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Bis(triphenylarsine oxide)hydrogen(I) Tetrachloroaurate(III)

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Abstract. $C_{36}H_{31}As_2O_2^+.AuCl_4^-$, $M_r = 984{\cdot}3$, monoclinic, $P2_1/n$, $a = 13{\cdot}659\ (5)$, $b = 9{\cdot}955\ (5)$, $c = 14{\cdot}481\ (5)$ Å, $\beta = 110{\cdot}98\ (3)°$, $U = 1838{\cdot}5$ Å^3, $Z = 2$, $D_x = 1{\cdot}78$ Mg m^{-3}, $F(000) = 952$, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 6{\cdot}1$ mm^{-1}, $T = 293$ K, final $R = 0{\cdot}072$ for 2095 unique observed reflections. The anions are associated with the centre of symmetry at 0,0·5,0·5, with Au–Cl 2·270, 2·280 (4) Å. The Ph_3AsO moieties of the cation are related across the symmetry centre 0,0,0; the proton that connects these *via* a hydrogen bond of 2·39 (2) Å was not located, but presumably lies on the origin.

Experimental. A yellow prism 0·25 × 0·15 × 0·1 mm was mounted in a glass capillary; 5320 profile-fitted intensities were measured on a Stoe–Siemens four-circle diffractometer using monochromated Mo $K\alpha$ radiation ($2\theta_{max}$ 50°, scan ratio $2\theta/\omega = 1$). Three check reflections showed no significant intensity change. An absorption correction based on ψ scans was performed; transmission factors lay in the range 0·69–0·84. Merging equivalents gave 3218 unique reflections (R_{int} 0·035; index ranges h −15 to 15, k 0 to 11, l 0 to 17), 2095 of which with $F > 4\sigma(F)$ were used for all calculations. Cell constants were refined from 2θ values of 68 reflections in the range 15–25°. The structure was solved by the heavy-atom method and subjected to anisotropic full-matrix least-squares refinement on F. H atoms were included using a riding model with C–H = 0·96 Å, except for the acidic H, which was not located (although it very probably lies on the origin). The final R value was 0·072, with wR 0·052. The weighting scheme was $w^{-1} = \sigma^2(F) + 0{\cdot}00015F^2$. 205 parameters; S 1·7; max. Δ/σ 0·013; max. $\Delta\rho$ features ±1·2 e Å^{-3}. Final atomic coordinates are presented in Table 1.† Selected bond lengths and angles are given in the *Abstract* and the caption to Fig. 1.

† Lists of structure factors, anisotropic thermal parameters, further bond lengths and angles and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51246 (16 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Atomic coordinates* (× 10^4) *and equivalent isotropic displacement parameters* (Å^2 × 10^3)

Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
As	62 (1)	1761 (1)	1276 (1)	50 (1)
Au	0	5000	5000	60 (1)
Cl(1)	1069 (3)	6779 (4)	5636 (3)	84 (2)
Cl(2)	1372 (3)	3797 (4)	4886 (3)	85 (2)
O	−352 (7)	1045 (8)	142 (5)	67 (4)
C(11)	1540 (10)	2070 (12)	1731 (7)	48 (5)
C(12)	2150 (11)	1442 (12)	1283 (9)	59 (6)
C(13)	3218 (13)	1630 (14)	1664 (11)	72 (7)
C(14)	3667 (12)	2424 (14)	2465 (12)	70 (7)
C(15)	3064 (13)	3051 (14)	2894 (10)	69 (7)
C(16)	1997 (11)	2916 (12)	2540 (9)	55 (6)
C(21)	−672 (9)	3407 (12)	1151 (8)	48 (5)
C(22)	−800 (11)	4017 (14)	1947 (10)	68 (7)
C(23)	−1336 (13)	5246 (18)	1818 (13)	94 (9)
C(24)	−1715 (12)	5835 (16)	909 (16)	93 (9)
C(25)	−1587 (12)	5244 (16)	120 (13)	90 (8)
C(26)	−1066 (11)	4013 (13)	225 (10)	70 (7)
C(31)	−224 (10)	646 (12)	2210 (8)	52 (5)
C(32)	490 (10)	506 (13)	3160 (9)	61 (6)
C(33)	257 (13)	−314 (13)	3830 (11)	73 (7)
C(34)	−683 (14)	−987 (15)	3536 (13)	80 (8)
C(35)	−1399 (12)	−881 (15)	2598 (13)	77 (8)
C(36)	−1154 (10)	−40 (15)	1927 (10)	71 (6)

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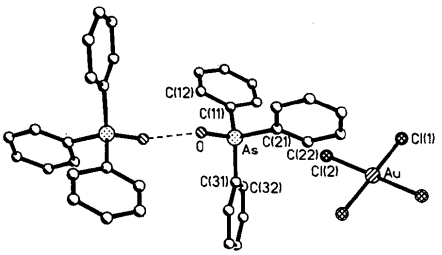

Fig. 1. Perspective view of a cation and anion of the title compound, showing the atomic numbering scheme. Radii are arbitrary and H atoms are omitted for clarity. The O···O hydrogen bond is indicated by a dashed line. Bond lengths and angles (see also *Abstract*): As–O 1·690 (7), As–C(11) 1·911 (12), As–C(21) 1·896 (12), As–C(31) 1·985 (12) Å, Cl(1)–Au–Cl(2) 90·8 (1), Cl(1^i)–Au–Cl(2) 89·2 (1), O–As–C(11) 110·4 (5), O–As–C(21) 106·9 (4), O–As–C(31) 111·3 (5), C(11)–As–C(21) 110·5 (5), C(11)–As–C(31) 108·1 (5), C(21)–As–C(31) 109·7 (6)°. Symmetry operator (i): $-x$, $1-y$, $1-z$.

Related literature. The preparation of the title compound has been described by Potts (1970) and more recently by Yuqiu & Shihua (1987). Structures of compounds with general formula $(RO)_2H^+.AuCl_4^-$ have been described by Jones & Sheldrick (1978) ($R = Ph_3P$; not isostructural with the title compound), Hussain & Schlemper (1982) (R = pyridine), Hussain & Al-Hamoud (1984) (R = α-picoline), Hussain & Al-Hamoud (1985) (R = 3-methylpyridine), Hussain & Al-Hamoud (1986) (R = 4-methylpyridine), and Drew, Glaves & Hudson (1985) (R = 2-nonylpyridine).

Calculations were performed with the program system *SHELX*76 (Sheldrick, 1976) locally modified by its author. We thank the Fonds der Chemischen Industrie for financial support.

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The Structure of 3′,5′-Di-*O*-acetyl-2′-deoxyadenosine

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Abstract. $C_{14}H_{17}N_5O_5$, $M_r = 335·3$, orthorhombic, $P2_12_12_1$, $a = 7·75$ (1), $b = 12·89$ (2), $c = 15·47$ (1) Å, $U = 1546$ Å^3, $Z = 4$, $D_x = 1·440$ Mg m^{-3}, Mo $K\alpha$ radiation, $\lambda = 0·71069$ Å, $\mu = 0·10$ mm^{-1}, $F(000) = 704$, $T = 293$ K, $R = 0·056$ for 919 unique observed [$F > 5\sigma(F)$] reflections. The N-glycosidic bond angle χ has a value of −86 (1)°, in the high *anti* range. The sugar pucker is $^2T_1$ with $P = 155$ (1)° and $\psi = 33$ (1)°. The C4′–C5′ conformation is *–sc* with $\gamma = -76$ (1)°. Symmetry-related molecules form self-base-paired hydrogen-bonded ribbons through N1···N6^i and N6···N7^{ii} contacts, both of 3·02 Å [(i) $-x$, $-\frac{1}{2}+y$, $-\frac{1}{2}-z$; (ii) $-1-x$, $-\frac{1}{2}+y$, $-\frac{1}{2}-z$]. This type of base-pairing is similar to that found for 2′,3′,5′-tri-*O*-acetylated adenosine molecules. The base pair shows a propeller twist, defined as the angle between the base planes about a line joining them, of 31 (2)°.

Experimental. Crystals were obtained from aqueous solution. Space group and initial cell dimensions were obtained from Weissenberg photographs. Data were collected on a Nicolet *P*3 (four-circle) diffractometer in Aberdeen by RAH. The crystal had dimensions 0·9 × 0·26 × 0·08 mm. Cell parameters were measured

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