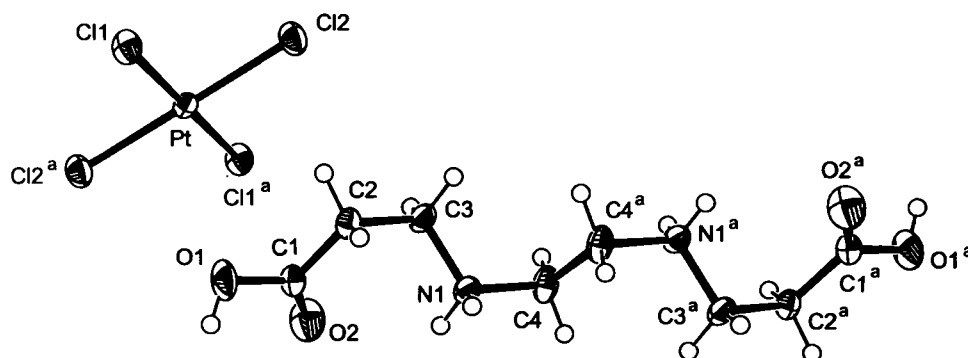


Crystal structure of ethylenediammonium-*N,N'*-di-3-propionic acid tetrachloroplatinate(II), $(\text{CH}_2\text{NH}_2(\text{CH}_2)_2\text{COOH})_2[\text{PtCl}_4]$

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Received June 22, 2006, accepted and available on-line August 28, 2006; CCDC no. 1267/1822



Abstract

$\text{C}_8\text{H}_{18}\text{Cl}_4\text{N}_2\text{O}_4\text{Pt}$, monoclinic, $P12_1/n1$ (no. 14), $a = 8.181(3) \text{ \AA}$, $b = 10.303(5) \text{ \AA}$, $c = 9.073(6) \text{ \AA}$, $\beta = 103.2(1)^\circ$, $V = 744.6 \text{ \AA}^3$, $Z = 2$, $R_{\text{gt}}(F) = 0.080$, $wR_{\text{ref}}(F^2) = 0.247$, $T = 293 \text{ K}$.

Source of material

Potassium tetrachloroplatinate(II) (0.200 g, 0.482 mmol) and ethylenediamine-*N,N'*-di-3-propanoic acid dihydrochloride (0.133 g, 0.482 mmol) were dissolved in 20 ml of water. The reaction mixture was left at room temperature for a few days. After one week, orange crystals were formed from the mother liquor. Upon crystallization crystals were filtered off.

Experimental details

The relatively large R values can be explained by rather bad quality of single crystals.

Discussion

Only one crystal structure with the ethylenediammonium-*N,N'*-di-3-propanoic acid counter to a metal complex anion is described in the literature, (ethylenediammonium-*N,N'*-di-3-propanoic acid) tetrachloropalladate(II) complex [1], $\text{H}_4\text{eddp}[\text{PdCl}_4]$. The title complex consists of two entities: the anion $[\text{PtCl}_4]^{2-}$ and dication $\text{H}_4\text{eddp}^{2+}$. The $[\text{PtCl}_4]^{2-}$ anion exhibits a square-planar coordination with slight deviations from ideal values of 90° with respect to *cis*-coordinated Cl atoms. The $\text{H}_4\text{eddp}^{2+}$ ion is nearly linear. The β -alaninate part of the cation forms *gauche* conformation ($\angle \text{N1}-\text{C3}-\text{C2}-\text{C1} = -64.9(8)^\circ$). The $\text{C4}-\text{N1}-\text{C3}-\text{C2}$ torsion angle of $-171(1)^\circ$ shows a nearly *antiperiplanar* conformation of the $\text{H}_4\text{eddp}^{2+}$ ion. Deviation in the $\text{Cl}-\text{Pt}-\text{Cl}$ angle can be explained by intermolecular hydrogen bond interactions between $\text{N1}-\text{H1}\cdots\text{Cl1}$. Structural fragment $-\text{C}(3)\text{H}_2-\text{C}(2)\text{H}_2-\text{C}(1)\text{OOH}$ is nearly planar and its plane is parallel with the $[\text{PtCl}_4]$ coordina-

tion plane. Every $[\text{PtCl}_4]$ species is located between two above-mentioned fragments. It is interesting to note that one of two H atoms from the $\text{C}(2)\text{H}_2$ group is directed to the Pt atom occupying approximately axial position. The $\text{Pt}-\text{H}$ distance is $3.012(2) \text{ \AA}$ that is shorter than sum of the van der Waals radii. The $\text{C2}-\text{H}\cdots\text{Pt}$ angle is $127.2(5)^\circ$. In this way the Pt atom is situated in a deformed octahedral surrounding formed by four equatorial Cl and two H atoms located on the axial positions. Isostructural complexes, $\text{H}_4\text{eddp}[\text{PtCl}_4]$ and $\text{H}_4\text{eddp}[\text{PdCl}_4]$, have nearly equal $M-L$ bond distances and corresponding angles. This is in agreement with the ionic radii of the central atom.

Table 1. Data collection and handling.

Crystal:	orange prism, size $0.12 \times 0.56 \times 0.56 \text{ mm}$
Wavelength:	Mo K_α radiation ($0.71073 \text{ \AA}$)
μ :	101.50 cm^{-1}
Diffraction, scan mode:	Enraf-Nonius CAD4, $\omega/2\theta$
$2\theta_{\text{max}}$:	52°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	1562, 1461
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1332
$N(\text{param})_{\text{refined}}$:	89
Programs:	SHELXS-97 [2], SHELXL-97 [3], ORTEP-3 [4]

Table 2. Atomic coordinates and displacement parameters (in $\text{\AA}^2$).

Atom	Site	x	y	z	U_{iso}
H(1N1)	4e	0.7005	0.4124	-0.0292	0.029
H(2N1)	4e	0.8499	0.3334	0.0211	0.029
H(1O1)	4e	0.4129	0.1557	0.1701	0.062
H(22)	4e	0.7225	0.3320	0.3569	0.029
H(12)	4e	0.7771	0.2411	0.2384	0.029
H(13)	4e	0.7312	0.5103	0.1973	0.031
H(23)	4e	0.9077	0.4448	0.2523	0.031
H(24)	4e	0.8837	0.5104	-0.1407	0.035
H(14)	4e	0.8814	0.5996	-0.0006	0.035

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Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Pt	2b	½	½	½	0.0256(6)	0.0139(6)	0.0206(7)	0.0008(1)	0.0095(4)	−0.0013(1)
Cl(1)	4e	0.5805(2)	0.3380(2)	0.6767(2)	0.034(1)	0.021(1)	0.035(1)	−0.0005(7)	0.0075(8)	0.0094(7)
Cl(2)	4e	0.7682(2)	0.5845(2)	0.5517(2)	0.030(1)	0.031(1)	0.038(1)	−0.0073(8)	0.0068(9)	0.0060(7)
N(1)	4e	0.8053(8)	0.4122(6)	0.0294(7)	0.033(3)	0.019(3)	0.023(3)	−0.005(3)	0.011(3)	−0.001(2)
O(1)	4e	0.4617(9)	0.2062(7)	0.2353(8)	0.039(3)	0.040(4)	0.045(4)	−0.014(3)	0.012(3)	0.017(3)
O(2)	4e	0.4560(9)	0.3641(7)	0.0647(8)	0.042(3)	0.048(4)	0.051(4)	0.002(3)	0.009(3)	0.019(3)
C(1)	4e	0.5329(9)	0.2994(7)	0.1711(9)	0.022(3)	0.017(3)	0.030(4)	0.002(3)	0.009(3)	0.004(3)
C(2)	4e	0.715(1)	0.3192(7)	0.2497(9)	0.026(3)	0.022(3)	0.027(4)	−0.001(3)	0.012(3)	0.002(3)
C(3)	4e	0.796(1)	0.4323(8)	0.1902(9)	0.035(4)	0.023(3)	0.024(4)	−0.004(3)	0.015(3)	−0.004(3)
C(4)	4e	0.909(3)	0.514(1)	−0.031(3)	0.033(8)	0.020(5)	0.040(8)	0.002(4)	0.020(6)	0.006(5)

Acknowledgment. The authors are grateful to the Ministry of Science and Environmental Protection of the Republic of Serbia for financial support (grant no. 142010).

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