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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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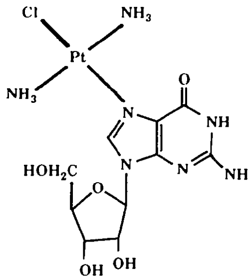
Abstract

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.

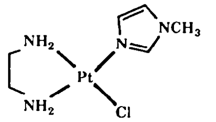
Comment

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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between the ribose O atoms (O2′ and O3′) and the N atom of a Pt-bound amine (N12). Finally, there exists the possibility of an amine H atom (N11) forming a bond to the carbonyl O atom (O6) of a second molecule.

The structure of (II) contains the typical distortions from square-planar geometry that are found for [Pt(en)] complexes (Gellert & Bau, 1975). As such, the bond angle between Pt and the two N atoms of the en ligand is only 83.4 (4)°, while the remaining ligand–Pt–ligand angles are just slightly greater than 90°. The distances to coordinated atoms are in the expected ranges for both Pt—N and Pt—Cl bonds.

The 1-methylimidazole (1-MeIm) moiety is planar and there are no deviations from the least-squares plane through the five ring atoms greater than 0.023 Å. The Pt atom and the methyl C atom (C1) are displaced from the imidazole plane by 0.040 and 0.014 Å, respectively. The dihedral angle between the plane of the Pt-coordination sphere and the imidazole ring system is 36.5 (5)°. In the similar complexes *cis*-$[PtCl_2(1\text{-}MeIm)_2]$ and *trans*-$[Pt(1\text{-}MeIm)_2(NH_3)_2]^{2+}$ this dihedral angle is reported to be 41.7 (Graves, Hodson, van Kralingen & Reedijk, 1978) and 49.2° (Carmichael, Chan, Cordes, Fair & Johnson, 1972), respectively.

The packing arrangement involves hydrogen bonding between the metal complex and the nitrate counter ion. Specifically, a nitrate ion connects the cations *via* hydrogen bonding to N—H groups of the en ligands, with the N···C contact distances ranging from 2.89 (2) to 3.02 (2) Å. There are no interactions between the cations.

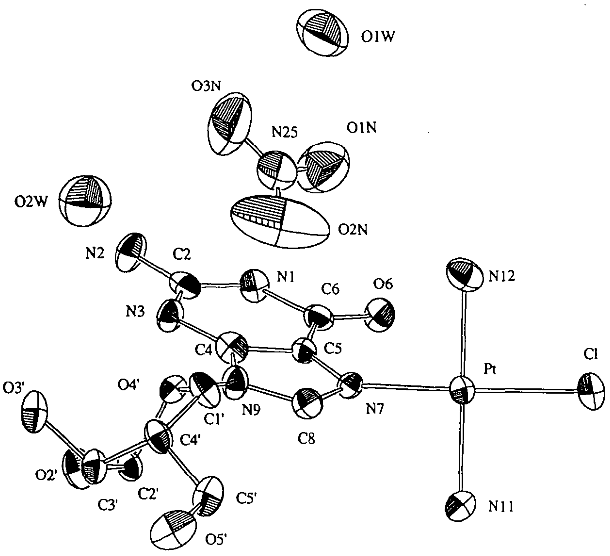

Fig. 1. Structure of compound (I) showing the atom-labeling scheme and 50% probability displacement ellipsoids.

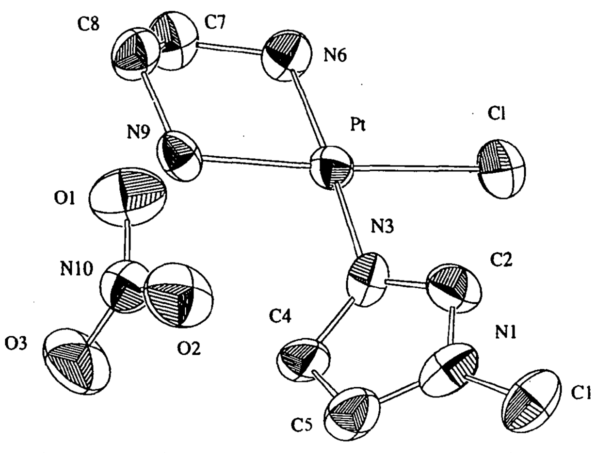

Fig. 2. Structure of compound (II) showing the atom-labeling scheme and 50% probability displacement ellipsoids.

Experimental

300 mg (1 mmol) of *trans*-diamminedichloroplatinum(II) was dissolved in 30 ml of dimethylformamide. 169 mg (1 mmol) of $AgNO_3$ was added and the solution was stirred overnight in the dark. AgCl was filtered off and 283 mg (1 mmol) of guanosine hydrate was added. After 14 h the solvent was evaporated and the complex was precipitated by adding CH_2Cl_2. The light yellow powder was crystallized from water to yield 442 mg of compound (I). X-ray quality crystals were obtained by slow evaporation from water. Analysis calculated (found) for $C_{10}H_{19}ClN_8O_8Pt.H_2O$: C 19.13 (19.08), H 3.37 (3.67), N 17.85% (17.79%). The same procedure was carried out on 326 mg of $[PtCl_2(en)]$ resulting in 255 mg of compound (II). Crystals were obtained from water. Analysis calculated (found) for $C_6H_{14}ClN_5O_3Pt$: C 16.57 (16.66), H 3.22 (3.11), N 16.11% (15.98%).

Compound (I)

Crystal data

$[PtCl(NH_3)_2(C_{10}H_{13}N_5O_5)]$-$NO_3.2H_2O$
$M_r = 645.88$
Orthorhombic
$P2_12_12_1$
$a = 6.988\ (5)$ Å
$b = 17.760\ (8)$ Å
$c = 15.929\ (7)$ Å
$V = 1978\ (2)$ Å^3
$Z = 4$
$D_x = 2.170$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.7107$ Å
Cell parameters from 25 reflections
$\theta = 10.0$–$26.0°$
$\mu = 7.62$ mm^{-1}
$T = 294$ K
Lathe
0.38 × 0.06 × 0.05 mm
Yellow

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: empirical
$T_{min} = 0.5630$, $T_{max} = 0.6813$
6332 measured reflections
5081 independent reflections
3898 observed reflections
$[F > 4.0\sigma(F)]$

$R_{int} = 0.0384$
$\theta_{max} = 30.0°$
$h = 0 \rightarrow 9$
$k = 0 \rightarrow 24$
$l = -22 \rightarrow 22$
3 standard reflections
frequency: 120 min
intensity variation: none

Refinement

Refinement on F
$R = 0.048$
$wR = 0.045$
3898 reflections
271 parameters
H-atom parameters not refined
Calculated weights $w = 1.175/[\sigma^2(F) + 0.0009F^2]$

$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 3.5$ e Å^{-3}
$\Delta\rho_{\min} = -0.4$ e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

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

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

	x	y	z	$U_{\rm eq}$
Pt	0.87041 (6)	0.74564 (2)	0.42474 (2)	0.0231 (2)
Cl	0.8473 (6)	0.8620 (2)	0.4866 (2)	0.040 (2)
N11	0.8680 (18)	0.6945 (5)	0.5392 (5)	0.034 (5)
N12	0.8726 (18)	0.7973 (5)	0.3097 (6)	0.040 (5)
N7	0.8894 (14)	0.6459 (4)	0.3670 (5)	0.024 (4)
C5	1.0207 (16)	0.6234 (6)	0.3081 (6)	0.023 (5)
C6	1.1909 (17)	0.6579 (6)	0.2782 (7)	0.029 (5)
O6	1.2659 (12)	0.7177 (4)	0.3032 (5)	0.034 (4)
N1	1.2757 (13)	0.6156 (5)	0.2142 (6)	0.029 (5)
C2	1.2106 (19)	0.5495 (6)	0.1827 (7)	0.033 (6)
N2	1.3145 (16)	0.5174 (6)	0.1220 (6)	0.040 (6)
N3	1.0508 (14)	0.5167 (5)	0.2097 (6)	0.029 (5)
C4	0.9642 (16)	0.5556 (6)	0.2734 (8)	0.031 (6)
C8	0.7544 (17)	0.5931 (6)	0.3690 (7)	0.030 (6)
N9	0.7966 (15)	0.5374 (5)	0.3128 (6)	0.031 (5)
C1′	0.6740 (16)	0.4728 (6)	0.2925 (7)	0.028 (6)
C2′	0.7110 (16)	0.4031 (5)	0.3481 (7)	0.026 (5)
O2′	0.8673 (14)	0.3609 (4)	0.3233 (5)	0.040 (4)
C3′	0.5181 (17)	0.3630 (6)	0.3355 (8)	0.031 (6)
O3′	0.5106 (12)	0.3301 (4)	0.2543 (5)	0.035 (4)
C4′	0.3781 (19)	0.4286 (5)	0.3379 (7)	0.030 (5)
C5′	0.2886 (17)	0.4447 (7)	0.4230 (8)	0.037 (6)
O5′	0.1380 (14)	0.3935 (5)	0.4420 (5)	0.046 (5)
O4′	0.4850 (11)	0.4942 (4)	0.3111 (5)	0.032 (4)
O1*W*	0.735 (2)	0.783 (1)	−0.040 (1)	0.085 (9)
O2*W*	0.740 (2)	0.523 (1)	0.561 (1)	0.087 (10)
N25	0.759 (2)	0.665 (1)	0.120 (1)	0.062 (9)
O1N	0.886 (2)	0.714 (1)	0.135 (1)	0.094 (9)
O2N	0.658 (2)	0.641 (1)	0.174 (1)	0.160 (16)
O3N	0.772 (4)	0.644 (1)	0.051 (1)	0.155 (18)

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

Pt—Cl	2.295 (3)	C6—N1	1.399 (14)
Pt—N11	2.037 (9)	N1—C2	1.354 (14)
Pt—N12	2.050 (9)	C2—N2	1.34 (2)
Pt—N7	2.000 (8)	C2—N3	1.33 (2)
N7—C5	1.373 (14)	N3—C4	1.37 (2)
N7—C8	1.330 (14)	C4—N9	1.37 (2)
C5—C6	1.42 (2)	C8—N9	1.37 (2)
C5—C4	1.38 (2)	N9—C1′	1.468 (14)
C6—O6	1.250 (13)		
O6···Cl$^{\rm i}$	3.679 (9)	O3′···N12$^{\rm iii}$	2.92 (1)
O6···N11$^{\rm i}$	3.04 (1)	O5′···O1*W*$^{\rm iii}$	2.67 (2)
N1···O4′$^{\rm ii}$	3.03 (1)	O1*W*···O1N$^{\rm iv}$	2.87 (2)
N1···O2N$^{\rm ii}$	2.79 (2)	O2*W*···O3N$^{\rm v}$	2.97 (2)
O2′···O5′$^{\rm ii}$	2.74 (1)		
N12—Pt—N7	89.2 (3)	O6—C6—N1	121 (1)
N11—Pt—N7	91.0 (3)	C6—N1—C2	126 (1)
N11—Pt—N12	179.9 (4)	N1—C2—N3	123 (1)
Cl—Pt—N7	178.0 (2)	N1—C2—N2	117 (1)
Cl—Pt—N12	88.9 (3)	N2—C2—N3	120 (1)
Cl—Pt—N11	91.0 (3)	C2—N3—C4	113 (1)
Pt—N7—C8	124.5 (7)	C5—C4—N3	128 (1)
Pt—N7—C5	128.1 (7)	N3—C4—N9	127 (1)
C5—N7—C8	106.6 (8)	C5—C4—N9	105 (1)
N7—C5—C4	109.6 (9)	N7—C8—N9	110 (1)
N7—C5—C6	131.6 (9)	C4—N9—C8	108 (1)
C6—C5—C4	119 (1)	C8—N9—C1′	126 (1)
C5—C6—N1	111.6 (9)	C4—N9—C1′	126 (1)
C5—C6—O6	128 (1)		
N12—Pt—N7—C5	52.7 (9)	C6—C5—C4—N9	−179 (1)
N11—Pt—N7—C5	−127.3 (9)	O4′—C1′—C2′—O2′	163.0 (9)
N3 C4 N9 –C8	−176 (1)	C6—C5—C4—N3	−2 (2)
N12—Pt—N7—C8	−115.2 (9)	C1′—C2′—C3′—O3′	74 (1)
C5—C4—N9—C8	0 (1)	C4—C5—C6—N1	1 (1)
N11—Pt—N7—C8	64.7 (9)	C1′—C2′—C3′—C4′	−40 (1)
N7—C8—N9—C4	0 (1)	C4—C5—C6—O6	−178 (1)
Pt—N7—C8—N9	170.1 (7)	O2′—C2′—C3′—O3′	−46 (1)
N7—C8—N9—C1′	−175 (1)	C5—C6—N1—C2	0 (2)
Pt—N7—C5—C6	9 (2)	O2′—C2′—C3′—C4′	−161.1 (9)
C8—N9—C1′—C2′	−90 (1)	O6—C6—N1—C2	179 (1)
Pt—N7—C5—C4	−169.5 (8)	C2′—C3′—C4′—C5′	−95 (1)
C4—N9—C1′—C2′	96 (1)	C6—N1—C2—N2	−179 (1)
C5—N7—C8—N9	0 (1)	C2′—C3′—C4′—O4′	26 (1)
C8—N9—C1′—O4′	25 (1)	C6—N1—C2—N3	1 (2)
C8—N7—C5—C4	0 (1)	O3′—C3′—C4′—C5′	150 (1)
C4—N9—C1′—O4′	−149 (1)	N1—C2—N3—C4	−2 (2)
C8—N7—C5—C6	178 (1)	O3′—C3′—C4′—O4′	−90 (1)
N9—C1′—O4′—C4′	−148.3 (8)	N2—C2—N3—C4	178 (1)
N7—C5—C4—N9	0 (1)	C3′—C4′—O4′—C1′	0 (1)
N9—C1′—C2′—O2′	−81 (1)	C2—N3—C4—C5	2 (2)
N7—C5—C4—N3	176 (1)	C5′—C4′—O4′—C1′	125.5 (9)
N9—C1′—C2′—C3′	158.5 (9)	C2—N3—C4—N9	178 (1)
N7—C5—C6—O6	4 (2)	C3′—C4′—C5′—O5′	−78 (1)
C2′—C1′—O4′—C4′	−27 (1)	N3—C4—N9—C1′	−2 (2)
N7—C5—C6—N1	−177 (1)	O4′—C4′—C5′—O5′	162.5 (9)
O4′—C1′—C2′—C3′	42 (1)	C5—C4—N9—C1′	175 (1)

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

Compound (II)

Crystal data

$[\mathrm{PtCl(C_2H_8N_2)(C_4H_6N_2)}]$-$\mathrm{NO_3}$
$M_r = 434.75$
Monoclinic
$C2/c$
$a = 31.875$ (4) Å
$b = 5.118$ (2) Å
$c = 15.398$ (2) Å
$\beta = 106.14$ (1)°
$V = 2413.0$ (6) Å^3
$Z = 8$
$D_x = 2.411$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.7107$ Å
Cell parameters from 25 reflections
$\theta = 14.0$–$26.0°$
$\mu = 11.98$ mm^{-1}
$T = 294$ K
Lathe
0.18 × 0.10 × 0.10 mm
Yellow

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: empirical
$T_{\min} = 0.378$, $T_{\max} = 0.497$
4076 measured reflections
3795 independent reflections
2002 observed reflections $[F > 4.0\sigma(F)]$

$R_{\rm int} = 0.0117$
$\theta_{\max} = 30.0°$
$h = -42 \rightarrow 42$
$k = 0 \rightarrow 7$
$l = 0 \rightarrow 21$
3 standard reflections
frequency: 120 min
intensity variation: none

Refinement

Refinement on F
$R = 0.086$
$wR = 0.064$

$(\Delta/\sigma)_{\max} = 0.062$
$\Delta\rho_{\max} = 1.8$ e Å^{-3}
$\Delta\rho_{\min} = -1.6$ e Å^{-3}

2002 reflections
148 parameters
H-atom parameters not refined
Calculated weights $w = 2.555/[\sigma^2(F) + 0.0009F^2]$

Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 3. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for* (II)

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

	x	y	z	$U_{\rm eq}$
Pt	0.37244 (2)	0.3629 (1)	0.06687 (3)	0.0331 (2)
Cl	0.3083 (1)	0.3996 (9)	−0.0482 (2)	0.051 (2)
N9	0.4316 (3)	0.350 (2)	0.1617 (7)	0.036 (5)
N6	0.4050 (3)	0.591 (2)	−0.0014 (7)	0.042 (6)
C8	0.4657 (4)	0.421 (3)	0.1172 (9)	0.045 (7)
C7	0.4491 (5)	0.654 (3)	0.058 (1)	0.047 (7)
N3	0.3437 (3)	0.128 (2)	0.1395 (7)	0.037 (5)
C2	0.3143 (5)	−0.051 (3)	0.109 (1)	0.047 (8)
C4	0.3521 (4)	0.131 (4)	0.2322 (8)	0.055 (8)
C5	0.3283 (5)	−0.061 (4)	0.257 (1)	0.056 (9)
N1	0.3033 (3)	−0.169 (2)	0.1774 (9)	0.051 (7)
C1	0.2717 (5)	−0.384 (3)	0.168 (1)	0.058 (9)
N10	0.4408 (5)	−0.186 (2)	0.3393 (8)	0.044 (7)
O1	0.4543 (4)	−0.119 (3)	0.2752 (8)	0.074 (8)
O2	0.4408 (5)	−0.044 (3)	0.4032 (9)	0.079 (9)
O3	0.4240 (4)	−0.410 (2)	0.3362 (9)	0.073 (8)

Table 4. *Selected geometric parameters* (Å, °) *for* (II)

Pt—Cl	2.312 (3)	N3—C4	1.38 (2)
Pt—N9	2.041 (9)	C2—N1	1.34 (2)
Pt—N6	2.039 (12)	C4—C5	1.36 (3)
Pt—N3	2.024 (12)	C5—N1	1.38 (2)
N3—C2	1.30 (2)	N1—C1	1.47 (2)
Pt···C2^{i}	3.68 (1)	Cl···C1^{i}	3.97 (2)
Pt···N1^{i}	3.95 (1)	Cl···C1^{iv}	3.77 (2)
Cl···C2^{i}	3.68 (2)	Cl···C1^{ii}	3.66 (2)
Cl···C2^{ii}	3.83 (1)	N9···O3^{i}	3.02 (2)
Cl···C5^{iii}	3.67 (2)	N6···O3^{iii}	2.89 (2)
Cl···N1^{ii}	3.82 (1)		
N9—Pt—N3	93.2 (4)	N3—C2—N1	111 (1)
N9—Pt—N6	83.4 (4)	N3—C4—C5	109 (1)
Cl—Pt—N3	91.8 (3)	C4—C5—N1	106 (1)
Cl—Pt—N6	91.6 (3)	C2—N1—C5	108 (1)
C2—N3—C4	107 (1)	C2—N1—C1	125 (1)
N9—Pt—N3—C2	−143 (1)	N9—C8—C7—N6	−53 (1)
Cl—Pt—N3—C2	37 (1)	Pt—N3—C2—N1	179.3 (9)
N9—Pt—N3—C4	37 (1)	Pt—N3—C4—C5	−177 (1)
Cl—Pt—N3—C4	−143 (1)	C2—N3—C4—C5	3 (2)
N9—Pt—N6—C7	−8.6 (9)	C4—N3—C2—N1	−1 (2)
Cl—Pt—N6—C7	171.5 (8)	N3—C2—N1—C1	−179 (1)
N6—Pt—N9—C8	−20.1 (8)	N3—C2—N1—C5	−2 (2)
N3—Pt—N9—C8	158.9 (8)	N3—C4—C5—N1	−4 (2)
Pt—N9—C8—C7	44 (1)	C4—C5—N1—C2	3 (2)
Pt—N6—C7—C8	35 (1)	C4—C5—N1—C1	−180 (1)

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

Systematic absences showed that the space group of compound (I) was $P2_12_12_1$. For (I), the atomic coordinates for the Pt atom were obtained from a three-dimensional Patterson synthesis using *SHELXS*86 (Sheldrick, 1985). The remaining non-H atoms were found in a series of successive difference Fourier maps. All non-H atoms were refined with anisotropic displacement parameters by full-matrix least squares using *SHELX*76 (Sheldrick, 1976). H atoms were refined with a common isotropic displacement parameter of 6 Å^2 and, except those at N11, N2, O2′, O3′, O5′, O1*W* and O2*W* (which were placed at calculated positions and fixed), were considered as riding atoms at a distance of 0.95 Å.

For compound (II), systematic absences and statistical distribution of $|E|$ suggested the space group $C2/c$; this was confirmed by the final model. Solution and refinement methods were the same as for compound (I). The C_{sp} an N_{sp^2} H atoms were included as riding atoms placed in their calculated positions (C—H = 0.95 Å) with a common isotropic displacement parameter of 6 Å^2. H atoms of the methyl C atom (C1) were calculated as a rigid group (C—H = 0.95 Å) and included in refinement with isotropic displacement parameters of 9 Å^2.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989). Cell refinement: *CAD*-4 *Software* (Enraf–Nonius, 1989). Data reduction: *MolEN* (Fair, 1990). Program(s) used to solve structure: *SHELXS*86. Program(s) used to refine structure: *SHELX*76. Software used to prepare material for publication: local program.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: CD1054). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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