

## Dichloridobis[*N*-(diphenylphosphino)-isopropylamine- $\kappa$ P]platinum(II) chloroform solvate

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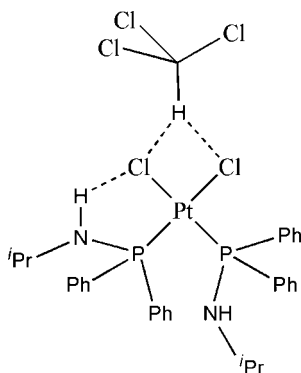
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Key indicators: single-crystal X-ray study;  $T = 150$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.022;  $wR$  factor = 0.043; data-to-parameter ratio = 22.0.

The *cis* isomer of the square-planar title complex has been crystallized as the chloroform solvate,  $[\text{PtCl}_2(\text{C}_{15}\text{H}_{18}\text{NP})_2] \cdot \text{CHCl}_3$ . Comparison of the Pt—P and Pt—Cl bond lengths and the Cl—Pt—Cl and P—Pt—P angles with the known compounds *cis*- $\{\text{Ph}_2\text{PN}(\text{H})\text{R}'\}_2\text{PtCl}_2$  reveals that the  $\text{R}'$  substituents have negligible effects on these structural parameters. Intramolecular N—H $\cdots$ Cl and intermolecular Pt—Cl $\cdots$ H—CCl<sub>3</sub> hydrogen bonds are evident in the title structure.

### Related literature

Functionalized tertiary phosphines with secondary amine groups have been used in coordination and organometallic chemistry (see Gaw *et al.*, 1999; Kühl *et al.*, 2001). For structures of square-planar dichloroplatinum(II) complexes with similar ligands, see also: Slawin *et al.* (2005); Priya *et al.* (2003). For related literature, see: Bergamini *et al.* (2004); Browning & Farrar (1995); Burrows *et al.* (2000); Clarke *et al.* (2003); Lindner *et al.* (2000); Ly *et al.* (1997); Slawin *et al.* (1999).



### Experimental

#### Crystal data

$[\text{PtCl}_2(\text{C}_{15}\text{H}_{18}\text{NP})_2] \cdot \text{CHCl}_3$   
 $M_r = 871.91$   
 Monoclinic,  $P2_1/n$   
 $a = 11.5142$  (4) Å  
 $b = 14.5440$  (5) Å  
 $c = 21.5825$  (8) Å  
 $\beta = 104.795$  (2)°  
 $V = 3494.4$  (2) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 4.51$  mm<sup>-1</sup>  
 $T = 150$  (2) K  
 $0.34 \times 0.24 \times 0.14$  mm

#### Data collection

Bruker SMART 1000 CCD diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 2003)  
 $T_{\min} = 0.287$ ,  $T_{\max} = 0.531$   
 26733 measured reflections  
 8350 independent reflections  
 6863 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.027$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.022$   
 $wR(F^2) = 0.044$   
 $S = 1.04$   
 8350 reflections  
 380 parameters  
 2 restraints  
 H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 1.14$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.75$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1 $\cdots$ Cl1	0.815 (17)	2.32 (2)	3.000 (2)	141 (3)
C31—H31 $\cdots$ Cl1	1.00	2.65	3.435 (3)	136
C31—H31 $\cdots$ Cl2	1.00	2.69	3.521 (3)	141

**Table 2**

Selected geometric parameters (Å, °) for (I) and a comparison with (II) and (III).

	(I)	(II)	(III)
Pt—P	2.2565 (6) 2.2416 (6)	2.2625 (10) 2.251 (9)	2.221 (2) [2.253 (2)] 2.254 (2) [2.239 (2)]
Pt—Cl	2.3779 (6) 2.3503 (6)	2.3644 (10) 2.3649 (12)	2.348 (2) [2.254 (2)] 2.362 (2) [2.353 (2)]
P—N	1.647 (2) 1.665 (2)	1.663 (3) 1.660 (4)	1.667 (8) [1.634 (8)] 1.686 (9) [1.669 (8)]
P—Pt—P	96.03 (2)	98.81 (4)	102.3 (1) [95.4 (1)]
Cl—Pt—Cl	84.75 (2)	84.53 (4)	86.6 (1) [86.6 (1)]

Notes: (I) this work ( $R = \text{iPr}$ ); (II) Slawin *et al.* (2005) ( $R = \text{CH}_2\text{CH}=\text{CH}_2$ ); (III) Priya *et al.* (2003), two molecules present in the asymmetric unit; values in square brackets are for the second molecule in the asymmetric unit ( $R = \text{Ph}$ ).

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Bruker, 2000); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and local programs.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2039).

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**supplementary materials**

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## Dichloridobis[*N*-(diphenylphosphino)isopropylamine- $\kappa$ P]platinum(II) chloroform solvate

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### Comment

Secondary aminophosphines are useful ligands in coordination and organometallic chemistry (Gaw *et al.*, 1999). Depending on the *R'* group these phosphorus(III) ligands may either be *P*-monodentate,  $R_2PN(H)R'$ , (Clarke *et al.*, 2003; Slawin *et al.*, 2005; Slawin *et al.*, 1999) or *P/P'*-didentate,  $R_2PN(H)R'N(H)PR_2$ , (Bergamini *et al.*, 2004; Lindner *et al.*, 2000; Ly *et al.*, 1997). For many of these ligands the  $Ph_2P$  group has been widely employed whereas *R'* has been various substituents *e.g.*  $CH_2CH=CH_2$  (II),  $CH(CH_3)C(O)OCH_3$  (III), Ph (Priya *et al.*, 2003; Slawin *et al.*, 1999, 2005). These ligands coordinate readily to  $d^8$  square-planar metal centres including palladium(II) and platinum(II). Both *cis*- and *trans*- geometric isomers of  $\{R_2PN(H)R'\}_2MCl_2$  have previously been structurally characterized (Browning & Farrar, 1995; Burrows *et al.*, 2000; Priya *et al.*, 2003; Slawin *et al.*, 2005; Slawin *et al.*, 1999). For *trans*- $\{R_2PN(H)R'\}_2MCl_2$  complexes two intramolecular H-bonds between both NH moieties and terminal chlorides are observed. Some of these ligands *e.g.*  $Ph_2PN(H)R$  ( $R = Ph, ^tBu$ ) complex also with Group 6 metals to give *cis*- and/or *trans*- $\{Ph_2PN(H)R\}_2M(CO)_4$  ( $M = Cr, Mo, W$ ) but with the more sterically hindered aminophosphine (2,4,6-Me<sub>3</sub>C<sub>6</sub>H<sub>2</sub>)<sub>2</sub>PN(H)Ph no coordination was observed (Kühl *et al.*, 2001; Priya *et al.*, 2003).

The structure of (I) (Fig. 1 and Table 2) exhibits an essentially square-planar, *cis*- geometry comprising two chloride and two  $Ph_2PN(H)^iPr$  ligands around the platinum(II) metal centre. In (I) the Pt—P and Pt—Cl bond lengths are typical and compare favourably with those reported for the related complexes (II) and (III) (Table 2). The angles around the platinum coordination sphere in (I) vary from 84.75 (2)° [Cl—Pt—Cl] to 96.03 (2)° [P—Pt—P]. The P—N bond distances for (I) are similar to those in (II) and (III) and are shorter than those expected for a single P—N bond. This suggests some delocalization of electron density. Complex (I) displays an intramolecular H-bond between the secondary amine and a terminal bound chloride ligand. This leads to disparity between the Pt(1)—P(1)—N(1) and Pt(1)—P(2)—N(2) bond angles [109.00 (8)° *versus*. 116.04 (8)° respectively]. The chloroform hydrogen forms a bifurcated H-bond to the two Pt-coordinated chlorides.

In summary, we have shown that the aminophosphine  $Ph_2PN(H)^iPr$  complexes to platinum(II) to afford the *cis*-isomer  $\{Ph_2PN(H)^iPr\}_2PtCl_2$  with typical Pt—P/Pt—Cl/P—N bond lengths and Cl—Pt—Cl/P—Pt—P bond angles.

### Experimental

Preparation of (I). To a  $CH_2Cl_2$  (10 ml) solution of  $PtCl_2(cod)$  (0.046 g, 0.123 mmol) was added  $Ph_2PN(H)^iPr$  (0.066 g, 0.244 mmol). The solution was stirred for 1 h and the volume reduced to *ca* 2 ml under reduced pressure. Addition of petroleum ether (b.p. 60–80 °C, 20 ml) gave (I) which was collected by suction filtration and dried *in vacuo*. Yield: 0.045 g, 49%. Selected data:  $^{31}P\{^1H\}/(CDCl_3)$ : 30.4 p.p.m.,  $^1J(PtP)$  3952 Hz.  $^1H/(CDCl_3)$ : 7.61–7.27 (m, arom. H), 3.89 [t,  $^2J(PH)$  21 Hz, NH], 2.65 (m, CH), 0.69 [d,  $^3J(HH)$  6.4 Hz, CH<sub>3</sub>] p.p.m.. FT—IR/(KBr pellet):  $\nu_{NH}$  3363, 3262,  $\nu_{PtCl}$  310, 284

## supplementary materials

$\text{cm}^{-1}$ . Found: C, 44.41; H, 4.24; N, 3.26.  $\text{C}_{30}\text{H}_{36}\text{Cl}_2\text{N}_2\text{P}_2\text{Pt}\cdot\text{CH}_2\text{Cl}_2$  requires C, 44.51; H, 4.58; N, 3.35%. Colourless block crystals of (I) were obtained by slow diffusion of petroleum ether (b.p. 60–80 °C) into a  $\text{CHCl}_3$  solution.

### Refinement

Aromatic H atoms were placed in geometric positions (C—H distance = 0.95 Å for aryl H; 0.98 Å for methyl H; and 1.00 Å for methine H) using a riding model. NH coordinates were freely refined.  $U_{\text{iso}}$  values were set to  $1.2U_{\text{eq}}$  ( $1.5U_{\text{eq}}$  for methyl H and NH).

### Figures

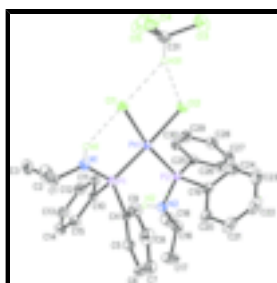


Fig. 1. A perspective view of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. Hydrogen bonds are shown as dashed lines.

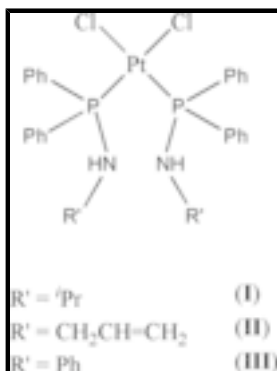


Fig. 2. The schematic structures of some *cis*- $\{\text{Ph}_2\text{PN}(\text{H})\text{R}'\}_2\text{PtCl}_2$  compounds.

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#### Crystal data

$[\text{PtCl}_2(\text{C}_{15}\text{H}_{18}\text{NP})_2]\cdot\text{CHCl}_3$

$M_r = 871.91$

Monoclinic,  $P2_1/n$

Hall symbol:  $-P\ 2_1n$

$a = 11.5142$  (4) Å

$b = 14.5440$  (5) Å

$c = 21.5825$  (8) Å

$\beta = 104.795$  (2)°

$V = 3494.4$  (2) Å<sup>3</sup>

$Z = 4$

$F_{000} = 1720$

$D_x = 1.657$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 13577 reflections

$\theta = 2.3$ – $28.9$ °

$\mu = 4.51$  mm<sup>-1</sup>

$T = 150$  (2) K

Block, colourless

$0.34 \times 0.24 \times 0.14$  mm

*Data collection*

Bruker SMART 1000 CCD diffractometer	8350 independent reflections
Radiation source: sealed tube	6863 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.027$
$T = 150(2)$ K	$\theta_{\text{max}} = 29.0^\circ$
$\omega$ rotation with narrow frames scans	$\theta_{\text{min}} = 1.7^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	$h = -14 \rightarrow 15$
$T_{\text{min}} = 0.287$ , $T_{\text{max}} = 0.531$	$k = -18 \rightarrow 17$
26733 measured reflections	$l = -27 \rightarrow 29$

*Refinement*

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: geom except NH coords freely refined
$R[F^2 > 2\sigma(F^2)] = 0.022$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.044$	$w = 1/[\sigma^2(F_o^2) + (0.0136P)^2 + 2.3257P]$
$S = 1.04$	where $P = (F_o^2 + 2F_c^2)/3$
8350 reflections	$(\Delta/\sigma)_{\text{max}} = 0.002$
380 parameters	$\Delta\rho_{\text{max}} = 1.14 \text{ e } \text{\AA}^{-3}$
2 restraints	$\Delta\rho_{\text{min}} = -0.75 \text{ e } \text{\AA}^{-3}$
Primary atom site location: heavy-atom method	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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Pt1	0.610678 (8)	0.266739 (7)	0.607682 (4)	0.01569 (3)
Cl1	0.40601 (5)	0.23034 (5)	0.59963 (3)	0.02215 (13)
Cl2	0.62839 (6)	0.27216 (5)	0.71855 (3)	0.02706 (14)
P1	0.58363 (5)	0.25957 (4)	0.50050 (3)	0.01643 (13)

## supplementary materials

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P2	0.81064 (6)	0.28418 (4)	0.63150 (3)	0.01808 (14)
N1	0.4412 (2)	0.23747 (16)	0.46669 (10)	0.0239 (5)
H1	0.397 (2)	0.237 (2)	0.4910 (12)	0.036*
C1	0.3803 (2)	0.23277 (19)	0.39797 (12)	0.0249 (6)
H1A	0.4430	0.2293	0.3734	0.030*
C2	0.3042 (3)	0.1459 (2)	0.38439 (14)	0.0401 (8)
H2A	0.3552	0.0920	0.3986	0.060*
H2B	0.2670	0.1412	0.3383	0.060*
H2C	0.2414	0.1485	0.4076	0.060*
C3	0.3063 (3)	0.3187 (2)	0.37732 (13)	0.0373 (7)
H3A	0.2467	0.3248	0.4024	0.056*
H3B	0.2652	0.3143	0.3317	0.056*
H3C	0.3592	0.3726	0.3846	0.056*
C4	0.6650 (2)	0.16705 (17)	0.47293 (11)	0.0191 (5)
C5	0.7616 (2)	0.17847 (19)	0.44604 (12)	0.0236 (6)
H5	0.7901	0.2385	0.4409	0.028*
C6	0.8167 (3)	0.1026 (2)	0.42654 (13)	0.0300 (7)
H6	0.8820	0.1111	0.4076	0.036*
C7	0.7766 (3)	0.0151 (2)	0.43462 (14)	0.0345 (7)
H7	0.8141	-0.0366	0.4210	0.041*
C8	0.6825 (3)	0.0023 (2)	0.46236 (14)	0.0350 (7)
H8	0.6559	-0.0581	0.4684	0.042*
C9	0.6266 (3)	0.07774 (19)	0.48150 (13)	0.0280 (6)
H9	0.5617	0.0687	0.5006	0.034*
C10	0.6209 (2)	0.36412 (17)	0.46285 (11)	0.0180 (5)
C11	0.6288 (2)	0.44695 (18)	0.49622 (12)	0.0220 (6)
H11	0.6239	0.4471	0.5395	0.026*
C12	0.6440 (2)	0.52958 (19)	0.46646 (14)	0.0275 (6)
H12	0.6491	0.5857	0.4895	0.033*
C13	0.6516 (3)	0.53001 (19)	0.40386 (14)	0.0296 (7)
H13	0.6615	0.5865	0.3837	0.036*
C14	0.6449 (2)	0.44817 (19)	0.37024 (13)	0.0278 (6)
H14	0.6513	0.4486	0.3272	0.033*
C15	0.6288 (2)	0.36561 (19)	0.39924 (12)	0.0237 (6)
H15	0.6232	0.3098	0.3758	0.028*
N2	0.86725 (19)	0.31830 (16)	0.57158 (10)	0.0215 (5)
H2	0.822 (2)	0.3539 (17)	0.5452 (12)	0.032*
C16	0.9961 (2)	0.3428 (2)	0.58081 (13)	0.0298 (6)
H16	1.0437	0.3106	0.6201	0.036*
C17	1.0398 (3)	0.3090 (3)	0.52374 (16)	0.0471 (9)
H17A	1.0278	0.2423	0.5191	0.071*
H17B	1.1254	0.3231	0.5307	0.071*
H17C	0.9942	0.3397	0.4847	0.071*
C18	1.0154 (3)	0.4455 (2)	0.59066 (16)	0.0452 (9)
H18A	0.9664	0.4784	0.5535	0.068*
H18B	1.1004	0.4600	0.5955	0.068*
H18C	0.9920	0.4644	0.6293	0.068*
C19	0.8767 (2)	0.17142 (18)	0.65314 (12)	0.0220 (6)
C20	0.9065 (2)	0.11735 (19)	0.60665 (14)	0.0285 (6)

H20	0.9026	0.1424	0.5655	0.034*
C21	0.9421 (3)	0.0269 (2)	0.61997 (16)	0.0379 (8)
H21	0.9621	-0.0098	0.5878	0.046*
C22	0.9486 (3)	-0.0103 (2)	0.67930 (17)	0.0394 (8)
H22	0.9731	-0.0724	0.6880	0.047*
C23	0.9196 (3)	0.0426 (2)	0.72611 (16)	0.0369 (8)
H23	0.9248	0.0170	0.7672	0.044*
C24	0.8827 (2)	0.1333 (2)	0.71358 (14)	0.0284 (6)
H24	0.8616	0.1693	0.7458	0.034*
C25	0.8729 (2)	0.36076 (18)	0.69854 (12)	0.0205 (5)
C26	0.9837 (2)	0.34360 (19)	0.74212 (12)	0.0246 (6)
H26	1.0236	0.2868	0.7407	0.030*
C27	1.0353 (3)	0.4093 (2)	0.78732 (13)	0.0305 (7)
H27	1.1102	0.3971	0.8169	0.037*
C28	0.9783 (3)	0.4925 (2)	0.78963 (13)	0.0301 (6)
H28	1.0138	0.5373	0.8208	0.036*
C29	0.8696 (3)	0.5102 (2)	0.74632 (13)	0.0306 (7)
H29	0.8312	0.5678	0.7473	0.037*
C30	0.8164 (2)	0.44455 (19)	0.70155 (13)	0.0257 (6)
H30	0.7407	0.4569	0.6727	0.031*
C31	0.3502 (3)	0.2155 (2)	0.74824 (13)	0.0354 (7)
H31	0.4102	0.2101	0.7221	0.042*
Cl3	0.42136 (9)	0.18738 (8)	0.82838 (4)	0.0609 (3)
Cl4	0.23036 (8)	0.13999 (7)	0.71669 (4)	0.0556 (2)
Cl5	0.29746 (8)	0.32944 (6)	0.74342 (4)	0.0493 (2)

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Pt1	0.01498 (5)	0.01740 (5)	0.01464 (5)	-0.00012 (4)	0.00371 (3)	0.00047 (4)
Cl1	0.0184 (3)	0.0288 (3)	0.0201 (3)	-0.0045 (3)	0.0065 (2)	-0.0015 (3)
Cl2	0.0228 (3)	0.0432 (4)	0.0154 (3)	-0.0049 (3)	0.0052 (2)	-0.0001 (3)
P1	0.0161 (3)	0.0173 (3)	0.0157 (3)	0.0000 (2)	0.0036 (2)	-0.0004 (3)
P2	0.0161 (3)	0.0212 (4)	0.0169 (3)	0.0001 (3)	0.0042 (2)	0.0006 (3)
N1	0.0203 (11)	0.0353 (13)	0.0162 (10)	-0.0040 (10)	0.0050 (9)	-0.0020 (10)
C1	0.0213 (13)	0.0349 (15)	0.0166 (12)	-0.0032 (12)	0.0012 (10)	-0.0002 (12)
C2	0.0420 (19)	0.044 (2)	0.0284 (16)	-0.0153 (15)	-0.0019 (14)	-0.0034 (14)
C3	0.0355 (17)	0.048 (2)	0.0226 (14)	0.0060 (14)	-0.0025 (13)	-0.0002 (14)
C4	0.0219 (13)	0.0183 (13)	0.0162 (12)	0.0028 (10)	0.0033 (10)	-0.0008 (10)
C5	0.0250 (14)	0.0233 (15)	0.0217 (13)	0.0029 (11)	0.0044 (11)	-0.0015 (11)
C6	0.0291 (15)	0.0351 (18)	0.0270 (15)	0.0092 (13)	0.0092 (12)	-0.0015 (13)
C7	0.0412 (18)	0.0295 (17)	0.0299 (16)	0.0142 (14)	0.0039 (14)	-0.0067 (13)
C8	0.0440 (19)	0.0194 (16)	0.0387 (17)	0.0017 (13)	0.0051 (14)	-0.0034 (13)
C9	0.0312 (16)	0.0236 (16)	0.0296 (15)	-0.0017 (12)	0.0087 (12)	0.0014 (12)
C10	0.0157 (12)	0.0196 (14)	0.0181 (12)	0.0001 (10)	0.0033 (10)	0.0018 (10)
C11	0.0210 (13)	0.0253 (15)	0.0202 (13)	0.0009 (11)	0.0062 (11)	0.0011 (11)
C12	0.0313 (16)	0.0177 (15)	0.0353 (16)	0.0023 (12)	0.0117 (13)	0.0001 (12)
C13	0.0330 (16)	0.0224 (15)	0.0370 (16)	0.0038 (12)	0.0153 (13)	0.0098 (13)



## supplementary materials

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C14	0.0319 (16)	0.0326 (17)	0.0204 (13)	0.0026 (12)	0.0095 (12)	0.0056 (12)
C15	0.0269 (14)	0.0241 (15)	0.0210 (13)	0.0000 (11)	0.0075 (11)	-0.0005 (11)
N2	0.0176 (11)	0.0263 (13)	0.0206 (11)	-0.0017 (9)	0.0047 (9)	0.0021 (9)
C16	0.0205 (14)	0.0417 (18)	0.0282 (15)	-0.0060 (12)	0.0082 (12)	-0.0008 (13)
C17	0.0329 (18)	0.069 (2)	0.046 (2)	-0.0164 (17)	0.0225 (15)	-0.0153 (18)
C18	0.0405 (19)	0.049 (2)	0.052 (2)	-0.0213 (16)	0.0220 (16)	-0.0053 (17)
C19	0.0156 (12)	0.0220 (14)	0.0270 (14)	-0.0005 (10)	0.0030 (11)	0.0003 (11)
C20	0.0224 (14)	0.0292 (16)	0.0316 (15)	0.0082 (12)	0.0028 (12)	0.0002 (12)
C21	0.0268 (16)	0.0337 (18)	0.048 (2)	0.0099 (13)	-0.0002 (14)	-0.0082 (15)
C22	0.0229 (15)	0.0242 (16)	0.065 (2)	0.0033 (12)	0.0002 (15)	0.0080 (16)
C23	0.0244 (15)	0.0379 (19)	0.0449 (19)	-0.0013 (13)	0.0024 (14)	0.0177 (15)
C24	0.0232 (14)	0.0304 (17)	0.0316 (15)	-0.0022 (12)	0.0071 (12)	0.0043 (13)
C25	0.0198 (13)	0.0232 (14)	0.0187 (12)	-0.0004 (11)	0.0053 (10)	-0.0007 (11)
C26	0.0228 (14)	0.0248 (15)	0.0254 (14)	0.0009 (11)	0.0047 (11)	-0.0010 (11)
C27	0.0229 (14)	0.0396 (18)	0.0254 (14)	-0.0025 (12)	-0.0006 (12)	-0.0023 (13)
C28	0.0323 (16)	0.0312 (17)	0.0257 (14)	-0.0085 (13)	0.0050 (12)	-0.0082 (13)
C29	0.0343 (17)	0.0245 (16)	0.0335 (16)	0.0019 (12)	0.0096 (13)	-0.0043 (13)
C30	0.0220 (14)	0.0287 (16)	0.0251 (14)	0.0024 (11)	0.0034 (11)	0.0005 (12)
C31	0.0321 (16)	0.051 (2)	0.0259 (15)	-0.0043 (14)	0.0136 (13)	-0.0023 (14)
Cl3	0.0603 (6)	0.0896 (8)	0.0323 (4)	0.0058 (5)	0.0105 (4)	0.0095 (5)
Cl4	0.0532 (5)	0.0645 (6)	0.0539 (5)	-0.0265 (5)	0.0226 (4)	-0.0134 (5)
Cl5	0.0398 (5)	0.0538 (6)	0.0555 (5)	-0.0010 (4)	0.0145 (4)	-0.0067 (4)

### *Geometric parameters (Å, °)*

Pt1—P2	2.2417 (6)	C14—C15	1.388 (4)
Pt1—P1	2.2564 (6)	C14—H14	0.9500
Pt1—C12	2.3503 (6)	C15—H15	0.9500
Pt1—C11	2.3780 (6)	N2—C16	1.489 (3)
P1—N1	1.648 (2)	N2—H2	0.845 (17)
P1—C4	1.824 (3)	C16—C18	1.517 (4)
P1—C10	1.826 (3)	C16—C17	1.526 (4)
P2—N2	1.666 (2)	C16—H16	1.0000
P2—C19	1.818 (3)	C17—H17A	0.9800
P2—C25	1.821 (3)	C17—H17B	0.9800
N1—C1	1.471 (3)	C17—H17C	0.9800
N1—H1	0.815 (17)	C18—H18A	0.9800
C1—C3	1.514 (4)	C18—H18B	0.9800
C1—C2	1.523 (4)	C18—H18C	0.9800
C1—H1A	1.0000	C19—C20	1.385 (4)
C2—H2A	0.9800	C19—C24	1.403 (4)
C2—H2B	0.9800	C20—C21	1.386 (4)
C2—H2C	0.9800	C20—H20	0.9500
C3—H3A	0.9800	C21—C22	1.374 (4)
C3—H3B	0.9800	C21—H21	0.9500
C3—H3C	0.9800	C22—C23	1.377 (5)
C4—C5	1.389 (3)	C22—H22	0.9500
C4—C9	1.399 (4)	C23—C24	1.392 (4)
C5—C6	1.391 (4)	C23—H23	0.9500

C5—H5	0.9500	C24—H24	0.9500
C6—C7	1.380 (4)	C25—C30	1.391 (4)
C6—H6	0.9500	C25—C26	1.401 (3)
C7—C8	1.378 (4)	C26—C27	1.386 (4)
C7—H7	0.9500	C26—H26	0.9500
C8—C9	1.387 (4)	C27—C28	1.384 (4)
C8—H8	0.9500	C27—H27	0.9500
C9—H9	0.9500	C28—C29	1.381 (4)
C10—C11	1.395 (4)	C28—H28	0.9500
C10—C15	1.399 (3)	C29—C30	1.385 (4)
C11—C12	1.394 (4)	C29—H29	0.9500
C11—H11	0.9500	C30—H30	0.9500
C12—C13	1.376 (4)	C31—C15	1.758 (3)
C12—H12	0.9500	C31—C14	1.759 (3)
C13—C14	1.386 (4)	C31—C13	1.763 (3)
C13—H13	0.9500	C31—H31	1.0000
P2—Pt1—P1	96.03 (2)	C13—C14—C15	120.2 (3)
P2—Pt1—C12	86.89 (2)	C13—C14—H14	119.9
P1—Pt1—C12	177.05 (2)	C15—C14—H14	119.9
P2—Pt1—C11	169.29 (2)	C14—C15—C10	120.4 (2)
P1—Pt1—C11	92.29 (2)	C14—C15—H15	119.8
C12—Pt1—C11	84.75 (2)	C10—C15—H15	119.8
N1—P1—C4	104.36 (12)	C16—N2—P2	122.79 (18)
N1—P1—C10	106.61 (11)	C16—N2—H2	112 (2)
C4—P1—C10	105.69 (11)	P2—N2—H2	114 (2)
N1—P1—Pt1	108.91 (8)	N2—C16—C18	111.0 (2)
C4—P1—Pt1	114.87 (8)	N2—C16—C17	109.7 (2)
C10—P1—Pt1	115.54 (8)	C18—C16—C17	111.3 (3)
N2—P2—C19	104.32 (12)	N2—C16—H16	108.2
N2—P2—C25	106.38 (12)	C18—C16—H16	108.2
C19—P2—C25	107.08 (12)	C17—C16—H16	108.2
N2—P2—Pt1	116.00 (8)	C16—C17—H17A	109.5
C19—P2—Pt1	107.13 (8)	C16—C17—H17B	109.5
C25—P2—Pt1	115.09 (8)	H17A—C17—H17B	109.5
C1—N1—P1	128.26 (17)	C16—C17—H17C	109.5
C1—N1—H1	116 (2)	H17A—C17—H17C	109.5
P1—N1—H1	115 (2)	H17B—C17—H17C	109.5
N1—C1—C3	110.2 (2)	C16—C18—H18A	109.5
N1—C1—C2	109.6 (2)	C16—C18—H18B	109.5
C3—C1—C2	112.0 (2)	H18A—C18—H18B	109.5
N1—C1—H1A	108.3	C16—C18—H18C	109.5
C3—C1—H1A	108.3	H18A—C18—H18C	109.5
C2—C1—H1A	108.3	H18B—C18—H18C	109.5
C1—C2—H2A	109.5	C20—C19—C24	119.1 (3)
C1—C2—H2B	109.5	C20—C19—P2	119.4 (2)
H2A—C2—H2B	109.5	C24—C19—P2	120.9 (2)
C1—C2—H2C	109.5	C19—C20—C21	120.2 (3)
H2A—C2—H2C	109.5	C19—C20—H20	119.9
H2B—C2—H2C	109.5	C21—C20—H20	119.9

## supplementary materials

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C1—C3—H3A	109.5	C22—C21—C20	120.7 (3)
C1—C3—H3B	109.5	C22—C21—H21	119.7
H3A—C3—H3B	109.5	C20—C21—H21	119.7
C1—C3—H3C	109.5	C21—C22—C23	119.8 (3)
H3A—C3—H3C	109.5	C21—C22—H22	120.1
H3B—C3—H3C	109.5	C23—C22—H22	120.1
C5—C4—C9	118.7 (2)	C22—C23—C24	120.4 (3)
C5—C4—P1	125.5 (2)	C22—C23—H23	119.8
C9—C4—P1	115.8 (2)	C24—C23—H23	119.8
C4—C5—C6	120.5 (3)	C23—C24—C19	119.7 (3)
C4—C5—H5	119.7	C23—C24—H24	120.2
C6—C5—H5	119.7	C19—C24—H24	120.2
C7—C6—C5	120.0 (3)	C30—C25—C26	118.8 (2)
C7—C6—H6	120.0	C30—C25—P2	118.63 (19)
C5—C6—H6	120.0	C26—C25—P2	122.0 (2)
C8—C7—C6	120.3 (3)	C27—C26—C25	120.2 (3)
C8—C7—H7	119.8	C27—C26—H26	119.9
C6—C7—H7	119.8	C25—C26—H26	119.9
C7—C8—C9	119.9 (3)	C28—C27—C26	120.4 (3)
C7—C8—H8	120.0	C28—C27—H27	119.8
C9—C8—H8	120.0	C26—C27—H27	119.8
C8—C9—C4	120.6 (3)	C29—C28—C27	119.6 (3)
C8—C9—H9	119.7	C29—C28—H28	120.2
C4—C9—H9	119.7	C27—C28—H28	120.2
C11—C10—C15	118.8 (2)	C28—C29—C30	120.5 (3)
C11—C10—P1	118.78 (19)	C28—C29—H29	119.8
C15—C10—P1	122.08 (19)	C30—C29—H29	119.8
C12—C11—C10	120.4 (2)	C29—C30—C25	120.5 (3)
C12—C11—H11	119.8	C29—C30—H30	119.7
C10—C11—H11	119.8	C25—C30—H30	119.7
C13—C12—C11	120.2 (3)	C15—C31—C14	109.92 (17)
C13—C12—H12	119.9	C15—C31—C13	110.11 (16)
C11—C12—H12	119.9	C14—C31—C13	110.91 (17)
C12—C13—C14	120.1 (3)	C15—C31—H31	108.6
C12—C13—H13	120.0	C14—C31—H31	108.6
C14—C13—H13	120.0	C13—C31—H31	108.6
P2—Pt1—P1—N1	175.27 (9)	P1—C10—C11—C12	-172.9 (2)
C11—Pt1—P1—N1	2.01 (10)	C10—C11—C12—C13	-0.2 (4)
P2—Pt1—P1—C4	58.67 (10)	C11—C12—C13—C14	-0.3 (4)
C11—Pt1—P1—C4	-114.59 (9)	C12—C13—C14—C15	0.9 (4)
P2—Pt1—P1—C10	-64.82 (9)	C13—C14—C15—C10	-0.9 (4)
C11—Pt1—P1—C10	121.92 (9)	C11—C10—C15—C14	0.3 (4)
P1—Pt1—P2—N2	18.14 (10)	P1—C10—C15—C14	173.2 (2)
C12—Pt1—P2—N2	-162.27 (10)	C19—P2—N2—C16	-69.1 (2)
C11—Pt1—P2—N2	159.01 (14)	C25—P2—N2—C16	43.9 (2)
P1—Pt1—P2—C19	-97.86 (9)	Pt1—P2—N2—C16	173.29 (18)
C12—Pt1—P2—C19	81.73 (9)	P2—N2—C16—C18	-94.6 (3)
C11—Pt1—P2—C19	43.02 (16)	P2—N2—C16—C17	141.9 (2)
P1—Pt1—P2—C25	143.22 (10)	N2—P2—C19—C20	-29.7 (2)

C12—Pt1—P2—C25	-37.19 (10)	C25—P2—C19—C20	-142.2 (2)
C11—Pt1—P2—C25	-75.90 (16)	Pt1—P2—C19—C20	93.8 (2)
C4—P1—N1—C1	-61.4 (3)	N2—P2—C19—C24	159.1 (2)
C10—P1—N1—C1	50.2 (3)	C25—P2—C19—C24	46.6 (2)
Pt1—P1—N1—C1	175.5 (2)	Pt1—P2—C19—C24	-77.4 (2)
P1—N1—C1—C3	-103.9 (3)	C24—C19—C20—C21	-0.2 (4)
P1—N1—C1—C2	132.4 (2)	P2—C19—C20—C21	-171.5 (2)
N1—P1—C4—C5	130.0 (2)	C19—C20—C21—C22	-0.2 (4)
C10—P1—C4—C5	17.7 (3)	C20—C21—C22—C23	0.0 (5)
Pt1—P1—C4—C5	-110.9 (2)	C21—C22—C23—C24	0.5 (5)
N1—P1—C4—C9	-51.5 (2)	C22—C23—C24—C19	-0.9 (4)
C10—P1—C4—C9	-163.73 (19)	C20—C19—C24—C23	0.7 (4)
Pt1—P1—C4—C9	67.7 (2)	P2—C19—C24—C23	172.0 (2)
C9—C4—C5—C6	1.7 (4)	N2—P2—C25—C30	84.6 (2)
P1—C4—C5—C6	-179.8 (2)	C19—P2—C25—C30	-164.3 (2)
C4—C5—C6—C7	-0.9 (4)	Pt1—P2—C25—C30	-45.4 (2)
C5—C6—C7—C8	-0.4 (4)	N2—P2—C25—C26	-86.8 (2)
C6—C7—C8—C9	0.9 (4)	C19—P2—C25—C26	24.3 (2)
C7—C8—C9—C4	0.0 (4)	Pt1—P2—C25—C26	143.23 (19)
C5—C4—C9—C8	-1.2 (4)	C30—C25—C26—C27	0.1 (4)
P1—C4—C9—C8	-179.9 (2)	P2—C25—C26—C27	171.5 (2)
N1—P1—C10—C11	102.8 (2)	C25—C26—C27—C28	-0.4 (4)
C4—P1—C10—C11	-146.55 (19)	C26—C27—C28—C29	-0.3 (4)
Pt1—P1—C10—C11	-18.4 (2)	C27—C28—C29—C30	1.3 (4)
N1—P1—C10—C15	-70.1 (2)	C28—C29—C30—C25	-1.5 (4)
C4—P1—C10—C15	40.5 (2)	C26—C25—C30—C29	0.8 (4)
Pt1—P1—C10—C15	168.73 (18)	P2—C25—C30—C29	-170.9 (2)
C15—C10—C11—C12	0.2 (4)		

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>
N1—H1...C11	0.815 (17)	2.32 (2)	3.000 (2)	141 (3)
C31—H31...C11	1.00	2.65	3.435 (3)	136
C31—H31...C12	1.00	2.69	3.521 (3)	141

**Table 2**

Selected geometric parameters (Å, °) for (I) and a comparison with (II) and (III)

	(I)	(II)	(III)
Pt—P	2.2565 (6), 2.2416 (6)	2.2625 (10), 2.251 (9)	2.221 (2) [2.253 (2)] 2.254 (2) [2.239 (2)]
Pt—Cl	2.3779 (6), 2.3503 (6)	2.3644 (10), 2.3649 (12)	2.348 (2) [2.254 (2)] 2.362 (2) [2.353 (2)]
P—N	1.647 (2), 1.665 (2)	1.663 (3), 1.660 (4)	1.667 (8) [1.634 (8)] 1.686 (9) [1.669 (8)]
P—Pt—P	96.03 (2)	98.81 (4)	102.3 (1) [95.4 (1)]
Cl—Pt—Cl	84.75 (2)	84.53 (4)	86.6 (1) [86.6 (1)]

# supplementary materials

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Notes: (I) this work ( $R = i\text{Pr}$ ); (II) Slawin *et al.* (2005) ( $R = \text{CH}_2\text{CH}=\text{CH}_2$ ); (III) Priya *et al.* (2003), two molecules present in the asymmetric unit ( $R = \text{Ph}$ ).

Fig. 1

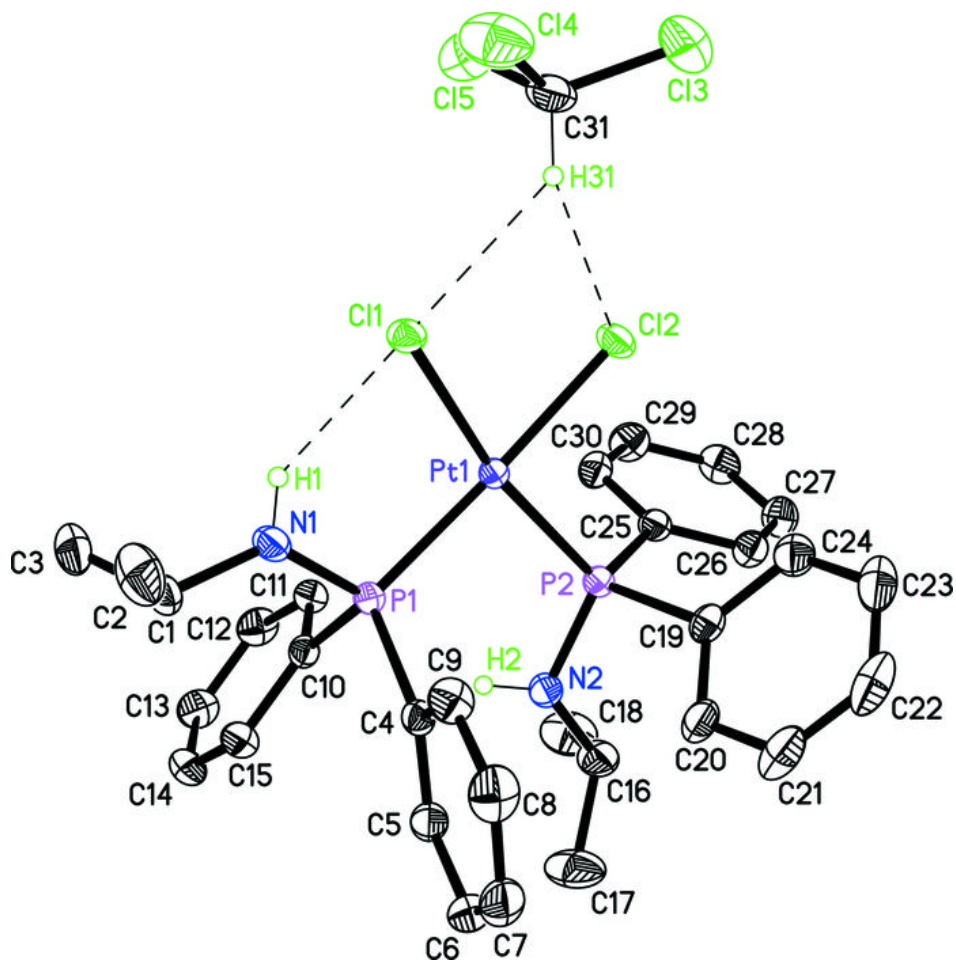


Fig. 2

