

cis-Dichloridobis(triisopropoxyphosphine)platinum(II)

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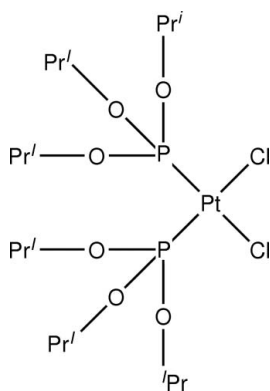
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Key indicators: single-crystal X-ray study; $T = 125$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.024; wR factor = 0.038; data-to-parameter ratio = 18.2.

The title compound, $[\text{PtCl}_2(\text{C}_9\text{H}_{21}\text{O}_3\text{P})_2]$, was obtained from a solution of $\text{PtCl}_2(\text{COD})$ ($\text{COD} = 1,5$ -cyclooctadiene) and triisopropylphosphite in dichloromethane. The complex features a Pt(II) atom coordinated by two Cl and two P atoms, yielding a slightly distorted *cis* square-planar geometry.

Related literature

For the structure of *cis*-bis(trimethoxyphosphite)dichlorido-platinum, see: Bao *et al.* (1987), for *cis*-dichloridobis(dimethoxyphenylphosphino)platinum(II), see: Slawin *et al.* (2007a); for dichloridobis(methoxydiphenylphosphino)platinum(II), see: Slawin *et al.* (2007b) and for *cis*-bis(trimethoxyphosphite)-dichloridopalladium(II), see Slawin *et al.* (2009).



Experimental

Crystal data

$[\text{PtCl}_2(\text{C}_9\text{H}_{21}\text{O}_3\text{P})_2]$
 $M_r = 682.47$
Monoclinic, $P2_1/c$
 $a = 10.8962$ (4) Å
 $b = 18.9114$ (8) Å
 $c = 14.2754$ (6) Å
 $\beta = 104.7461$ (10)°

$V = 2844.7$ (2) Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 5.24$ mm⁻¹
 $T = 125$ K
 $0.22 \times 0.22 \times 0.13$ mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan
(*ABSCOR*; Higashi, 1995)
 $T_{\min} = 0.356$, $T_{\max} = 0.506$

24157 measured reflections
4995 independent reflections
4473 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.040$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.024$
 $wR(F^2) = 0.038$
 $S = 1.11$
4995 reflections

275 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.57$ e Å⁻³
 $\Delta\rho_{\min} = -0.49$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Pt1—Cl1	2.3548 (7)	Pt1—P1	2.2176 (7)
Pt1—Cl2	2.3547 (9)	Pt1—P2	2.2117 (8)
Cl1—Pt1—Cl2	87.18 (2)	Cl2—Pt1—P1	85.34 (2)
Cl1—Pt1—P1	171.35 (2)	Cl2—Pt1—P2	175.09 (3)
Cl1—Pt1—P2	90.80 (2)	P1—Pt1—P2	96.99 (3)

Data collection: *SCXmini* (Rigaku, 2006); cell refinement: *PROCESS-AUTO* (Rigaku, 1998); data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalStructure* (Rigaku, 2006); software used to prepare material for publication: *CrystalStructure*.

We are grateful to the EPSRC for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FI2086).

References

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supplementary materials

Acta Cryst. (2009). E65, m1392 [doi:10.1107/S1600536809042226]

***cis*-Dichloridobis(triisopropoxyphosphine)platinum(II)**

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Comment

The title complex can be compared to similar platinum dichloride complexes containing trimethoxy phosphite; [PtCl₂(P(OMe)₃)₂] (Bao *et al.*, 1987). When compared to the structure of [PtCl₂(P(OMe)Ph₂)₂] and [PtCl₂(P(OMe)₂Ph)₂] (Slawin *et al.*, 2007*a*, 2007*b*) we note that the title compound has marginally shorter coordination bond lengths and significantly reduced Cl—Pt—Cl and P—Pt—P angles. Cl(1)—Pt(1)—Cl(2) 87.18?(2)°, P(1)—Pt(1)—P(2) 96.99?(3)°

Experimental

0.5 g (1.34 mmol) of PtCl₂(COD) was dissolved in the minimum volume of dichloromethane in a round-bottomed flask. To this 0.52 mL (2.67 mmol) of triisopropylphosphite was added. The solution was stirred for 0.5 h at room temperature. The product was precipitated *via* slow diffusion of hexane and the product was filtered off and dried under vacuum, [PtCl₂(P(OⁱPr)₃)₂](0.82 mmol, *ca* 63%). ³¹P-¹H}NMR: δ 61.7 p.p.m.. *J*{Pt—P} 5812 Hz.

Refinement

All H atoms were included in calculated positions (C—H distances are 0.98 Å for methyl H atoms, 1.00 Å for methylene H atoms) and were refined as riding atoms with *U*_{iso}(H) = 1.2 *U*_{eq}(parent atom, methylene H atoms) or *U*_{iso}(H) = 1.5 *U*_{eq}(parent atom, methyl H atoms). The highest peak in the difference map is 1.23 Å from atom Pt1.

Figures

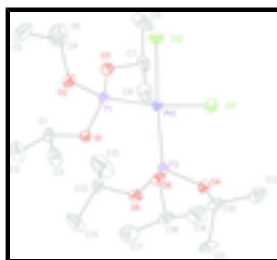


Fig. 1. The structure of (1) with displacement ellipsoids drawn at the 50% probability level, hydrogen atoms omitted for clarity.

***cis*-Dichloridobis(triisopropoxyphosphine)platinum(II)**

Crystal data

[PtCl₂(C₉H₂₁O₃P)₂]

M_r = 682.47

Monoclinic, *P*2₁/*c*

Hall symbol: -*P* 2ybc

*F*₀₀₀ = 1360.00

D_x = 1.593 Mg m⁻³

Mo *K*α radiation, λ = 0.71075 Å

Cell parameters from 27042 reflections

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$a = 10.8962$ (4) Å	$\theta = 3.0\text{--}27.5^\circ$
$b = 18.9114$ (8) Å	$\mu = 5.24$ mm ⁻¹
$c = 14.2754$ (6) Å	$T = 125$ K
$\beta = 104.7461$ (10)°	Chip, colourless
$V = 2844.7$ (2) Å ³	$0.22 \times 0.22 \times 0.13$ mm
$Z = 4$	

Data collection

Rigaku SCXmini diffractometer	4995 independent reflections
Radiation source: fine-focus sealed tube	4473 reflections with $F^2 > 2\sigma(F^2)$
Detector resolution: 6.85 pixels mm ⁻¹	$R_{\text{int}} = 0.040$
$T = 125$ K	$\theta_{\text{max}} = 25.0^\circ$
ω scans	$\theta_{\text{min}} = 2.1^\circ$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -12 \rightarrow 12$
$T_{\text{min}} = 0.356$, $T_{\text{max}} = 0.506$	$k = -22 \rightarrow 22$
24157 measured reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.024$	$w = 1/[\sigma^2(F_o^2) + (0.0077P)^2 + 2.3925P]$
$wR(F^2) = 0.038$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.11$	$(\Delta/\sigma)_{\text{max}} = 0.001$
4995 reflections	$\Delta\rho_{\text{max}} = 0.57$ e Å ⁻³
275 parameters	$\Delta\rho_{\text{min}} = -0.49$ e Å ⁻³
	Extinction correction: none

Special details

Geometry. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY

Refinement. Refinement was performed using all reflections. The weighted R -factor (wR) and goodness of fit (S) are based on F^2 . R -factor (gt) are based on F . The threshold expression of $F^2 > 2.0 \sigma(F^2)$ is used only for calculating R -factor (gt).

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Pt(1)	0.111011 (11)	0.242171 (6)	0.268469 (9)	0.01376 (4)
Cl(1)	0.15473 (8)	0.36409 (4)	0.26788 (6)	0.02227 (18)
Cl(2)	-0.09964 (8)	0.27341 (4)	0.26386 (7)	0.0280 (2)
P(1)	0.04057 (8)	0.13168 (4)	0.25627 (6)	0.01632 (18)
P(2)	0.31368 (8)	0.21699 (4)	0.28526 (6)	0.01501 (17)
O(1)	0.14345 (19)	0.07376 (10)	0.25384 (16)	0.0175 (5)
O(2)	-0.0612 (2)	0.11456 (11)	0.15873 (16)	0.0234 (5)

O(3)	-0.0298 (2)	0.10821 (11)	0.33539 (17)	0.0221 (5)
O(4)	0.4129 (2)	0.27767 (10)	0.32742 (15)	0.0180 (5)
O(5)	0.3566 (2)	0.19463 (12)	0.19174 (17)	0.0256 (5)
O(6)	0.3592 (2)	0.15798 (11)	0.36474 (16)	0.0200 (5)
C(1)	0.1080 (3)	-0.00243 (16)	0.2408 (2)	0.0216 (8)
C(2)	0.1982 (3)	-0.04269 (17)	0.3196 (2)	0.0326 (9)
C(3)	0.1142 (4)	-0.02438 (18)	0.1407 (2)	0.0384 (10)
C(4)	-0.1988 (3)	0.12485 (18)	0.1375 (2)	0.0311 (9)
C(5)	-0.2575 (3)	0.0519 (2)	0.1211 (3)	0.0587 (14)
C(6)	-0.2359 (4)	0.1716 (2)	0.0491 (3)	0.0513 (12)
C(7)	0.0033 (3)	0.13724 (18)	0.4343 (2)	0.0279 (8)
C(8)	0.1093 (3)	0.0943 (2)	0.4968 (2)	0.0382 (10)
C(9)	-0.1176 (3)	0.1367 (2)	0.4670 (3)	0.0449 (11)
C(10)	0.4641 (3)	0.32852 (17)	0.2685 (2)	0.0228 (8)
C(11)	0.5885 (3)	0.29936 (19)	0.2570 (2)	0.0315 (9)
C(12)	0.4805 (3)	0.39815 (17)	0.3221 (2)	0.0321 (9)
C(13)	0.2760 (3)	0.16206 (17)	0.1040 (2)	0.0225 (8)
C(14)	0.3629 (4)	0.1203 (2)	0.0582 (3)	0.0442 (11)
C(15)	0.2054 (4)	0.2179 (2)	0.0382 (2)	0.0534 (12)
C(16)	0.4941 (3)	0.13800 (17)	0.3989 (2)	0.0253 (8)
C(17)	0.5077 (3)	0.0630 (2)	0.3695 (3)	0.0533 (13)
C(18)	0.5323 (3)	0.1501 (2)	0.5057 (2)	0.0466 (11)
H(1)	0.0195	-0.0089	0.2473	0.026*
H(2)	0.2847	-0.0377	0.3120	0.039*
H(3)	0.1744	-0.0928	0.3155	0.039*
H(4)	0.1945	-0.0239	0.3828	0.039*
H(5)	0.0548	0.0043	0.0924	0.046*
H(6)	0.0912	-0.0744	0.1306	0.046*
H(7)	0.2005	-0.0173	0.1338	0.046*
H(8)	-0.2217	0.1481	0.1937	0.037*
H(9)	-0.2317	0.0288	0.0677	0.070*
H(10)	-0.3501	0.0560	0.1049	0.070*
H(11)	-0.2286	0.0237	0.1802	0.070*
H(12)	-0.1912	0.2169	0.0627	0.062*
H(13)	-0.3277	0.1799	0.0326	0.062*
H(14)	-0.2128	0.1484	-0.0054	0.062*
H(15)	0.0324	0.1872	0.4322	0.034*
H(16)	0.0835	0.0446	0.4955	0.046*
H(17)	0.1283	0.1119	0.5636	0.046*
H(18)	0.1850	0.0984	0.4721	0.046*
H(19)	-0.1809	0.1667	0.4239	0.054*
H(20)	-0.1007	0.1547	0.5334	0.054*
H(21)	-0.1500	0.0882	0.4648	0.054*
H(22)	0.4031	0.3342	0.2035	0.027*
H(23)	0.6462	0.2918	0.3210	0.038*
H(24)	0.6265	0.3331	0.2204	0.038*
H(25)	0.5733	0.2543	0.2219	0.038*
H(26)	0.3979	0.4146	0.3288	0.038*
H(27)	0.5160	0.4332	0.2857	0.038*

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H(28)	0.5383	0.3918	0.3864	0.038*
H(29)	0.2141	0.1293	0.1225	0.027*
H(30)	0.4276	0.1518	0.0444	0.053*
H(31)	0.3135	0.0991	-0.0023	0.053*
H(32)	0.4041	0.0829	0.1026	0.053*
H(33)	0.1510	0.2441	0.0712	0.064*
H(34)	0.1530	0.1959	-0.0205	0.064*
H(35)	0.2660	0.2505	0.0208	0.064*
H(36)	0.5458	0.1693	0.3674	0.030*
H(37)	0.4570	0.0321	0.4000	0.064*
H(38)	0.5971	0.0490	0.3902	0.064*
H(39)	0.4778	0.0589	0.2989	0.064*
H(40)	0.5205	0.2001	0.5192	0.056*
H(41)	0.6217	0.1373	0.5311	0.056*
H(42)	0.4797	0.1209	0.5367	0.056*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt(1)	0.01280 (7)	0.01280 (7)	0.01598 (7)	0.00090 (6)	0.00422 (5)	0.00039 (6)
Cl(1)	0.0217 (4)	0.0136 (4)	0.0319 (5)	-0.0003 (3)	0.0075 (4)	0.0018 (3)
Cl(2)	0.0155 (4)	0.0193 (4)	0.0505 (6)	0.0030 (3)	0.0111 (4)	-0.0011 (3)
P(1)	0.0143 (4)	0.0152 (4)	0.0197 (5)	-0.0008 (3)	0.0047 (3)	0.0000 (3)
P(2)	0.0131 (4)	0.0171 (4)	0.0152 (4)	0.0002 (3)	0.0043 (3)	-0.0004 (3)
O(1)	0.0145 (12)	0.0139 (11)	0.0237 (13)	-0.0001 (8)	0.0044 (10)	-0.0013 (9)
O(2)	0.0168 (12)	0.0244 (12)	0.0254 (14)	-0.0020 (10)	-0.0012 (11)	-0.0037 (10)
O(3)	0.0226 (13)	0.0195 (12)	0.0279 (14)	-0.0059 (9)	0.0131 (11)	-0.0031 (10)
O(4)	0.0178 (12)	0.0175 (11)	0.0187 (12)	-0.0038 (9)	0.0046 (10)	0.0006 (9)
O(5)	0.0174 (13)	0.0394 (14)	0.0214 (13)	-0.0001 (10)	0.0076 (11)	-0.0091 (10)
O(6)	0.0140 (12)	0.0178 (11)	0.0258 (14)	0.0004 (9)	0.0004 (10)	0.0073 (9)
C(1)	0.0244 (19)	0.0115 (16)	0.030 (2)	-0.0046 (14)	0.0082 (17)	-0.0032 (13)
C(2)	0.046 (2)	0.0159 (18)	0.034 (2)	0.0017 (17)	0.008 (2)	0.0006 (16)
C(3)	0.059 (2)	0.023 (2)	0.031 (2)	-0.0006 (18)	0.008 (2)	-0.0051 (16)
C(4)	0.017 (2)	0.0241 (19)	0.044 (2)	0.0016 (15)	-0.0071 (18)	-0.0037 (17)
C(5)	0.027 (2)	0.035 (2)	0.103 (4)	-0.0081 (19)	-0.005 (2)	-0.005 (2)
C(6)	0.046 (2)	0.041 (2)	0.052 (3)	0.010 (2)	-0.015 (2)	0.002 (2)
C(7)	0.040 (2)	0.0227 (19)	0.026 (2)	-0.0053 (16)	0.0177 (19)	-0.0063 (15)
C(8)	0.053 (2)	0.036 (2)	0.026 (2)	-0.0003 (19)	0.013 (2)	-0.0005 (17)
C(9)	0.057 (3)	0.041 (2)	0.052 (3)	0.007 (2)	0.042 (2)	0.002 (2)
C(10)	0.0162 (19)	0.0271 (19)	0.026 (2)	-0.0051 (14)	0.0073 (16)	0.0091 (15)
C(11)	0.017 (2)	0.041 (2)	0.038 (2)	-0.0048 (16)	0.0108 (18)	0.0048 (18)
C(12)	0.027 (2)	0.024 (2)	0.045 (2)	-0.0072 (16)	0.0079 (19)	0.0070 (17)
C(13)	0.027 (2)	0.0254 (19)	0.0166 (19)	-0.0076 (15)	0.0085 (16)	-0.0053 (14)
C(14)	0.054 (2)	0.047 (2)	0.036 (2)	0.014 (2)	0.019 (2)	-0.011 (2)
C(15)	0.074 (3)	0.065 (3)	0.021 (2)	0.030 (2)	0.012 (2)	0.004 (2)
C(16)	0.0150 (19)	0.0242 (19)	0.034 (2)	0.0035 (14)	0.0006 (17)	0.0058 (15)
C(17)	0.034 (2)	0.039 (2)	0.076 (3)	0.014 (2)	-0.004 (2)	-0.009 (2)
C(18)	0.030 (2)	0.060 (2)	0.041 (2)	0.012 (2)	-0.006 (2)	0.003 (2)

Geometric parameters (Å, °)

Pt(1)—Cl(1)	2.3548 (7)	C(4)—H(8)	1.000
Pt(1)—Cl(2)	2.3547 (9)	C(5)—H(9)	0.980
Pt(1)—P(1)	2.2176 (7)	C(5)—H(10)	0.980
Pt(1)—P(2)	2.2117 (8)	C(5)—H(11)	0.980
P(1)—O(1)	1.574 (2)	C(6)—H(12)	0.980
P(1)—O(2)	1.577 (2)	C(6)—H(13)	0.980
P(1)—O(3)	1.582 (2)	C(6)—H(14)	0.980
P(2)—O(4)	1.587 (2)	C(7)—H(15)	1.000
P(2)—O(5)	1.580 (2)	C(8)—H(16)	0.980
P(2)—O(6)	1.579 (2)	C(8)—H(17)	0.980
O(1)—C(1)	1.491 (3)	C(8)—H(18)	0.980
O(2)—C(4)	1.466 (4)	C(9)—H(19)	0.980
O(3)—C(7)	1.472 (4)	C(9)—H(20)	0.980
O(4)—C(10)	1.477 (4)	C(9)—H(21)	0.980
O(5)—C(13)	1.470 (3)	C(10)—H(22)	1.000
O(6)—C(16)	1.475 (3)	C(11)—H(23)	0.980
C(1)—C(2)	1.500 (4)	C(11)—H(24)	0.980
C(1)—C(3)	1.506 (5)	C(11)—H(25)	0.980
C(4)—C(5)	1.513 (5)	C(12)—H(26)	0.980
C(4)—C(6)	1.509 (5)	C(12)—H(27)	0.980
C(7)—C(8)	1.505 (4)	C(12)—H(28)	0.980
C(7)—C(9)	1.505 (6)	C(13)—H(29)	1.000
C(10)—C(11)	1.510 (5)	C(14)—H(30)	0.980
C(10)—C(12)	1.510 (4)	C(14)—H(31)	0.980
C(13)—C(14)	1.504 (5)	C(14)—H(32)	0.980
C(13)—C(15)	1.490 (5)	C(15)—H(33)	0.980
C(16)—C(17)	1.497 (5)	C(15)—H(34)	0.980
C(16)—C(18)	1.491 (5)	C(15)—H(35)	0.980
C(1)—H(1)	1.000	C(16)—H(36)	1.000
C(2)—H(2)	0.980	C(17)—H(37)	0.980
C(2)—H(3)	0.980	C(17)—H(38)	0.980
C(2)—H(4)	0.980	C(17)—H(39)	0.980
C(3)—H(5)	0.980	C(18)—H(40)	0.980
C(3)—H(6)	0.980	C(18)—H(41)	0.980
C(3)—H(7)	0.980	C(18)—H(42)	0.980
Cl(2)···C(11) ⁱ	3.410 (3)	H(19)···H(12) ⁱⁱ	2.981
C(7)···C(15) ⁱⁱ	3.591 (5)	H(19)···H(23) ⁱ	3.144
C(11)···Cl(2) ⁱⁱⁱ	3.410 (3)	H(19)···H(36) ⁱ	2.880
C(15)···C(7) ^{iv}	3.591 (5)	H(19)···H(38) ⁱ	3.233
Pt(1)···H(34) ⁱⁱ	3.155	H(19)···H(41) ⁱ	2.992
Pt(1)···H(35) ⁱⁱ	3.571	H(20)···Cl(2) ⁱⁱ	3.557
Cl(1)···H(1) ^v	3.035	H(20)···C(2) ^{vi}	3.340
Cl(1)···H(3) ^v	3.574	H(20)···H(3) ^{vi}	2.748
Cl(1)···H(6) ^v	3.551	H(20)···H(4) ^{vi}	3.036

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Cl(1)···H(11) ^v	3.162	H(20)···H(12) ⁱⁱ	2.693
Cl(1)···H(17) ^{iv}	2.893	H(20)···H(33) ⁱⁱ	3.275
Cl(1)···H(31) ⁱⁱ	3.369	H(20)···H(41) ⁱ	3.034
Cl(1)···H(34) ⁱⁱ	3.231	H(21)···C(2) ^{vi}	3.364
Cl(2)···H(3) ^v	2.807	H(21)···C(8) ^{vi}	3.505
Cl(2)···H(6) ^v	3.238	H(21)···H(3) ^{vi}	3.215
Cl(2)···H(20) ^{iv}	3.557	H(21)···H(4) ^{vi}	2.643
Cl(2)···H(23) ⁱ	3.099	H(21)···H(16) ^{vi}	2.635
Cl(2)···H(24) ⁱ	3.101	H(21)···H(36) ⁱ	3.595
Cl(2)···H(25) ⁱ	3.479	H(21)···H(38) ⁱ	2.791
P(2)···H(35) ⁱⁱ	3.584	H(21)···H(41) ⁱ	3.024
O(4)···H(30) ⁱⁱ	3.339	H(22)···C(18) ^{iv}	3.473
O(4)···H(35) ⁱⁱ	3.567	H(22)···H(17) ^{iv}	3.309
O(6)···H(35) ⁱⁱ	3.185	H(22)···H(40) ^{iv}	3.269
C(2)···H(20) ^{vi}	3.340	H(22)···H(42) ^{iv}	2.845
C(2)···H(21) ^{vi}	3.364	H(23)···Cl(2) ⁱⁱⁱ	3.099
C(2)···H(24) ^{vii}	3.170	H(23)···C(6) ^{xii}	3.256
C(2)···H(41) ^{viii}	3.076	H(23)···H(12) ^{xii}	3.457
C(3)···H(5) ^{ix}	3.389	H(23)···H(13) ^{xii}	3.010
C(3)···H(9) ^{ix}	3.526	H(23)···H(14) ^{xii}	2.801
C(3)···H(14) ^{ix}	3.383	H(23)···H(19) ⁱⁱⁱ	3.144
C(5)···H(26) ^x	3.186	H(24)···Cl(2) ⁱⁱⁱ	3.101
C(5)···H(31) ^{ix}	3.298	H(24)···C(2) ^{xiii}	3.170
C(6)···H(23) ^{xi}	3.256	H(24)···C(18) ^{iv}	2.992
C(6)···H(28) ^{xi}	3.159	H(24)···H(2) ^{xiii}	2.711
C(6)···H(40) ^{xi}	3.542	H(24)···H(3) ^{xiii}	2.739
C(7)···H(33) ⁱⁱ	3.138	H(24)···H(40) ^{iv}	2.879
C(7)···H(34) ⁱⁱ	3.535	H(24)···H(41) ^{iv}	2.747
C(7)···H(35) ⁱⁱ	3.525	H(24)···H(42) ^{iv}	2.839
C(8)···H(16) ^{vi}	3.382	H(25)···Cl(2) ⁱⁱⁱ	3.479
C(8)···H(21) ^{vi}	3.505	H(25)···C(18) ^{iv}	3.507
C(8)···H(33) ⁱⁱ	3.230	H(25)···H(8) ⁱⁱⁱ	3.106
C(8)···H(35) ⁱⁱ	3.369	H(25)···H(13) ⁱⁱⁱ	3.455
C(9)···H(3) ^{vi}	3.420	H(25)···H(40) ^{iv}	2.933
C(9)···H(4) ^{vi}	3.281	H(25)···H(41) ^{iv}	3.554
C(9)···H(12) ⁱⁱ	3.277	H(25)···H(42) ^{iv}	3.497
C(9)···H(16) ^{vi}	3.475	H(26)···C(5) ^v	3.186
C(9)···H(38) ⁱ	3.447	H(26)···C(14) ⁱⁱ	3.456
C(9)···H(41) ⁱ	3.199	H(26)···H(9) ^v	3.390
C(10)···H(42) ^{iv}	3.489	H(26)···H(10) ^v	2.928
C(11)···H(40) ^{iv}	3.285	H(26)···H(11) ^v	2.748

C(11)···H(41) ^{iv}	3.543	H(26)···H(30) ⁱⁱ	3.263
C(11)···H(42) ^{iv}	3.416	H(26)···H(31) ⁱⁱ	2.802
C(12)···H(10) ^v	3.574	H(27)···C(17) ^{xiii}	3.273
C(12)···H(13) ^{xii}	3.519	H(27)···H(2) ^{xiii}	2.916
C(12)···H(30) ⁱⁱ	3.497	H(27)···H(7) ^{xiii}	3.151
C(12)···H(31) ⁱⁱ	3.453	H(27)···H(10) ^v	3.541
C(12)···H(39) ^{xiii}	3.582	H(27)···H(32) ^{xiii}	3.257
C(14)···H(9) ^{ix}	3.453	H(27)···H(37) ^{xiii}	3.318
C(14)···H(10) ⁱⁱⁱ	3.262	H(27)···H(38) ^{xiii}	3.323
C(14)···H(26) ^{iv}	3.456	H(27)···H(39) ^{xiii}	2.675
C(14)···H(28) ^{iv}	3.479	H(28)···C(6) ^{xii}	3.159
C(15)···H(15) ^{iv}	2.759	H(28)···C(14) ⁱⁱ	3.479
C(15)···H(17) ^{iv}	3.369	H(28)···H(7) ^{xiii}	3.399
C(15)···H(18) ^{iv}	3.591	H(28)···H(9) ^{xii}	3.454
C(16)···H(19) ⁱⁱⁱ	3.510	H(28)···H(10) ^{xii}	3.201
C(17)···H(27) ^{vii}	3.273	H(28)···H(13) ^{xii}	2.603
C(18)···H(2) ^{viii}	3.554	H(28)···H(14) ^{xii}	2.862
C(18)···H(13) ^{xii}	3.538	H(28)···H(30) ⁱⁱ	2.934
C(18)···H(22) ⁱⁱ	3.473	H(28)···H(31) ⁱⁱ	3.245
C(18)···H(24) ⁱⁱ	2.992	H(30)···O(4) ^{iv}	3.339
C(18)···H(25) ⁱⁱ	3.507	H(30)···C(12) ^{iv}	3.497
C(18)···H(35) ⁱⁱ	3.510	H(30)···H(10) ⁱⁱⁱ	2.971
H(1)···Cl(1) ^x	3.035	H(30)···H(13) ⁱⁱⁱ	2.766
H(2)···C(18) ^{viii}	3.554	H(30)···H(26) ^{iv}	3.263
H(2)···H(24) ^{vii}	2.711	H(30)···H(28) ^{iv}	2.934
H(2)···H(27) ^{vii}	2.916	H(30)···H(40) ^{iv}	3.031
H(2)···H(41) ^{viii}	2.905	H(31)···Cl(1) ^{iv}	3.369
H(2)···H(42) ^{viii}	3.302	H(31)···C(5) ^{ix}	3.298
H(3)···Cl(1) ^x	3.574	H(31)···C(12) ^{iv}	3.453
H(3)···Cl(2) ^x	2.807	H(31)···H(9) ^{ix}	2.663
H(3)···C(9) ^{vi}	3.420	H(31)···H(10) ^{ix}	3.348
H(3)···H(20) ^{vi}	2.748	H(31)···H(11) ^{ix}	3.390
H(3)···H(21) ^{vi}	3.215	H(31)···H(26) ^{iv}	2.802
H(3)···H(24) ^{vii}	2.739	H(31)···H(28) ^{iv}	3.245
H(3)···H(41) ^{viii}	2.821	H(32)···H(9) ^{ix}	3.403
H(4)···C(9) ^{vi}	3.281	H(32)···H(10) ⁱⁱⁱ	2.718
H(4)···H(20) ^{vi}	3.036	H(32)···H(27) ^{vii}	3.257
H(4)···H(21) ^{vi}	2.643	H(33)···C(7) ^{iv}	3.138
H(4)···H(38) ^{viii}	3.484	H(33)···C(8) ^{iv}	3.230
H(4)···H(41) ^{viii}	2.978	H(33)···H(15) ^{iv}	2.448
H(5)···C(3) ^{ix}	3.389	H(33)···H(17) ^{iv}	2.734

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H(5)···H(5) ^{ix}	2.610	H(33)···H(18) ^{iv}	3.358
H(5)···H(6) ^{ix}	3.442	H(33)···H(20) ^{iv}	3.275
H(5)···H(9) ^{ix}	3.402	H(34)···Pt(1) ^{iv}	3.155
H(6)···Cl(1) ^x	3.551	H(34)···Cl(1) ^{iv}	3.231
H(6)···Cl(2) ^x	3.238	H(34)···C(7) ^{iv}	3.535
H(6)···H(5) ^{ix}	3.442	H(34)···H(6) ^{ix}	3.563
H(6)···H(14) ^{ix}	2.849	H(34)···H(15) ^{iv}	2.572
H(6)···H(34) ^{ix}	3.563	H(35)···Pt(1) ^{iv}	3.571
H(7)···H(9) ^{ix}	2.989	H(35)···P(2) ^{iv}	3.584
H(7)···H(14) ^{ix}	3.107	H(35)···O(4) ^{iv}	3.567
H(7)···H(27) ^{vii}	3.151	H(35)···O(6) ^{iv}	3.185
H(7)···H(28) ^{vii}	3.399	H(35)···C(7) ^{iv}	3.525
H(8)···H(25) ⁱ	3.106	H(35)···C(8) ^{iv}	3.369
H(9)···C(3) ^{ix}	3.526	H(35)···C(18) ^{iv}	3.510
H(9)···C(14) ^{ix}	3.453	H(35)···H(15) ^{iv}	2.797
H(9)···H(5) ^{ix}	3.402	H(35)···H(17) ^{iv}	3.139
H(9)···H(7) ^{ix}	2.989	H(35)···H(18) ^{iv}	3.018
H(9)···H(26) ^x	3.390	H(35)···H(40) ^{iv}	2.932
H(9)···H(28) ^{xi}	3.454	H(35)···H(42) ^{iv}	3.335
H(9)···H(31) ^{ix}	2.663	H(36)···H(19) ⁱⁱⁱ	2.880
H(9)···H(32) ^{ix}	3.403	H(36)···H(21) ⁱⁱⁱ	3.595
H(10)···C(12) ^x	3.574	H(37)···H(27) ^{vii}	3.318
H(10)···C(14) ⁱ	3.262	H(37)···H(37) ^{viii}	3.023
H(10)···H(26) ^x	2.928	H(37)···H(38) ^{viii}	3.544
H(10)···H(27) ^x	3.541	H(37)···H(41) ^{viii}	3.520
H(10)···H(28) ^{xi}	3.201	H(37)···H(42) ^{viii}	3.056
H(10)···H(30) ⁱ	2.971	H(38)···C(9) ⁱⁱⁱ	3.447
H(10)···H(31) ^{ix}	3.348	H(38)···H(4) ^{viii}	3.484
H(10)···H(32) ⁱ	2.718	H(38)···H(19) ⁱⁱⁱ	3.233
H(11)···Cl(1) ^x	3.162	H(38)···H(21) ⁱⁱⁱ	2.791
H(11)···H(26) ^x	2.748	H(38)···H(27) ^{vii}	3.323
H(11)···H(31) ^{ix}	3.390	H(38)···H(37) ^{viii}	3.544
H(12)···C(9) ^{iv}	3.277	H(38)···H(42) ^{viii}	3.542
H(12)···H(19) ^{iv}	2.981	H(39)···C(12) ^{vii}	3.582
H(12)···H(20) ^{iv}	2.693	H(39)···H(27) ^{vii}	2.675
H(12)···H(23) ^{xi}	3.457	H(40)···C(6) ^{xii}	3.542
H(12)···H(40) ^{xi}	3.425	H(40)···C(11) ⁱⁱ	3.285
H(12)···H(41) ^{xi}	3.390	H(40)···H(12) ^{xii}	3.425
H(13)···C(12) ^{xi}	3.519	H(40)···H(13) ^{xii}	2.787
H(13)···C(18) ^{xi}	3.538	H(40)···H(22) ⁱⁱ	3.269
H(13)···H(23) ^{xi}	3.010	H(40)···H(24) ⁱⁱ	2.879

H(13)···H(25) ⁱ	3.455	H(40)···H(25) ⁱⁱ	2.933
H(13)···H(28) ^{xi}	2.603	H(40)···H(30) ⁱⁱ	3.031
H(13)···H(30) ⁱ	2.766	H(40)···H(35) ⁱⁱ	2.932
H(13)···H(40) ^{xi}	2.787	H(41)···C(2) ^{viii}	3.076
H(13)···H(41) ^{xi}	3.501	H(41)···C(9) ⁱⁱⁱ	3.199
H(14)···C(3) ^{ix}	3.383	H(41)···C(11) ⁱⁱ	3.543
H(14)···H(6) ^{ix}	2.849	H(41)···H(2) ^{viii}	2.905
H(14)···H(7) ^{ix}	3.107	H(41)···H(3) ^{viii}	2.821
H(14)···H(23) ^{xi}	2.801	H(41)···H(4) ^{viii}	2.978
H(14)···H(28) ^{xi}	2.862	H(41)···H(12) ^{xii}	3.390
H(15)···C(15) ⁱⁱ	2.759	H(41)···H(13) ^{xii}	3.501
H(15)···H(33) ⁱⁱ	2.448	H(41)···H(19) ⁱⁱⁱ	2.992
H(15)···H(34) ⁱⁱ	2.572	H(41)···H(20) ⁱⁱⁱ	3.034
H(15)···H(35) ⁱⁱ	2.797	H(41)···H(21) ⁱⁱⁱ	3.024
H(16)···C(8) ^{vi}	3.382	H(41)···H(24) ⁱⁱ	2.747
H(16)···C(9) ^{vi}	3.475	H(41)···H(25) ⁱⁱ	3.554
H(16)···H(16) ^{vi}	2.508	H(41)···H(37) ^{viii}	3.520
H(16)···H(21) ^{vi}	2.635	H(42)···C(10) ⁱⁱ	3.489
H(17)···Cl(1) ⁱⁱ	2.893	H(42)···C(11) ⁱⁱ	3.416
H(17)···C(15) ⁱⁱ	3.369	H(42)···H(2) ^{viii}	3.302
H(17)···H(22) ⁱⁱ	3.309	H(42)···H(22) ⁱⁱ	2.845
H(17)···H(33) ⁱⁱ	2.734	H(42)···H(24) ⁱⁱ	2.839
H(17)···H(35) ⁱⁱ	3.139	H(42)···H(25) ⁱⁱ	3.497
H(18)···C(15) ⁱⁱ	3.591	H(42)···H(35) ⁱⁱ	3.335
H(18)···H(33) ⁱⁱ	3.358	H(42)···H(37) ^{viii}	3.056
H(18)···H(35) ⁱⁱ	3.018	H(42)···H(38) ^{viii}	3.542
H(19)···C(16) ⁱ	3.510		
Cl(1)—Pt(1)—Cl(2)	87.18 (2)	C(4)—C(6)—H(12)	109.5
Cl(1)—Pt(1)—P(1)	171.35 (2)	C(4)—C(6)—H(13)	109.5
Cl(1)—Pt(1)—P(2)	90.80 (2)	C(4)—C(6)—H(14)	109.5
Cl(2)—Pt(1)—P(1)	85.34 (2)	H(12)—C(6)—H(13)	109.5
Cl(2)—Pt(1)—P(2)	175.09 (3)	H(12)—C(6)—H(14)	109.5
P(1)—Pt(1)—P(2)	96.99 (3)	H(13)—C(6)—H(14)	109.5
Pt(1)—P(1)—O(1)	115.04 (8)	O(3)—C(7)—H(15)	109.0
Pt(1)—P(1)—O(2)	114.47 (8)	C(8)—C(7)—H(15)	109.0
Pt(1)—P(1)—O(3)	115.43 (8)	C(9)—C(7)—H(15)	109.0
O(1)—P(1)—O(2)	100.50 (11)	C(7)—C(8)—H(16)	109.5
O(1)—P(1)—O(3)	107.34 (12)	C(7)—C(8)—H(17)	109.5
O(2)—P(1)—O(3)	102.31 (12)	C(7)—C(8)—H(18)	109.5
Pt(1)—P(2)—O(4)	116.80 (8)	H(16)—C(8)—H(17)	109.5
Pt(1)—P(2)—O(5)	117.90 (8)	H(16)—C(8)—H(18)	109.5
Pt(1)—P(2)—O(6)	110.65 (9)	H(17)—C(8)—H(18)	109.5
O(4)—P(2)—O(5)	101.20 (12)	C(7)—C(9)—H(19)	109.5

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O(4)—P(2)—O(6)	100.33 (10)	C(7)—C(9)—H(20)	109.5
O(5)—P(2)—O(6)	108.15 (12)	C(7)—C(9)—H(21)	109.5
P(1)—O(1)—C(1)	120.80 (19)	H(19)—C(9)—H(20)	109.5
P(1)—O(2)—C(4)	127.4 (2)	H(19)—C(9)—H(21)	109.5
P(1)—O(3)—C(7)	122.4 (2)	H(20)—C(9)—H(21)	109.5
P(2)—O(4)—C(10)	125.05 (18)	O(4)—C(10)—H(22)	109.9
P(2)—O(5)—C(13)	126.2 (2)	C(11)—C(10)—H(22)	109.9
P(2)—O(6)—C(16)	121.6 (2)	C(12)—C(10)—H(22)	109.9
O(1)—C(1)—C(2)	107.3 (2)	C(10)—C(11)—H(23)	109.5
O(1)—C(1)—C(3)	108.2 (2)	C(10)—C(11)—H(24)	109.5
C(2)—C(1)—C(3)	113.1 (3)	C(10)—C(11)—H(25)	109.5
O(2)—C(4)—C(5)	106.3 (2)	H(23)—C(11)—H(24)	109.5
O(2)—C(4)—C(6)	107.0 (3)	H(23)—C(11)—H(25)	109.5
C(5)—C(4)—C(6)	113.1 (3)	H(24)—C(11)—H(25)	109.5
O(3)—C(7)—C(8)	109.3 (2)	C(10)—C(12)—H(26)	109.5
O(3)—C(7)—C(9)	105.9 (2)	C(10)—C(12)—H(27)	109.5
C(8)—C(7)—C(9)	114.4 (3)	C(10)—C(12)—H(28)	109.5
O(4)—C(10)—C(11)	107.7 (2)	H(26)—C(12)—H(27)	109.5
O(4)—C(10)—C(12)	107.0 (2)	H(26)—C(12)—H(28)	109.5
C(11)—C(10)—C(12)	112.3 (2)	H(27)—C(12)—H(28)	109.5
O(5)—C(13)—C(14)	106.6 (2)	O(5)—C(13)—H(29)	109.3
O(5)—C(13)—C(15)	109.9 (2)	C(14)—C(13)—H(29)	109.4
C(14)—C(13)—C(15)	112.3 (3)	C(15)—C(13)—H(29)	109.3
O(6)—C(16)—C(17)	108.1 (2)	C(13)—C(14)—H(30)	109.5
O(6)—C(16)—C(18)	107.1 (3)	C(13)—C(14)—H(31)	109.5
C(17)—C(16)—C(18)	114.2 (3)	C(13)—C(14)—H(32)	109.5
O(1)—C(1)—H(1)	109.4	H(30)—C(14)—H(31)	109.5
C(2)—C(1)—H(1)	109.4	H(30)—C(14)—H(32)	109.5
C(3)—C(1)—H(1)	109.4	H(31)—C(14)—H(32)	109.5
C(1)—C(2)—H(2)	109.5	C(13)—C(15)—H(33)	109.5
C(1)—C(2)—H(3)	109.5	C(13)—C(15)—H(34)	109.5
C(1)—C(2)—H(4)	109.5	C(13)—C(15)—H(35)	109.5
H(2)—C(2)—H(3)	109.5	H(33)—C(15)—H(34)	109.5
H(2)—C(2)—H(4)	109.5	H(33)—C(15)—H(35)	109.5
H(3)—C(2)—H(4)	109.5	H(34)—C(15)—H(35)	109.5
C(1)—C(3)—H(5)	109.5	O(6)—C(16)—H(36)	109.1
C(1)—C(3)—H(6)	109.5	C(17)—C(16)—H(36)	109.1
C(1)—C(3)—H(7)	109.5	C(18)—C(16)—H(36)	109.1
H(5)—C(3)—H(6)	109.5	C(16)—C(17)—H(37)	109.5
H(5)—C(3)—H(7)	109.5	C(16)—C(17)—H(38)	109.5
H(6)—C(3)—H(7)	109.5	C(16)—C(17)—H(39)	109.5
O(2)—C(4)—H(8)	110.1	H(37)—C(17)—H(38)	109.5
C(5)—C(4)—H(8)	110.1	H(37)—C(17)—H(39)	109.5
C(6)—C(4)—H(8)	110.1	H(38)—C(17)—H(39)	109.5
C(4)—C(5)—H(9)	109.5	C(16)—C(18)—H(40)	109.5
C(4)—C(5)—H(10)	109.5	C(16)—C(18)—H(41)	109.5
C(4)—C(5)—H(11)	109.5	C(16)—C(18)—H(42)	109.5
H(9)—C(5)—H(10)	109.5	H(40)—C(18)—H(41)	109.5
H(9)—C(5)—H(11)	109.5	H(40)—C(18)—H(42)	109.5

H(10)—C(5)—H(11)	109.5	H(41)—C(18)—H(42)	109.5
Cl(1)—Pt(1)—P(2)—O(4)	21.21 (10)	Pt(1)—P(2)—O(4)—C(10)	-93.9 (2)
Cl(1)—Pt(1)—P(2)—O(5)	-99.70 (10)	Pt(1)—P(2)—O(5)—C(13)	-25.7 (2)
Cl(1)—Pt(1)—P(2)—O(6)	135.11 (9)	Pt(1)—P(2)—O(6)—C(16)	-172.06 (19)
Cl(2)—Pt(1)—P(1)—O(1)	179.48 (10)	O(4)—P(2)—O(5)—C(13)	-154.4 (2)
Cl(2)—Pt(1)—P(1)—O(2)	63.79 (11)	O(5)—P(2)—O(4)—C(10)	35.4 (2)
Cl(2)—Pt(1)—P(1)—O(3)	-54.62 (9)	O(4)—P(2)—O(6)—C(16)	-48.1 (2)
P(1)—Pt(1)—P(2)—O(4)	-162.57 (9)	O(6)—P(2)—O(4)—C(10)	146.5 (2)
P(1)—Pt(1)—P(2)—O(5)	76.52 (10)	O(5)—P(2)—O(6)—C(16)	57.4 (2)
P(1)—Pt(1)—P(2)—O(6)	-48.67 (9)	O(6)—P(2)—O(5)—C(13)	100.7 (2)
P(2)—Pt(1)—P(1)—O(1)	-4.85 (10)	P(1)—O(1)—C(1)—C(2)	-129.3 (2)
P(2)—Pt(1)—P(1)—O(2)	-120.55 (11)	P(1)—O(1)—C(1)—C(3)	108.3 (2)
P(2)—Pt(1)—P(1)—O(3)	121.04 (9)	P(1)—O(2)—C(4)—C(5)	-115.5 (3)
Pt(1)—P(1)—O(1)—C(1)	-176.87 (19)	P(1)—O(2)—C(4)—C(6)	123.5 (2)
Pt(1)—P(1)—O(2)—C(4)	-86.4 (2)	P(1)—O(3)—C(7)—C(8)	-87.0 (3)
Pt(1)—P(1)—O(3)—C(7)	-31.2 (2)	P(1)—O(3)—C(7)—C(9)	149.3 (2)
O(1)—P(1)—O(2)—C(4)	149.7 (2)	P(2)—O(4)—C(10)—C(11)	-94.7 (2)
O(2)—P(1)—O(1)—C(1)	-53.4 (2)	P(2)—O(4)—C(10)—C(12)	144.3 (2)
O(1)—P(1)—O(3)—C(7)	98.5 (2)	P(2)—O(5)—C(13)—C(14)	-153.8 (2)
O(3)—P(1)—O(1)—C(1)	53.2 (2)	P(2)—O(5)—C(13)—C(15)	84.3 (3)
O(2)—P(1)—O(3)—C(7)	-156.2 (2)	P(2)—O(6)—C(16)—C(17)	-114.9 (3)
O(3)—P(1)—O(2)—C(4)	39.2 (2)	P(2)—O(6)—C(16)—C(18)	121.6 (2)

Symmetry codes: (i) $x-1, y, z$; (ii) $x, -y+1/2, z+1/2$; (iii) $x+1, y, z$; (iv) $x, -y+1/2, z-1/2$; (v) $-x, y+1/2, -z+1/2$; (vi) $-x, -y, -z+1$; (vii) $-x+1, y-1/2, -z+1/2$; (viii) $-x+1, -y, -z+1$; (ix) $-x, -y, -z$; (x) $-x, y-1/2, -z+1/2$; (xi) $x-1, -y+1/2, z-1/2$; (xii) $x+1, -y+1/2, z+1/2$; (xiii) $-x+1, y+1/2, -z+1/2$.

Fig. 1

