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(1,3-Diaminopropan-2-ol-κ²N,N′)(3-hydroxycyclobutane-1,1-dicarboxylato-κ²O,O′)platinum(II) monohydrate

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The reaction of 2-hydroxy-1,3-diaminopropane and 1,1-cyclobutanedicarboxylic acid with potassium tetrachloroplatinate(II) yielded the monomeric title complex, $[Pt(C_6H_6O_5)(C_3H_6N_2O)]\cdot H_2O$. The Pt^{II} atom, coordinated by two N atoms of diaminopropane and two O atoms of carboxylato groups, is in a sqare-planar environment. O—H⋯O hydrogen bonds between the ligands and the solvent water molecule create a three-dimensional network.

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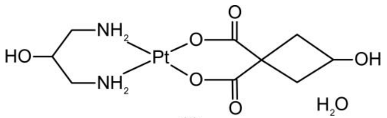
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.010 Å
R factor = 0.033
wR factor = 0.088
Data-to-parameter ratio = 17.4

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

Comment

Carboplatin [*cis*-Diamine(1,1-cyclobutanedicarboxylato)-platinum(II)] is commonly used for the treatment of testicular and ovarian cancer, and for cervical, bladder, head and neck tumors. It has proven to be the only second-generation platinum complex commercially available worldwide at present (Jakuper *et al.*, 2003). However, the application of carboplatin in therapy is limited by the dose-dependent nephrotoxicity and other side effects. The search for new potent platinum complexes possessing high antitumor activity and lack of cross-resistance is therefore continuing. It has been reported that platinum complexes with different amine carriers such as 1,2-diminocyclohexane could overcome some cross-resistance of carboplatin (Ho *et al.*, 2003). The title compound, (I), is a new soluble carboplatin analogue containing an asymmetric chelating diammine 2-hydroxy-1,3-diaminopropane as its carrier and anticancer tests are in progress.



(I)

The title complex consists of discrete monomeric molecules. The Pt^{II} atom has the expected square planar-geometry exhibiting the usual structural features (Fig. 1). The square plane is constituted by the 2-hydroxy-1,3-diaminopropane molecule which acts as a tetradentate ligand through its 2-hydroxy-1,3-diaminopropane N atoms and 1,1-cyclobutanedicarboxylate O atoms. The 2-hydroxy-1,3-diaminopropane ligand has already been used in the dichloroplatinum complex (Oksanen *et al.*, 1991). The 1,1-cyclobutanedicarboxylate ligand displays a similar geometry to those described in the literature (Tu *et al.*, 2004; Zhang *et al.*, 2002; Ali *et al.*, 2002). The two six-membered chelate rings that the ligands 2-hydroxy-1,3-diaminopropane and 1,1-cyclobutanedicarboxylate form with the Pt^{II} atom adopt the boat conformation, and the

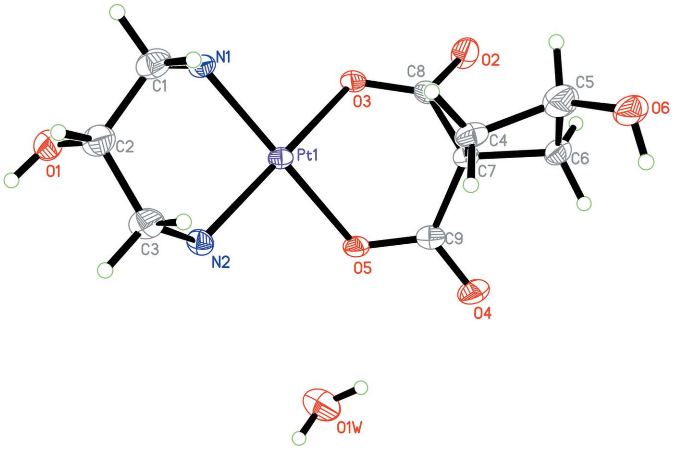


Figure 1
The molecular structure of (I) with the atomic labeling scheme. Displacement ellipsoids are drawn at the 30% probability level.

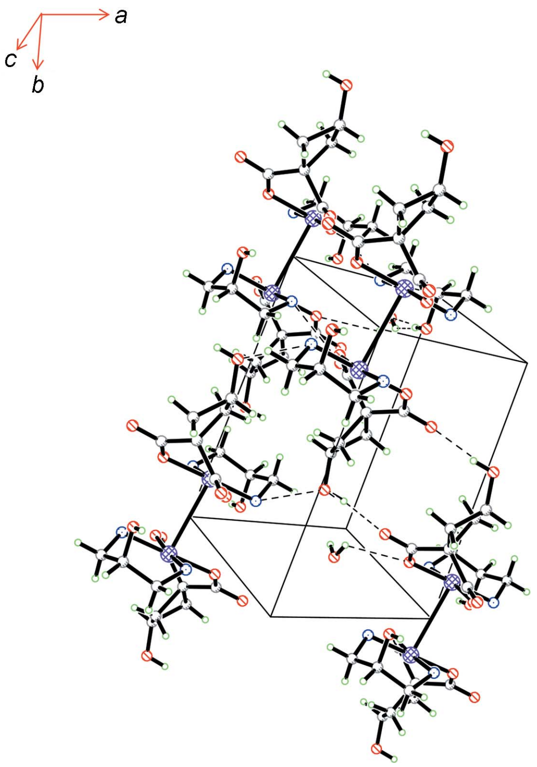


Figure 2
The crystal packing, showing the O—H···O hydrogen-bond network. Only the H atoms involved in hydrogen bonding are shown. Hydrogen bonds are shown as dashed lines.

cyclobutane ring is nearly perpendicular to the Pt^{II} coordination plane. O—H···O hydrogen bonds involving 1,1-cyclobutanedicarboxylate, 2-hydroxy-1,3-diaminopropane and the solvent water molecule (Table 2 and Fig. 2) generate a three-dimensional network.

Experimental

Potassium tetrachloroplatinate(II) (5 g, 12 mmol) was dissolved in water (50 ml) and treated with KI (12 g, 72 mmol). After leaving the solution in the dark for 30 min at room temperature, a solution of 2-hydroxy-1,3-diaminopropane (1.08 g, 12 mmol in 50 ml water) was added dropwise. The mixture was stirred for 4 h and the yellow precipitate was filtered off. To a suspension of bis(2-hydroxy-1,3-diaminopropane)PtI$_2$ (2.5 g, 0.044 mmol) in 75 ml water was added (1.36 g, 3.65 mmol) disilver 1,1-cyclobutanedicarboxylate, and the reaction mixture was stirred at 323 K for 72 h. The AgI formed was filtered off and the filtrate was condensed at 313 K under reduced pressure to 5 ml; a white crystalline product was precipitated. The compound was crystallized from water to obtain crystals suitable for X-ray structure analysis.

Crystal data

$[Pt(C_6H_6O_5)(C_3H_6N_2O)]\cdot H_2O$
$M_r = 457.31$
Triclinic, $P\overline{1}$
$a = 7.4903\ (5)$ Å
$b = 9.9299\ (7)$ Å
$c = 10.5580\ (8)$ Å
$\alpha = 76.3630\ (10)^\circ$
$\beta = 70.3950\ (10)^\circ$
$\gamma = 68.9720\ (10)^\circ$
$V = 684.52\ (8)$ Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 10.28$ mm^{-1}
$T = 298\ (2)$ K
$0.35 \times 0.21 \times 0.09$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
$T_{\min} = 0.086$, $T_{\max} = 0.397$
5674 measured reflections
3035 independent reflections
2820 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.025$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.088$
$S = 1.03$
3035 reflections
174 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{\max} = 2.19$ e Å^{-3}
$\Delta\rho_{\min} = -1.95$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O6—H6C···O4$^{\rm i}$	0.82	1.94	2.752 (7)	172
O1W—H1WB···O1$^{\rm ii}$	0.85	2.07	2.820 (8)	147
O1W—H1WA···O4	0.85	2.59	3.391 (8)	157
O1W—H1WA···O5	0.85	2.53	3.011 (7)	117
O1—H1D···O1$W^{\rm ii}$	0.82	2.01	2.820 (8)	172

Symmetry codes: (i) $-x, -y+1, -z-1$; (ii) $-x-1, -y, -z$.

All H atoms were initially located in a difference Fourier map. The H atoms bonded to carbon and nitrogen were placed at calculated positions (C—H = 0.96–0.97 Å and N—H = 0.90 Å) and were included in the refinement in the riding model approximation, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C,N})$. The H atoms of the water molecules were located in a difference Fourier map and were refined with distance restraints [O—H = 0.85 (1) Å]; their displacement parameters were refined. The largest peak in the final difference Fourier map is about about 1 Å from atom Pt1.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

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