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(2,2′-Bipyridine-5,5′-dicarboxylic acid)-tetrachloroplatinum(IV) monohydrate

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In the mononuclear title compound, $[PtCl_4(C_{12}H_8N_2O_4)]\cdot H_2O$, the Pt^{IV} atom is six-coordinated in octahedral configuration by two N atoms from the 2,2′-bipyridine-5,5′-dicarboxylic acid ligand and four terminal Cl atoms. In the crystal structure, the molecules are linked together through extensive intermolecular hydrogen bonding, forming a three-dimensional structure.

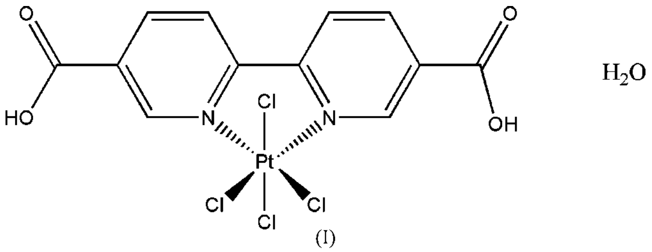
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.028
wR factor = 0.070
Data-to-parameter ratio = 15.2

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

Comment

In recent years, there has been an extensive growth in the research activity on the design and synthesis of metal-organic frameworks (MOFs) (Férey, 2001; Kim *et al.*, 2001; Rowsell & Yaghi, 2004; Côte *et al.*, 2005; Sudik *et al.*, 2005). These materials are constructed by connecting rigid rod-like organic molecules with inorganic clusters called secondary building units. The size and chemical environment of the resulting void spaces are defined by the length and functionality of the organic unit. There is a large number of reported organic molecules that can act as linkers in the synthesis of metal-organic frameworks (Vodak *et al.*, 2001; Chen *et al.*, 2001; Chae *et al.*, 2001; Eddaoudi *et al.*, 2002). However, the title compound, (I), has not yet been reported as a building block in the design of MOFs. We present here the crystal structure of (I), which can be used as a linking unit in MOF synthesis.



(I)

The molecular structure of (I) is shown in Fig. 1. The molecules of (I) are linked together *via* an extensive net of hydrogen bonds into a three-dimensional network. The network consists of layers running parallel to the b axis. Molecules within one layer are connected through O—H···O hydrogen bonds (Fig. 2), while O—H···Cl—Pt hydrogen bonds act between the layers (Fig. 3). Water molecules constitute an important part of the structure. They take part in hydrogen bonding both within and across the layers, giving the structure a three-dimensional character. The Pt—N and Pt—Cl bond distances and N—Pt—Cl, N—Pt—N and Cl—Pt—Cl angles are comparable to those in analogous Pt^{IV} complexes (Casas *et al.* 2005) and in similar square-planar Pt^{II} complexes (Kato & Ikemori, 2003; Connick *et al.*, 1996).

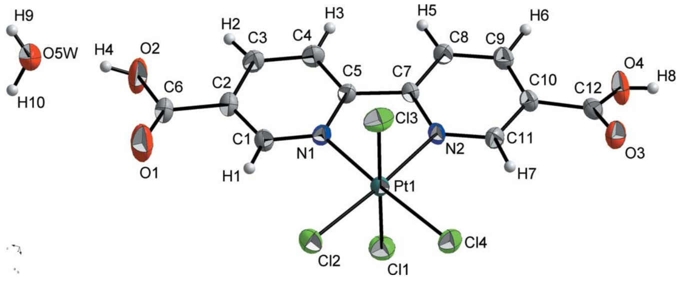


Figure 1

The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

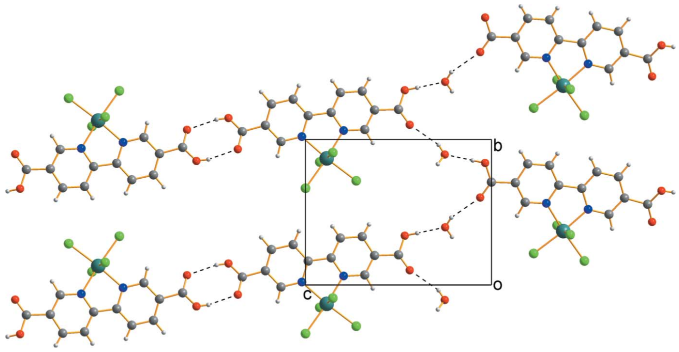


Figure 2

The crystal packing of (I), viewed along the *a* axis. Only one layer is shown for clarity. Dashed lines indicate hydrogen bonds.

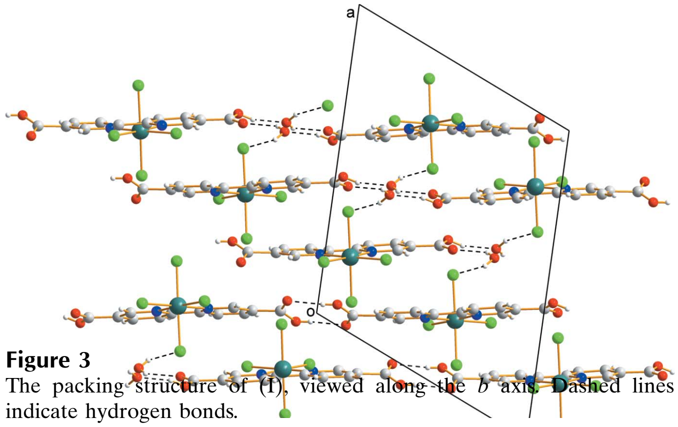


Figure 3

The packing structure of (I), viewed along the *b* axis. Dashed lines indicate hydrogen bonds.

Experimental

K_2PtCl_6 (0.10 g), 2,2′-bipyridine-5,5′-dicarboxylic acid (0.05 g), $CoCl_2\cdot 6H_2O$ (0.15 g) and distilled water (9.7 g) were mixed in a Teflon-lined vessel. The mixture was stirred at ambient temperature for 15 min. The vessel was placed in a sealed autoclave, heated to 373 K (heating rate: 53 K min^{-1}), and kept at this temperature for 12 h without stirring. The mixture was left to cool at room temperature and the pure product, consisting of yellow plate-shaped crystals, was isolated by filtration through an isopore membrane filter with pore size of 5.0 µm (Millipore, TMTP type). The isolated product was washed with distilled water and dried in air at ambient temperature.

Crystal data

$[PtCl_4(C_{12}H_8N_2O_4)]\cdot H_2O$
$M_r = 599.11$
Monoclinic, $P2_1/c$
$a = 15.905$ (3) Å
$b = 8.9969$ (18) Å
$c = 12.512$ (3) Å
$\beta = 113.12$ (3)°
$V = 1646.6$ (6) Å^3
$Z = 4$
$D_x = 2.417$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5858 reflections
$\theta = 2.7$–28.3°
$\mu = 9.20$ mm^{-1}
$T = 298$ (2) K
Plate, yellow
0.22 × 0.22 × 0.05 mm

Data collection

Siemens SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
$T_{\min} = 0.231$, $T_{\max} = 0.656$
10397 measured reflections
3903 independent reflections
3318 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.049$
$\theta_{\max} = 28.3°$
$h = -20 \rightarrow 20$
$k = -12 \rightarrow 7$
$l = -16 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.070$
$S = 1.03$
3903 reflections
257 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0282P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.002$
$\Delta\rho_{\max} = 1.53$ e Å^{-3}
$\Delta\rho_{\min} = -1.44$ e Å^{-3}

Table 1

Selected geometric parameters (Å, °).

Pt1—N2	2.044 (3)	Pt1—Cl4	2.3010 (12)
Pt1—N1	2.058 (3)	Pt1—Cl3	2.3196 (13)
Pt1—Cl2	2.2955 (11)	Pt1—Cl1	2.3212 (14)
N2—Pt1—N1	80.69 (13)	Cl2—Pt1—Cl3	90.60 (5)
N2—Pt1—Cl2	175.75 (10)	Cl4—Pt1—Cl3	91.84 (5)
N1—Pt1—Cl2	95.07 (10)	N2—Pt1—Cl1	88.01 (11)
N2—Pt1—Cl4	95.36 (10)	N1—Pt1—Cl1	88.50 (11)
N1—Pt1—Cl4	175.89 (9)	Cl2—Pt1—Cl1	92.25 (5)
Cl2—Pt1—Cl4	88.89 (5)	Cl4—Pt1—Cl1	90.26 (5)
N2—Pt1—Cl3	89.00 (11)	Cl3—Pt1—Cl1	176.48 (4)
N1—Pt1—Cl3	89.21 (11)		

Table 2

Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H4···O5W	0.81 (7)	1.76 (7)	2.553 (5)	164 (8)
O5W—H10···Cl1$^{\rm i}$	0.87 (7)	2.32 (7)	3.157 (5)	163 (6)
O4—H8···O3$^{\rm ii}$	0.75 (6)	1.93 (6)	2.667 (5)	167 (6)
O5W—H9···O1$^{\rm iii}$	0.75 (7)	2.18 (7)	2.848 (6)	150 (7)

Symmetry codes: (i) $-x+1, -y+2, -z+1$; (ii) $-x, -y+2, -z-1$; (iii) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$.

All H atoms were refined independently using an isotropic model; X—H distances are in the range 0.75–0.98 Å. In the final difference Fourier map, small peaks of 1.53, 1.43, 1.23 and 1.10 e Å^{-3} were found close to the Pt1 atom (0.96, 0.91, 0.85 and 0.87 Å, respectively). The deepest hole was also associated with the Pt1 atom (0.77 Å).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXL97*.

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