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Key indicators

Single-crystal X-ray study

$T = 178$ K

Mean $\sigma(\text{C}-\text{C}) = 0.010$ Å

R factor = 0.034

wR factor = 0.087

Data-to-parameter ratio = 16.0

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

{*N*-[*tert*-Butyl(phenyl)phosphino]-*N'*-diphenylphosphino-*N,N'*-dimethylurea-*P,P'*}dichloro-platinum(II) chloroform solvate

In the title compound, $[\text{PtCl}_2(\text{C}_{25}\text{H}_{30}\text{N}_2\text{OP}_2)] \cdot \text{CHCl}_3$, the urea ligand is *P,P'*-coordinated, leading to square-planar geometry at the Pt atom [bond lengths Pt–P 2.2102 (19) Å to the Ph_2P moiety and 2.2275 (18) Å to $\text{'Bu}(\text{Ph})\text{P}$; Pt–Cl 2.3658 (16) and 2.3658 (18) Å]. The ligand bite angle is 89.41 (7)°. The chloroform molecule is associated with the metal complex via a hydrogen-bond system of the form $\text{C}-\text{H}(\cdots\text{Cl})_2$.

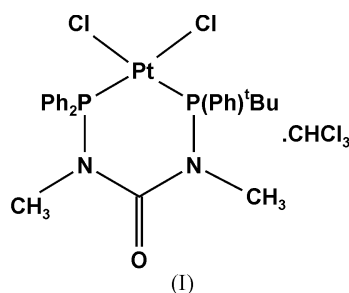
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Comment

The title compound, (I), formed part of a study of phosphorus-substituted *N,N'*-diorganylureas (Vogt, 1992). It crystallizes as a chloroform monosolvate.



The formula unit is shown in Fig. 1. The structure determination confirms the expected *P,P'*-bonding mode of the ligand; related derivatives of pentacarbonylchromium and -molybdenum unexpectedly proved to be *P,O*-bonded (Vogt *et al.*, 1991). The geometry at platinum is square planar; the Pt–Cl bond lengths are exactly equal, but the Pt–P bond to the Ph_2P moiety is slightly shorter than that to $\text{'Bu}(\text{Ph})\text{P}$ (Table 1). The P–N bond lengths display a similar qualitative difference, perhaps because of steric effects from the bulky *tert*-butyl group. The ligand bite angle is 89.41 (7)°. The chelate ring is not planar; torsion angles are given in Table 1.

The preparation and structures of several closely related compounds have recently been reported by Slawin *et al.* (2001). The dichloroplatinum complexes of $[\text{Ph}_2\text{PN}(\text{R})\text{C}(\text{O})\text{N}(\text{R})\text{PPh}_2]$ ($\text{R} = \text{Me}, \text{Et}$) display bond lengths and angles similar to those of the title compound.

The solvent molecule is associated with the metal complex by a three-centre hydrogen bond of the form $\text{C}-\text{H}(\cdots\text{Cl})_2$ (Table 2). The role of metal-bonded chlorine as a hydrogen-bond acceptor is well established for both 'classical' (Aullón *et al.*, 1998) and 'weak' (Freitag & Jones, 2000) hydrogen bonds.

Experimental

The title compound was prepared by treating (cyclooctadiene)PtCl₂ with the phosphinoureia ligand in dichloromethane (Vogt, 1992). Single crystals were obtained by evaporation from chloroform.

Crystal data

[PtCl₂(C₂₅H₃₀N₂OP₂)]·CHCl₃
M_r = 821.81
 Orthorhombic, *Pbca*
a = 16.380 (4) Å
b = 15.653 (3) Å
c = 24.074 (4) Å
V = 6172 (2) Å³
Z = 8
D_x = 1.769 Mg m⁻³

Data collection

Nicolet R3 diffractometer
 ω scans
 Absorption correction: ψ scan
 (XEMP; Nicolet, 1987)
T_{min} = 0.506, *T_{max}* = 0.999
 10 607 measured reflections
 5419 independent reflections
 3612 reflections with *I* > 2 σ (*I*)

Refinement

Refinement on *F*²
R[*F*² > 2 σ (*F*²)] = 0.034
wR(*F*²) = 0.087
S = 1.05
 5419 reflections
 339 parameters
 H-atom parameters constrained

Mo *K* α radiation
 Cell parameters from 50 reflections
 θ = 10–11.5°
 μ = 5.11 mm⁻¹
T = 178 (2) K
 Tablet, colourless
 0.40 × 0.40 × 0.15 mm

R_{int} = 0.043
 θ_{max} = 25.0°
h = 0 → 19
k = -18 → 18
l = -28 → 0
 3 standard reflections
 every 147 reflections
 intensity decay: 2%

$w = 1/[\sigma^2(F_o^2) + (0.0367P)^2 + 1.8493P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.006$
 $\Delta\rho_{\text{max}} = 2.40 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.85 \text{ e \AA}^{-3}$

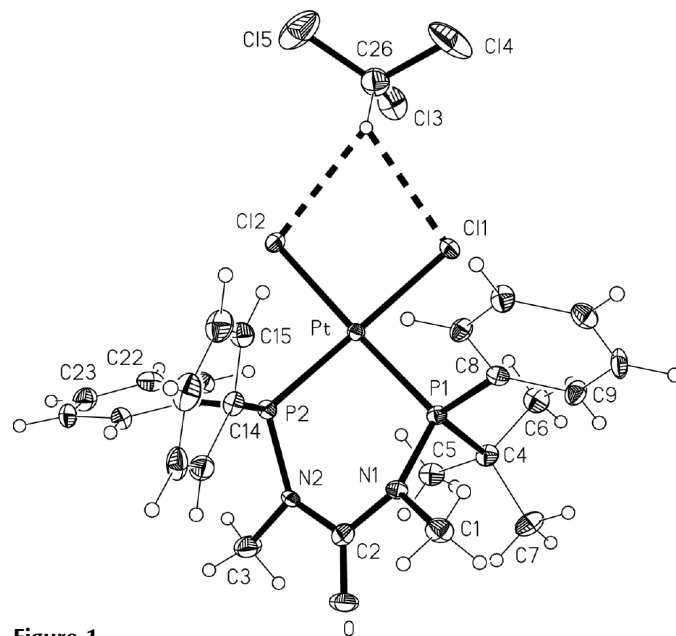


Figure 1

The formula unit of the title compound in the crystal. Ellipsoids represent 30% probability levels. H-atom radii are arbitrary.

Methyl H atoms were identified in difference syntheses, idealized and then refined allowing rigid methyl groups to rotate but not tip. The maxima at C1 and C3 were indistinct, which may indicate disorder or appreciable rotation of these methyl groups. Other H atoms were included using a riding model with fixed C–H bond lengths (aromatic 0.95, methyl 0.98 and methine 1.00 Å); *U_{iso}*(H) values were fixed at 1.2 times the *U_{eq}* of the parent atom. Three significant difference peaks (the largest 2.4 e Å⁻³) do not lie near the Pt atom. They may be caused by a minor but unidentified twinning or disorder component.

Data collection: *P3* (Nicolet, 1987); cell refinement: *P3*; data reduction: *XDISK* (Nicolet, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXL97*.

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Table 1

Selected geometric parameters (Å, °).

Pt–P2	2.2102 (19)	P2–C20	1.806 (7)
Pt–P1	2.2275 (18)	P2–C14	1.812 (7)
Pt–Cl2	2.3658 (16)	N1–C2	1.400 (9)
Pt–Cl1	2.3658 (18)	N1–C1	1.491 (8)
P1–N1	1.739 (6)	N2–C2	1.387 (8)
P1–C8	1.814 (7)	N2–C3	1.482 (9)
P1–C4	1.874 (6)	O–C2	1.212 (8)
P2–N2	1.711 (6)		
P2–Pt–P1	89.41 (7)	C20–P2–C14	108.0 (3)
P2–Pt–Cl2	92.05 (6)	N2–P2–Pt	114.4 (2)
P1–Pt–Cl2	176.43 (6)	C20–P2–Pt	116.5 (2)
P2–Pt–Cl1	175.87 (6)	C14–P2–Pt	109.9 (2)
P1–Pt–Cl1	89.86 (6)	C2–N1–C1	112.6 (6)
Cl2–Pt–Cl1	88.46 (6)	C2–N1–P1	123.0 (5)
N1–P1–C8	100.3 (3)	C1–N1–P1	120.0 (5)
N1–P1–C4	106.3 (3)	C2–N2–C3	114.2 (6)
C8–P1–C4	113.5 (3)	C2–N2–P2	121.5 (5)
N1–P1–Pt	112.6 (2)	C3–N2–P2	122.7 (4)
C8–P1–Pt	108.8 (2)	O–C2–N2	122.7 (7)
C4–P1–Pt	114.5 (2)	O–C2–N1	120.6 (6)
N2–P2–C20	102.0 (3)	N2–C2–N1	116.7 (6)
N2–P2–C14	105.2 (3)		
P2–Pt–P1–N1	–14.7 (2)	Pt–P2–N2–C2	63.5 (6)
P1–Pt–P2–N2	–31.0 (2)	P2–N2–C2–N1	–24.9 (8)
Pt–P1–N1–C2	60.9 (5)	P1–N1–C2–N2	–42.2 (8)

Table 2

Hydrogen-bonding 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>
C26–H26···Cl1	1.00	2.76	3.484 (9)	130
C26–H26···Cl2	1.00	2.76	3.579 (9)	139
C11–H11···Cl2 ⁱ	0.95	2.77	3.560 (7)	142

Symmetry code: (i) 1 – *x*, 1 – *y*, 1 – *z*.