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cis-Diammine(glycolato-κ^2O^1,O^2)-platinum(II)

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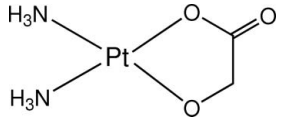
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.010 Å; R factor = 0.020; wR factor = 0.042; data-to-parameter ratio = 17.8.

The reaction of *cis*-$[Pt(NO_3)_2(NH_3)_2]$ and sodium glycolate yielded the title compound, $[Pt(C_2H_2O_3)(NH_3)_2]$. The Pt^{II} atom, coordinated by two N atoms of ammine and two O atoms of the carboxylate and oxido groups of the glycolate ligand, is in a square-planar environment. In the crystal structure, molecules are connected by intermolecular N—H···O hydrogen bonds, forming a three-dimensional network.

Related literature

The title compound is a second-generation platinum derivative that has an antitumour activity comparable to that of cisplatin, one of the most effective anti-cancer drugs for testicular, lung, bladder and other carcinomas, but which is less toxic to the kidney, see: Inuyama *et al.* (1992); Kameyama *et al.* (1990); Noda *et al.* (1992); Taguchi *et al.* (1992); Yamamoto *et al.* (2000). For related structures, see: Yuge & Miyamoto (1998); Griffith *et al.* (2007).



Experimental

Crystal data

$[Pt(C_2H_2O_3)(NH_3)_2]$
M_r = 303.19
Orthorhombic, $P2_12_12_1$
a = 5.6293 (6) Å
b = 7.2853 (8) Å
c = 14.1107 (16) Å
V = 578.70 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 24.17 mm^{-1}
T = 298 K
0.24 × 0.12 × 0.10 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.068, T_{max} = 0.196
3739 measured reflections
1354 independent reflections
1307 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.042
S = 0.99
1354 reflections
76 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.24 e Å^{-3}
$\Delta\rho_{min}$ = −1.10 e Å^{-3}
Absolute structure: Flack (1983), 489 Friedel pairs
Flack parameter: 0.013 (17)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1C···O2^{i}	0.89	2.01	2.883 (8)	167
N1—H1B···O2^{ii}	0.89	2.44	3.107 (7)	132
N1—H1B···O3^{iii}	0.89	2.45	3.049 (7)	125
N1—H1A···O3^{iv}	0.89	2.00	2.888 (7)	173
N2—H2C···O3^{v}	0.89	2.32	3.108 (7)	147
N2—H2B···O2^{ii}	0.89	2.21	3.014 (8)	150
N2—H2A···O3^{iii}	0.89	2.26	3.010 (7)	142

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RN2056).

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supporting information

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Qing-Kun Wang, Shao-Ping Pu, Yan-Wei Cong, Yong-Nian Li and Chun-Fang Luan

S1. Comment

Cis-diamminedichloro-platinum(II) (cisplatin) is one of the most effective anti-cancer drugs for testicular, lung, bladder and other carcinomas. However, the clinical usefulness of this drug has frequently been limited by serious nephrotoxicity and gastrointestinal toxicity and the development of acquired resistance. In an attempt to overcome these drawbacks of cisplatin, numerous analogues have been prepared and evaluated in a search for alternative active agents. Among these compounds, the title compound, *cis*-diammine(glycolato-o,o′)platinum(II), is a second-generation platinum derivative that has an antitumour activity comparable to cisplatin but is less toxic to the kidney (Kameyama *et al.*,1990), as seen in preclinical experiments. It produced promising response rates in phase II trials for treatment of squamous cell carcinoma arising from the head and neck (Inuyama *et al.*,1992), lung (Yamamoto *et al.*,2000), oesophagus (Taguchi *et al.*,1992), and uterine cervix (Noda *et al.*, 1992). For related structures see: (Yuge & Miyamoto, 1998; Griffith *et al.*, 2007) The compound forms a hydrogen-bonded structure (Fig. 2), in which one of the H atoms of ammonia serves as a donor to the O atom of the glycollate of an adjacent molecule and these hydrogen-bond interactions give rise to a three-dimensional network.

S2. Experimental

Cis-[$Pt(NO_3)_2(NH_3)_2$] (2.0 nmol) was dissolved in 50 ml water and sodium glycolate (2.0 mmol in 50 ml water) was added thereto. The mixture was adjusted to pH=7 with NaOH solution and stirred at 323k for 3 h. The solution was condensed at 313k under reduced pressure to 5 ml, then a yellow crystalline product was precipitated. The compound was crystallized from water to obtain crystals suitable for X-ray structure analysis.

S3. Refinement

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 = 0.97Å and N—H = 0.89 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) = 1.2Ueq(C), U_{iso}(H) = 1.5Ueq(N).

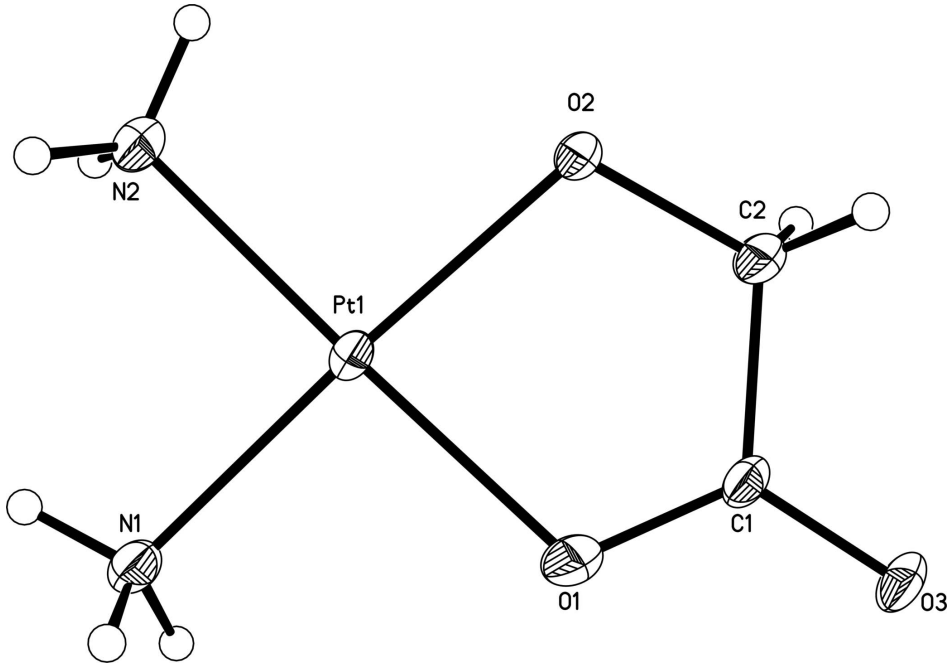

Figure 1

The molecular structure of title complex with the atomic labeling scheme. Displacement ellipsoids are drawn at the 30% probability level.

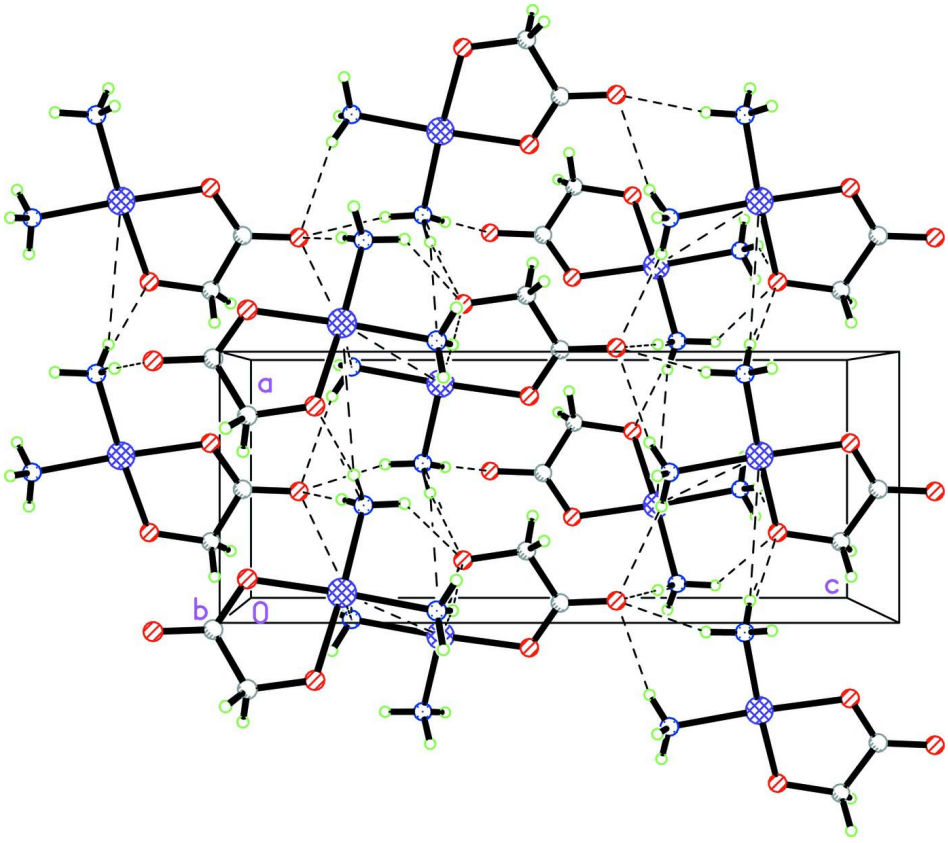

Figure 2

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

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$M_r = 303.19$
Orthorhombic, $P2_12_12_1$
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$b = 7.2853\ (8)$ Å
$c = 14.1107\ (16)$ Å
$V = 578.70\ (11)$ Å^3
$Z = 4$
$F(000) = 544$
$D_x = 3.480$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1354 reflections
$\theta = 2.9$–$28.3°$
$\mu = 24.17$ mm^{-1}
$T = 298$ K
Block, colourless
0.24 × 0.12 × 0.10 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
$T_{min} = 0.068$, $T_{max} = 0.196$
3739 measured reflections
1354 independent reflections
1307 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.9°$
$h = -6 \rightarrow 7$
$k = -9 \rightarrow 9$
$l = -17 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.020$
$wR(F^2) = 0.042$
$S = 0.99$
1354 reflections
76 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0103P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.24$ e Å^{-3}
$\Delta\rho_{min} = -1.10$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0087 (3)
Absolute structure: Flack (1983), 489 Friedel pairs
Absolute structure parameter: 0.013 (17)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.
Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Pt1	0.10734 (4)	0.96205 (3)	0.178777 (16)	0.01860 (9)
N2	0.0429 (10)	0.9713 (9)	0.3193 (4)	0.0310 (12)
H2A	0.1574	1.0347	0.3479	0.047*
H2B	0.0392	0.8577	0.3424	0.047*
H2C	−0.0964	1.0256	0.3296	0.047*
N1	0.4267 (10)	0.8432 (8)	0.2082 (3)	0.0272 (13)
H1A	0.4471	0.7457	0.1711	0.041*
H1B	0.4298	0.8085	0.2686	0.041*
H1C	0.5427	0.9237	0.1976	0.041*
O1	0.1557 (8)	0.9447 (7)	0.0377 (3)	0.0308 (11)
O2	−0.2005 (8)	1.0830 (7)	0.1425 (3)	0.0263 (11)
C1	−0.0264 (12)	0.9948 (9)	−0.0099 (4)	0.0230 (15)
C2	−0.2372 (12)	1.0639 (11)	0.0439 (5)	0.0332 (17)
H2E	−0.2827	1.1823	0.0182	0.040*
H2D	−0.3688	0.9803	0.0337	0.040*
O3	−0.0334 (8)	0.9898 (7)	−0.0983 (3)	0.0288 (11)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.02166 (13)	0.02149 (13)	0.01266 (12)	−0.00028 (10)	−0.00029 (9)	0.00010 (9)
N2	0.030 (3)	0.043 (3)	0.020 (3)	0.003 (2)	0.001 (2)	−0.003 (3)

N1	0.033 (3)	0.036 (3)	0.012 (2)	0.010 (3)	0.005 (2)	0.003 (2)
O1	0.028 (3)	0.046 (3)	0.018 (2)	0.004 (2)	0.0023 (19)	−0.006 (2)
O2	0.027 (2)	0.038 (3)	0.014 (2)	0.008 (2)	−0.0030 (18)	−0.0067 (19)
C1	0.027 (3)	0.024 (4)	0.018 (3)	−0.003 (2)	0.003 (2)	0.003 (2)
C2	0.032 (4)	0.052 (5)	0.016 (3)	0.011 (3)	−0.002 (3)	−0.004 (3)
O3	0.036 (3)	0.038 (3)	0.012 (2)	−0.002 (2)	−0.0002 (18)	−0.0005 (19)

Geometric parameters (Å, º)

Pt1—O2	2.010 (5)	N1—H1B	0.8900
Pt1—O1	2.013 (4)	N1—H1C	0.8900
Pt1—N2	2.017 (5)	O1—C1	1.279 (8)
Pt1—N1	2.038 (5)	O2—C2	1.413 (7)
N2—H2A	0.8900	C1—O3	1.248 (8)
N2—H2B	0.8900	C1—C2	1.496 (9)
N2—H2C	0.8900	C2—H2E	0.9700
N1—H1A	0.8900	C2—H2D	0.9700
O2—Pt1—O1	83.82 (18)	Pt1—N1—H1C	109.5
O2—Pt1—N2	94.6 (2)	H1A—N1—H1C	109.5
O1—Pt1—N2	176.9 (2)	H1B—N1—H1C	109.5
O2—Pt1—N1	176.77 (19)	C1—O1—Pt1	113.2 (4)
O1—Pt1—N1	93.18 (18)	C2—O2—Pt1	109.5 (4)
N2—Pt1—N1	88.4 (2)	O3—C1—O1	122.8 (6)
Pt1—N2—H2A	109.5	O3—C1—C2	119.5 (6)
Pt1—N2—H2B	109.5	O1—C1—C2	117.7 (5)
H2A—N2—H2B	109.5	O2—C2—C1	114.7 (6)
Pt1—N2—H2C	109.5	O2—C2—H2E	108.6
H2A—N2—H2C	109.5	C1—C2—H2E	108.6
H2B—N2—H2C	109.5	O2—C2—H2D	108.6
Pt1—N1—H1A	109.5	C1—C2—H2D	108.6
Pt1—N1—H1B	109.5	H2E—C2—H2D	107.6
H1A—N1—H1B	109.5		
O2—Pt1—O1—C1	−6.9 (4)	Pt1—O1—C1—O3	−178.2 (5)
N2—Pt1—O1—C1	53 (5)	Pt1—O1—C1—C2	2.4 (8)
N1—Pt1—O1—C1	174.3 (5)	Pt1—O2—C2—C1	−11.1 (7)
O1—Pt1—O2—C2	9.7 (4)	O3—C1—C2—O2	−173.3 (6)
N2—Pt1—O2—C2	−167.7 (5)	O1—C1—C2—O2	6.1 (10)
N1—Pt1—O2—C2	31 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*C*···O2^{i}	0.89	2.01	2.883 (8)	167
N1—H1*B*···O2^{ii}	0.89	2.44	3.107 (7)	132
N1—H1*B*···O3^{iii}	0.89	2.45	3.049 (7)	125
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