

Related literature. Compared to Pt^{II} and Pd^{II}, the coordination chemistry of the d^8 metal ion Au^{III} has been studied considerably less extensively (Sadler, 1976). To date, structurally characterized examples of nucleobase complexes of Au^{III} are restricted to two models containing pyrimidine bases 1-methylcytosine (Holowczak, Stancl & Wong, 1985) and 1-methyluracil (Micklitz, Mikulcik, Müller, Riede & Lippert, 1989). No structurally characterized purine base complex of Au^{III} is presently available. Our attempts to prepare a 9-ethylguanine complex of Au^{III} in analogy to AuCl₃ (guanosine) (Hadjiliadis, Pneumatikakis & Basosi, 1981) have so far been unsuccessful. The structure of the cation closely resembles that of the related tetrachloroplatinate(II) analogue (Purnell & Hodgson, 1976). Even details such as the dihedral angle between the pyrimidine and the imidazole portions of the guaninium (3.9°) are very similar. The site of protonation is also N(7), as is evident from the increase of the internal ring angle at N(7) from 104° in neutral 9-ethylguanine (Destro, Kistenmacher & Marsh, 1974; Taylor & Kennard, 1982) to $108.2(6)^\circ$ in the title compound and the rather short [2.736 (7) Å] hydrogen bond of N(7)H to the water molecule. While the platinate salt displays this feature as well [N(7)H···OH₂ 2.650 Å], the other hydrogen bonds differ in both structures. Instead of N(3)···H₂N(2) hydrogen bonding in the platinate salt, the aurate

compound has pairs of intermolecular N(1)H···O(6) hydrogen bonds of 2.837 (8) Å, for example.

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trans-Bis(glycine-*N*)bis(methylamine)platinum(II) Dinitrate Dihydrate, *trans*-[(NH₂CH₃)₂(C₂H₅NO₂)₂Pt](NO₃)₂·2H₂O

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Abstract. C₆H₂₄N₆O₁₂Pt, $M_r = 567.38$, monoclinic, $P2_1/c$, $a = 9.125$ (2), $b = 12.860$ (3), $c = 7.752$ (2) Å, $\beta = 104.72$ (2)°, $V = 879.8$ (4) Å³, $Z = 2$, $D_x = 2.142$ Mg m⁻³, $\lambda(\text{Mo } K\alpha) = 0.71073$ Å, $\mu = 8.12$ mm⁻¹, $F(000) = 552$, $T = 291$ (1) K, final $R = 0.026$ for 1341 unique observed [$F \geq 3.0\sigma(F)$] diffractometer data. The centrosymmetric cation contains two methylamine and two neutral glycine ligands, each coordinated to Pt through the NH₂ group. The Pt has a square-planar coordination geometry without any unusual features. The geometry of the methylamine ligand is very similar to that found in

trans-(NH₂CH₃)₂PtCl₂ [Arpalahti, Lippert, Schöllhorn & Thewalt (1988). *Inorg. Chim. Acta*, **153**, 45–49] and two derivatives containing the model nucleobase 1-methylcytosine [Pesch, Preut & Lippert (1990). *Inorg. Chim. Acta*, **169**, 195–200]. The glycine ligands likewise have a geometry that is close to that observed in a related complex containing the anionic glycinato ligand, except for the carboxylato groups. Protonation of O(2) in the title compound expectedly causes significant differences in bond lengths between protonated [1.320 (7) Å] and non-protonated CO groups [1.207 (6) Å]. The acidic proton at O(2) forms

a rather strong hydrogen bond with the water molecule in the crystal lattice [$O(2) \cdots O(11)$ 2.626 (6) Å].

Experimental. The title compound was prepared by reaction of *trans*-[(NH₂CH₃)₂Pt(H₂O)₂](NO₃)₂, obtained *in situ* from *trans*-(NH₂CH₃)₂PtCl₂ (Ar-palahti *et al.*, 1988) and AgNO₃ with 2·3 equiv. of glycine (pH 6·5, 3 d, 323 K) and subsequent recrystallization of the precipitated *trans*-(NH₃)₂Pt(gly)₂ from dilute HNO₃ (pH 1·2). Slow evaporation at 277 K gave [Pt(NH₂CH₃)₂(C₂H₅NO₂)₂](NO₃)₂·2H₂O: calculated C 12·7, H 4·3, N 14·8%; found C 12·8, H 4·5, N 14·6%. Crystal size ~0·16 × 0·20 × 0·14 mm, D_m not determined, $\omega/2\theta$ scan, scan speed 3·00–14·65° min⁻¹ in θ , scan width (1·2 + dispersion); Nicolet R3m/V diffractometer, graphite-monochromated Mo K α radiation; lattice parameters from least-squares fit with 16 reflections up to 2 θ = 37·59°; ω scans of low-order reflections along the three crystal axes showed acceptable mosaicity; six standard reflections (400, 040, 004, 400, 040, 004) recorded every 2·5 h, only random deviations over

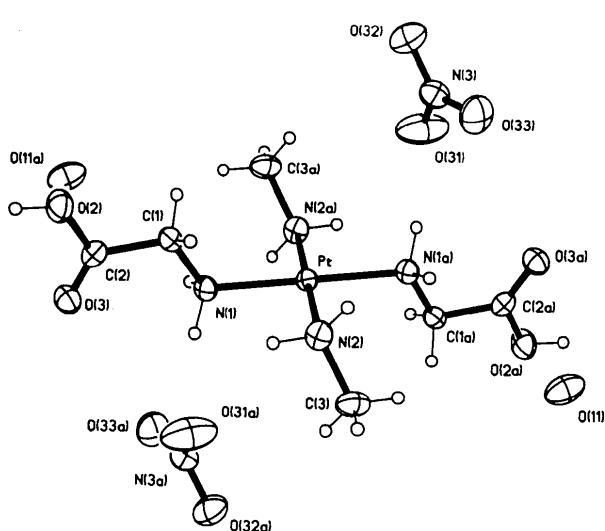


Fig. 1. General view (*SHELXTL-Plus* graphic) of the molecule, showing the atom-numbering scheme.

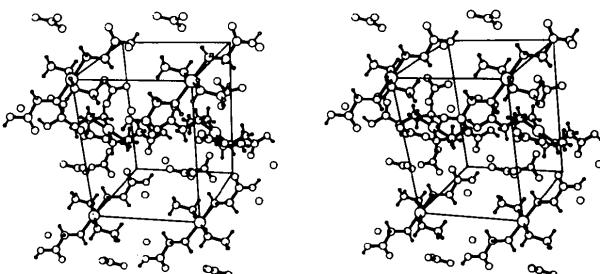


Fig. 2. Stereoscopic view (*SCHAKAL* graphic) of the unit cell (*a* horizontal, *b* nearly vertical).

Table 1. *Atomic coordinates and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^4$)*

$$U_{\text{eq}} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq}
Pt(1)	0.0	0.0	0.0	189 (1)
O(2)	-0.3682 (4)	-0.1388 (3)	0.3809 (5)	372 (14)
O(3)	-0.2455 (4)	-0.2621 (3)	0.2685 (5)	315 (12)
O(11)	0.5371 (4)	0.2131 (4)	0.0378 (5)	448 (13)
O(31)	-0.1400 (5)	0.2627 (4)	-0.2344 (7)	739 (20)
O(32)	-0.2860 (5)	0.3554 (3)	-0.1211 (6)	494 (16)
O(33)	-0.0450 (5)	0.3710 (4)	-0.0270 (5)	491 (15)
N(1)	-0.1093 (4)	-0.1175 (3)	0.0958 (5)	232 (13)
N(2)	0.1517 (6)	0.0131 (3)	0.2468 (7)	292 (17)
N(3)	-0.1568 (5)	0.3287 (3)	-0.1271 (6)	330 (17)
C(1)	-0.2123 (5)	-0.0832 (3)	0.2010 (6)	246 (15)
C(2)	-0.2754 (5)	-0.1720 (4)	0.2871 (6)	232 (17)
C(3)	0.3109 (8)	-0.0147 (4)	0.257 (1)	368 (22)

Table 2. Bond distances (\AA), bond angles ($^\circ$), torsion angles ($^\circ$) and hydrogen-bond geometry

$\text{Pt}(1)-\text{N}(1)$	2.051 (4)	$\text{O}(32)-\text{N}(3)$	1.240 (7)
$\text{Pt}(1)-\text{N}(2)$	2.064 (5)	$\text{O}(33)-\text{N}(3)$	1.240 (6)
$\text{O}(2)-\text{H}(2)$	0.850 (5)	$\text{N}(1)-\text{C}(1)$	1.467 (7)
$\text{O}(2)-\text{C}(2)$	1.320 (7)	$\text{N}(2)-\text{C}(3)$	1.479 (9)
$\text{O}(3)-\text{C}(2)$	1.207 (6)	$\text{C}(1)-\text{C}(2)$	1.505 (7)
$\text{O}(31)-\text{N}(3)$	2.225 (7)		
$\text{N}(1)-\text{Pt}(1)-\text{N}(2)$	89.9 (2)	$\text{O}(31)-\text{N}(3)-\text{O}(32)$	120.1 (5)
$\text{H}(2)-\text{O}(2)-\text{C}(2)$	108.8 (5)	$\text{N}(1)-\text{C}(1)-\text{C}(2)$	112.8 (4)
$\text{Pt}(1)-\text{N}(1)-\text{C}(1)$	115.0 (3)	$\text{O}(3)-\text{C}(2)-\text{C}(1)$	123.7 (5)
$\text{Pt}(1)-\text{N}(2)-\text{C}(3)$	116.6 (4)	$\text{O}(2)-\text{C}(2)-\text{C}(1)$	111.4 (4)
$\text{O}(32)-\text{N}(3)-\text{O}(33)$	119.7 (5)	$\text{O}(2)-\text{C}(2)-\text{O}(3)$	124.9 (5)
$\text{O}(31)-\text{N}(3)-\text{O}(33)$	120.3 (5)		
$\text{N}(1)-\text{Pt}(1)-\text{N}(2)-\text{C}(3)$	114.2 (4)	$\text{Pt}(1)-\text{N}(1)-\text{C}(1)-\text{C}(2)$	-172.8 (3)
$\text{N}(2)-\text{Pt}(1)-\text{N}(1)-\text{C}(1)$	79.7 (3)	$\text{N}(1)-\text{C}(1)-\text{C}(2)-\text{O}(3)$	-1.5 (7)
$\text{H}(2)-\text{O}(2)-\text{C}(2)-\text{O}(3)$	-14.4 (8)	$\text{N}(1)-\text{C}(1)-\text{C}(2)-\text{O}(2)$	179.9 (4)
$\text{H}(2)-\text{O}(2)-\text{C}(2)-\text{C}(1)$	164.2 (5)		
$\text{O}(2)\cdots\text{O}(11^{\circ})$	2.626 (6)	$\text{H}(2)\cdots\text{O}(11^{\circ})$	
		$\text{O}(2)-\text{H}(2)\cdots\text{O}(11^{\circ})$	
		1.779 (6)	
		173.5 (5)	

Symmetry code: (i) $-x, y - 0.5, 0.5 - z$.

42.20 h of X-ray exposure; 3963 reflections measured
 $2.0 \leq 2\theta \leq 50.0^\circ$, $-10 \leq h \leq 10$, $-16 \leq k \leq 16$,
 $-11 \leq l \leq 11$; after averaging ($R_{\text{int}} = 0.023$):
 1553 unique reflections, 1341 with $F \geq 3.0\sigma(F)$;
 Lorentz-polarization correction and absorption
 correction via ψ scans, max./min. transmission
 $0.99/0.89$; systematic absences ($h0l$) $l = 2n + 1$, ($0k0$)
 $k = 2n + 1$ conform to space group $P2_1/c$; structure
 solution via direct methods and ΔF syntheses. Full-
 matrix least-squares refinement with anisotropic tem-
 perature factors for all non-H atoms and a common
 isotropic temperature factor for H atoms, which
 were placed in geometrically calculated positions
 (C—H 0.96 Å) except H(2) which was localized in a
 ΔF map; refinement on F with 1341 reflections and
 116 refined parameters; $w = 1.0 / [\sigma^2(F) + (0.0003F^2)]$
 which led to featureless analysis of variance in terms
 of $\sin\theta$ and F_o ; $S = 1.40$, $R = 0.026$, $wR = 0.028$,
 $(\Delta/\sigma)_{\text{max}} = 0.003$, no extinction correction; largest
 peak in final ΔF map ± 0.7 (3) e Å⁻³ near Pt; atomic

scattering factors for neutral atoms and real and imaginary dispersion terms from *International Tables for X-ray Crystallography* (1974). Programs: *PARST* (Nardelli, 1983), *SHELXTL-Plus* (Sheldrick, 1987), *PCK83* (Williams, 1984), *PLATON* (Spek, 1982), *MISSYM* (Le Page, 1987), *SCHAKAL* (Keller, 1986). The molecule, which is on a center of symmetry, and the numbering are shown in Fig. 1 and a stereoscopic view is in Fig. 2. Positional parameters and U_{eq} values for the non-H atoms are given in Table 1.* Bond lengths, bond angles, torsion angles, least-squares planes, dihedral angles and hydrogen-bond geometry are given in Table 2.

Related literature. The coordination chemistry of amino acids and Pt electrophiles has been the subject of numerous studies (Volshtain, 1975; Beck, 1988). The simplest amino acid, glycine (glyH), has been used particularly often. Of the various binding modes of deprotonated glycine (gly), both chelate formation (N, O) (Freeman & Golomb, 1969; Iakovidis, Hadjiliadis, Schöllhorn, Thewalt & Trötscher, 1989) and binding via the terminal amino group (Baidina, Podberezskaya, Borisov, Shestakova, Kuklina & Mal'chikov, 1979; Pesch, Preut & Lippert, 1990) have been established by X-ray analysis. In acidic medium, neutral glycine can bind both through oxygen and through nitrogen (Appleton,

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, least-squares-planes data and complete hydrogen-bond geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52576 (10 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Hall & Ralph, 1985; Schwarz, Lippert, Iakovidis & Hadjiliadis, 1990).

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Structure of Potassium Isocyanato[N-salicylidene-DL-alaninato(2-)]cuprate(II)

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Abstract. $\text{K}[\text{Cu}(\text{NCO})(\text{C}_{10}\text{H}_9\text{NO}_3)]$, $M_r = 335.84$, monoclinic, $P2_1/c$, $a = 7.925$ (3), $b = 17.144$ (8), $c = 9.231$ (5) Å, $\beta = 104.53$ (5)°, $V = 1214.0$ (8) Å³, $Z = 4$, $D_m = 1.84$ (1), $D_x = 1.837$ Mg m⁻³, $\lambda(\text{Cu } K\alpha) =$

1.54178 Å, $\mu = 4.76$ mm⁻¹, $F(000) = 676$, $T = 293$ K, final $R = 0.045$ for 1397 observed reflections. The Cu coordination can be described as square planar (with Cu bonded to the heteroatoms of the