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

Cu(1)—Cu(1^{i})	3.395 (3)	N(5)—C(4)	1.350 (10)
Cu(1)—Cl(1)	2.183 (3)	N(5)—C(6)	1.290 (10)
Cu(1)—Cl(2)	2.197 (3)	N(21)—C(2)	1.324 (10)
Cu(1)—Cl(3)	2.317 (3)	N(21)—C(22)	1.463 (10)
Cu(1)—Cl(3^{i})	2.313 (3)	N(21)—C(26)	1.466 (10)
O(1)—C(2)	1.361 (9)	N(41)—C(4)	1.321 (10)
O(1)—C(6)	1.339 (10)	N(41)—C(42)	1.460 (10)
O(24)—C(23)	1.411 (10)	N(41)—C(46)	1.464 (11)
O(24)—C(25)	1.415 (10)	C(6)—C(61)	1.456 (11)
O(44)—C(43)	1.401 (12)	C(22)—C(23)	1.502 (12)
O(44)—C(45)	1.420 (12)	C(25)—C(26)	1.493 (12)
N(3)—C(2)	1.321 (10)	C(42)—C(43)	1.497 (13)
N(3)—C(4)	1.336 (10)	C(45)—C(46)	1.495 (13)
Cl(1)—Cu(1)—Cl(2)	98.2 (1)	O(1)—C(2)—N(3)	124.1 (8)
Cl(1)—Cu(1)—Cl(3)	96.6 (1)	O(1)—C(2)—N(21)	115.9 (8)
Cl(2)—Cu(1)—Cl(3)	146.8 (1)	N(3)—C(2)—N(21)	120.0 (8)
Cl(1)—Cu(1)—Cl(3^{i})	146.5 (1)	N(3)—C(4)—N(5)	123.9 (8)
Cl(2)—Cu(1)—Cl(3^{i})	97.7 (1)	N(3)—C(4)—N(41)	118.9 (8)
Cl(3)—Cu(1)—Cl(3^{i})	85.7 (1)	N(5)—C(4)—N(41)	117.2 (8)
Cu(1)—Cl(3)—Cu(1^{i})	94.3 (1)	O(1)—C(6)—N(5)	123.5 (7)
C(2)—O(1)—C(6)	115.9 (7)	O(1)—C(6)—C(61)	115.5 (8)
C(23)—O(24)—C(25)	110.3 (8)	N(5)—C(6)—C(61)	121.0 (8)
C(43)—O(44)—C(45)	110.0 (8)	N(21)—C(22)—C(23)	109.3 (8)
C(2)—N(3)—C(4)	114.8 (7)	O(24)—C(23)—C(22)	111.6 (8)
C(4)—N(5)—C(6)	117.1 (7)	O(24)—C(25)—C(26)	111.5 (8)
C(2)—N(21)—C(22)	121.1 (7)	N(21)—C(26)—C(25)	109.6 (7)
C(2)—N(21)—C(26)	123.6 (7)	N(41)—C(42)—C(43)	109.8 (8)
C(22)—N(21)—C(26)	114.7 (7)	O(44)—C(43)—C(42)	111.8 (9)
C(4)—N(41)—C(42)	121.7 (8)	O(44)—C(45)—C(46)	111.5 (9)
C(4)—N(41)—C(46)	122.9 (8)	N(41)—C(46)—C(45)	109.2 (8)
C(42)—N(41)—C(46)	114.8 (7)		

Symmetry code: (i) $1-x, 2-y, 3-z$.

ψ scans indicated that absorption was negligible in this case (minimum transmission factor 0.96, average 0.98). The H atoms were placed geometrically (C—H distance 1.00 Å) and treated as riding atoms with a fixed $U_{\rm iso}$ = 0.08 Å^2. MSC/AFC software was used for data collection and cell determination, and *TEXSAN* software (Molecular Structure Corporation, 1989) for data reduction. The structure was solved by direct methods using *SHELXS*86 programs (Sheldrick, 1990), refined by full-matrix least squares and prepared for publication using the *CRYSTALS* program (Watkin, Carruthers & Betteridge, 1990). Molecular graphics were prepared using *SHELXTL-Plus* (Sheldrick, 1989).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: MU1126). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Dichloro(ethylenediamine)platinum(II)

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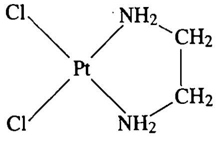
Abstract

The crystal structure of a new polymorph of dichloro(1,2-ethanediamine)platinum(II), $[PtCl_2(C_2H_8N_2)]$, has been determined and is described. Average Pt—N and Pt—Cl bond lengths are 2.032 and 2.318 Å, respectively.

Comment

Two crystal products were obtained from the reaction of $[Pt(en)Cl_2(OH)_2]$ with acetic anhydride in dichloromethane (en = ethylenediamine). One was the expected compound, $[Pt(en)Cl_2(OCOCH_3)_2]$ (Ellis, Er & Hambley, unpublished work), and the other was found to be a new polymorph of $[Pt(en)Cl_2]$ and is described herein.



(I)

$[Pt(en)Cl_2]$ is a close analogue of the widely used anticancer drug cisplatin {*cis*-$[Pt(NH_3)_2Cl_2]$} and has similar anticancer activity (Cleare & Hoeschele, 1973). In the structure of the previously reported polymorph, the complex was found to lie on a twofold axis in the orthorhombic space group $C222_1$

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(Iball, MacDougall & Scrimgeour, 1975). In the presently described polymorph, the complex is located at a general site in the triclinic space group $P\bar{1}$. There is extensive intermolecular hydrogen bonding between the chloro ligands and the H(amine) atoms. The two chloro ligands, the two N(amine) atoms and the Pt atom do not deviate significantly from a square-planar arrangement. The Pt—Cl and Pt—N bond lengths determined for this structure are more consistent with those observed in other platinum(II) complexes, such as *cis*-diamminedichloroplatinum(II) (Milburn & Truter, 1966), than those in the structure reported by Iball *et al.* (1975).

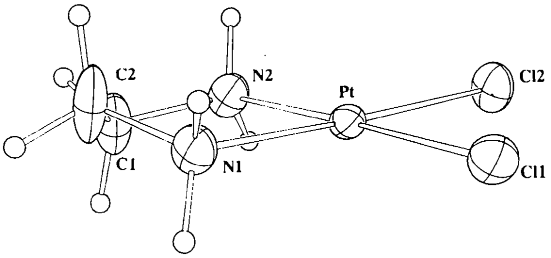

Fig. 1. *ORTEP* (Johnson, 1965) drawing of the title compound showing the atomic labelling scheme. Displacement ellipsoids are drawn at the 30% level.

Experimental

Crystal data

$[PtCl_2(C_2H_8N_2)]$
$M_r = 326.08$
Triclinic
$P\bar{1}$
$a = 6.549\ (2)$ Å
$b = 6.918\ (3)$ Å
$c = 8.040\ (4)$ Å
$\alpha = 83.22\ (4)°$
$\beta = 68.64\ (4)°$
$\gamma = 68.70\ (3)°$
$V = 316.0\ (3)$ Å^3
$Z = 2$
$D_x = 3.43$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 25 reflections
$\theta = 8–12°$
$\mu = 23.17$ mm^{-1}
$T = 294$ K
Needles
0.20 × 0.04 × 0.009 mm
Yellow

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: by integration from crystal shape
$T_{min} = 0.215$, $T_{max} = 0.639$
1192 measured reflections
1073 independent reflections
1010 observed reflections $[I > 2.5\sigma(I)]$

$R_{int} = 0.026$
$\theta_{max} = 25°$
$h = -7 \rightarrow 7$
$k = -8 \rightarrow 8$
$l = 0 \rightarrow 9$
3 standard reflections
frequency: 60 min
intensity variation: <1%

Refinement

Refinement on F
$R = 0.020$
$wR = 0.024$
$S = 1.03$
1010 reflections
67 parameters
Only H-atom U's refined
$w = 0.87/[\sigma^2(F_o) + 0.00045F_o^2]$
$(\Delta/\sigma)_{max} = 0.003$

$\Delta\rho_{max} = 1.6$ e Å^{-3}
$\Delta\rho_{min} = -1.2$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV), *SHELX*76 (Sheldrick, 1976) and *SDP* (Enraf–Nonius, 1985)

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

$$B_{eq} = (8\pi^2/3)\Sigma_i\Sigma_jU_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
Pt	1.00903 (3)	0.24492 (3)	0.99085 (2)	2.02 (2)
Cl1	0.7467 (3)	0.2976 (3)	0.8455 (2)	3.10 (7)
Cl2	1.3306 (3)	0.1575 (3)	0.7283 (2)	3.34 (8)
N1	0.7457 (9)	0.3129 (9)	1.2318 (7)	3.2 (2)
N2	1.2124 (10)	0.2040 (10)	1.1409 (7)	3.0 (2)
C1	0.8464 (14)	0.2470 (15)	1.3745 (8)	5.3 (4)
C2	1.0703 (13)	0.2730 (13)	1.3265 (9)	4.7 (5)

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

Pt—Cl1	2.314 (2)	C1—N1	1.473 (8)
Pt—Cl2	2.322 (2)	C1—C2	1.447 (10)
Pt—N1	2.034 (5)	C2—N2	1.468 (8)
Pt—N2	2.031 (5)		
N1—Pt—Cl1	91.4 (2)	N2—Pt—Cl2	92.4 (2)
N1—Pt—Cl2	175.4 (1)	C1—N1—Pt	109.0 (4)
N1—Pt—N2	83.1 (2)	C1—C2—N2	109.9 (6)
Cl1—Pt—Cl2	93.2 (1)	C2—N2—Pt	111.3 (4)
N2—Pt—Cl1	174.5 (1)	C2—C1—N1	112.3 (6)

H atoms were included at sites calculated assuming tetrahedral geometry, with C—H and N—H = 0.97 Å. Data reduction was carried out using *SDP* (Enraf–Nonius, 1985) and the structure was solved and refined using *SHELX*76 (Sheldrick, 1976).

We wish to thank the Australian Research Council and the Sydney University Cancer Research Fund for financial support of this work.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and least-squares-planes data have been deposited with the IUCr (Reference: OH1064). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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