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(2,2′-Biquinoline-$\kappa^2 N,N'$)dichloroplatinum(II)–2,2′-biquinoline (2/1)

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In the structure of the title complex, $2[PtCl_2(C_{18}H_{12}N_2)]\cdot C_{18}H_{12}N_2$, the metal complex and a free 2,2′-biquinoline molecule are present in a 2:1 ratio. The cocrystallized molecule of 2,2′-biquinoline lies about a center of symmetry. The four-coordinate Pt atom has a distorted *cis*-square-planar geometry and is bonded by the two N atoms of a 2,2′-biquinoline ligand and two anionic Cl^- ions. The overall structure of the metal complex is not planar, and the Pt and Cl atoms deviate significantly from the plane of the 2,2′-biquinoline ligand.

Key indicators

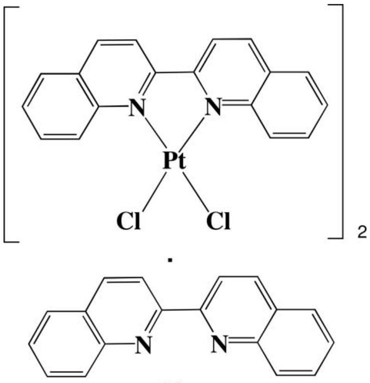
Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.015 Å
R factor = 0.038
wR factor = 0.097
Data-to-parameter ratio = 17.3

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

Comment

Cisplatin [*cis*-diamminedichloroplatinum(II)] is well known as one of the most potent anticancer drugs, and many studies have been performed to synthesize new platinum(II) complexes analogous to cisplatin with antitumor, antimicrobial and antiviral activity (Corbi *et al.*, 2005; Giovagnini *et al.*, 2005). Recently, palladium(II) and platinum(II) complexes with a heterocyclic 2,2′-dipyridylamine (dpa) ligand instead of the ammine ligands of cisplatin have been synthesized and their structures determined (Rauterkus *et al.*, 2003). The DNA-binding ability and cytotoxic activity of platinum(II)–dpa have also been reported (Tu *et al.*, 2004).

In a previous study (Muranishi *et al.*, 2005), we have synthesized and determined the crystal structures of palladium(II), copper(II) and zinc(II) complexes of the 2,2′-biquinoline (biq) ligand with structures analogous to cisplatin. We report here the synthesis and structure of the platinum(II) complex, $[Pt(biq)Cl_2]$, which cocrystallized with free 2,2′-biquinoline in a 2:1 molar ratio to give crystals of the title compound, (I).



(I)

In the crystal structure, the 2,2′-biquinoline molecule lies about a center of symmetry. The four-coordinate Pt atom has a

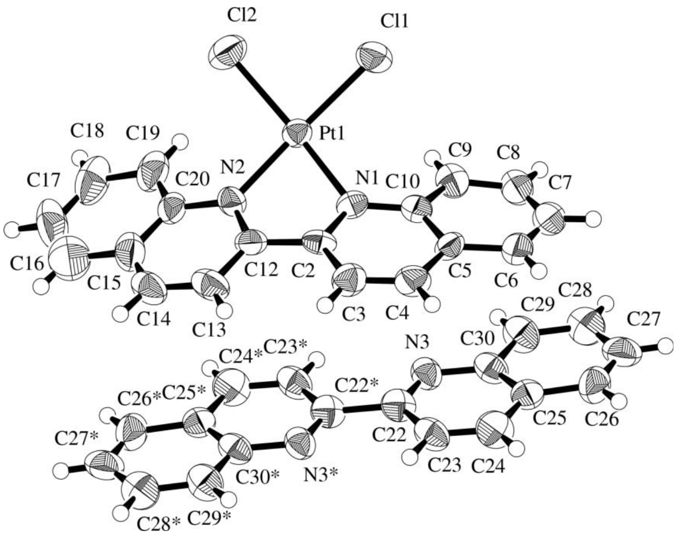


Figure 1
Molecular structure of (I), showing the atom-numbering scheme with displacement ellipsoids drawn at the 50% probability level. The suffix * indicates the symmetry position $2 - x$, $1 - y$, $2 - z$.

distorted *cis*-square planar geometry in which the Pt atom is bonded by the two N atoms of the biq ligand and two Cl atoms in *cis* positions (Fig. 1, and Tables 1 and 2). The platinum(II) complex, [Pt(biq)Cl_2], in (I) has a similar structure to that of the palladium(II) complex, [Pd(biq)Cl_2], (II) (Muranishi *et al.*, 2005), although free biq does not cocrystallize in (II). Bond-length and angle data for (I) and (II) are compared in Table 2.

Both the free and the coordinated biq molecules in (I) are essentially planar, with a dihedral angle between the two quinoline rings of the coordinated biq molecule of 15.7 (4)°. However the overall structure of the metal complex is not planar. The deviations from the mean plane through atoms N1, C2, C12 and N2 (r.m.s. deviation 0.0136) are 0.55 (3), 1.42 (5) and 1.67 (5) Å for atoms Pt1, Cl1 and Cl2, respectively, in the same direction. The five-membered ring (Pt/N1/C2/C12/N2) forms an envelope with the Pt atom as the flap, just as in (II).

Experimental

2,2′-Biquinoline [5.0 mg dissolved in 2 ml of dimethylsulfoxide (DMSO)] was mixed with potassium tetrachloroplatinate(II) [$K_2(PtCl_4)$] (8.1 mg in 2 ml of DMSO) at room temperature (molar ratio 1:1). This mixture was allowed to stand at room temperature to yield red rod-like crystals of (I) over a period of days.

Crystal data

$2[PtCl_2(C_{18}H_{12}N_2)]\cdot C_{18}H_{12}N_2$
$M_r = 1300.84$
Monoclinic, $P2_1/n$
$a = 8.123$ (2) Å
$b = 16.650$ (2) Å
$c = 16.658$ (2) Å
$\beta = 95.35$ (2)°
$V = 2243.1$ (7) Å^3
$Z = 2$

$D_x = 1.926$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 13.5$–14.9°
$\mu = 6.52$ mm^{-1}
$T = 296.2$ K
Rod, red
0.40 × 0.10 × 0.10 mm

Data collection

Rigaku AFC-5*R* diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.410$, $T_{\max} = 0.521$
5706 measured reflections
5158 independent reflections
2327 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.047$
$\theta_{\max} = 27.5°$
$h = 0 \rightarrow 10$
$k = 0 \rightarrow 21$
$l = -21 \rightarrow 21$
3 standard reflections every 150 reflections intensity decay: 0.5%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.097$
$S = 0.96$
5158 reflections
298 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 1.01$ e Å^{-3}
$\Delta\rho_{\min} = -0.82$ e Å^{-3}

Table 1
Selected bond angles (°).

Cl1—Pt1—N1	95.9 (2)	Cl2—Pt1—N1	170.0 (2)
Cl1—Pt1—N2	170.9 (2)	Cl2—Pt1—N2	96.9 (2)

Table 2
Comparative selected geometric parameters (Å, °).

M = Pt or Pd	I(Pt)	II(Pd)[a]
M—Cl1	2.296 (3)	2.2819 (10)
M—Cl2	2.294 (3)	2.2878 (13)
M—N1	2.032 (7)	2.067 (3)
M—N2	2.031 (7)	2.032 (2)
Cl1—*M*—Cl2	86.39 (10)	86.74 (3)
N1—*M*—N2	79.4 (3)	79.24 (10)

Reference: (*a*) Muranishi (2005).

All H atoms were located fin difference Fourier maps, and then were treated as riding, with a C—H distance of 0.93 Å and $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(carrier atom). The highest density peak is located between atoms Pt1 and N2.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1992); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 2000); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *TEXSAN*.

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