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2,2′:6′,2″-Terpyridine(1-methylimidazole-N^3)platinum(II) Perchlorate Acetonitrile Solvate

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Abstract

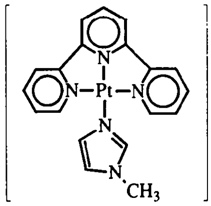
The title compound, $[Pt(C_{15}H_{11}N_3)(C_4H_6N_2)](ClO_4)_2.C_2H_3N$, is formed by reaction of chloro-2,2′:6′,2″-terpyridineplatinum(II) chloride dihydrate with 1-methylimidazole in the presence of excess amounts of $NaClO_4$. The platinum center is approximately square-planar N_4-coordinated to the tridentate terpyridine and monodentate 1-methylimidazole with Pt—N 1.943 (7)–2.026 (7) Å. The imidazole ring forms a dihedral angle of 66.5 (2)° with the planar Pt–terpyridine ring system. The crystal packing is dominated by π–π stacking interactions with the absence of any short metal···metal interactions.

Comment

A primary interest in Pt^{II} complexes derives from the finding that a number of its amine complexes possess antitumor properties, accounting for the large number of investigations into its coordination properties with biological molecules such as DNA (*e.g.* Pasini & Zunino, 1987, and references therein).

Complexes of the type $[Pt(tpy)X]^{n+}$ (tpy = 2,2′:6′,2″-terpyridine) belong to the class of compounds referred to as metallo-intercalators (Lippard, 1978). Intercalation of a Pt–tpy moiety into DNA occurs between two Watson–Crick base pairs, unwinding the DNA helix and puckering the deoxyribose rings (Wang, Nathans, van der Marel, van Boom & Rich, 1978). However, other modes of interaction with DNA by Pt-based drugs also involve direct covalent binding (Pasini & Zunino, 1987).

As part of an investigation into metal-ion–biomolecule interactions (Buncel, Joly & Jones, 1986; Buncel, Joly & Yee, 1989; Buncel, Clement & Onyido, 1994; Buncel & Clement, 1995; Clement, Roszak & Buncel, 1996) we have studied the complex formed between [Pt(tpy)Cl]Cl and 1-methylimidazole (MeIm) as a model for the interaction of Pt^{II} complexes with DNA. In this case the nitrogen base (MeIm) displaces chlorine and binds covalently to the terpyridineplatinum(II) cation. We report here the crystal and molecular structure of the acetonitrile solvate of the resulting complex, $[Pt(tpy)(MeIm)](ClO_4)_2.MeCN$, (I).



(I)

Fig. 1 shows the cation of (I) viewed perpendicularly to the PtN_4 coordination plane. The dihedral angle between the least-squares Pt–terpyridine plane and the plane of the imidazole ring is 66.5 (2)°, which is probably a result of steric interactions between the C16 and C18 H atoms of imidazole and the C1 and C15 H atoms of terpyridine. The restricted bite angle of the tridentate terpyridine ligand has caused a small distortion at the Pt atom from square-planar geometry. The *cis* N1—Pt—N2 and N2—Pt—N3 angles are less than 90° [80.5 (3) and 81.3 (3)°, respectively], as is commonly observed in terpyridine complexes (*e.g.* Bailey, Catalano & Gray, 1993; Yip, Cheng, Cheung & Che, 1993; Jennette, Gill, Sadownick & Lippard, 1976; Aldridge, Stacy & McMillin, 1994). The

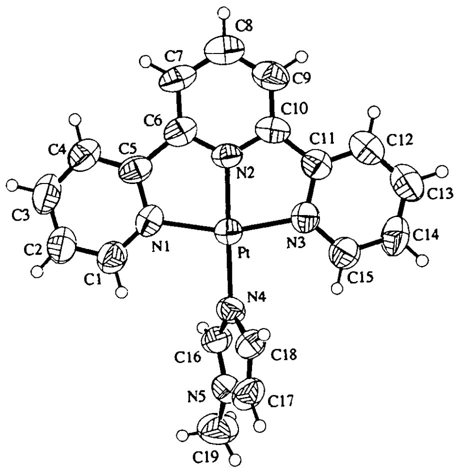


Fig. 1. Molecular structure of the title cation with the atom-numbering scheme. The displacement ellipsoids are drawn at the 50% probability level and H atoms are drawn as unlabeled spheres of arbitrary size.

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Pt—N2 distance [1.943 (7) Å] is significantly shorter than the Pt—N1 and Pt—N3 distances [2.016 (7) and 2.026 (7) Å, respectively], which also result from the geometrical constraints imposed by the tpy ligand. The major difference between the tricoordinated terpyridine ligand in this complex and the free tpy ligand in the solid state (Bessel, See, Jameson, Churchill & Takeuchi, 1992) is the *cis,cis* ligand conformation in the complex as opposed to the *trans,trans* conformation of the free ligand. The greatest distortion upon coordination is observed for exocyclic bond angles at the C5, C6, C10 and C11 atoms (numbering from the present structure), which are significantly decreased on the side of the Pt atom [112.2–115.6° in (I) *versus* 116.7–121.7° in the free tpy ligand], and for the endocyclic angle at atom N2, which is increased from 117.5 (5)° in the free ligand to 122.7 (8)° in $[Pt(tpy)(MeIm)]^+$. Similar changes in the terpyridine ligand upon coordination to a metal centre were observed for the ruthenium complex (Bessel *et al.*, 1992).

The Pt—N4 distance, 2.021 (6) Å, is in good agreement with the expected value of 2.017 Å, which is the average Pt—N(imidazole) distance for 20 cases of *N*-alkylimidazole-platinum(II) tetracoordinated compounds [sample standard deviation 0.014 Å (Orpen *et al.*, 1992)]. The dimensions of the MeIm ligand are somewhat more deviated from expected values with the main difference being the relative lengths of two bonds to atom C16: the formally double bond N4—C16 is longer than the formally single bond N5—C16 [1.343 (10) *versus* 1.306 (10) Å, respectively], while the expected values for these two bonds are 1.320 and 1.346 Å (Orpen *et al.*, 1992). A similar inverted situation was found in the structure of *trans*-diamminebis(*N*-methylimidazole)-platinum(II) [1.36 (4) *versus* 1.27 (4) Å, respectively; Carmichael, Chan, Cordes, Fair & Johnson, 1972]. On the other hand, these bonds are as expected in *cis*-dichlorobis(*N*-methylimidazole)platinum(II) [1.301 (10) and 1.345 (10) Å, respectively; Graves, Hodgson, van Kralingen & Reedijk, 1978] and in tetrakis(1-methyl-imidazole)platinum(II) [1.322 (10) *versus* 1.339 (11) Å, and 1.331 (10) *versus* 1.348 (11) Å in two independent imidazole ligands; Clement *et al.*, 1996].

The title cations are packed in the crystal lattice approximately parallel to the *ac*-face diagonal and to the *b* axis, and form rows along the *c* axis (Fig. 2*a*). Adjacent molecules in these rows interact by partial π–π stacking between the outer pyridine rings of the tpy ligands. Fig. 2(*b*) shows four neighboring cations viewed perpendicular to terpyridine ring systems; two of them (3 and 4) are above and one (2) below the plane of the central cation 1. An estimated distance between the overlapping pyridine rings of the tpy ligands 2 and 1 (and by symmetry between 3 and 1) is 3.48 (4) Å. The distance between the pyridine rings of tpy 1 and tpy 4, which overlap only at the edge, is 3.543 (3) Å. The limited overlap observed is probably due to the out-of-plane orientation of 1-methylimidazole. In contrast, much more extensive overlap and formation of head-to-tail dimers was observed in the structure of 2-hydroxy-ethanethiolato(2,2′,2″-terpyridine)platinum(II) (Jennette *et al.*, 1976), where the mercaptoethanol ligand is present on one side of the tpy plane and does not interfere with stacking. The perchlorate ions and the acetonitrile molecules are packed tightly between the complex cations (Fig. 2*a*). The N6 atom of acetonitrile is in short contact with H1 of the terpyridine ligand (bonded to C1); this contact could be interpreted as a C—H···N hydrogen bond (Table 2). The closest Pt···Pt distance in (I) is 7.575 (1) Å.

As a result of the almost perpendicular orientation of the MeIm ligand with respect to the Pt–tpy plane, it is

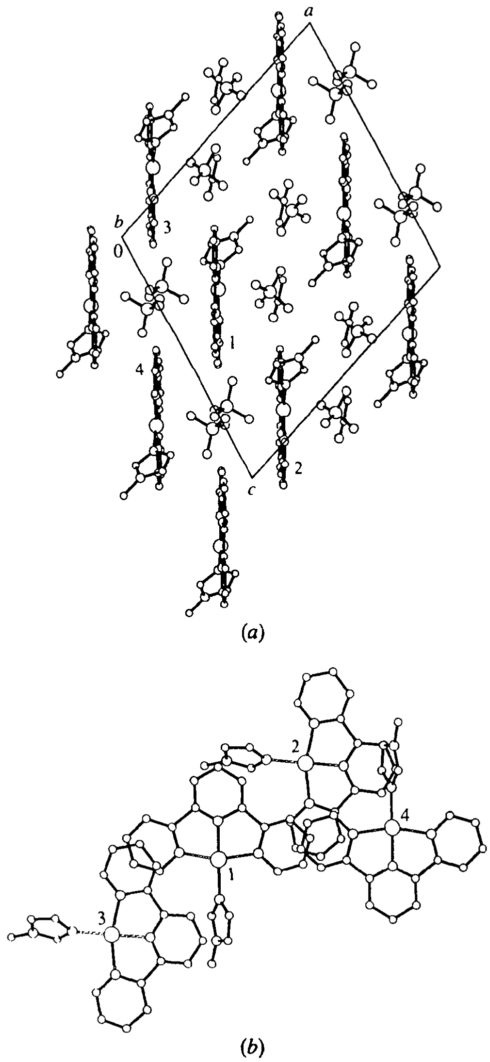

Fig. 2. Crystal packing of the title structure: (*a*) view along the *b* axis, with the molecule of acetonitrile overlapped by one of the perchlorates; (*b*) view perpendicular to the terpyridine ring system showing only four adjacent cations involved in the π–π stacking; symmetry codes: (1) x, y, z; (2) $x, \frac{1}{2} - y, \frac{1}{2} + z$; (3) $x, \frac{1}{2} - y, -\frac{1}{2} + z$; (4) $-x, -y, 1 - z$.

anticipated that covalent binding of $[Pt(tpy)Cl]^+$ to DNA bases may place the tpy rings in a similar orientation with respect to the coordinating nucleic base. Such an orientation will probably lead to a mode of disruption to the DNA helix different from that by intercalation (see above). This is pertinent with respect to the molecular mechanism of drug action by Pt^{II} complexes, which has implicated covalent adduct formation between Pt^{II} and DNA bases (Farrell *et al.*, 1995).

Experimental

The stoichiometric reaction of chloro-2,2′:6′,2″-terpyridine-platinum(II) chloride dihydrate, $[Pt(tpy)Cl].2H_2O$, with 1-methylimidazole (MeIm) in the presence of excess amounts of $NaClO_4$, yielded a reddish brown crystalline product that was shown to be 2,2′:6′,2″-terpyridine(1-methylimidazole)-platinum(II) perchlorate, $[Pt(tpy)(MeIm)](ClO_4)_2$, (I), by analysis. Single crystals of (I) as an acetonitrile solvate were obtained by vapor diffusion of anhydrous diethyl ether into an acetonitrile solution of the complex, at room temperature (24 h).

Crystal data

$[Pt(C_{15}H_{11}N_3)(C_4H_6N_2)]$-$(ClO_4)_2.C_2H_3N$
$M_r = 750.42$
Monoclinic
$P2_1/c$
$a = 15.754\,(4)$ Å
$b = 11.468\,(4)$ Å
$c = 15.084\,(3)$ Å
$\beta = 108.97\,(2)°$
$V = 2577.2\,(12)$ Å^3
$Z = 4$
$D_x = 1.934$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 25 reflections
$\theta = 15–18°$
$\mu = 5.71$ mm^{-1}
$T = 293\,(2)$ K
Prism
0.50 × 0.20 × 0.12 mm
Orange–brown

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: refined from ΔF (*DIFABS*; Walker & Stuart, 1983)
$T_{min} = 0.34$, $T_{max} = 0.50$
5834 measured reflections
5615 independent reflections

2923 observed reflections $[I > 2\sigma(I)]$
$R_{int} = 0.0313$
$\theta_{max} = 26.99°$
$h = -20 \rightarrow 19$
$k = 0 \rightarrow 14$
$l = 0 \rightarrow 19$
3 standard reflections
frequency: 60 min
intensity variation: 3%%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0382$
$wR(F^2) = 0.1239$
$S = 1.006$
5615 reflections
335 parameters
H atoms riding, C—H = 0.93–0.96 Å
$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.022$
$\Delta\rho_{max} = 0.919$ e Å^{-3}
$\Delta\rho_{min} = -0.840$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 1. *Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)*

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}/U_{iso}
Pt	0.22521 (2)	0.21900 (3)	0.41475 (2)	0.05541 (13)
N1	0.2602 (4)	0.3577 (6)	0.3521 (5)	0.060 (2)
N2	0.1758 (4)	0.3432 (7)	0.4707 (5)	0.060 (2)
N3	0.1724 (4)	0.1202 (7)	0.4952 (4)	0.059 (2)
N4	0.2766 (4)	0.0887 (6)	0.3576 (4)	0.055 (2)
N5	0.3700 (5)	−0.0297 (7)	0.3260 (5)	0.070 (2)
C1	0.3039 (6)	0.3580 (9)	0.2881 (6)	0.070 (2)
C2	0.3210 (6)	0.4576 (9)	0.2497 (7)	0.076 (3)
C3	0.2958 (7)	0.5618 (10)	0.2753 (8)	0.091 (3)
C4	0.2517 (6)	0.5646 (8)	0.3408 (7)	0.074 (3)
C5	0.2346 (5)	0.4617 (8)	0.3779 (6)	0.061 (2)
C6	0.1845 (5)	0.4516 (8)	0.4480 (6)	0.064 (2)
C7	0.1534 (6)	0.5410 (9)	0.4874 (7)	0.075 (3)
C8	0.1108 (6)	0.5122 (10)	0.5529 (7)	0.081 (3)
C9	0.1018 (6)	0.3991 (11)	0.5741 (6)	0.079 (3)
C10	0.1335 (6)	0.3128 (9)	0.5326 (6)	0.065 (3)
C11	0.1310 (6)	0.1855 (8)	0.5454 (6)	0.065 (2)
C12	0.0916 (6)	0.1333 (11)	0.6024 (7)	0.080 (3)
C13	0.0901 (6)	0.0132 (12)	0.6092 (7)	0.090 (3)
C14	0.1321 (7)	−0.0497 (10)	0.5585 (7)	0.083 (3)
C15	0.1724 (6)	0.0040 (8)	0.5013 (6)	0.068 (2)
C16	0.3635 (6)	0.0644 (7)	0.3721 (6)	0.063 (2)
C17	0.2842 (7)	−0.0705 (9)	0.2788 (7)	0.077 (3)
C18	0.2286 (6)	0.0034 (7)	0.2990 (6)	0.063 (2)
C19	0.4544 (7)	−0.0848 (10)	0.3283 (8)	0.101 (3)
N6	0.3572 (10)	0.1806 (15)	0.1484 (8)	0.158 (6)
C20	0.4013 (8)	0.1374 (13)	0.1199 (9)	0.099 (4)
C21	0.4539 (9)	0.0727 (13)	0.0778 (10)	0.140 (5)
Cl1	−0.04405 (15)	0.2742 (2)	0.2579 (2)	0.0654 (5)
O11	0.0026 (5)	0.3805 (7)	0.2847 (5)	0.107 (3)
O12	−0.0938 (5)	0.2815 (7)	0.1611 (5)	0.114 (3)
O13	−0.1057 (7)	0.2552 (7)	0.3060 (7)	0.119 (3)
O14	0.0156 (6)	0.1827 (7)	0.2684 (7)	0.128 (3)
Cl2	0.3912 (2)	−0.2226 (3)	0.5719 (2)	0.0830 (7)
O21*A*†	0.3657 (17)	−0.255 (2)	0.4745 (13)	0.190 (4)
O22*A*†	0.4760 (13)	−0.2696 (19)	0.6209 (17)	0.190 (4)
O23*A*†	0.3935 (16)	−0.0972 (14)	0.5749 (17)	0.190 (4)
O24*A*†	0.3246 (15)	−0.258 (2)	0.6038 (17)	0.190 (4)
O21*B*†	0.3378 (17)	−0.3180 (19)	0.5705 (19)	0.190 (4)
O22*B*†	0.4232 (17)	−0.176 (2)	0.6661 (13)	0.190 (4)
O23*B*†	0.3580 (18)	−0.128 (2)	0.5120 (18)	0.190 (4)
O24*B*†	0.4656 (16)	−0.260 (2)	0.549 (2)	0.190 (4)

† Disordered site; U_{iso} (see below).

Table 2. *Selected geometric parameters (Å, °)*

Pt—N1	2.016 (7)	N3—C11	1.371 (10)
Pt—N2	1.943 (7)	N3—C15	1.336 (11)
Pt—N3	2.026 (7)	N4—C16	1.343 (10)
Pt—N4	2.021 (6)	N4—C18	1.370 (10)
N1—C1	1.355 (10)	N5—C16	1.306 (10)
N1—C5	1.356 (10)	N5—C17	1.388 (11)
N2—C6	1.309 (11)	N5—C19	1.462 (11)
N2—C10	1.357 (11)	C17—C18	1.323 (12)
N1—Pt—N2	80.5 (3)	Pt—N3—C11	112.7 (6)
N1—Pt—N3	161.8 (3)	Pt—N3—C15	127.5 (6)
N1—Pt—N4	100.1 (3)	C11—N3—C15	119.8 (8)
N2—Pt—N3	81.3 (3)	Pt—N4—C16	127.8 (6)
N2—Pt—N4	179.4 (3)	Pt—N4—C18	126.1 (5)
N3—Pt—N4	98.1 (3)	C16—N4—C18	106.1 (7)
Pt—N1—C1	128.0 (6)	C16—N5—C17	108.7 (8)
Pt—N1—C5	114.1 (6)	C16—N5—C19	124.9 (9)
C1—N1—C5	118.0 (8)	C17—N5—C19	126.4 (8)
Pt—N2—C6	119.5 (6)	N4—C16—N5	109.6 (8)
Pt—N2—C10	117.8 (7)	N5—C17—C18	105.9 (8)
C6—N2—C10	122.7 (8)	C17—C18—N4	109.8 (8)
N1—Pt—N4—C16	68.4 (7)	N1—Pt—N4—C18	−114.9 (7)
N3—Pt—N4—C16	−112.2 (7)	N3—Pt—N4—C18	64.5 (7)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···N6	0.96	2.42	3.231 (16)	146

The structure was solved by the heavy-atom method. Of two perchlorate anions, one was found disordered (Cl2) and was refined with two positions of its O atoms, the geometry of which with respect to the Cl2 atom was restrained to be similar to the geometry of the ordered anion (Cl1). O atoms of the disordered perchlorate were refined isotropically with a common U_{iso} value. The occupation factors of O atoms in two positions converged to 0.550 (9) and 0.450 (9) for those O atoms with labels appended by *A* and *B*, respectively. The absorption correction transmission factors derived from ΔF are in good agreement with those obtained *via* ψ scan method.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989). Cell refinement: *CAD*-4 *Software*. Data reduction: *Xtal*3.0 (Hall & Stewart, 1990). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ORTEP*II (Johnson, 1976), *PLUTO* (Motherwell & Clegg, 1978). Software used to prepare material for publication: *SHELXL*93.

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Lists of structure factors, least-squares-planes data, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: FG1115). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Bis[2-(2-pyridylmethylaminomethyl)-phenol]copper(II) Diacetate Trihydrate $[Cu(HBPA)_2](CH_3COO)_2.3H_2O$

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Abstract

The mononuclear $[Cu(HBPA)_2]^{2+}$ cation within the title compound, $[Cu(C_{13}H_{14}N_2O)_2](CH_3COO)_2.3H_2O$, has a tetragonally elongated coordination polyhedron and represents a rare example of a copper complex in which two phenolic O atoms are axially coordinated to the Cu^{II} centre without deprotonation.

Comment

In recent years copper complexes of ligands containing phenolic hydroxy groups have received a great deal of attention because of their relevance to copper enzymes such as tyrosinate (Himmelwright, Eickman, LuBien, Lerch & Solomon, 1980) and galactose oxidase (Kosman, 1984). Recently, the crystal structure of galactose oxidase (Ito *et al.*, 1991) was determined. The geometry of the active site reveals a unique mononuclear copper site with two histidine N atoms, a tyrosine O atom and an acetate ion forming an almost perfect square and another tyrosine O atom in the axial position completing the square pyramid. In this work, we report the synthesis

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