0.11$ mm

Data collection

Bruker APEX DUO 4K CCD
diffractometer

Graphite monochromator

Detector resolution: 8.4 pixels mm⁻¹

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2008)

$T_{\min} = 0.679$, $T_{\max} = 0.746$

31470 measured reflections

5799 independent reflections

5763 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.042$

$\theta_{\max} = 28.4^\circ$, $\theta_{\min} = 1.9^\circ$

$h = -13 \rightarrow 14$

$k = -14 \rightarrow 14$

$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.019$
 $wR(F^2) = 0.040$
 $S = 1.04$
 5799 reflections
 282 parameters
 0 restraints
 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
 $w = 1/[\sigma^2(F_o^2) + (0.016P)^2 + 0.4415P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.68 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.51 \text{ e } \text{\AA}^{-3}$

Special details

Experimental. The intensity data was collected on a Bruker Apex DUO 4 K CCD diffractometer using an exposure time of 20 s/frame. A total of 2352 frames were collected with a frame width of 0.5° covering up to $\theta = 28.66^\circ$ with 99.3% completeness accomplished.

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

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

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Pt1	0.5	0.5	0.5	0.00927 (3)
Cl1	0.52266 (5)	0.28766 (4)	0.49934 (4)	0.01424 (9)
P1	0.49557 (5)	0.49994 (4)	0.29769 (5)	0.01069 (9)
O2	0.31108 (15)	0.97824 (13)	0.08244 (15)	0.0210 (3)
O3	0.06877 (15)	0.21272 (14)	0.30254 (14)	0.0212 (3)
O1	1.08770 (15)	0.32059 (15)	-0.12406 (14)	0.0225 (3)
O1S	0.08106 (17)	0.10043 (16)	0.63614 (17)	0.0353 (4)
C20	0.4006 (2)	0.32915 (18)	0.19434 (19)	0.0146 (4)
H20	0.4908	0.3216	0.1189	0.017*
C6	0.7760 (2)	0.35873 (19)	0.1910 (2)	0.0190 (4)
H6	0.7519	0.3277	0.2769	0.023*
C19	0.2972 (2)	0.26563 (18)	0.1987 (2)	0.0174 (4)
H19	0.3177	0.2136	0.1272	0.021*
C18	0.1634 (2)	0.27795 (18)	0.3078 (2)	0.0153 (4)
C5	0.9129 (2)	0.3196 (2)	0.0926 (2)	0.0220 (5)
H5	0.9821	0.2622	0.1112	0.026*
C17	0.1346 (2)	0.35162 (18)	0.4140 (2)	0.0160 (4)
H17	0.0441	0.3598	0.4891	0.019*
C1	0.67224 (19)	0.44348 (17)	0.16598 (18)	0.0128 (4)
C8	0.43388 (19)	0.64708 (17)	0.23846 (18)	0.0123 (4)
C3	0.8488 (2)	0.44858 (19)	-0.06024 (19)	0.0165 (4)
H3	0.8737	0.4804	-0.1459	0.02*

C15	0.37324 (19)	0.40419 (17)	0.29972 (18)	0.0124 (4)
C12	0.4759 (2)	0.84717 (19)	0.14382 (19)	0.0171 (4)
H12	0.5356	0.9077	0.1135	0.02*
C11	0.3432 (2)	0.86913 (18)	0.13752 (19)	0.0149 (4)
C16	0.2402 (2)	0.41291 (18)	0.40867 (19)	0.0141 (4)
H16	0.221	0.4624	0.4817	0.017*
C10	0.2547 (2)	0.78264 (19)	0.1844 (2)	0.0183 (4)
H10	0.1631	0.7982	0.1827	0.022*
C7	1.1264 (2)	0.3620 (2)	-0.2550 (2)	0.0215 (4)
H7A	1.0643	0.3361	-0.2886	0.032*
H7B	1.2276	0.326	-0.3104	0.032*
H7C	1.1137	0.4525	-0.2561	0.032*
C4	0.9497 (2)	0.36409 (18)	-0.03364 (19)	0.0158 (4)
C1S	0.2096 (2)	0.0584 (2)	0.5897 (2)	0.0253 (5)
C9	0.3009 (2)	0.67246 (18)	0.2342 (2)	0.0164 (4)
H9	0.2397	0.613	0.2661	0.02*
C14	0.1812 (2)	0.9985 (2)	0.0649 (2)	0.0245 (5)
H14A	0.1845	0.9306	0.0121	0.037*
H14B	0.1726	1.0769	0.0201	0.037*
H14C	0.0975	1.002	0.1507	0.037*
C2	0.7115 (2)	0.48623 (19)	0.03891 (19)	0.0165 (4)
H2	0.6423	0.5428	0.0196	0.02*
C13	0.5205 (2)	0.73802 (18)	0.19384 (19)	0.0151 (4)
H13	0.6107	0.7241	0.1982	0.018*
C21	-0.0678 (2)	0.2190 (2)	0.4155 (2)	0.0253 (5)
H21A	-0.0516	0.1871	0.4915	0.038*
H21B	-0.126	0.169	0.3992	0.038*
H21C	-0.119	0.3052	0.4327	0.038*
C2S	0.2949 (3)	0.0285 (2)	0.4466 (2)	0.0388 (7)
H2S1	0.2289	0.0343	0.4057	0.058*
H2S2	0.3517	-0.0557	0.4346	0.058*
H2S3	0.3602	0.0873	0.4056	0.058*
C3S	0.2896 (3)	0.0339 (2)	0.6725 (3)	0.0385 (6)
H3S1	0.2234	0.0597	0.7632	0.058*
H3S2	0.3685	0.0805	0.6393	0.058*
H3S3	0.3295	-0.0548	0.6693	0.058*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.00961 (5)	0.00951 (5)	0.00805 (5)	-0.00186 (3)	-0.00334 (4)	0.00087 (4)
Cl1	0.0185 (2)	0.0105 (2)	0.0130 (2)	-0.00282 (17)	-0.00628 (18)	0.00104 (17)
P1	0.0110 (2)	0.0113 (2)	0.0095 (2)	-0.00231 (18)	-0.00417 (18)	0.00079 (18)
O2	0.0229 (7)	0.0151 (7)	0.0244 (8)	-0.0027 (6)	-0.0113 (6)	0.0078 (6)
O3	0.0204 (7)	0.0245 (8)	0.0227 (8)	-0.0114 (6)	-0.0098 (6)	-0.0001 (6)
O1	0.0129 (7)	0.0352 (9)	0.0120 (7)	0.0017 (6)	-0.0010 (6)	-0.0017 (6)
O1S	0.0215 (8)	0.0367 (10)	0.0382 (10)	-0.0019 (7)	-0.0049 (8)	-0.0059 (8)
C20	0.0154 (9)	0.0151 (10)	0.0121 (9)	-0.0033 (7)	-0.0050 (8)	0.0009 (7)

C6	0.0204 (10)	0.0200 (11)	0.0131 (10)	0.0004 (8)	-0.0062 (8)	0.0029 (8)
C19	0.0227 (10)	0.0158 (10)	0.0157 (10)	-0.0039 (8)	-0.0097 (8)	-0.0013 (8)
C18	0.0174 (9)	0.0133 (9)	0.0196 (10)	-0.0060 (7)	-0.0113 (8)	0.0048 (8)
C5	0.0180 (10)	0.0261 (12)	0.0160 (10)	0.0057 (8)	-0.0062 (8)	0.0004 (9)
C17	0.0145 (9)	0.0168 (10)	0.0165 (10)	-0.0039 (7)	-0.0065 (8)	0.0018 (8)
C1	0.0114 (8)	0.0132 (9)	0.0135 (9)	-0.0038 (7)	-0.0043 (7)	-0.0004 (7)
C8	0.0136 (9)	0.0129 (9)	0.0097 (9)	-0.0014 (7)	-0.0048 (7)	0.0007 (7)
C3	0.0174 (9)	0.0199 (10)	0.0092 (9)	-0.0028 (8)	-0.0034 (8)	0.0004 (8)
C15	0.0131 (8)	0.0116 (9)	0.0133 (9)	-0.0029 (7)	-0.0066 (7)	0.0024 (7)
C12	0.0192 (10)	0.0166 (10)	0.0160 (10)	-0.0074 (8)	-0.0070 (8)	0.0026 (8)
C11	0.0179 (9)	0.0131 (9)	0.0112 (9)	-0.0006 (7)	-0.0050 (8)	0.0004 (7)
C16	0.0160 (9)	0.0140 (9)	0.0125 (9)	-0.0027 (7)	-0.0062 (8)	-0.0002 (7)
C10	0.0152 (9)	0.0177 (10)	0.0228 (11)	-0.0028 (8)	-0.0098 (8)	0.0040 (8)
C7	0.0166 (10)	0.0268 (12)	0.0142 (10)	-0.0046 (8)	0.0001 (8)	-0.0028 (9)
C4	0.0121 (9)	0.0187 (10)	0.0141 (10)	-0.0024 (7)	-0.0030 (8)	-0.0037 (8)
C1S	0.0250 (11)	0.0141 (10)	0.0307 (13)	-0.0049 (9)	-0.0064 (10)	0.0028 (9)
C9	0.0158 (9)	0.0147 (10)	0.0182 (10)	-0.0055 (8)	-0.0065 (8)	0.0043 (8)
C14	0.0261 (11)	0.0195 (11)	0.0297 (12)	0.0009 (9)	-0.0167 (10)	0.0052 (9)
C2	0.0147 (9)	0.0192 (10)	0.0144 (10)	-0.0003 (8)	-0.0064 (8)	0.0008 (8)
C13	0.0156 (9)	0.0166 (10)	0.0133 (9)	-0.0043 (8)	-0.0060 (8)	0.0003 (8)
C21	0.0204 (10)	0.0275 (12)	0.0306 (13)	-0.0112 (9)	-0.0108 (10)	0.0027 (10)
C2S	0.0381 (14)	0.0278 (14)	0.0300 (14)	0.0102 (11)	-0.0042 (11)	0.0084 (11)
C3S	0.0387 (14)	0.0326 (14)	0.0456 (16)	-0.0033 (11)	-0.0208 (13)	-0.0010 (12)

Geometric parameters (Å, °)

Pt1—Cl1 ⁱ	2.3075 (5)	C3—C4	1.386 (3)
Pt1—Cl1	2.3075 (5)	C3—H3	0.95
Pt1—P1	2.3196 (5)	C15—C16	1.390 (3)
Pt1—P1 ⁱ	2.3197 (5)	C12—C13	1.378 (3)
P1—C15	1.8110 (19)	C12—C11	1.396 (3)
P1—C1	1.8151 (19)	C12—H12	0.95
P1—C8	1.8185 (19)	C11—C10	1.380 (3)
O2—C11	1.366 (2)	C16—H16	0.95
O2—C14	1.433 (2)	C10—C9	1.391 (3)
O3—C18	1.361 (2)	C10—H10	0.95
O3—C21	1.435 (3)	C7—H7A	0.98
O1—C4	1.366 (2)	C7—H7B	0.98
O1—C7	1.426 (2)	C7—H7C	0.98
O1S—C1S	1.212 (3)	C1S—C3S	1.492 (3)
C20—C19	1.386 (3)	C1S—C2S	1.495 (3)
C20—C15	1.397 (3)	C9—H9	0.95
C20—H20	0.95	C14—H14A	0.98
C6—C5	1.381 (3)	C14—H14B	0.98
C6—C1	1.401 (3)	C14—H14C	0.98
C6—H6	0.95	C2—H2	0.95
C19—C18	1.394 (3)	C13—H13	0.95
C19—H19	0.95	C21—H21A	0.98

C18—C17	1.391 (3)	C21—H21B	0.98
C5—C4	1.390 (3)	C21—H21C	0.98
C5—H5	0.95	C2S—H2S1	0.98
C17—C16	1.387 (3)	C2S—H2S2	0.98
C17—H17	0.95	C2S—H2S3	0.98
C1—C2	1.390 (3)	C3S—H3S1	0.98
C8—C9	1.388 (3)	C3S—H3S2	0.98
C8—C13	1.406 (3)	C3S—H3S3	0.98
C3—C2	1.384 (3)		
Cl1 ⁱ —Pt1—Cl1	180.0000 (10)	C17—C16—C15	122.03 (18)
Cl1 ⁱ —Pt1—P1	91.984 (16)	C17—C16—H16	119
Cl1—Pt1—P1	88.016 (16)	C15—C16—H16	119
Cl1 ⁱ —Pt1—P1 ⁱ	88.016 (16)	C11—C10—C9	119.42 (18)
Cl1—Pt1—P1 ⁱ	91.984 (16)	C11—C10—H10	120.3
P1—Pt1—P1 ⁱ	180	C9—C10—H10	120.3
C15—P1—C1	107.86 (9)	O1—C7—H7A	109.5
C15—P1—C8	103.27 (8)	O1—C7—H7B	109.5
C1—P1—C8	103.77 (9)	H7A—C7—H7B	109.5
C15—P1—Pt1	110.80 (6)	O1—C7—H7C	109.5
C1—P1—Pt1	112.70 (6)	H7A—C7—H7C	109.5
C8—P1—Pt1	117.60 (6)	H7B—C7—H7C	109.5
C11—O2—C14	116.83 (16)	O1—C4—C3	124.33 (18)
C18—O3—C21	117.38 (16)	O1—C4—C5	115.86 (17)
C4—O1—C7	116.81 (15)	C3—C4—C5	119.80 (18)
C19—C20—C15	120.62 (18)	O1S—C1S—C3S	121.7 (2)
C19—C20—H20	119.7	O1S—C1S—C2S	121.3 (2)
C15—C20—H20	119.7	C3S—C1S—C2S	117.0 (2)
C5—C6—C1	120.95 (18)	C8—C9—C10	121.71 (18)
C5—C6—H6	119.5	C8—C9—H9	119.1
C1—C6—H6	119.5	C10—C9—H9	119.1
C20—C19—C18	120.17 (18)	O2—C14—H14A	109.5
C20—C19—H19	119.9	O2—C14—H14B	109.5
C18—C19—H19	119.9	H14A—C14—H14B	109.5
O3—C18—C17	124.15 (18)	O2—C14—H14C	109.5
O3—C18—C19	115.85 (18)	H14A—C14—H14C	109.5
C17—C18—C19	119.99 (18)	H14B—C14—H14C	109.5
C6—C5—C4	120.14 (18)	C3—C2—C1	121.79 (17)
C6—C5—H5	119.9	C3—C2—H2	119.1
C4—C5—H5	119.9	C1—C2—H2	119.1
C16—C17—C18	118.99 (18)	C12—C13—C8	120.71 (17)
C16—C17—H17	120.5	C12—C13—H13	119.6
C18—C17—H17	120.5	C8—C13—H13	119.6
C2—C1—C6	117.78 (17)	O3—C21—H21A	109.5
C2—C1—P1	121.60 (14)	O3—C21—H21B	109.5
C6—C1—P1	120.56 (15)	H21A—C21—H21B	109.5
C9—C8—C13	117.93 (17)	O3—C21—H21C	109.5
C9—C8—P1	121.10 (14)	H21A—C21—H21C	109.5

C13—C8—P1	120.97 (14)	H21B—C21—H21C	109.5
C2—C3—C4	119.52 (18)	C1S—C2S—H2S1	109.5
C2—C3—H3	120.2	C1S—C2S—H2S2	109.5
C4—C3—H3	120.2	H2S1—C2S—H2S2	109.5
C16—C15—C20	118.19 (17)	C1S—C2S—H2S3	109.5
C16—C15—P1	117.96 (14)	H2S1—C2S—H2S3	109.5
C20—C15—P1	123.68 (15)	H2S2—C2S—H2S3	109.5
C13—C12—C11	120.23 (18)	C1S—C3S—H3S1	109.5
C13—C12—H12	119.9	C1S—C3S—H3S2	109.5
C11—C12—H12	119.9	H3S1—C3S—H3S2	109.5
O2—C11—C10	124.34 (17)	C1S—C3S—H3S3	109.5
O2—C11—C12	115.70 (17)	H3S1—C3S—H3S3	109.5
C10—C11—C12	119.96 (18)	H3S2—C3S—H3S3	109.5
C11 ⁱ —Pt1—P1—C15	-133.32 (7)	C1—P1—C15—C16	166.68 (14)
C11—Pt1—P1—C15	46.68 (7)	C8—P1—C15—C16	-83.88 (16)
C11 ⁱ —Pt1—P1—C1	105.72 (7)	Pt1—P1—C15—C16	42.91 (16)
C11—Pt1—P1—C1	-74.28 (7)	C1—P1—C15—C20	-18.18 (18)
C11 ⁱ —Pt1—P1—C8	-14.92 (7)	C8—P1—C15—C20	91.26 (17)
C11—Pt1—P1—C8	165.08 (7)	Pt1—P1—C15—C20	-141.95 (14)
C15—C20—C19—C18	1.2 (3)	C14—O2—C11—C10	-4.5 (3)
C21—O3—C18—C17	-1.4 (3)	C14—O2—C11—C12	175.03 (18)
C21—O3—C18—C19	177.40 (17)	C13—C12—C11—O2	-177.95 (18)
C20—C19—C18—O3	179.52 (17)	C13—C12—C11—C10	1.6 (3)
C20—C19—C18—C17	-1.6 (3)	C18—C17—C16—C15	0.8 (3)
C1—C6—C5—C4	-0.1 (3)	C20—C15—C16—C17	-1.2 (3)
O3—C18—C17—C16	179.38 (17)	P1—C15—C16—C17	174.19 (15)
C19—C18—C17—C16	0.6 (3)	O2—C11—C10—C9	177.62 (19)
C5—C6—C1—C2	0.3 (3)	C12—C11—C10—C9	-1.8 (3)
C5—C6—C1—P1	-176.99 (17)	C7—O1—C4—C3	-2.8 (3)
C15—P1—C1—C2	88.16 (17)	C7—O1—C4—C5	178.13 (18)
C8—P1—C1—C2	-20.94 (18)	C2—C3—C4—O1	179.84 (19)
Pt1—P1—C1—C2	-149.22 (14)	C2—C3—C4—C5	-1.1 (3)
C15—P1—C1—C6	-94.64 (17)	C6—C5—C4—O1	179.66 (19)
C8—P1—C1—C6	156.27 (16)	C6—C5—C4—C3	0.5 (3)
Pt1—P1—C1—C6	27.99 (18)	C13—C8—C9—C10	1.7 (3)
C15—P1—C8—C9	14.06 (18)	P1—C8—C9—C10	-177.47 (16)
C1—P1—C8—C9	126.52 (16)	C11—C10—C9—C8	0.2 (3)
Pt1—P1—C8—C9	-108.28 (16)	C4—C3—C2—C1	1.3 (3)
C15—P1—C8—C13	-165.06 (16)	C6—C1—C2—C3	-0.9 (3)
C1—P1—C8—C13	-52.59 (17)	P1—C1—C2—C3	176.36 (16)
Pt1—P1—C8—C13	72.60 (17)	C11—C12—C13—C8	0.4 (3)
C19—C20—C15—C16	0.2 (3)	C9—C8—C13—C12	-2.0 (3)
C19—C20—C15—P1	-174.93 (15)	P1—C8—C13—C12	177.19 (15)

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

Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C6—H6···C11	0.95	2.7	3.493 (2)	142
C10—H10···O1S ⁱⁱ	0.95	2.57	3.235 (3)	127
C12—H12···O2 ⁱⁱⁱ	0.95	2.53	3.357 (2)	146

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