metal-organic papers

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Key indicators

Single-crystal X-ray study T = 85 K Mean σ (C–C) = 0.003 Å R factor = 0.014 wR factor = 0.036 Data-to-parameter ratio = 18.8

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

Bis(2,2'-bipyridine- $\kappa^2 N, N'$)platinum(II) bis(perchlorate)

The title complex, $[Pt(C_{10}H_8N_2)_2](ClO_4)_2$, adopts a squareplanar geometry in which all four N-atom donors are strictly coplanar as the Pt ion lies on an inversion centre. However, the 2,2'-bipyridine ligand deviates significantly from planarity, as demonstrated by the angle of 20.52 (11)° between the mean planes of the two pyridine rings.

Comment

The title complex, (I) (Fig. 1), was obtained during a study of the reactivity of $[Pt(C_{10}H_8N_2)_2]^{2+}$ in aqueous alkaline solution (McInnes *et al.*, 2003). Complex (I) crystallizes in the triclinic space group *P*1 with the Pt ion lying on an inversion centre, thus requiring it to be strictly coplanar with the four attached N atoms. The Pt—N distances [2.0227 (18) and 2.0292 (17) Å] are similar to those found in $[Pt(C_{10}H_8N_2)_2](NO_3)_2 \cdot H_2O$ (Hazell *et al.*, 1986) and $[Pt(C_{10}H_8N_2)_2](CF_3SO_3)_2$ (Fedotova *et al.*, 2003), and are typical of those found in Pt complexes containing pyridine ligands (mean = 2.064 Å, SD = 0.074 Å for 997 structurally characterized complexes and 2214 individual Pt—N distances; Cambridge Structural Database, Version 5.26 of November 2004 (Allen, 2002)].



The 2,2'-bipyridine ligands display a bow distortion (Fig. 2) with a remarkably large angle of 20.52 (11)° between the mean planes of the two rings (Hazell, 2004). A similar distortion is seen in the trifluoromethanesulfonate salt of the complex (Fedotova *et al.*, 2003) and presumably prevents the close inter-ligand approach of atoms H1 and H10 (attached to C1 and C10, respectively). It is tempting to speculate that the strain inherent in such a distortion is responsible for the unusual behaviour of $[Pt(C_{10}H_8N_2)_2]^{2+}$ in aqueous alkaline solution, allowing facile coordination of hydroxide ion to give a pseudo-five-coordinate complex (McInnes *et al.*, 2003).

There are weak π -stacking interactions throughout the three-dimensional structure (Fig. 3), with centroid-to-centroid distances between the pyridine rings of 3.703 (3) (-1 - x, -y,

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Figure 1

The structure of the cation of (I), with displacement ellipsoids drawn at the 50% probability level. [Symmetry code for unlabelled atoms: -x, -y, -z.]



Figure 2

View of the cation of (I), emphasizing the bow distortion of the 2,2'bipyridine ligands.



Figure 3

Packing, viewed down the a axis. Close interactions are indicated as dashed lines.

-z) and 3.924 (3) Å (-x, -y, 1 - z). The perchlorate ions are also involved in an ion- π interactions, with O1-centroid (at 1 + x, y, 1 + z and O4-centroid (at -x, 1 - y, 1 - z) distances of 3.064 (3) and 3.356 (3) Å, respectively.

Experimental

Complex (I) precipitated on addition of one drop of 6 M NaClO₄(aq) to a solution of $[Pt(C_{10}H_8N_2)_2](NO_3)_2 \cdot H_2O$ (53 mg), prepared according to McInnes et al. (2003) in water (1 ml) to which one equivalent of 1 M NaOH(aq) (84 µl) had been added. Dilution to approximately 20 ml with hot water and subsequent slow cooling gave (I) as small pale-yellow crystals.

Crystal data

$[Pt(C_{10}H_8N_2)_2](ClO_4)_2$	Z = 1
$M_r = 706.35$	$D_x = 2.227 \text{ Mg m}^{-3}$
Triclinic, P1	Mo $K\alpha$ radiation
a = 7.811 (5) Å	Cell parameters from 5
b = 8.621 (5) Å	reflections
c = 9.054 (5) Å	$\theta = 2.4 - 33.0^{\circ}$
$\alpha = 72.972 \ (5)^{\circ}$	$\mu = 6.97 \text{ mm}^{-1}$
$\beta = 86.553 \ (5)^{\circ}$	T = 85 (2) K
$\gamma = 64.960 \ (5)^{\circ}$	Plate, pale-yellow
$V = 526.7 (5) \text{ Å}^3$	$0.32 \times 0.16 \times 0.08 \text{ mm}$

Data collection

Bruker Kappa-APEX-II areadetector diffractometer φ and ω scans Absorption correction: multi-scan (SADABS; Bruker, 2001) $T_{\min} = 0.361, T_{\max} = 0.572$ 11349 measured reflections

Refinement

Refinement on F^2 $R[F^2 > 2\sigma(F^2)] = 0.014$ wR(F²) = 0.036 S = 1.083010 reflections 160 parameters H-atom parameters constrained 3010 independent reflections 3010 reflections with $I > 2\sigma(I)$ $R_{\rm int} = 0.028$ $\theta_{\rm max} = 33.2^{\circ}$ $h = -7 \rightarrow 10$ $k = -11 \rightarrow 12$

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 $w = 1/[\sigma^2(F_0^2) + (0.0182P)^2]$ + 0.2101P] where $P = (F_0^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\rm max} < 0.001$ $\Delta \rho_{\rm max} = 1.19 \text{ e} \text{ Å}^{-3}$ $\Delta \rho_{\rm min} = -1.34 \text{ e} \text{ Å}^{-3}$

 $l = -13 \rightarrow 13$

All H atoms were included in the riding-model approximation, with C-H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The highest residual peak in the difference map is 0.79 Å from atom Pt1 and the deepest hole is 0.81 Å from atom Pt1.

Data collection: APEXII (Bruker, 2004); cell refinement: APEXII and SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SIR97 (Altomare et al., 1999); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP3 (Farrugia, 1997) and SHELXTL (Bruker, 2001); software used to prepare material for publication: WinGX (Farrugia, 1999).

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