C(12)	0.0327 (6)	0.2276 (6)	0.6593 (5)	0.0722 (14)
C(13)	−0.1379 (7)	0.1261 (7)	0.5550 (6)	0.091 (2)
C(21)	0.3533 (5)	0.6685 (5)	0.7091 (4)	0.0508 (10)
C(22)	0.5300 (6)	0.8001 (6)	0.7866 (5)	0.0698 (14)
C(23)	0.5773 (8)	0.9398 (6)	0.7354 (6)	0.084 (2)
C(31)	0.3058 (5)	0.5413 (5)	0.8735 (4)	0.0492 (10)
C(32)	0.1969 (7)	0.6122 (7)	0.9051 (5)	0.0663 (13)
C(33)	0.2264 (6)	0.6386 (6)	1.0406 (4)	0.0657 (13)
C(41)	0.4137 (5)	0.4356 (5)	0.7364 (4)	0.0470 (10)
C(42)	0.4342 (7)	0.3974 (7)	0.6152 (4)	0.0678 (13)
C(43)	0.5478 (7)	0.3194 (7)	0.6235 (5)	0.0753 (15)

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

Cu(1)—Cl(2)	2.1979 (14)	C(11)—C(12)	1.514 (6)
Cu(1)—Cl(3)	2.1983 (15)	C(12)—C(13)	1.504 (7)
Cu(1)—Cl(1)	2.3076 (14)	C(21)—C(22)	1.496 (6)
Cu(1)—Cl(1^i)	2.3241 (13)	C(22)—C(23)	1.503 (7)
N(1)—C(41)	1.516 (5)	C(31)—C(32)	1.513 (6)
N(1)—C(11)	1.517 (5)	C(32)—C(33)	1.511 (7)
N(1)—C(31)	1.518 (5)	C(41)—C(42)	1.506 (6)
N(1)—C(21)	1.529 (5)	C(42)—C(43)	1.503 (7)
Cl(2)—Cu(1)—Cl(3)	98.91 (6)	C(11)—N(1)—C(21)	105.8 (3)
Cl(2)—Cu(1)—Cl(1)	96.17 (5)	C(31)—N(1)—C(21)	111.3 (3)
Cl(3)—Cu(1)—Cl(1)	147.64 (6)	C(12)—C(11)—N(1)	116.5 (4)
Cl(2)—Cu(1)—Cl(1^i)	145.99 (6)	C(13)—C(12)—C(11)	109.9 (4)
Cl(3)—Cu(1)—Cl(1^i)	97.37 (6)	C(22)—C(21)—N(1)	116.2 (4)
Cl(1)—Cu(1)—Cl(1^i)	85.48 (5)	C(21)—C(22)—C(23)	111.0 (4)
Cu(1)—Cl(1)—Cu(1^i)	94.52 (5)	C(32)—C(31)—N(1)	117.0 (3)
C(41)—N(1)—C(11)	111.7 (3)	C(33)—C(32)—C(31)	109.0 (4)
C(41)—N(1)—C(31)	105.2 (3)	C(42)—C(41)—N(1)	116.5 (3)
C(11)—N(1)—C(31)	111.6 (3)	C(43)—C(42)—C(41)	110.1 (4)
C(41)—N(1)—C(21)	111.3 (3)		

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

Data collection, cell refinement and data reduction: *SHELXL XSCANS* (Sheldrick, 1994). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*. Molecular graphics: *SHELXL XP*. Software used to prepare material for publication: *SHELXL*.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: BR1067). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Battaglia, L. P., Bonamartini Corradi, A., Marcotrigiano, G., Menabue, L. & Pellacani, G. C. (1980). *Inorg. Chem.* **19**, 125–129.

Colombo, A., Menabue, L., Motori, A., Pellacani, G. C., Porzio, W., Sandrolini, F. & Willett, R. D. (1985). *Inorg. Chem.* **24**, 2900–2905.

Harlow, R. L., Wells, W. J., Watt, G. W. & Simonsen, S. H. (1974). *Inorg. Chem.* **13**, 2860–2863.

Murray-Rust, P. (1975). *Acta Cryst.* **B31**, 1771–1772.

Roberts, S. A., Bloomquist, D. R., Willett, R. D. & Dodgen, H. W. (1981). *J. Am. Chem. Soc.* **103**, 2606–2610.

Sheldrick, G. M. (1990). *Acta Cryst.* **A46**, 467–473.

Sheldrick, G. M. (1994). *J. Appl. Cryst.* In preparation.

Sheldrick, W. S. (1981). *Acta Cryst.* **B37**, 945–946.

Textor, M., Dubler, E. & Oswald, H. R. (1974). *Inorg. Chem.* **13**, 1361–1365.

Vossos, P. H., Fitzwater, D. R. & Rundle, R. E. (1963). *Acta Cryst.* **16**, 1037–1045.

Willett, R. D. (1966). *J. Chem. Phys.* **44**, 39–42.

Willett, R. D. & Chow, C. (1974). *Acta Cryst.* **B30**, 207–214.

Willett, R. D., Dwiggins, C., Kruh, R. F. & Rundle, R. E. (1963). *J. Chem. Phys.* **38**, 2429–2436.

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cis-Ammine(benzoylhydrazine-*N*)-dichloroplatinum(II)

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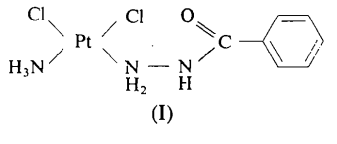
Abstract

In the title compound, *cis*-ammine(benzohydrazide-*N'*)-dichloroplatinum(II), *cis*-$[PtCl_2(C_7H_8N_2O)(NH_3)]$, the benzoylhydrazine ligand is bonded to the Pt atom through its amino group. The Pt—Cl and Pt—N distances are in the ranges 2.293 (5)–2.318 (5) and 2.01 (1)–2.08 (1) Å, respectively. The arrangement of molecules in the monoclinic unit cell approximates $P2_1/c$ space-group patterns; however, the true space-group symmetry is $P2_1$. The two crystallographically independent molecules have significantly different conformations about the Pt—N(hydrazine) bond. The structure is held together by a complicated network of N—H···O and N—H···Cl hydrogen bonds.

Comment

The considerable success of *cis*-$[PtCl_2(NH_3)_2]$ (cisplatin) in the clinical treatment of tumours (Carter, 1984) has stimulated the design of analogous complexes with modified ligands (Hides & Russell, 1988; Lippert, 1992). Recently, Dodoff, Grancharov, Gugova & Spassovska (1994) described the preparation, characterization and *in vitro* cytotoxic effects of a series of Pt^{II} complexes of benzoylhydrazine and 3-methoxybenzoylhydrazine. Crystals could be obtained only for the title compound (I).



(I)

The asymmetric unit of the title compound contains two *cis*-$[PtCl_2(bh)(NH_3)]$ (bh = benzoylhydrazine) molecules (Fig. 1) related by a pseudo symmetry centre at $(0,0,\frac{1}{4})$. Corresponding atoms of the two independent molecules are labelled identically, except those of the second molecule are distinguished by primes (see

Table 1). The two molecules have very similar geometries but differ in their conformation around the Pt—N2 bond (Fig. 2). The torsion angle Cl1—Pt—N2—N1 is −39 (1)° for the 'unprimed' molecule and 70 (1)° for the 'primed' molecule. The PtN_2Cl_2 moieties are planar to within 0.02 (2) (unprimed) and 0.05 (2) Å (primed), as are the N2, N1, C, O, C1*a* fragments and phenyl rings [to within 0.09 (2) and 0.03 (2) Å, respectively, for the unprimed molecule, and 0.04 (2) and 0.03 (2) Å, respectively, for the primed molecule]. The dihedral angles between the two planar parts of the bh ligand are 22 (1) (unprimed) and 28 (1)° (primed). The molecules are held together by an extensive system of hydrogen bonds of the N—H···Cl and N—H···O types (Fig. 3). The latter are weak and link H—N—C=O peptide moieties in different molecules.

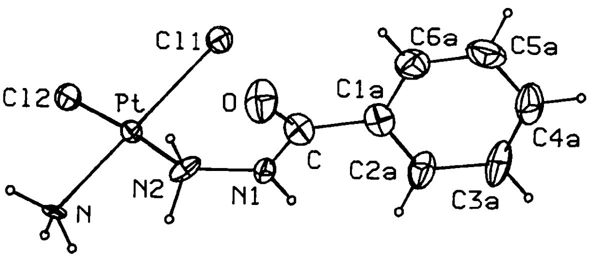


Fig. 1. A view of the $[PtCl_2(bh)(NH_3)]$ molecule showing the atom-numbering scheme and 30% probability displacement ellipsoids. H atoms are represented by spheres of arbitrary size.

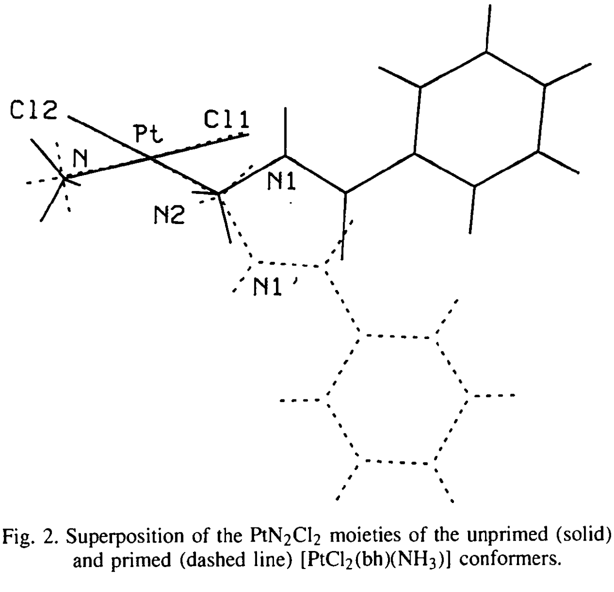


Fig. 2. Superposition of the PtN_2Cl_2 moieties of the unprimed (solid) and primed (dashed line) $[PtCl_2(bh)(NH_3)]$ conformers.

The geometry of the bh ligand can be compared with that of isonicotinic acid hydrazide (Bhat, Singh & Vijayan, 1974). The platinum coordination geometry is similar to those found for *cis*-$[PtCl_2(NH_3)_2]$ (Milburn & Truter, 1966) and *cis*-$[PtCl_2(CH_3NH_3)_2]$ (Wimmer, Wimmer, Jaud, Johnson & Castan, 1988). The shortest Pt···Pt′ distance of 3.384 (1) Å relates PtN_2Cl_2 fragments, which make a dihedral angle of only 6 (2)° with each other; the next shortest Pt···Pt($-x$, $\frac{1}{2}+y$, $-z$) distance is 5.299 (1) Å. In cisplatin, the molecules are ordered in stacks with Pt···Pt distances of 3.372 (2) and 3.409 (2) Å (Milburn & Truter, 1966).

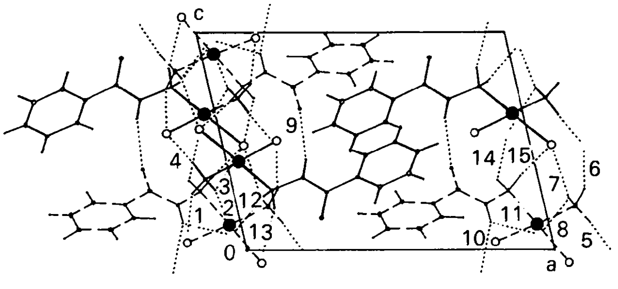


Fig. 3. Projection of part of the structure down the *b* axis. The two independent $[PtCl_2(bh)(NH_3)]$ molecules are distinguished by full and broken lines. Hydrogen bonds, represented by dotted lines, are numbered as in Table 3.

Experimental

The starting complex, $[PtCl_2(bh)(NH_3)].0.5H_2O$, was prepared according to Dodoff, Grancharov, Gugova & Spassovska (1994). A solution of 0.15 g (1.10 mmol) benzoylhydrazine in 10 ml water was added, under stirring, to a solution of 0.40 g (1.12 mmol) $K[PtCl_3(NH_3)]$ in 10 ml of water. The reaction mixture was left overnight. The yellow precipitate which formed was filtered off, washed with water and ethanol and dried under vacuum (70% yield, 0.33 g). 50 mg of the complex was dissolved in 1 ml of freshly distilled dimethylformamide and 4 ml ethanol was added. Crystals of $[PtCl_2(bh)(NH_3)]$ formed after three weeks.

Crystal data

$[PtCl_2(C_7H_8N_2O)(NH_3)]$
M_r = 419.18
Monoclinic
$P2_1$
a = 13.132 (2) Å
b = 9.433 (3) Å
c = 9.414 (2) Å
β = 103.09 (1)°
V = 1135.8 (8) Å^3
Z = 4
D_x = 2.451 Mg m^{-3}

Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 22 reflections
θ = 20.13–20.84°
μ = 12.93 mm^{-1}
T = 292 K
Plate
0.13 × 0.06 × 0.01 mm
Yellow transparent

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans [Δw = (0.80 + 0.40tanθ)°]
Absorption correction: spherical
T_{min} = 0.277, T_{max} = 0.294
ψ scan (North, Phillips & Mathews, 1968)
T_{min} = 0.717, T_{max} = 0.999

5545 measured reflections
5323 independent reflections
3093 observed reflections [$I > 3.0\sigma(I)$]
R_{int} = 0.034
θ_{max} = 28.0°
$h = 0 \rightarrow 17$
$k = -12 \rightarrow 12$
$l = -12 \rightarrow 12$
3 standard reflections
frequency: 120 min
intensity variation: −3.3%

Refinement

Refinement on F
$R = 0.038$
$wR = 0.038$
$S = 1.121$
3093 reflections
252 parameters
H atoms riding

$w = 1/[\sigma^2(F) + (0.010F)^2]$
$(\Delta/\sigma)_{\max} = 0.51$
$\Delta\rho_{\max} = 1.62$ e Å^{-3}
$\Delta\rho_{\min} = -2.14$ e Å^{-3}
Atomic scattering factors from *SDP/PDP* (Enraf–Nonius, 1985)

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

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
Pt	0.03650 (5)	0.12000†	0.38456 (7)	0.0297 (1)
Pt′	−0.03802 (5)	−0.12026 (7)	0.11404 (6)	0.0294 (1)
Cl1	0.1738 (3)	−0.0328 (5)	0.4763 (5)	0.040 (1)
Cl1′	−0.1871 (4)	0.0115 (5)	0.0373 (5)	0.051 (1)
Cl2	−0.0665 (3)	0.0264 (4)	0.5316 (4)	0.039 (1)
Cl2′	0.0379 (3)	−0.0188 (5)	−0.0578 (5)	0.045 (1)
O	0.262 (1)	0.120 (2)	0.125 (1)	0.072 (4)
O′	−0.2758 (8)	−0.220 (1)	0.369 (1)	0.040 (3)
N	−0.0844 (9)	0.251 (1)	0.308 (1)	0.023 (3)
N′	0.100 (1)	−0.231 (2)	0.195 (2)	0.061 (5)
N1	0.233 (1)	0.238 (1)	0.314 (1)	0.034 (4)
N1′	−0.191 (1)	−0.305 (1)	0.201 (1)	0.033 (3)
N2	0.123 (1)	0.214 (1)	0.256 (1)	0.036 (4)
N2′	−0.107 (1)	−0.214 (2)	0.266 (2)	0.047 (4)
C	0.299 (1)	0.176 (2)	0.246 (2)	0.046 (5)
C′	−0.271 (2)	−0.305 (2)	0.269 (2)	0.045 (5)
C1*a*	0.411 (1)	0.178 (2)	0.315 (2)	0.046 (5)
C1*a*′	−0.362 (1)	−0.398 (2)	0.202 (2)	0.036 (4)
C2*a*	0.453 (2)	0.277 (2)	0.418 (2)	0.061 (6)
C2*a*′	−0.345 (1)	−0.525 (2)	0.138 (2)	0.052 (5)
C3*a*	0.561 (2)	0.284 (2)	0.478 (2)	0.065 (6)
C3*a*′	−0.427 (2)	−0.609 (2)	0.083 (2)	0.074 (7)
C4*a*	0.623 (2)	0.186 (2)	0.429 (2)	0.071 (7)
C4*a*′	−0.528 (1)	−0.578 (2)	0.084 (2)	0.075 (6)
C5*a*	0.580 (2)	0.085 (2)	0.328 (3)	0.077 (8)
C5*a*′	−0.543 (2)	−0.448 (3)	0.153 (2)	0.079 (8)
C6*a*	0.476 (1)	0.086 (2)	0.267 (2)	0.064 (7)
C6*a*′	−0.461 (1)	−0.369 (2)	0.212 (2)	0.055 (6)

† Coordinate fixed to define origin.

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

Pt—Cl1	2.318 (4)	N1—N2	1.44 (2)
Pt—Cl2	2.318 (5)	N1—C	1.33 (2)
Pt—N	2.01 (1)	N1′—N2′	1.42 (2)
Pt—N2	2.04 (1)	N1′—C′	1.35 (3)
Pt′—Cl1′	2.293 (5)	C—O	1.24 (2)
Pt′—Cl2′	2.293 (5)	C—C1*a*	1.47 (2)
Pt′—N′	2.08 (1)	C′—O′	1.25 (2)
Pt′—N2′	2.06 (2)	C′—C1*a*′	1.50 (2)
Cl1—Pt—Cl2	92.9 (2)	N′—Pt′—N2′	90.9 (6)
Cl1—Pt—N	178.8 (4)	N2—N1—C	117 (1)
Cl1—Pt—N2	90.2 (4)	N2′—N1′—C′	114 (1)
Cl2—Pt—N	85.9 (4)	Pt—N2—N1	119.0 (9)
Cl2—Pt—N2	176.4 (4)	Pt′—N2′—N1′	112 (1)
N—Pt—N2	91.0 (5)	O—C—N1	118 (2)
Cl1′—Pt′—Cl2′	91.6 (2)	O—C—C1*a*	123 (2)
Cl1′—Pt′—N′	176.4 (5)	N1—C—C1*a*	119 (1)
Cl1′—Pt′—N2′	88.3 (4)	O′—C′—N1′	122 (2)
Cl2′—Pt′—N′	89.2 (5)	O′—C′—C1*a*′	122 (2)
Cl2′—Pt′—N2′	179.1 (4)	N1′—C′—C1*a*′	116 (1)

Table 3. *Hydrogen-bonding geometry* (Å, °)

No.*	D—H···A	D—H	H···A	D···A	D—H···A
1	N—H1···Cl1′	0.95	2.60	3.446 (11)	149
2	N—H2···Cl2′$^{\rm i}$	0.95	2.45	3.357 (12)	159
3	N—H2···Cl2$^{\rm ii}$	0.95	2.94	3.403 (11)	112
4	N—H3···Cl1$^{\rm ii}$	0.95	2.39	3.275 (13)	155
5	N′—H1′···Cl1′$^{\rm iii}$	0.95	2.92	3.619 (18)	132
6	N′—H2′···Cl1	0.95	2.32	3.211 (17)	155
7	N′—H3′···Cl2$^{\rm iv}$	0.95	2.74	3.547 (18)	143
8	N′—H3′···Cl2′$^{\rm iii}$	0.95	2.72	3.352 (15)	125
9	N1—H11···O′$^{\rm ii}$	0.95	2.15	2.934 (17)	139
10	N1′—H11′···O$^{\rm iii}$	0.95	2.28	3.087 (17)	142
11	N1′—H11′···Cl2′$^{\rm iii}$	0.95	2.64	3.336 (14)	130
12	N2—H21···Cl2′$^{\rm ii}$	0.95	2.66	3.533 (13)	153
13	N2—H22···Cl2′	0.95	2.74	3.651 (12)	162
14	N2′—H21′···Cl2	0.95	2.56	3.324 (15)	137
15	N2′—H22′···Cl2$^{\rm iv}$	0.95	2.67	3.587 (14)	163

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

* The hydrogen-bond numbering relates to Fig. 3.

Data were collected using *CAD*-4 *Software* (Enraf–Nonius, 1988). Data reduction was performed using *SDP/PDP* (Enraf–Nonius, 1985). The initial structure solution was carried out in the centrosymmetric space group $P2_1/c$. The position of the Pt atom was found from the Patterson function and the rest of the [$PtCl_2(bh)(NH_3)$] molecule was found from difference Fourier maps. The structural motif was refined by full-matrix least squares to $R(F) = 0.061$ for 1510 (3σ) reflections (the unique data set was initially under $2/m$ symmetry) with fixed isotropic displacement parameters for the O, N and C atoms. Further analysis of the refinement results, along with the indications of statistical tests (*SDP/PDP NORMAL*, *NZTEST*; Enraf–Nonius, 1985), led us to choose the non-centrosymmetric space group $P2_1$, in which convergence was reached. The positions of the H atoms were calculated and left riding on their attached atoms (N—H 0.95 Å) with fixed U values [U(H) = 0.063 Å^2]. No attempts were made to establish the absolute structure. The maximum residual peaks on the $\Delta\rho$ maps were ripples close to the Pt atom. *ORTEP*II (Johnson, 1976) was used for molecular graphics; the material for publication was prepared using *KAPPA* (Macíček, 1992, unpublished).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry including H-atom geometry and torsion angles have been deposited with the IUCr (Reference: MU1101). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Bhat, T. N., Singh, T. P. & Vijayan, M. (1974). *Acta Cryst.* **B30**, 291–292.

Carter, S. K. (1984). In *Platinum Coordination Complexes in Cancer Chemotherapy*, edited by M. P. Hacker, E. B. Douple & I. H. Krakoff. Boston: Martinus Nijhoff.

Dodoff, N., Grancharov, K., Gugova, R. & Spassovska, N. (1994). *J. Inorg. Biochem.* In the press.

Enraf–Nonius (1985). *Structure Determination Package. SDP/PDP User's Guide.* Version 3.0. Enraf–Nonius, Delft, The Netherlands.

Enraf–Nonius (1988). *CAD*-4 *Manual.* Version 5.0. Enraf–Nonius, Delft, The Netherlands.

Hides, P. C. & Russell, M. J. H. (1988). *Cancer Metastasis Rev.* **7**, 67–89.

Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

Lippert, B. (1992). *BioMetals*, **5**, 195–208.

Milburn, G. H. W. & Truter, M. R. (1966). *J. Chem. Soc. A*, pp. 1609–1616.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Wimmer, S., Wimmer, F., Jaud, J., Johnson, N. P. & Castan, P. (1988). *Inorg. Chim. Acta*, **144**, 25–30.

Acta Cryst. (1994). C**50**, 1217–1220

Platinum(II) Triamine Complexes: *cis*-$[PtCl(NH_3)_2(C_{10}H_{13}N_5O_5)]NO_3.2H_2O$ and $[PtCl(C_2H_8N_2)(C_4H_6N_2)]NO_3$

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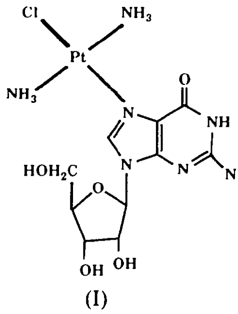
Abstract

The structures of *cis*-diamminechloro(guanosine-N^7)-platinum(II) nitrate dihydrate, *cis*-$[PtCl(NH_3)_2(C_{10}H_{13}N_5O_5)]NO_3.2H_2O$, (I), and chloro(ethylenediamine)(1-methylimidazole-N^3)platinum(II) nitrate, $[Pt(C_2H_8N_2)(C_4H_6N_2)Cl]NO_3$, $[PtCl(en)(1\text{-}MeIm)]NO_3$, (II), were determined by single-crystal X-ray diffraction. The former complex crystallized in the orthorhombic system and the latter in the monoclinic system. In compound (I), water molecules were found to connect the metal complex with the nitrate counter ions *via* hydrogen bonding.

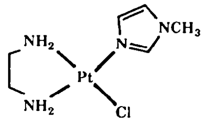
Comment

We have undertaken a study of model complexes for the formation of platinum(II) mediated protein–DNA crosslinks. The nitrate salts of the triaminechloroplatinum(II) compounds described here were prepared as precursors for our preliminary model systems. Syntheses were accomplished following the methods of Lippert (Lippert, Lock & Speranzini, 1981) and Hollis (Hollis, Amundsen & Stern, 1989).

The crystal structure of (I) confirms the expected coordination of guanosine to Pt through the N7 atom. Furthermore, the geometry about Pt is square planar with Pt deviating −0.0039 Å from the mean plane of the Cl and three N atoms. The angles around Pt are near 90° and the distances to coordinated atoms fall within the range of typical values for Pt—N and Pt—Cl bonds.



(I)



(II)

The purine group is planar with no atom deviating more than 0.03 Å from the mean plane, which makes an angle of 58.8 (2)° with the Pt coordination plane. Overall, the geometry of the purine ring system is similar to that found in other guanine and guanosine Pt complexes (Faggiani, Lippert, Lock & Speranzini, 1982; Schollhorn, Raudaschl-Sieber, Muller, Thewalt & Lippert, 1985). Thus, the variations of 105 (1)–110 (1)° for the bond angles of the five-membered ring and 112 (1)–128 (1)° for those of the six-membered ring are reasonable for this complex. Typically, the internal ring angle at an N atom is greater if that atom is covalently bound to an extra-annular H atom than if it has no extra annular attachment (Singh, 1965); in (I), C6—N1—C2 is found to be 126 (1)° while C2—N3—C4 is 113 (1)°. As one might expect, the angle C8—N7—C5 is a few degrees larger than that observed for free guanosine (Taylor & Kennard, 1982*a*) and is close to those values observed for structures which are protonated (Taylor & Kennard, 1982*b*) or platinated (Melanson & Rochon, 1979) at N7.

The glycosyl bond is normal at 1.47 (1) Å and the ribose ring angles are close to tetrahedral. The orientation of the purine base relative to the ribose ring within the nucleotide is expressed as χ, the glycosyl torsion angle O4′–C1′–N9—C4, which in this case is −149 (1)° and falls within the '*anti*' range (Saenger, 1984). The sugar puckering is described by the pseudorotation angle *P*, calculated from the ribose torsion angles ν_0–ν_4 (Altona & Sundaralingam, 1972). In the case of (I), the molecule can be classified as C2′-*endo*.

Intermolecular interactions which take the form of hydrogen bonding mainly involving nitrate ions and water molecules, appear to dictate the packing in (I). In the strongest interactions O1*W* connects O5′ with a pair of nitrate ions. The second water molecule interacts with both a nitrate ion and the Cl atom. The role of the amine ligands on Pt in the hydrogen-bonding system is less evident. Weaker hydrogen bonds form contacts

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