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[*N*,*N*-Bis(diphenylphosphanyl)-(*R*)-1,2,3,4-tetrahydro-1-naphthylamine-κ^2P,P']dichloroplatinum(II)

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Key indicators

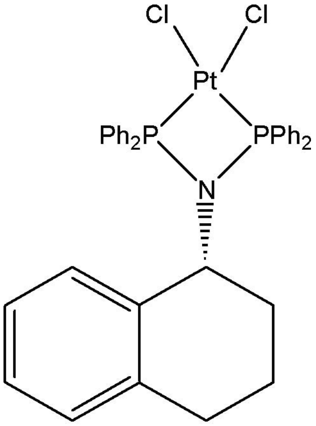
Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.009 Å
R factor = 0.034
wR factor = 0.054
Data-to-parameter ratio = 19.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $[PtCl_2(C_{34}H_{31}NP_2)]$, crystallizes with four crystallographically independent molecules. All four molecules have the same *R* chirality, with P—Pt—P bite angles ranging from 72.14 (5) to 72.38 (5)°.

Comment

The structure determination of the title compound, (I), was carried out in order to determine and study its coordination geometry and P—Pt—P bite angles. The asymmetric unit was found to contain four crystallographically independent molecules with the expected *R* chirality but with slightly differing conformations of the ring systems (Fig. 1). The metal is in a slightly distorted square-planar environment (Table 1). The chelating ligand forms a four-membered ring with Pt. The geometry of (I) is in close agreement with that of the *sec*-butylamine analogue (Calabrò *et al.*, 2004).



(I)

The packing diagram (Fig. 2) illustrates the pseudo-translation symmetry in the *c*-axis direction. About 83% of the atoms in the unit cell are, within 0.4 Å, related by this pseudo-translation. C—H···Cl short interactions are listed in Table 2.

Experimental

N,*N*-Bis(diphenylphosphanyl)-(*R*)-1,2,3,4-tetrahydro-1-naphthylamine (72 mg, 140 µmol), prepared following the procedure described by Kuhlmann *et al.* (2006) was reacted with $Pt(cod)Cl_2$ (52 mg, 139 µmol) in dichloromethane (5 ml). After 1 h of stirring at room temperature, the solvent was removed *in vacuo*. The white solid was washed twice with additional dichloromethane to remove traces of remaining cyclooctadiene. Colorless crystals were obtained by diffusion of Et_2O into a $CHCl_3$ solution. ^{31}P NMR ($CDCl_3$): δ 19.9 (*s*, $^1J_{Pt-P}$ = 3281 Hz).

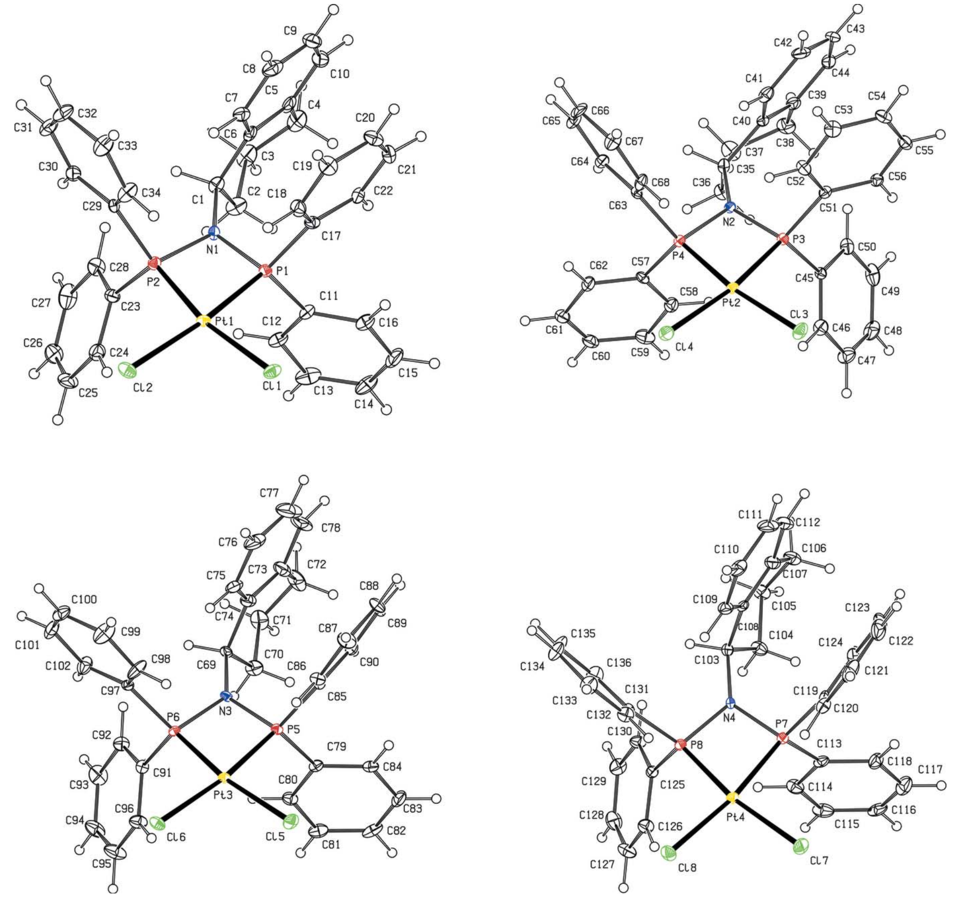


Figure 1
The structures of the four crystallographically independent molecules of the title compound with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

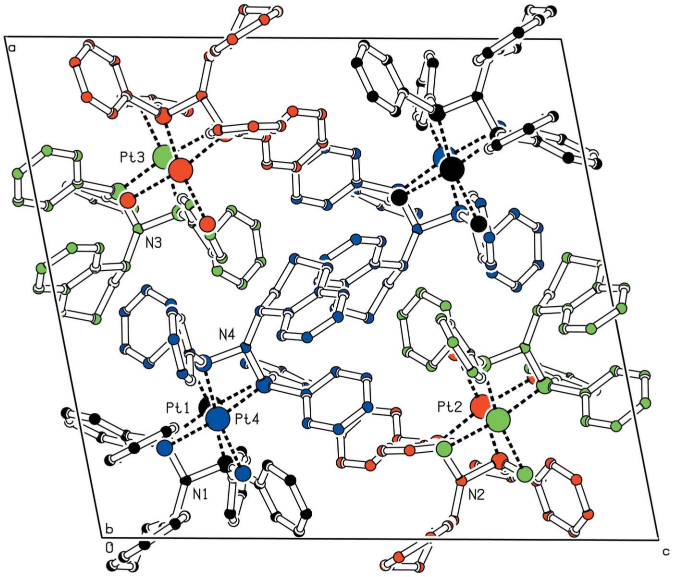


Figure 2
Packing diagram, viewed down the monoclinic b axis. The four independent molecules are colour-coded as black, red, green and blue. H atoms have been omitted.

Crystal data

$[PtCl_2(C_{34}H_{31}NP_2)]$
$M_r = 781.53$
Monoclinic, $P2_1$
$a = 19.107$ (1) Å
$b = 15.9176$ (7) Å
$c = 20.8122$ (11) Å
$\beta = 101.266$ (5)°
$V = 6207.8$ (5) Å^3
$Z = 8$
$D_x = 1.672$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 4.82$ mm^{-1}
$T = 150$ K
Block, colourless
0.33 × 0.13 × 0.06 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
$T_{\min} = 0.44$, $T_{\max} = 0.75$
151899 measured reflections
28340 independent reflections
21447 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.065$
$\theta_{\max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.054$
$S = 1.01$
28340 reflections
1441 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0146P)^2 + 3.8989P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.002$
$\Delta\rho_{\max} = 1.42$ e Å^{-3}
$\Delta\rho_{\min} = -0.87$ e Å^{-3}
Absolute structure: Flack (1983), 13646 Friedel pairs
Flack parameter: −0.021 (3)

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Table 1
Selected geometric parameters (Å, °).

Pt1—Cl1	2.3580 (16)	Pt3—Cl5	2.3673 (16)
Pt1—Cl2	2.3613 (15)	Pt3—Cl6	2.3577 (13)
Pt1—P1	2.2061 (15)	Pt3—P6	2.2128 (14)
Pt1—P2	2.2087 (14)	Pt3—P5	2.2040 (13)
Pt2—Cl3	2.3644 (14)	Pt4—P8	2.2158 (14)
Pt2—Cl4	2.3521 (13)	Pt4—Cl8	2.3575 (13)
Pt2—P3	2.2171 (13)	Pt4—Cl7	2.3617 (16)
Pt2—P4	2.1964 (14)	Pt4—P7	2.2142 (13)
Cl1—Pt1—Cl2	92.22 (5)	P5—Pt3—P6	72.38 (5)
P1—Pt1—P2	72.33 (5)	Cl5—Pt3—Cl6	91.69 (5)
P3—Pt2—P4	72.37 (5)	P7—Pt4—P8	72.14 (5)
Cl3—Pt2—Cl4	91.34 (5)	Cl7—Pt4—Cl8	91.21 (5)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15···Cl4^{i}	0.95	2.72	3.635 (6)	162
C24—H24···Cl2	0.95	2.78	3.626 (6)	149
C38—H38*B*···Cl6^{ii}	0.99	2.78	3.624 (5)	144
C54—H54···Cl6^{iii}	0.95	2.83	3.573 (6)	136
C59—H59···Cl6^{iv}	0.95	2.78	3.518 (6)	136
C92—H92···Cl1	0.95	2.77	3.658 (6)	155
C116—H116···Cl2	0.95	2.80	3.689 (7)	156
C130—H130···Cl3^{iii}	0.95	2.82	3.706 (6)	155

Symmetry codes: (i) $x, y, z-1$; (ii) $x-1, y, z$; (iii) $-x+1, y+\frac{1}{2}, -z+1$; (iv) $-x+1, y-\frac{1}{2}, -z+1$.

All H atoms were placed at geometrically idealized positions (C—H = 0.95 Å for C*sp*^{2}, C—H = 0.99 Å for methylene and C—H = 1.00 Å for tertiary) and constrained to ride on their parent atoms, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C). The absolute configuration is as expected from that of the starting material; the data set contains a 99.8% coverage of Friedel pairs

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DIRAX* (Duisenberg, 1992); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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