±0·6 (4) e Å^{-3} in the remaining parts of the cell; no extinction correction; atomic scattering factors for neutral atoms and real and imaginary dispersion terms from *International Tables for X-ray Crystallography* (1974); programs: Enraf–Nonius *Structure Determination Package* (Frenz, 1985), *PARST* (Nardelli, 1983), *SHELXTL-PLUS* (Sheldrick, 1987), *SCHAKAL* (Keller, 1986), *PCK*83 (Williams, 1984), *PLATON* (Spek, 1982), *MISSYM* (Le Page, 1987). The molecules and the numbering scheme are shown in Fig. 1 and a stereoscopic view of the unit cell in Fig. 2. Positional parameters and the equivalent values of the displacement parameters are given in Table 1.* Bond lengths and angles, torsion angles and short intermolecular distances are given in Table 2.

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9-Ethylguaninium Tetrachloroaurate(III) Hydrate

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Abstract. 2-Amino-9-ethyl-6-oxo-1,6-dihydro-7*H*$^+$,9*H*-purinium tetrachloroaurate(III) hydrate, $C_7H_{10}N_5O^+.AuCl_4^-.H_2O$, M_r = 536·98, monoclinic, $P2_1/n$, a = 7·345 (2), b = 14·976 (4), c = 13·366 (5) Å, β = 93·35 (3)°, V = 1467·7 (8) Å^3, Z = 4, D_x = 2·430 Mg m^{-3}, $F(000)$ = 1008, λ(Mo $K\alpha$) = 0·71073 Å, μ = 10·74 mm^{-1}, T = 291 (1) K, final R = 0·039 for 2378 unique observed [$F \geq 3{\cdot}0\sigma(F)$] diffractometer data. The title compound consists of discrete 9-ethylguaninium cations, tetrachloroaurate(III) anions and water molecules. The $[AuCl_4]^-$ anion is planar with Au—Cl distances in the range 2·277 (2)–2·283 (2) Å.

Experimental. Orange-yellow needles of the title compound were obtained in 81% yield by cocrystallization of 9-ethylguanine and $NaAuCl_4$ in 0·1 *M* HCl and subsequent recrystallization from water at 276 K. A crystal of size ~0·26 × 0·04 × 0·12 mm was used, D_m was not determined. Intensity data were collected with $\omega/2\theta$ scans, scan speed 4–15° min^{-1} in θ and scan width 1·2° + dispersion. A Nicolet *R3m/V* diffractometer with graphite-monochromated Mo $K\alpha$ radiation was used. The lattice parameters were determined from least-squares fit of 28 reflections with $2\theta \leq 33{\cdot}09°$; ω scans of low-order reflections along the three crystal axes showed acceptable mosaicity. Six standard reflections (200, 020, 002, $\bar{2}00$, $0\bar{2}0$, $00\bar{2}$) were recorded every 2·5 h, only random deviations were detected during 158 h of X-ray exposure; 10023 reflections with $3{\cdot}0 \leq 2\theta \leq 50{\cdot}0°$, $-9 \leq h \leq 9$, $-18 \leq k \leq 18$, $-16 \leq l \leq 16$ were measured. The data were corrected for Lorentz–polarization and absorption effects, the latter *via* ψ scans; the max./min. transmission factors were 1·00/0·53. The intensities were averaged ($R_{\rm int}$ = 0·065) to 2593 unique reflections, 2378 of which had $F \geq 3{\cdot}0\sigma(F)$. The systematic absences ($h0l$) $h + l = 2n + 1$, ($0k0$) $k = 2n + 1$ conform to space group $P2_1/n$. The structure was solved from Patterson function and $\Delta\rho$ maps. It was refined (on F) using full-matrix least squares with anisotropic temperature factors for

Table 1. *Atomic coordinates and equivalent isotropic displacement parameters* (Å^2 × 10^4)

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

	x	y	z	U_{eq}
Au(1)	0·14666 (4)	0·02999 (2)	0·22209 (2)	345
Cl(1)	0·2011 (3)	0·1768 (1)	0·2576 (2)	526
Cl(2)	0·2121 (4)	0·0550 (1)	0·0596 (1)	560
Cl(3)	0·0747 (3)	0·0052 (2)	0·3831 (2)	591
Cl(4)	0·1001 (4)	−0·1176 (2)	0·1876 (2)	704
O(2)	0·4604 (8)	0·1311 (3)	0·8703 (4)	440
N(1)	0·1281 (8)	0·4105 (4)	0·9435 (4)	331
C(2)	0·191 (1)	0·3257 (5)	0·9372 (5)	319
N(2)	0·215 (1)	0·2811 (4)	1·0251 (4)	494
N(3)	0·2271 (8)	0·2862 (4)	0·8529 (4)	312
C(4)	0·1981 (9)	0·3408 (4)	0·7728 (5)	280
C(5)	0·149 (1)	0·4296 (5)	0·7739 (5)	296
C(6)	0·101 (1)	0·4706 (5)	0·8657 (5)	330
O(6)	0·0373 (7)	0·5450 (3)	0·8765 (4)	393
N(7)	0·1447 (9)	0·4606 (4)	0·6785 (5)	371
C(8)	0·183 (1)	0·3921 (5)	0·6176 (6)	433
N(9)	0·2185 (9)	0·3188 (4)	0·6740 (4)	339
C(9′)	0·261 (1)	0·2278 (5)	0·6381 (5)	458
C(9″)	0·230 (1)	0·2187 (6)	0·5275 (5)	565

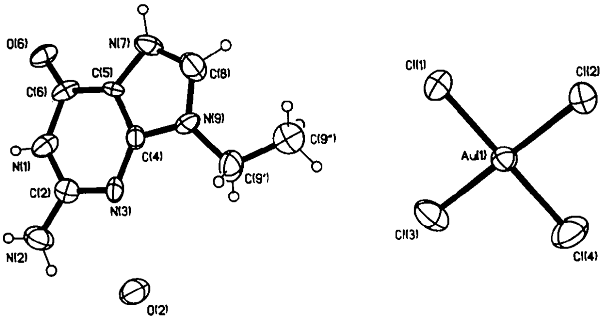

Fig. 1. General view (*SHELXTL-PLUS*) of the ethylguaninium cation and the tetrachloroaurate(III) anion, with atomic numbering scheme.

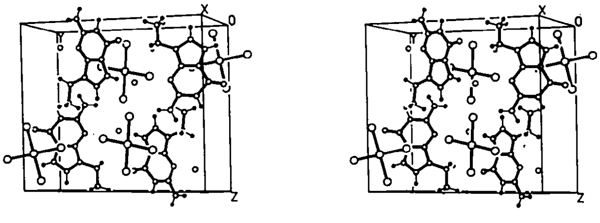

Fig. 2. Stereoscopic view (*SHELXTL-PLUS*) of the unit cell.

Table 2. *Bond distances* (Å), *bond angles* (°), *torsion angles* (°), *least-squares planes and dihedral angles* (°)

Au(1)—Cl(1)	2·280 (2)	C(4)—C(5)	1·378 (9)
Au(1)—Cl(2)	2·283 (2)	C(4)—N(9)	1·377 (8)
Au(1)—Cl(3)	2·277 (2)	C(5)—C(6)	1·43 (1)
Au(1)—Cl(4)	2·280 (2)	C(5)—N(7)	1·355 (9)
N(1)—C(2)	1·356 (9)	C(6)—O(6)	1·219 (9)
N(1)—C(6)	1·382 (9)	N(7)—C(8)	1·350 (9)
C(2)—N(2)	1·354 (9)	C(8)—N(9)	1·348 (9)
C(2)—N(3)	1·312 (9)	N(9)—C(9′)	1·484 (9)
N(3)—C(4)	1·355 (8)	C(9′)—C(9″)	1·49 (1)

Cl(3)—Au(1)—Cl(4)	89·6 (1)	C(5)—C(4)—N(9)	106·6 (6)
Cl(2)—Au(1)—Cl(4)	90·2 (1)	C(4)—C(5)—N(7)	108·2 (6)
Cl(2)—Au(1)—Cl(3)	178·7 (1)	C(4)—C(5)—C(6)	120·0 (6)
Cl(1)—Au(1)—Cl(4)	178·5 (1)	C(6)—C(5)—N(7)	131·7 (6)
Cl(1)—Au(1)—Cl(3)	90·44 (9)	N(1)—C(6)—C(5)	109·5 (6)
Cl(1)—Au(1)—Cl(2)	89·77 (8)	C(5)—C(6)—O(6)	127·4 (6)
C(2)—N(1)—C(6)	126·7 (6)	N(1)—C(6)—O(6)	123·1 (6)
N(1)—C(2)—N(3)	124·2 (6)	C(5)—N(7)—C(8)	108·2 (6)
N(1)—C(2)—N(2)	115·8 (6)	N(7)—C(8)—N(9)	108·8 (6)
N(2)—C(2)—N(3)	120·0 (6)	C(4)—N(9)—C(8)	108·2 (6)
C(2)—N(3)—C(4)	112·1 (6)	C(8)—N(9)—C(9′)	127·1 (6)
N(3)—C(4)—N(9)	126·3 (6)	C(4)—N(9)—C(9′)	124·6 (6)
N(3)—C(4)—C(5)	127·1 (6)	N(9)—C(9′)—C(9″)	112·6 (6)

C(8)—N(9)—C(9′)—C(9″)	−9 (1)	C(4)—N(9)—C(9′)—C(9″)	165·7 (7)

No.	Plane through atoms	Equation of the plane (x along **a**; y in the plane ab; z along **c**)	χ^2
1	N(1), C(2), N(3), C(4), C(5), C(6)	$-0{\cdot}9419x - 0{\cdot}308y - 0{\cdot}135z = 3{\cdot}79$ Å	62·92
2	C(4), C(5), N(7), C(8), N(9)	$-0{\cdot}9625x - 0{\cdot}249y - 0{\cdot}107z = -3{\cdot}19$ Å	7·86

Dihedral angle 1,2: 3·9 (2)°

Possible hydrogen bonds

Donor···Acceptor	H···Acceptor	Donor—H···Acceptor
N(1)···O(6^{i})	H(1)···O(6^{i})	N(1)—H(1)···O(6^{i})
2·837 (8)	1·972 (8)	160·6 (6)
N(2)···Cl(2^{ii})	H(22)···Cl(2^{ii})	N(2)—H(22)···Cl(2^{ii})
3·417 (7)	2·606 (7)	150·3 (7)
N(7)···O(2^{iii})	H(7)···O(2^{iii})	N(7)—H(7)···O(2^{iii})
2·736 (7)	1·841 (7)	172·5 (7)

Symmetry codes: (i) $-x, -y+1, -z+2$; (ii) $+x, +y, +z+1$; (iii) $-x+1/2, +y+1/2, -z+1/2+1$.

all non-H atoms and a common isotropic temperature factor for H atoms, which were placed in geometrically calculated positions (C—H, N—H 0·96 Å). The water H atoms were not included in the refinement. 173 parameters were refined. Weights $w = 1{\cdot}0/[\sigma^2(F) + (0{\cdot}000985F^2)]$ led to a featureless analysis of variance in terms of $\sin\theta$ and F_o. The refinement converged to $S = 0{\cdot}91$, $R = 0{\cdot}039$, $wR = 0{\cdot}034$, and $\Delta/\sigma \leq 0{\cdot}06$ (no extinction correction). The largest peak and trough in the final $\Delta\rho$ map were ± 1·1 (5) e Å^{-3}. Atomic scattering factors for neutral atoms and real and imaginary dispersion terms were taken from *International Tables for X-ray Crystallography* (1974). The programs used were *PARST* (Nardelli, 1983), *SHELXTL-PLUS* (Sheldrick, 1987), *PLATON* (Spek, 1982) and *MISSYM* (Le Page, 1987). The molecule and numbering scheme are shown in Fig. 1 and a stereoscopic view of the unit-cell content in Fig. 2. Positional parameters and the equivalent values of the anisotropic temperature factors for the non-H atoms are given in Table 1.* Selected bond lengths, bond angles, torsion angles, least-squares planes and dihedral angles and possible hydrogen-bond geometries are given in Table 2.

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52621 (13 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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 $AuCl_3$ (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)° 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···OH_2 2·650 Å], the other hydrogen bonds differ in both structures. Instead of N(3)···$H_2N(2)$ 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*-$[(NH_2CH_3)_2(C_2H_5NO_2)_2Pt](NO_3)_2.2H_2O$

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Abstract. $C_6H_{24}N_6O_{12}Pt$, $M_r = 567·38$, 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) Å^3, $Z = 2$, $D_x = 2·142$ Mg m^{-3}, λ(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 NH_2 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*-$(NH_2CH_3)_2PtCl_2$ [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

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